All-sky Radiative Transfer and Characterisation for Cosmic Structures

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I, Jennifer Yik Ham Chan, confirm that the work presented in this thesis is my own. Where information has been derived from other sources, I confirm that this has been indicated in the thesis. This thesis is based on my research in collaboration with Prof. Jason Ewen, Prof. Kinwah Wu, Prof. Tom Kitching, Alvina On, Dr. David Barnes, Dr. Custis Saxton, Prof. Lidia van Driel-Gesztelyi, and Dr. Boris Leistedt.

Abstract

This thesis focuses on providing a solid theoretical foundation and the associated methodologies for the studies of cosmic magnetism and cosmological reionisation. It develops covariant formalisms of cosmological radiative transport of (i) polarised continuum radiation, and (ii) 21-cm line of neutral hydrogen that calculate, from first principles, the polarisation arising from the emergence and evolution of cosmic magnetic fields and the tomographic 21-cm line signals associated with cosmological reionisation, respectively. The two formalisms, namely the cosmological polarised radiative transfer (CPRT) and the cosmological 21-cm line radiative transfer (C21LRT), self-consistently account for the relevant radiation processes, relativistic and cosmological effects along a ray transported in an expanding, evolving Universe. Their all-sky algorithms adopt a ray-tracing method and a post-processing approach by which complex physical models, such as those obtained from cosmological simulations, can be accounted for in the radiative transfer calculations. The power of the CPRT calculations to compute unambiguous point-to-point polarisation of largescale structures, such as a 3D simulated galaxy cluster and a modelled magnetised universe, is demonstrated. The ability of the C21LRT formulation to calculate the 21-cm line spectra across cosmic time, with full accounts of the essential cosmological radiative transfer effects, is verified. Furthermore, a new spherical curvelet transform for efficient extraction of directional, elongated features within spherical data is constructed. It is particularly useful for the studies in wide-field astronomical research, such as analyses of the data of continuum polarisation and the structured 21-cm line from all-sky surveys or from the CPRT and C21LRT calculations. The formulations, methodologies and techniques developed in this work together establish a solid framework within which reliable theoretical predictions and robust data characterisation can be made, ultimately laying a foundation for the meaningful physical interpretation of observations and studying the structural evolution of the

magnetic ionised Universe.

Impact Statement

(1) Impacts on understanding large-scale cosmic magnetism and cosmological reionisation

This thesis research provides a solid theoretical foundation and the associated methodology underpinning two core sciences, cosmic magnetism and cosmological reionisation, of the Square Kilometre Array (SKA), the most powerful radio telescope in the coming decade for the study of the fundamental aspects of astrophysics and cosmology. The all-sky cosmological polarised radiative transfer (CPRT) formulation makes it possible for the first time to compute unambiguous theoretical point-to-point polarisation across the entire sky. The cosmological 21-cm line radiative transfer (C21LRT) formulation provides a reliable theoretical framework that account for the essential cosmological and astrophysical effects correctly and selfconsistently for the calculations of the tomographic 21-cm hyperfine line spectrum. The new-generation spherical curvelets give an efficient representation of oriented, elongated features within all-sky (spin) data, thus is a useful tool to extract and characterise structural information in cosmological magnetic fields and cosmological reionisation observations.

(2) Impacts on broader astrophysics and other sciences

The CPRT and C21LRT are generic formulations derived from first principles. They provide a theoretical framework for the derivation of other cosmological radiative transfer formulation for scientific explorations beyond cosmic magnetism and cosmological reionisation. The CPRT formulation can be used, without much modification, for the calculations of polarised emission from sources (locally) through magnetised line-of-sight medium (globally) with velocity, density, magnetic structures in an expanding Universe. Examples are polarised radiation from background point sources, e.g. quasars or FRB, through a line-of-sight magnetised medium and synchrotron radiation from jets or galactic outflows. Similarly, the C21LRT can be used for the calculations of line emission from systems with velocity, density and thermodynamic structures in an expanding Universe, and an examples is the Lyman- α emission from distant quasars or galaxies. The spherical curvelets are well-suited to investigate any spherical data, not only those from wide-sky astrophysical and cosmpological surveys. Examples of applications are in remote-sensing in geophysics and planetary science (collected over spherical planetary surfaces), 360-degree videos in computer vision (taken by omnidirectional cameras) and medical imaging (such as brain scans). Addition examples include data compression and processing (e.g. noise reduction, inpainting, segmentation, etc) in scientific and non-scientific disciplines.

(3) Impacts in a broader community

This thesis has contributed to the human endeavour of understanding how the Universe that we live in came into being today. More specifically, it responds to our philosophical and curiosity quests on how the Universe acquired its magnetic fields and how it began to manufacture stars and galaxies. The thesis has also provided an educational opportunity for two undergraduate students, whom I supervised, to conduct real-life scientific research and produced frontier scientific material for STEM outreach and public engagement activities, in particular, in my outreach talks, in the featuring of the SKA telescope at the New Scientist Live Festival, and in several scientific blogs for laypersons.

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Lists of Acronyms and Symbols

| Abbreviation/ | Definition |
|---------------|---|
| Acronym | |
| ATCA | The Australia Telescope Compact Array |
| ASKAP | The Australian SKA Pathfinder |
| BBN | Big Bang Nucleosynthesis |
| C21LRT | Cosmological 21-cm Line Radiative Transfer |
| CDM | Cold Dark Matter |
| CHIME | The Canadian Hydrogen Intensity Mapping Experiment |
| CMB | Cosmic Microwave Background |
| CPRT | Cosmological Polarised Radiative Transfer |
| DARE | The Dark Ages Radio Explorer |
| EoR | Epoch of Reionisation |
| EDGES | The Experiment to Detect the Global EoR Signature |
| EVLA | The Expanded Very Large Array |
| FAST | Five hundred meter Aperture Spherical Telescope |
| FFT | Fast Fourier Transform |
| FRW | Friedmann-Robertson-Walker |
| FWHM | Full-Width-Half-Maximum |
| GCMHD+ | Galactic Chemodynamics smoothed particle MagnetoHy- |
| | droDynamic (code) |
| GLEAM | GaLactic and Extragalactic All-sky MWA Survey |
| GRRT | General Relativistic Radiative Transfer |
| GRPRT | General Relativistic Polarised Radiative Transfer |

Abbreviation and acronym glossary

| Acronym | Definition |
|----------|---|
| HEALPix | Hierarchical Equal Area isoLatitude Pixelation of a 2- |
| | sphere |
| HERA | The Hydrogen Epoch of Reionization Array |
| ICM | Intracluster medium |
| IGM | Intergalactic medium |
| ISM | Interstellar medium |
| LCP, RCP | Left-handed and right-handed circular polarisation |
| LOFAR | The LOw-Frequency ARray |
| MeerKAT | Originally the Karoo Array Telescope (MeerKAT means |
| | "more KAT") |
| MHD | Magnetohydrodynamics |
| MIGHTEE | MeerKAT International GigaHertz Tiered Extragalactic |
| | Exploration survey |
| MSSS | The Multi-frequency Snapshot Sky Survey (on LOFAR) |
| MWA | The Murchison Widefield Array |
| PAPER | The Precision Array for Probing the Epoch of Reionisation |
| | (also known as HERA phase I) |
| POSSUM | The POlarisation Sky Survey of the Universe's Magnetism |
| | (on ASKAP) |
| PRT | Polarised Radiative Transfer |
| RK | Runge-Kutta (method or differential equation solver) |
| RM | Rotation Measure(s) |
| RMF | Rotation Measure Fluctuations |
| SARAS | The Shaped Antenna measurement of the background RA- |
| | dio Spectrum |
| SPMHD | Smoothed Particle MagnetoHydroDynamics (code) |
| STFT | Short-time Fourier Transform |
| SKA | The Square Kilometre Array |

| Acronym | Definition |
|---------|---|
| VLA | The Karl G. Jansky Very Large Array (VLA) |
| VLASS | The Very Large Array Sky Survey |
| ΛCDM | Cold Dark Matter with a non-zero cosmological constant |
| | (dark energy with an equation of state of $w \equiv -1$) |

Symbol dictionary

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| Symbol | Units/Remarks | Definition |
|-------------------------------------|--|---|
| A _{ul} | [s ⁻¹] | Einstein A coefficient |
| b_{D} | | Doppler parameter |
| $B_{\rm ul}, B_{\rm lu}$ | [s ⁻¹] | Einstein B coefficients |
| B_{ν} | | Planck function |
| В | | Magnetic field |
| B | [G] | Magnetic field strength |
| $C_{\rm lu}, C_{\rm ul}$ | | Collisional excitation and de-excitation rates, respec- |
| | | tively |
| $d_{mn}^\ell(eta)$ | | Wigner small-D function |
| $D_{mn}^\ell, D_{mn}^{\ell*}$ | | Wigner <i>D</i> -function and its conjugate |
| $\mathrm{d}\varrho(\rho)$ | $\sin\beta d\alpha d\beta d\gamma$ | Invariant measure on the rotation group |
| $\mathrm{d}\Omega(\omega)$ | $\sin\theta \mathrm{d}\theta \mathrm{d}\phi$ | Invariant measure of the sphere |
| е | 4.8032068 × | Elementary charge |
| | 10^{-10} esu | |
| eps | | Error tolerance level of the RK-solver |
| ð, ð | (Eth) | Spin-raising and spin-lowering operators |
| f_{ν} | $[cm^{-1}]$ | Faraday rotation coefficient |
| $f(\boldsymbol{x}, \boldsymbol{p})$ | | Photon distribution function |
| $f_{\rm nt}$ | | Non-thermal electron fraction |
| \mathcal{F}_{nt} | | Fraction of non-thermal electrons |

| Symbol | Remarks | Definition |
|---|--|--|
| <i>g</i> I | ≈ 5.58569 | Nuclear g-factor of proton |
| g_i | | Statistical weight of level <i>i</i> |
| g_{ν}, h_{ν} | $[cm^{-1}]$ | Faraday conversion coefficients (in the PRT context) |
| h | 6.6260755 × | Planck constant |
| | 10^{-27} erg s | |
| \hbar | $h/2\pi$ | Reduced Planck constant |
| $H_0, H(z)$ | $[\mathrm{km}\mathrm{s}^{-1}\mathrm{Mpc}^{-1}]$ | Hubble constant and Hubble parameter |
| h | | Dimensionless (Hubble) parameter where H_0 = |
| | | $100h [\rm km s^{-1} Mpc^{-1}]$ |
| H(q, x) | | Voigt function |
| i | | Inclination angle of a disk galaxy |
| $i_z, i_{\rm ray}$ | | Indices of the CPRT algorithm |
| ind ^{refine} | | Cell index used in the refinement scheme of the CPRT |
| | | algorithm |
| I_{ν} | $[\mathrm{erg}\mathrm{s}^{-1}\mathrm{cm}^{-2}$ | Specific intensity |
| | $Hz^{-1} str^{-1}$] | |
| $I_{\nu}, Q_{\nu}, U_{\nu}, V_{\nu}$ | $e^{-1} \mathrm{cm}^{-2}$ | Comoving Stokes parameters |
| | $Hz^{-1} str^{-1}$] | |
| $I_{ m v}, Q_{ m v}, {\cal U}_{ m v}, {\cal V}$ | $V_{\nu}[\mathrm{erg}\mathrm{s}^{-1}\mathrm{cm}^{-2}]$ | Invariant Stokes parameters |
| | $Hz^{-4} str^{-1}$] | |
| $\kappa_{\nu}, q_{\nu}, u_{\nu}, v_{\nu}$ | $[cm^{-1}]$ | Comoving absorption coefficients |
| j | | Wavelet scale |
| J_0 | | Minimum scale to be probed by curvelets |
| $k_{\rm B}$ | 1.380658×10^{-1} | ¹ Boltzmann constant |
| | $erg K^{-1}$ | |
| \boldsymbol{k} | | Radiation propagation direction |
| k^{α} | | Photon 4-momentum |

| Symbol | Remarks | Definition |
|------------------------|---------------------|---|
| $k_{\lambda}(t)$ | | Mathematical function defined in curvelet construc- |
| | | tion |
| ł | | Degree of a spherical harmonic function, or known as |
| | | multipole. Higher values of ℓ corresponds to smaller |
| | | angular scales (for reference: $\ell \sim 100$ corresponds to |
| | | an angular scale of about 1 degree) |
| L | | Band-limit |
| m ^{emp} | | Power-law index of the ratio of the output peak inten- |
| | | sities of the two profiles |
| m | | Order of a spherical harmonic function |
| m _e | 9.1093897 × | Mass of an electron |
| | 10 ⁻²⁸ g | |
| m _p | 1.6726231 × | Mass of a proton |
| | $10^{-24} { m g}$ | |
| $m_{\rm H}$ | 1.6737236 × | Mass of a hydrogen atom |
| | 10 ⁻²⁴ g | |
| n _e | | Electron number density |
| n _H | | Hydrogen number density |
| $n_{ m HI}$ | | Neutral hydrogen number density |
| $n_{\rm l}, n_{\rm u}$ | | Number density of neutral hydrogen atoms in the lower |
| | | and upper hyperfine states, respectively |
| N _{cell} | | Total number of discretised cells across the light-travel |
| | | distance in the CPRT algorithm |
| Neqn | | Total number of (coupled) differential equations to be |
| | | solved by the RK-solver |
| N _{step} | | Total number of steps for the RK solver |
| N _{ray} | | Total number of rays |
| \bar{n}_b^c | | Comoving baryon number density |

| Symbol | Remarks | Definition |
|--------------------------|-------------------------|---|
| 0 | | Order of magnitude |
| р | | Power-law index of the non-thermal electrons' energy |
| | | spectrum |
| $P_{\rm lu}, P_{\rm ul}$ | | Radiative excitation and de-excitation rates, respec- |
| | | tively, due to $Ly\alpha$ scattering |
| P(k) | | Power spectrum |
| $\Pr(\cdot)$ | | Probability distribution |
| q | | The Voigt parameter quantifying the relative strength |
| | | of the damping broadening to the Doppler broadening |
| r | | Radial component |
| $r_I^{\rm emp}$ | | Empirical value of intensity ratio defined by |
| | | $I_{\rm peak}^{\rm in}/I_{\rm peak,0}$ |
| res_{x} | | Residual of quantity x |
| R_{∞} | | Rydberg constant |
| $R_{ m H}$ | 1.09678×10^{5} | Hydrogen Rydberg constant |
| | cm^{-1} | |
| $R_{\rm H}c$ | 3.28805 × | Hydrogen Rydberg frequency |
| | 10 ¹⁵ Hz | |
| $\mathcal R$ | | Rotation measure variable |
| $\mathcal{R}_ ho$ | | Rotation operator parameterised by the Euler angles |
| | | $\rho = (\alpha, \beta, \gamma) \in \mathrm{SO}(3)$ |
| \mathcal{R}_{ω} | | Rotation operator parameterised by $\mathcal{R}_{\omega} = \mathcal{R}_{(\phi,\theta,0)}$ |
| S | [cm] | Light-travel distance (in radiative transfer) |
| S | $\in \mathbb{Z}$ | Spin (in signal analysis and curvelet context) |
| $_{s}S, _{s}S_{\ell m}$ | | Directional component of spin curvelets and its har- |
| | | monic components |
| $S_{ u}$ | | Specific Source function |
| \mathcal{S}_{ν} | $= S_{\nu}/\nu^3$ | Lorentz-invariant specific source function |

| Symbol | Remarks | Definition |
|---|-----------------|---|
| $s_{\lambda}(t)$ | | Infinitely differentiable Schwartz function |
| $sf_{\ell m}$ | | Spin spherical harmonic functions (= $\langle sf, sY_{\ell m} \rangle$) |
| $_{s}Y_{\ell m}, _{s}Y^{*}_{\ell m}$ | | Spin spherical harmonics and its conjugate |
| t | | Time |
| $\Delta t_{21 \mathrm{cm}}$ | ~ 11 Myr | Mean lifetime of the hyperfine 21-cm transition |
| T _e | | Temperature of thermal electrons |
| T _b | | Brightness temperature |
| T_{lpha} | | Colour temperature of the Ly α radiation field |
| $T_{\rm k}$ | | Gas kinetic temperature |
| T _r | | Temperature of the radiation |
| $T_{\rm s}$ | | Spin temperature |
| $T_{\rm CMB}(z)$ | 2.73(1+z) K | CMB temperature at redshift z |
| T_{\star} | 0.0682 K | Characteristic 21-cm temperature: $T_{\star} = hc/k_{\rm B}\lambda_{21\rm cm}$ |
| U_{B} | $[erg cm^{-3}]$ | Magnetic energy density which equals to $ \mathbf{B} ^2/8\pi$ |
| v | | 3-velocity |
| v^{eta} | | Photon comoving 4-velocity |
| v_{\parallel} | | Velocity component along the line-of-sight |
| $W^{s\psi^{(j)}}$ | | Curvelet coefficients of a spin function ${}_s f \in L^2(\mathbb{S}^2)$ |
| $\left(W^{s^{\psi^{(j)}}}\right)_{mn}^{\ell}$ | | Wigner coefficients of curvelet coefficients defined as |
| | | $\langle W^{_{s}\psi^{(j)}},\ D_{mn}^{\ell*} angle$ |
| $\widetilde{W}^{s\widetilde{\psi}^{(j)}}$ | | Unrotated curvelet coefficients of a spin function de- |
| | | fined as $\langle {}_{s}f, \mathcal{R}_{\rho} {}_{s}\widetilde{\psi}^{(j)} \rangle$ |
| $\left(\widetilde{W}^{s\widetilde{\psi}^{(j)}} ight)_{mn}^\ell$ | | Wigner coefficients of unrotated curvelets which offset |
| | | from the North pole |
| $W^{s\Phi}(\omega)$ | | Scaling coefficients |
| $(W^{s\Phi})_{\ell m}$ | | Spherical harmonic coefficient of scaling coefficients |
| | | defined as $\langle W^{s\Phi}, _{0}Y_{\ell m} \rangle$ |
| <i>w</i> (<i>m</i> ') | | Weighting function to $X_{mnm''}$ in evaluating $\mathcal{Y}_{mnm'}$ |

| Symbol | Remarks | Definition |
|---|------------------------|--|
| x _c | | Collisional coupling coefficient for T_s |
| $x_{\rm tot}$ | | Total coupling coefficient for T_s |
| x_{lpha} | | Wouthuysen-Field coupling coefficient for T_s |
| $x_{\rm HI}$ | | Neutral fraction |
| x _i | | Ionisation fraction |
| $X_{mn}(\beta_b)$ | | Fourier transform is performed over Euler angles α |
| | | and γ |
| $\overline{\mathcal{X}}_{mn}(eta_b)$ | | $X_{mn}(\beta_b)$ extended to the domain $[0, 2\pi)$ |
| $X_{mnm'}$ | | Fourier transform of $\overline{X}_{mn}(\beta_b)$ in β |
| Y _{He} | 0.25 | Helium mass fraction |
| $Y_{\ell m}$ | | Spherical harmonic functions |
| $\mathcal{Y}_{mnm'}$ | | Exact quadrature for integration over β |
| Z. | | Redshift |
| $z_{equality}$ | ≈ 3371 | Redshift of radiation-matter equality |
| α | = (p - 1)/2 | Synchrotron radiation power-law spectrum index |
| γ_i | | Electrons' low energy cut off specified by the Lorentz |
| | | factor |
| $\Gamma_{\rm rad}$ | | Radiative damping parameter |
| $\Gamma_{damping}$ | | Total damping line width |
| $\delta_{ m b}$ | | Fractional baryonic matter overdensity |
| Δv_D | | Doppler width |
| Δ_{mn}^ℓ | | Scaled small-d Wigner function defined as $d_{mn}^{\ell}(\pi/2)$ |
| $\epsilon_{\scriptscriptstyle \mathcal{V}}$ | $[erg s^{-1} cm^{-3}]$ | Comoving emission coefficient at frequency v |
| | $Hz^{-1} str^{-1}$] | |
| ζν | $= \nu \kappa_{\nu}$ | Lorentz-invariant absorption coefficient |

| Symbol | Remarks | Definition |
|-----------------------------|---|--|
| $\zeta(p, \gamma_{\rm i})$ | $= \left(\frac{\ln \gamma_i}{\gamma_i^2}\right) \times$ | Weighting function of Faraday rotation contribution |
| | $\left(\frac{(p-1)(p+2)}{(p+1)}\right)$ | by non-thermal electrons with power-law energy spec- |
| | | trum of index p and the Lorentz factor of low-energy |
| | | cut-off γ_i |
| Θ | $= 1 - \mathcal{F}_{nt}(1 - $ | Electron contribution weighting factor to the total |
| | $\zeta(p, \gamma_{\rm i}))$ | Faraday rotation effect |
| К | [cm ⁻¹] | Absorption coefficient |
| $\kappa_{10}^{\text{coll}}$ | $[cm^{-1}]$ | Collisional spin de-excitation rate coefficient |
| $\kappa^{(j)}$ | | Angular localisation kernel of the <i>j</i> -th scale curvelet |
| λ | | Wavelength (in radiative transfer context) |
| λ | | Dilation parameter determining the compact support |
| | | of curvelets and also the angular scale at where |
| | | curvelets peak |
| $\lambda_{21 \mathrm{cm}}$ | 21.1 cm | Wavelength of hyperfine 21-cm line of neutral hydro- |
| | | gen |
| λ_{a} | | Mathematical affine parameter |
| Λ | | Cosmological constant or vacuum energy |
| $\mu_{ m B}$ | 9.27401×10^{-2} | ²¹ Bohr magneton |
| | ${\rm erg}{\rm G}^{-1}$ | |
| ν | | Radiation frequency |
| v_{21cm} | 1.42 GHz | Rest frequency of hyperfine 21-cm line of neutral hy- |
| | | drogen |
| ξ_{v} | $=\epsilon_{\nu}/\nu^2$ | Lorentz-invariant emission coefficient |
| Ξ | $= \frac{n_{\mathrm{u}}}{n_{\mathrm{l}}} \frac{g_{\mathrm{l}}}{g_{\mathrm{u}}}$ | Stimulated emission correction factor |
| Π_l, Π_c, Π_{tot} | | Linear, circular, or total polarisation fraction |
| ρ = | | Euler angles |
| (α, β, γ) | | |
| ρ^{\star} | | Euler angle describing the rotation to the North pole |

| Symbol | Remarks | Definition |
|--|------------------------------------|---|
| $(\alpha_a, \beta_b, \gamma_g)$ | | Sample positions of the adopted equiangular sam- |
| | | pling, where a, b , and g are indices of the Euler angles |
| Q | | Pitch angle of the emission |
| σ | | Standard deviation |
| $	au_{ u}$ | | Optical depth evaluated at frequency v |
| $\phi_{ u}$ | | Line profile function |
| Φ_{s} | | Scaling functions of curvelets capturing the low- |
| | | frequency content of signal |
| $arphi,\Deltaarphi$ | [rad] | Polarisation angle and its change |
| X | | Angle defined in Fig. A.1 |
| ${}_{s}\psi^{(j)}, {}_{s}\psi^{(j)}_{\ell m}$ | | Scale-discretised spin curvelets and its harmonic com- |
| | | ponents |
| ${}_s\widetilde{\psi}^{(j)}_{\ell m}$ | | Constructed scale-discretised spin curvelets centred at |
| | | colatitude $\vartheta^j = \cos^{-1}\left(\frac{-s}{\lambda^j}\right)$ |
| ω | $=2\pi\nu$ | Angular frequency |
| $\omega_{ m B}$ | | Electron angular gyro-frequency |
| $\omega_{ m p}$ | | Plasma frequency |
| $\omega_{ m R}$ | $=\omega_{\rm p}^2/\omega_{\rm B}$ | Razin frequency |
| $\Omega_{\rm m}, \Omega_{\rm r}, \Omega_{\Lambda}$ | | Density of matter, radiation, and cosmological con- |
| | | stant or vacuum energy, respectively |
| (x, y, z) | | Cartesian coordinates |
| $(\tilde{x}, \tilde{y}, \tilde{z})$ | | Cartesian basis defined in local system such as using |
| | | magnetic field |
| (a,b) | | Cartesian basis for "observer's" (or polarimeter's) sys- |
| | | tem |
| (r, θ, ϕ) | | Spherical coordinates |
| $\boldsymbol{\omega} = (\theta, \phi)$ | | Sky coordinates, where colatitude $\theta \in [0, \pi]$, and |
| | | longitude $\phi \in [0, 2\pi)$ |

| Symbol | Remarks | | Definition |
|---------------------------------|--------------|---|--|
| L ² -space | forms | a | The set of square-integrable L ² -functions. A function |
| | Hilbert spac | e | $f(x)$ is square-integrable if $\int_{-\infty}^{\infty} f(x) ^2 dx$ is finite |
| N | | | Naturals (positive integers including 0) |
| \mathbb{R}^+ | | | Positive real numbers |
| \mathbb{S}^2 | | | 2-sphere (the ordinary sphere, i.e. 2-dimensional |
| | | | spherical surface embedded in a 3-dimensional space) |
| SO(3) | | | Special orthogonal group in 3 dimensions, also known |
| | | | as the rotation group |
| \mathbb{Z} | | | Integers |
| δ_{ij} | | | Kronecker delta |
| $\delta(\cdot)$ | | | Dirac delta function |
| $\langle (\cdot) \rangle$ | | | Ensemble average |
| $\langle (\cdot, \cdot) angle$ | | | Inner products |
| [·], [·] | | | Floor and ceiling functions |
| .* | | | Complex conjugation (in curvelet context) |
| $\tilde{\cdot}$ | | | Unrotated quantity in curvelet construction |
| • | | | Denoting the line-of-sight component of the quantity |
| ·_ | | | Denoting the component perpendicular to the line-of- |
| | | | sight |
| •0 | | | Quantity measured at the present epoch (i.e. $z = 0$) |
| ·abs | | | Denoting quantity related to absorption |
| •ana | | | Denoting analytic value |
| ·central | | | Denoting the central value |
| ·centre | | | Denoting the line centre value |
| ·co | | | Denoting quantity measured in the comoving frame |
| ·coll | | | Denoting the collisional (pressure) damping |
| ·C | | | Denoting quantity related to continuum radiation |
| ·e | | | Denoting quantity related to electron |

| Symbol | Remarks | Definition |
|---------|---------|---|
| ·eq | | Denoting equal partition |
| •emi | | Denoting quantity related to emission |
| ·emp | | Denoting empirical value |
| ·HI | | Denoting quantity related to neutral hydrogen |
| 'init | | Denoting the initial quantity |
| ·1 | | Denoting quantity at the lower hyperfine level |
| ·L | | Denoting quantity related to a spectral line |
| •nt | | Denoting the non-thermal component of the quantity |
| ·obs | | Denoting the quantity measured at the observer frame |
| •ori | | Denoting quantity originating from a certain redshift |
| ·peak | | Denoting the peak value |
| ·rms | | Denoting the root-mean-square value |
| •rot | | Denoting quantity related to rotation |
| •sti | | Denoting quantity related to stimulated emission |
| •tot | | Denoting the total amount of the quantity |
| •th | | Denoting the thermal component of the quantity |
| •turb | | Denoting quantity related to turbulence |
| ·refine | | Denoting quantity used in the refinement scheme of |
| | | the CPRT algorithm |
| 'rad | | Denoting the radiative damping |
| ·u | | Denoting quantity at the upper hyperfine level |
| ·u | | Denoting quantity related to the transition from the |
| | | upper to the lower hyperfine level |
| ·v | | Denoting quantity that is velocity dependent |
| ·v | | Denoting quantity that is frequency dependent |

Preface

"You are all right. But you are all wrong too.

For each of you touched only one part of the animal."

– Karen Backstein,

Blind Men And The Elephant (The lo S Seis Ciegos Y El Elefante).

Chapter 1

Introduction

1.1 Thesis Overview

An important goal of astrophysics and cosmology is to understand how structures in the Universe formed and evolved over the cosmic history to the current state. The Universe is a complicated system. Today, it is predominantly filled with ionised plasmas, threaded by large-scale magnetic fields. The objective of my thesis is to understand these two important aspects: ionisation and magnetism in the Universe on the largest possible scales. These are two inter-related frontiers in fundamental astrophysics, namely **cosmic magnetism** and **cosmological reionisation**. They are underpinned by, and also somewhat underpin, the structural evolution of the Universe that we live in. Cosmic magnetism and cosmological reionisation are the research themes that form a number of key science projects for the upcoming unprecedentedly powerful radio telescope, the Square Kilometre Array (SKA). The scientific formulation, the methodologies, and the techniques developed in my research will enable astrophysicists to utilise the SKA observations for advancing our understanding of the structure evolution of the ionised, magnetised Universe.

This thesis focuses on providing a solution to each of the following immediate research questions:

- How to compute the polarisation, determine its statistical properties, and make reliable predictions of the continuum radio emission associated with magnetism that co-evolves with the structural evolution of the Universe?
- How to properly calculate the 21-cm hyperfine line of neutral hydrogen from an expanding, evolving Universe with broad ranges of length scales and time scales over cosmic time, as the Universe proceeded from a neutral phase to an

ionised phase?

• How to extract and characterise the structural information encoded in the data defined on a sphere, in particular the all-sky and wide-sky observational survey data that may carry spin information?

1.2 Thematic Sciences and Scientific Contexts

Charged particles interact with magnetic field, and the Universe is mostly ionised. Magnetic activities, therefore, are present everywhere, from substellar objects (e.g. Vallée 1998), stars (e.g. Parker 1970; Schrijver and Zwaan 2008; Vallée 2011), stellar systems (e.g. Feinstein et al. 2008; Landecker et al. 2010; Vallée 2011) and stellar remnants (e.g. Milne and Dickel 1974; Angel 1978; Putney 1997; Brogan et al. 2000; Taverna et al. 2015) to galaxies and the interstellar space (e.g. Beck 2008; Fletcher et al. 2011; Jones et al. 2012; Beck and Wielebinski 2013; Carretti et al. 2013; Iacobelli et al. 2013; Planck Collaboration XLIV 2016), to groups and clusters of galaxies (e.g. Carilli and Taylor 2002; Clarke 2004; Govoni and Feretti 2004) and the intergalactic and intercluster gas, (e.g. Xu et al. 2006; Ravi et al. 2016), and to cosmic filaments and voids (Neronov and Vovk 2010; Taylor et al. 2011).

Magnetic fields are important on the scales of galaxies and above. They contribute to the energy content of diffuse media such as interstellar gases (e.g. Beck 2003; Beck and Wielebinski 2013; McBride 2014; Rodrigues et al. 2015), intracluster medium (e.g. Carilli and Taylor 2002; Govoni and Feretti 2004), and intergalactic medium (e.g. Kronberg et al. 2001; Kronberg 2010). They also have intriguing interplay between turbulence and cosmic rays (e.g. Fermi 1949; Biermann and Schlüter 1951; Giacalone and Jokipii 1999; Subramanian et al. 2006; Yan and Lazarian 2008; Lazarian et al. 2012; Xu and Lazarian 2018). Magnetic fields are essential in the structural formation processes on the stellar scales (e.g. Balbus and Hawley 1991; Krumholz and Federrath 2019). They also play non-negligible roles in the structure formation processes on the galactic scales and beyond (e.g. Marinacci et al. 2015, 2018). Despite the omnipresence of magnetism in the Universe, there remain many open question surrounding the origin, evolution, and structure of large-scale cosmic magnetic fields.

Our current knowledge of cosmic magnetism will be greatly advanced with the forthcoming SKA all-sky polarisation surveys. With its wide field-of-view and unprecedented spectro-polarimetric capabilities, the SKA permits studies of the detailed structure of galactic and extragalactic magnetic fields across the entire sky, and allows us to peer more deeply into the evolution of cosmic magnetism (Gaensler et al. 2004; Johnston-Hollitt et al. 2015). Measurements of the strength and structure of the large-scale magnetic fields will set constraints on their origin, by distinguishing whether they originated from astrophysical processes, or from cosmological mechanisms that operated before the structural formation epochs.

The Universe today is structured as a vast cosmic web, and it is filled with brightly lit plasmas. As the observations of the cosmic microwave background (CMB) reveal, the Universe was once generally smooth and filled with neutral gas, which is mainly hydrogen. The Universe must have undergone a drastic transition, which ushered the Universe from being neutral into being completely ionised. A frontier in astronomical research concerns the cosmological reionisation process, which transformed the intergalactic space from a diffuse fog of neutral hydrogen into an ionised plasma network that we see today.

This transitional period, known as the Epoch of Reionisation (EoR), is yet to be fully charted observationally (see e.g. Morales and Wyithe 2010; Pritchard and Loeb 2012; Pritchard et al. 2015; DeBoer et al. 2017). The drivers of the cosmological reionisation are believed to be the radiations from the first stars and galaxies, which carved out ionised bubbles around them by their UV radiation, as well as from the first quasars, which harbour accreting super-massive blackholes, where the strong X-rays they emit would easily ionise the ambient gas (Barkana and Loeb 2001; Barkana 2006; Loeb 2001, 2011; Zaroubi 2013). The subsequent generations of the first stars, first galaxies and first quasars also contributed to the ionisation. As more stars, galaxies, and quasars emerged, the ionised bubbles that they produced percolated and overlapped until the entire intergalactic space become almost completely ionised.

Tracing how the sizes, morphology, number and spatial distribution of ionised regions (and also the neutral regions) evolved since the first coming of luminous structures (the Cosmic Dawn) will map out the Universe's reionisation history (e.g. Madau et al. 1997; Furlanetto and Briggs 2004). Measurements of these properties will, in turn, provide information of the nature and properties of the different groups of these first luminous ionising sources at great distances. This information is crucial for advancing our understanding of the formation and evolution of structures in the Universe and for the construction of a proper theory to describe how the Universe began, have evolved and will end. The EoR statistics, which span a substantial fraction of volume of the observable Universe, is also a powerful means to set constraints on the cosmological models (see e.g. Loeb and Zaldarriaga 2004; Zaldarriaga et al. 2004; Morales and Hewitt 2004; Morales and Wyithe 2010; Pritchard et al. 2015).

1.3 The Evolving Universe

Our understanding of the early hot phase of the Universe was established mostly based on CMB observations. The CMB radiation has an almost perfect thermal blackbody spectrum, with a characteristic temperature of about 2.7 K (see Penzias and Wilson 1965; Mather et al. 1994; Spergel et al. 2003; Planck Collaboration XVI 2014). After subtracting the background radiation, there are anisotropy patterns on the small scales in the CMB sky map, in spite of it appearing generally smooth on a global scale. These patterns are miniature temperature fluctuations at a level of about 1 part in 10⁵ (Smoot et al. 1992; Bennett et al. 2013; Planck Collaboration XVI 2014). The CMB anisotropies provide a stringent test for the theories of the early Universe. The hot Big Bang scenario (see e.g. Peacock 2003) and the associated cosmological inflation¹ theory (Guth 1981; Sato 1981; Albrecht and Steinhardt

¹Inflation postulates a very brief period of exponential expansion of the Universe driven by a highly energetic set of scalar fields during the first $\sim 10^{-32}$ seconds after the Big Bang (Guth 1981). Such an expansion provides a resolution to several outstanding problems that the Big Bang theory alone did not address (Linde 1982). These outstanding problems include: (i) the horizon problem (why causally independent regions in the Universe give nearly the same value for CMB temperature if it is not by assumption that the Universe is homogeneous and isotropic on cosmological scales?), (ii) the flatness problem (why the Universe is flat if it is not assumed in a specific set of initial conditions, i.e. the critical density of the Universe was extremely close to unity?), and (iii) the monopole problem (why not a single of magnetic monopoles has ever been detected, nor created experimentally, if the Big Bang models predict an efficient generation of these monopoles in the very hot early universe and that these monopoles should be stable enough to exist and be observed today?). Inflation
1982; Linde 1982) has been widely recognised and stood observational tests so far (e.g. Komatsu 2010; Planck Collaboration XXIV 2014; Planck Collaboration XVII 2015).

The Big Bang Universe started with a hot, dense phase, and the Universe expands. There was an early energetic epoch when atomic matter could not exist, and the entire Universe was a "soup" of radiation, electrons and protons (i.e. a hot ionised plasma). Electromagnetic radiation (photons) and charged particles were strongly coupled in this infant Universe. Photons interact with free electrons via Thompson scattering (see e.g. Padmanabhan 1993), and the large Thomson optical depth made the Universe opaque to electromagnetic radiation. As the Universe continued to expand, it gradually cooled down. It came a time when the material in the Universe was not energetic enough for atoms to remain ionised. Protons and electrons began to combine to form neutral hydrogen, and recombination left the Universe as a neutral medium, and to the photons, which had also been decoupled from the cosmic gas at this stage, a transparent medium. These photons freely streamed through the Universe and emerged as the CMB radiation. The CMB that we observe today is a snapshot of the cosmic time when the coupling of photons and electrons disengaged. This occurred when the Universe was just about 380 thousand years old, corresponding to a redshift $z \approx 1100$ (Planck Collaboration XVI 2014; Planck Collaboration XIII 2016; Planck Collaboration VI 2018).

The anisotropies in the observed CMB are fossils of the density fluctuations before cosmological recombination. These fluctuations are believed to be of quantum origin. They arose during the inflation era (Guth and Pi 1982) and were recorded as temperature fluctuations in the CMB, through the coupling of photons with the baryonic fluids (see e.g. Padmanabhan 1993). At the time of recombination, photons and the baryons and electrons were decoupled, and the previous density fluctuations fossilised into the free-stream photons, that became the CMB that we observe to-

also provides a mechanism to produce the inhomogeneity in the universe (Guth and Pi 1982; Hawking 1982; Starobinsky 1982; Bardeen et al. 1983), and gives specific predictions about the spatial pattern (scale-invariant and follows Gaussian statistics) of primordial fluctuation. Their predictions generally agree with the CMB observations (Planck Collaboration I 2015).

day. Fluctuations in the CMB not only preserve the primordial information but also provide the initial conditions for the subsequent structural evolution, such as galaxy formation, in the Universe.

The recombination era commenced at redshift $z \approx 1100$. At this redshift, the CMB has a temperature $T = 2.7 (1 + z) \text{ K} \sim 3000 \text{ K}$. As the Universe expanded, the CMB temperature continued to drop. The CMB was gradually shifted to the lower frequencies and eventually dropped out from the optical waveband, letting the Dark Ages of the Universe set in (see Miralda-Escudé 2003; Loeb and Furlanetto 2013; Natarajan and Yoshida 2014, for review and reference therein). For a hundred million years, starting from $z \sim 200$ till $z \sim 30$, the Universe remained dark.

No objects were there to shine in the Dark Ages, as the first stars were yet to ignite, although their formation was underway. The seed density enhancements sown in the earlier epoch were growing under self-gravity. At $z \sim 15 - 30$, the first astrophysical objects began to take shape, signalling the start of the Cosmic Dawn. Over time, the small-scale, over-dense regions acquired more and more matter falling into their developing gravitational well (contributed also by dark matter). The trapped baryons eventually collapsed into stars, on the small scales, and the trapped baryons and dark matter eventually assembled into galaxies, all under gravity but regulated by non-gravitational processes, in particular, the radiative cooling of the baryonic gas. When the first stars and the first galaxies emerged, the UV radiation that they produced ionised the neutral hydrogen gas in their surroundings into a plasma. The strong X-rays emitted from the first quasars, which were penetrative and could reach longer distances, provided additional ionisation power. The ionised regions expanded with the growing populations of stars, galaxies and quasars. These expanding ionised regions conglomerated, and the intergalactic space was progressively filled, leaving only some "islands" of neutral hydrogen gas that were shielded from the ionising UV radiation and X-rays.

UV radiation is heavily absorbed by neutral hydrogen. The Lyman- α (Ly α) emission from an astrophysical source will therefore be strongly suppressed if a substantial amount of neutral hydrogen is present along the line-of-sight. The

striking forests of Lyman- α absorption features observed² in the spectra of high-z quasars (Fan et al. 2006) indicate that the intergalactic medium was predominantly neutral hydrogen before becoming almost entirely ionised at $z \sim 6$, corresponding to about a billion years after the last scattering that produced the CMB (see Fan et al. 2006). Observational integrated constraint on the reionisation history of the Universe provided by the Thomson scattering of the CMB also indicates that the reionisation might end by $z \sim 6$, with the Thomson scattering optical depth $\tau = 0.054 \pm 0.007$ and a model-dependent redshift mid-point at 7.82 ± 0.71 (Planck Collaboration VI 2018).

The Cold Dark Matter (CDM) model predicts that the formation of structure in the Universe is hierarchical (see e.g. White et al. 1987), with clustering of matter occuring on small scales first and non-linear structures of ever-increasing sizes developed by merging processes. The large structures further collapsed to form sheets and filamentary structures, resulting in the cosmic web observed in the largescale cosmological galaxy surveys (Jõeveer et al. 1978; Bond et al. 1996; York and SDSS Collaboration 2000; Colless et al. 2001; Aihara et al. 2011; Sarkar and Pandey 2019).

How the Universe, in particular, the larger structures such as super-clusters, cosmic filaments and voids, become magnetised is still an open question in fundamental astrophysics. The magneto-genesis could be a complex, multi-channel process. Nonetheless, it would involve at least a mechanism for the seed field generation and the subsequent processes that can efficiently amplify the seed field. There are a number of propositions for the seed-field generation. It has been argued that primordial magnetic fields (e.g. Turner and Widrow 1988; Grasso and Rubinstein 2001; Giovannini 2004; Widrow et al. 2012; Davies and Widrow 2000; Kobayashi et al. 2007; Subramanian 2008; Kandus et al. 2011; Durrer and Neronov 2013; Naoz and Narayan 2013; Ichiki et al. 2006; Kronberg 2016b; Subramanian 2016; Han 2017) were generated during inflation, and the subsequent radiation era

²The Ly α forests are measured at the frequencies from far-ultraviolet to near-infrared, corresponding to the redshifted frequencies of the Ly α line.

(> $z_{equality} = 3371$) before and during cosmological recombination ($z \approx 1100$). At a later structural formation stage magnetic fields could be created by a local Biermann battery process (Biermann 1950), when the density and pressure gradients are misaligned (often occurring in shocks, gravity-induced mergers and gravitational collapse). Magnetic fields could also be produced by the Weibel instability (Weibel 1959; Huntington et al. 2015; Huntington et al. 2017), which grow from anisotropies in the velocity distribution of plasma, such as those in relativistic jets and outflows.

Stars (e.g. the Sun) are known to be magnetised. When they evolve and die, part of their magnetic fields will be expelled into their surroundings, via stellar wind or more catastrophic events, such as supernova explosion. In the nearby Universe, galactic outflows driven by star-forming and/or AGN activities would deliver the magnetised material to the circum-galactic and intergalactic space. Similarly, during the Cosmic Dawn, supernova explosions of the very massive first stars (also known as the population-III stars) would eject magnetic fields into the interstellar medium (ISM). Magnetised galactic outflows, driven either by the early epochs of violent starformation or by the onset of accretion of the nuclear black holes in galaxies, would deliver galactic magnetic fields into the intergalactic medium (IGM), and into the intracluster medium (ICM; when galaxy clusters began to assemble) (see Kronberg et al. 1999; Völk and Atoyan 2000; Colgate and Li 2000). Despite this appealing qualitative scenario, the mixing of the magnetised gas injected from galaxies with the unmagnetised gas in the surrounding environments is still an issue yet to be resolved, needless to say whether the vast volume in the Universe is actually magnetised by galaxies.

Today, we see structures on various scales in the Universe, from stars and galaxies to cosmic filaments and voids. We also see diffuse media – the ISM, ICM and IGM – on various scales, and these diffuse media have different properties. ISM are multi-phase mixtures of ionised plasma, neutral atomic and molecular gas, and dust. They can be found in a more condensed form, i.e. molecular clouds. Molecular clouds are relatively cold gas condensates. They typically have a temperature $\sim 10 - 50$ K. This is in contrast to the temperatures of the ambient ISM, where the cold neutral medium has a temperature ~ 100 K, the warm neutral medium has a temperature ~ 5000 K, and the hot ionised medium has a temperature ~ $10^4 - 10^{5.5}$ K or even higher (Draine 2011). ICM are highly-ionised hot gases trapped inside galaxy clusters by gravity. The ICM temperature reflects the depth of the cluster gravitational well and the recent dynamical history of the host clusters. ICM are hot enough to emit X-rays in the 0.1 – 10 keV energy range. Spectroscopic X-ray observations of galaxy clusters showed that the ICM generally have a thermal temperature ~ $10^6 - 10^8$ K (see Fabian 1994; Böhringer and Werner 2010). IGM are also multiphase gases. Our knowledge of IGM is still very primitive. IGM are thought to be complex and diffuse, as their many aspects in the dynamics, thermodynamics and chemistry, are influenced by the history and activities in nearby galaxies and in the higher structural hierarchy where they reside. Current observations have identified a warm-hot component, which has a temperature between 10^5 and 10^7 K, in the filaments, and a cold component, which has a temperature of < 10^5 K, in the very tenuous diffuse regions (Ryden and Pogge 2016).

The missing big gaps in our knowledge of when the first structures formed, how the reionisation proceeded, and how the first magnetic fields developed, have left us many related open questions. To understand how the cosmos acquires its magnetisation on the large scales and how reionisation proceeded, proper theoretical tools in modelling and in analysis are needed, in addition to the collection of more data through observations and experiments. In the aspect of theoretical modelling of radiation and providing testable predictions to compare with observations, radiative transfer is an essential tool. In the context of understanding the physical processes in the development of the large-scale cosmic magnetic fields and in the progression of transforming the intergalactic gas from a neutral phase to a predominantly ionised phase, constructing a proper covariant cosmological radiative transfer formulation for the calculations of the radio polarised continuum radiation and of the 21-cm hyperfine line of neutral hydrogen is a necessity. The radiation that we observe has propagated through an evolving, expanding, structured Universe. On its journey from the distant past to us in the present day, radiation processes and varieties of astrophysical sources and intervening media can leave imprints on the radiation. The radiation itself is also subject to stretches in wavelengths due to the cosmological expansion of the Universe. The observed radio continuum polarisation and the 21-cm hyperline of neutral hydrogen are shaped by these processes. Meaningful comparisons between theories, models and observations require reliable quantification and characterisation of the data, and accurate information extraction from the data. The observational studies of large-scale cosmic magnetism and cosmological reionisation would require wide-sky and all-sky surveys, where the data would live on the celestial sphere. It is therefore a necessity to develop diagnostic tools to characterise and extract information from the data registered in a spherical geometry. The constructions of a covariant cosmological radiative transfer formulation and of a new spherical data analysis technique are, therefore, the technical foci of my thesis research.

1.4 Structure of the Thesis

Driven by the two key thematic sciences, cosmic magnetism and cosmological reionisation, this thesis focuses on developing a proper formalism and appropriate methodologies for the studies of the emergence and evolution of large-scale magnetic fields and for the proceeding of the reionisation of the Universe. More specifically, my thesis research provides a solid foundation for robust diagnostics of all-sky observations, based on a covariant formulation for cosmological radiative transfer in continuum polarised radiation and in 21-cm line radiation. My thesis work also includes the construction of data-characterisation tools, using wavelet-based techniques. These tools are newly derived and applied to test various physical scenarios against all-sky or wide-sky observational data. My thesis contains three main components, which are inter-connected to each other as illustrated in Fig. 1.1.

The remainder of the thesis is organised as follows. In **Chapter 2**, I show the derivation of the covariant cosmological polarised radiative transfer equation and provide an introduction to wavelet analysis. In **Chapter 3**, I show the computational algorithm that I develop to calculate the polarised continuum radiation arisen from



Fig. 1.1: This thesis concerns two aspects of the Universe: magnetism and reionisation. It presents formulations and methodologies, linking theory, models, and observation, in the context of forward modelling and backward modelling. For forward modelling, I develop covariant cosmological radiative transfer formalisms for both polarised continuum radiation and 21-cm line radiation. The covariant cosmological polarised radiative transfer calculates the all-sky polarisation of large-scale structures obtained from cosmological magnetohydrodynamic (MHD) simulations. The covariant cosmological 21-cm line radiative transfer calculates the radiative signals from the Epoch of Reionisation (or the preceding Dark Ages) to the present Universe. For inverse-problem applications, I construct a new curvelet transform on a sphere, which can efficiently extract and characterise elongated features in any natural spherical images, in particular, those obtained from the all-sky cosmological surveys or wide-sky astronomical observations.

sources in the Universe across the cosmic time. I also present an illustrative numerical calculation of all-sky polarisation. In **Chapter 4**, I show the derivation of a covariant formulation for cosmological radiative transfer of the 21-cm line, with the objective of acquiring a quantitative understanding of how the reionisation of the Universe proceeded over time. I also show the verification of numerical calculations in a local frame setting, by means of 21-cm galaxy tomography, and a demonstration in a global frame setting, which is essential for making theoretical models in 21-cm tomography. In **Chapter 5**, I show my construction of a new curvelet transform on the sphere for efficient extraction of features with elongated structures, e.g. edges and filaments. They are particularly useful for the studies in wide-field astronomical observations, such as those of the all-sky surveys of the continuum polarisation and of the structured 21-cm line. The applications of the curvelets that I construct are not restrictive to only astronomical research involving wide-field data on the celestial sphere. These curvelets are also applicable for the analysis of data on spheres in areas outside astrophysics. A brief summary of this thesis is given in **Chapter 6**.

1.5 Adopted Conventions

The conventions used in this thesis are declared below. Unless otherwise specified, the c.g.s. Guassian units are used. A [-, +, +, +] signature is adopted for the space-time metric.

Polarisation convention conforms to the IEEE/IAU standard described in Appendix B given the coordinate systems explicitly defined in Appendix A. Attentions are also drawn to the opposite sign (to the IAU standard) of Stokes parameter U of linear polarisation used in the CMB community³, as well as to the factors that alter the sign concerning Stokes parameter V of circular polarisation (see Appendix B for discussion).

The convention for the magnetic field is such that the field is positive when pointing towards the observer. This is opposite to the traditional astronomical convention (see Appendix B for relevant discussion). Geometry of the radiative transfer problems considered in Chapters 3 and 4 are specified in Appendix A, following similar coordinate systems as Huang and Shcherbakov (2011), such that consistency of the signs of the Stokes parameters and their corresponding transfer coefficients could be checked.

ACDM cosmology is assumed throughout this thesis. The maximum likelihood cosmological parameters obtained by Planck Collaboration XIII (2016) are considered: the present Hubble constant is $H_0 = 100 h_0 = 67.74 \text{ kms}^{-1} \text{Mpc}^{-1}$, the present matter density is $\Omega_{m,0} = 0.3089$, the baryonic density is $\Omega_{b,0} = 0.0223(h_0)^{-2}$, and the cosmological constant or vacuum density today is $\Omega_{\Lambda,0} = 0.6911$. The radiation density today is given by $\Omega_{r,0} = 4.1650 \times 10^{-5} (h_0)^{-2}$ (Wright 2006).

Rotation of functions on a sphere is specified by the Euler angles. The zyz Euler

³When spherical pixelisation scheme HEALPIX (Górski et al. 2005) is used to compute polarisation power spectra, which are widely adopted in the CMB studies, note that a sign flip of U is needed to bring the sign consistent to the IAU standard.

convention is adopted, corresponding to the rotation of a physical body in a fixed coordinate system about the *z*, *y* and *z* axes by the angles γ , β and α , respectively (see Sec. 2.5.2). The Condon-Shortley phase convention is adopted in the spin spherical harmonic functions (see Sec. 2.5.1 for its definition).

Chapter 2

Radiative Transfer and Wavelet Characterisation

This chapter reviews the theory of (i) cosmological radiative transfer, and (ii) wavelet transform on the sphere, concisely, and addresses the question of *why they are important*. For (i), it starts with summarising the classical description of radiative transfer theory, continues with the formal expressions for the covariant equation of cosmological radiative transport (Chan et al. 2019), and ends with the transfer of (a) polarised continuum radiation for studying large-scale cosmic magnetism, and (b) 21-cm line radiation for studying the Cosmic Dawn and the Epoch of Reionisation. For (ii), it begins with a brief introduction of wavelets, and follows by a discussion on curvelets and wavelet transform on a sphere (see Chan et al. 2017).

2.1 Radiative Transfer

As radiation (e.g. electromagnetic radiation) passes through matter, it may undergo absorption, emission, and scattering. These interactions will modify the radiation, and, in addition, leave imprints of the physical properties of the medium. Radiative transfer deals with how radiation propagates, and is modified through the interaction with matter. This leads to a critical question: *how do the overall properties of the radiation from astrophysical sources change on its course of travel to reach us?* This question is essential, as theories can only be tested against observations with confidence when we have a proper understanding of the information encoded in the radiation that we receive. This, in turn, affects the technical approaches that we would adopt for the forward modelling and the inverse modelling.

In forward modelling, one first calculates the radiation from the sources. The

pertinent physical properties of the material along the line-of-sight are specified first, and with which we calculate the radiation and determine how it is transported and hence the observable signatures in the radiation. This is facilitated by solving the radiative transfer equation (on a specific space-time), and hence the forward problem is essentially solving the transfer equation to predict the observables.

In inverse modelling, one deduces the properties of a medium or the emitter from the observed signals. Models are physical interpretations derived from the observational data. Many astrophysical problems are in fact of inverse modelling nature. Two examples are related to the core science of my thesis. The corresponding questions that I seek to answer are: (i) what does the emergent polarisation say about the characteristics of large-scale magnetic fields, and (ii) what does the spatial and spectral information encoded in tomographic observational data of the 21cm line emission say about the morphological progress of the cosmological reionisation?

I investigate the transfer of electromagnetic radiation (in the radio frequencies) emitted from the Universe spanning from a distant past to the present day. My focus is on (i) the polarised continuum radiation encoded with the information of largescale cosmological magnetic fields that co-evolved with the structural evolution of the Universe, and (ii) the 21-cm line associated with the hyperfine transition of neutral hydrogen at Cosmic Dawn and the Epoch of Reionisation. As these radiation travel over cosmological distances, they are modified accordingly, subject to global effects, such as cosmic expansion and cosmological structural evolution, and local effects, such as the ionisation state of the material along the line-of-sight and the presence of turbulence and local hydrodynamic flows. There are both observational aspects and theoretical aspects in the analyses of these radiation. However, the two kinds of aspects are not always separable, because inference is, by nature, an inverse process. In addition to the improvement in the statistical methods, constructing correct theoretical models and deriving a workable formalism for theoretical calculations are also an urgent necessity, given the advent of instruments, such as the Square Kilometre Array (SKA), which will collect a vast amount of observational data.

The studies of all-sky polarisation data and all-sky cosmological 21-cm data are still in an infant stage, although work has already started some decades ago. For reviews on polarised radio emission as diagnostics of cosmic magnetism, see e.g. Gardner and Whiteoak (1966); Asseo and Sol (1987); Saikia and Salter (1988); Kronberg (2016a); Widrow (2002); Widrow et al. (2012); Han (2017), and references therein. For reviews on using cosmological 21-cm line to probe the transitional epochs of the Universe, see e.g. Furlanetto et al. (2006); Morales and Wyithe (2010); Pritchard and Loeb (2012); Loeb and Furlanetto (2013); Glover et al. (2014); Furlanetto (2016), and references therein.

In current theoretical and observational studies of cosmic magnetism and cosmological reionisation, simplified models are often used, even though very advanced statistical methods are employed. For instance, rotation measure has been a workhorse for the diagnosis of the large-scale magnetic field, although this can be better achieved by a polarised radiative transfer (PRT) calculation. Note that rotation measure calculations are a simplification using a restricted form of polarised radiative transfer; see Appendix D. The use of rotation measure overlooks certain subtle complexity such as the contribution of density fluctuations and the convolution of density fluctuations and magnetic field fluctuations.

In the tomographic studies of 21-cm line associated with cosmological reionisation, theoretical universes are generated by numerical simulations employing a cubic comoving volume whose structure is allowed to evolve with the cosmological time. They also involve a separate prescription to take account for only the light from the past that can reach now (e.g. Ross et al. 2019, using a method of "light-cone construction"). Although the evolution of the simulation cube can be visualised on a computer screen, the visualisation is not a proper representation of the observation. The radiation that we observe is a convolution of the radiation arisen from different parts of the Universe at different cosmological epochs. They are not the same as the radiation arisen from the same part of the Universe at different cosmological epochs. Cross-correction of the radiation from a model universe using the same simulated cube would give artefacts. These false signals arise from correlating the same particular region in a universe at different stages of evolution, as the simulation is essentially a continuous self-mapping process, which is inevitably subject to Brouwer's fixed point theorem (see e.g. Starr 2011; Farmakis and Moskowitz 2013).

My study of the cosmological radiative transfer will provide a means to address all of these issues properly and so to derive methods to avoid the known serious pitfalls in the current approaches in theoretical modelling of the observables, while still taking the advantage of the vast resources in the sophisticated cosmological hydrodynamic simulations.

2.1.1 Polarised radiative transfer

From the conservation of energy, we may obtain an expression for the radiation transfer equation (neglecting scattering), in a local rest reference frame:

$$\frac{\mathrm{d}I_{\nu}}{\mathrm{d}s} = -\kappa_{\nu}I_{\nu} + \epsilon_{\nu} = -\kappa_{\nu}(I_{\nu} - S_{\nu}) \tag{2.1}$$

(see e.g. Mihalas 1978), where the subscript ν denotes the radiation frequency. Hence, I_{ν} is a specific intensity, and $S_{\nu} = \epsilon_{\nu}/\kappa_{\nu}$ is the specific source function. The radiative transfer equation describes the change in the specific intensity, dI_{ν} , over a path length ds passing through a medium with an emission coefficient, ϵ_{ν} , and absorption coefficient, κ_{ν} . The specific intensity at a location r, is the amount of energy dE_{ν} , in a frequency range $d\nu$, crossing an area dA of a normal \hat{n} , over the solid angle d\Omega around the direction \hat{s} in a time interval dt, i.e.

$$I_{\nu}(\boldsymbol{r},t)\Big|_{s} = \frac{\mathrm{d}E_{\nu}}{(\hat{\boldsymbol{s}}\cdot\hat{\boldsymbol{n}})\,\mathrm{d}A\,\mathrm{d}t\,\mathrm{d}\nu\,\mathrm{d}\Omega} \tag{2.2}$$

(see e.g., Rybicki and Lightman 1986). It has the units of erg s⁻¹ cm⁻² Hz⁻¹ str⁻¹. I_{ν} is a macroscopic quantity. It can be defined in a ray along which radiation propagates and is therefore often used to describe the energy transported by a bundle of photons of the same energy in a ray¹.

¹Note that quantum properties of light imposes certain restrictions for the ray approximation (Younsi 2013, PhD thesis, UCL). Firstly, due to the uncertainty principle, $dA d\Omega \gtrsim \lambda^2$, where λ is the wavelength of radiation, when $dA \sim \lambda^2$, one can no longer define the ray direction with accuracy. The concepts of ray would break down. Also, $dE dt \gtrsim \hbar$, hence $d\nu dt \gtrsim 1/2\pi$. When the wavelength of radiation exceeds atomic scales, Eqn. (2.2)

In the absence of emission ($\epsilon_v = 0$) and absorption ($\kappa_v = 0$), $dI_v/ds = 0$, and hence, I_v remains constant along a ray. If only emission is present (i.e. $\kappa_v = 0$ and $\epsilon_v \neq 0$), then the change in the intensity over a distance ds is simply $dI_v = \epsilon_v ds$, with the emission coefficient ² given by $\epsilon_v(\mathbf{r}, t)|_s = dE_v/((\hat{s} \cdot \hat{n}) dV dt dv d\Omega)$, which has a unit of erg s⁻¹ cm⁻³ Hz⁻¹ str⁻¹ (since [ds] = [dV]/[dA]). If only absorption is present (i.e. $\epsilon_v = 0$ but $\kappa_v > 0$), then $dI_v = -\kappa_v I_v ds < 0$. The absorption coefficient has a unit of cm⁻¹. Note that the absorption coefficient κ_v can take a negative value, resulting in $dI_v > 0$. This corresponds to a stimulated emission, which is effectively a negative absorption.

For a polarised radiation, the radiative transfer process involves not only the change in the energy due to gain by emission or loss by absorption, but also the interconversion between the polarisation components. The polarisation will modify as the radiation propagates, and the processes can be decomposed into Faraday rotation, which alters the angle of the plane of polarisation, and Faraday conversion, which involves the conversion between the linear and circular polarisation components. A commonly used formalism in astrophysics describes these effects in terms of the 4-Stokes parameters. From these, we can derive the according transfer coefficients within the 4-Stokes framework and obtain a polarised radiative transfer equation. This equation is conveniently expressed in terms of matrices, and it takes the form:

$$\frac{\mathrm{d}I_{i,\nu}}{\mathrm{d}s} = -\kappa_{ij,\nu}I_{j,\nu} + \epsilon_{i,\nu} \ . \tag{2.3}$$

In an explicit matrix representation, it is

$$\frac{\mathrm{d}}{\mathrm{d}s} \begin{bmatrix} I_{\nu} \\ Q_{\nu} \\ U_{\nu} \\ V_{\nu} \end{bmatrix} = -\begin{bmatrix} \kappa_{\nu} & q_{\nu} & u_{\nu} & v_{\nu} \\ q_{\nu} & \kappa_{\nu} & f_{\nu} & -g_{\nu} \\ u_{\nu} & -f_{\nu} & \kappa_{\nu} & h_{\nu} \\ v_{\nu} & g_{\nu} & -h_{\nu} & \kappa_{\nu} \end{bmatrix} \begin{bmatrix} I_{\nu} \\ Q_{\nu} \\ U_{\nu} \\ V_{\nu} \end{bmatrix} + \begin{bmatrix} \epsilon_{I,\nu} \\ \epsilon_{Q,\nu} \\ \epsilon_{U,\nu} \\ \epsilon_{V,\nu} \end{bmatrix}$$
(2.4)

using I_{ν} as a fundamental variable would no longer provide a good description of the interaction of light on atomic scales. Nonetheless, the standard description of radiative transfer theory is still valid macroscopically. ²Note that some of the literature denote ϵ_{ν} defined here as j_{ν} , and κ_{ν} here as α_{ν} .

(see Unno 1956; Sazonov 1969; Pacholczyk 1970; Jones and O'Dell 1977a; Pacholczyk 1977; Degl'innocenti and Degl'innocenti 1985; Huang and Shcherbakov 2011; Janett et al. 2017a,b; Janett and Paganini 2018). The indices *i* and *j* runs from 1 to 4, corresponding respectively to the components I_{ν} , Q_{ν} , U_{ν} and V_{ν} in the 4-Stokes parameter formulation.

The Stokes parameters are measurable with appropriate instrumental design and observational techniques. The first component I_v is the specific intensity of the radiation. It is contributed by all the polarisation components. Using it and the other Stokes parameter, we may construct useful quantities for describing the polarisation properties of the radiation. For instance, the total degree of polarisation at a particular frequency v is $\Pi_{tot} = \sqrt{Q_v^2 + U_v^2 + V_v^2}/I_v$. This quantity equals to 1 for fully polarised radiation, and it is less than 1 if the radiation is partially polarised. The degree of linear polarisation is given by $\Pi_1 = \sqrt{Q_v^2 + U_v^2}/I_v$, and the polarisation angle by $\varphi = (1/2) \tan^{-1}(U_v/Q_v)$. Thus, Q_v and U_v are the two parameters specifying the linear polarisation. The degree of circular polarisation $\Pi_c = V_v/I_v$, and hence V_v is the parameter specifying the circular polarisation (see e.g. Rybicki and Lightman 1986).

In the transfer equation, emission is specified by the emission coefficient $\epsilon_{i,v}$. Transfer effects are specified by the matrix $\kappa_{ij,v}$, analogous to the role of the absorption coefficient in the radiative transfer equation for non-polarised radiation. In $\kappa_{ij,v}$, the κ_v , q_v , u_v and v_v components account for the absorption of the corresponding Stokes parameters, the f_v component for Faraday rotation, and g_v and h_v components for the inter-conversion between linear and circular polarisation.

Faraday rotation is induced by circular birefringence due to the slight difference in the speeds that left and right circularly polarised radiation propagate in a magneto-ionic medium. This leads to a rotation of the angle of polarisation in the linear polarisation modes when the radiation propagates, resulting in the conversion $Q_{\nu} \leftrightarrow U_{\nu}$ in the 4-Stokes formulation. Faraday conversion is caused by linear birefringence, which is manifested in the inter-conversion between the linear and circular polarisation modes of the radiation. In the 4-Stokes formulation, it is $(Q_{\nu} \leftrightarrow V_{\nu}, U_{\nu} \leftrightarrow V_{\nu})$. The transfer matrix $\kappa_{ij,\nu}$ can be decomposed into a symmetric part and an anti-asymmetric part, and it contains ten independent components. The symmetric part consists of only the absorptive components, and hence, it governs the dissipation when the radiation propagates. The anti-symmetric part consists of the rotation and conversion components, and hence, it specifies the corresponding polarisation modulation in the propagation process. The polarised radiative transfer equation (presented above) in this form is applicable for radiative transport in weakly anisotropic medium (Sazonov and Tsytovich 1968; Sazonov 1969; Jones and O'Dell 1977a; Pacholczyk 1977).

Stokes parameters are dependent on the coordinate system, and each parameter alone is not invariant when undergoing a coordinate transformation. However, it is possible to derive invariant quantities with the linear combination of the Stokes parameters. For instance, the two linear polarisation Stokes parameters can be combined to a complex conjugate pair ($Q_v \pm i U_v$), which are invariant under coordinate transformation. This pair can be linearly transformed to the so-called the *E*- and *B*modes of the linear polarisation, corresponding to an odd-parity and an even-parity polarisation, respectively.

In the study of polarised properties of an astrophysical source using a Stokesparameter formulation, the coordinate system on which the specific representation is constructed, the exact definition of the polarisation and convention by which the polarisation is defined must be clearly stated. Otherwise, it will lead to ambiguities in the theoretical calculations and improper interpretations of the observations. For instance, the handedness of the coordinate system (left-handed or right-handed) will give rise to different signs in transfer coefficients in the polarised radiative transfer equations (cf. Sazonov 1969; Pacholczyk 1970; Melrose and McPhedran 1991; Huang and Shcherbakov 2011). This coordinate handedness is also manifested in the sign of the Stokes parameter V_{ν} , which specifies the circular polarisation. There are also different conventions in the definition of the polarisation angle³, the

³Investigations of the polarisation of the CMB adopt the opposite convention to the International Astronomical Union (IAU) standard, for which polarisation angle increases clockwise (counterclockwise) when looking at the source for the former (latter). To rectify the discrepancy, an opposite

handedness of circular polarisation, and the Stokes parameter V_{ν} (see Robishaw 2008, for a compilation of the conventions used in radio polarisation work). All of these must be clarified before carrying out polarised radiative transfer calculations of extracting information from observed polarisation data by means of a theoretical or simulated models.

In Appendix A, the coordinate systems and the underlying geometry considered in this study are shown, and in Appendix B, the intricacies of keeping a consistent polarisation convention is discussed. The Stokes parameter U_v and its associated coefficients, u_v , g_v and $\epsilon_{U,v}$, can be made to vanish by a choice of a local coordinate system (see Sazonov 1969; Pacholczyk 1977). This is illustrated in Fig. A.1 in Appendix A, where u_v , g_v and $\epsilon_{U,v}$ become zero in the basis (x, y), because the projection of the magnetic field onto the (x, y)-plane is parallel to y. In this representation, the circular polarisation Stokes parameter V_v couples only to one if the linear polarisation Stokes parameter U_v , but $V_v \leftrightarrow Q_v$.

2.1.2 Lorentz-invariant radiative transfer equations

The covariant formulation for radiative transfer without the consideration of polarisation were presented in Rybicki and Lightman (1986); Fuerst and Wu (2004); Younsi et al. (2012) for special relativistic and general relativistic settings. I elaborate the derivation of Lorentz-invariant radiative transfer equation here, following the approach adopted in Fuerst and Wu (2004) and Younsi et al. (2012), before I present a more general, fully covariant radiative transfer formulation and the cosmological radiative transfer equation. Consider a bundle of particles (presumably photons) filling a phase-space volume element $d\mathcal{V} \equiv d^3x d^3p$ (where the 3-spatial volume element $d^3x = dx dy dz$ and the 3-momentum volume element $d^3p = dp_x dp_y dp_z$ in the Cartesian coordinates) at a given time *t*. The Liouville's theorem states that $d\mathcal{V}/d\lambda_a = 0$ (Misner et al. 2017), implying that the phase-space volume element $d\mathcal{V}$ is an invariant quantity.

sign has to be applied to the Stokes parameter U_{ν} (see https://aas.org/posts/news/2015/12/ iau-calls-consistency-use-polarisation-angle).

The distribution function of the particles in the bundle is essentially the phase-space density and is given by f(x, p) = dN/dV, where dN is the number of particles in dV. Particle number is a scalar. Therefore dN/dV is Lorentz invariant. Hence f(x, p) is also Lorentz invariant.

Photons are massless relativistic particles with speed v = c. For a bundle of photons with energy E (= cp), the spatial and momentum volume elements in the phase-space are $d^3x = dAc dt$ and $c^3d^3p = E^2 dE d\Omega$, respectively, where dA is the area element through which the photons travel in the time interval dt and $d\Omega$ corresponds to the direction of photon propagation. This gives a distribution function

$$c^{-3}f(\boldsymbol{x},\boldsymbol{p}) = \frac{\mathrm{d}N}{\mathrm{d}A\,c\,\,\mathrm{d}t\,E^2\,\,\mathrm{d}E\,\,\mathrm{d}\Omega} \tag{2.5}$$

(cf. Fuerst and Wu 2004; Younsi et al. 2012). The specific intensity of the radiation, in terms of energy of the photons, E, may be expressed as

$$I_E = \frac{E \, \mathrm{d}N}{\mathrm{d}A \, \mathrm{d}t \, \mathrm{d}E \, \mathrm{d}\Omega} \,, \tag{2.6}$$

along the propagation of the ray and across a surface element dA perpendicular to the ray propagation. Thus,

$$\frac{I_E}{E^3} = c^{-2} f(x, p)$$
(2.7)

is invariant under Lorentz transformation. It follows that I_{ν}/ν^3 is a Lorentz-invariant quantity. Hence, we may define a Lorentz-invariant specific intensity

$$I_{\nu} \equiv \frac{I_{\nu}}{\nu^3} . \tag{2.8}$$

Note that the increment of the optical depth along a ray $d\tau_v (= \kappa_v ds)$ is a scalar, and hence it is invariant when undergoing a coordinate transformation. We may therefore expect the Lorentz-invariant radiative transfer equation to take this form:

$$\frac{\mathrm{d}I_{\nu}}{\mathrm{d}\tau_{\nu}} = -I_{\nu} + \mathcal{S}_{\nu} \tag{2.9}$$

(see Rybicki and Lightman 1986; Fuerst and Wu 2004). Here, S_{ν} is the Lorentzinvariant specific source function. We may obtain by a dimensional analysis the Lorentz-invariant absorption and emission coefficients, with respect to the Lorentzinvariant intensity, and they are $\zeta_{\nu} = \nu \kappa_{\nu}$ and $\xi_{\nu} = \epsilon_{\nu}/\nu^2$, respectively (see Fuerst and Wu 2004). Thus, the Lorentz-invariant specific source function is

$$S_{\nu} \equiv \frac{\xi_{\nu}}{\zeta_{\nu}} = \frac{1}{\nu^3} \left(\frac{\epsilon_{\nu}}{\kappa_{\nu}} \right) = \frac{S_{\nu}}{\nu^3} , \qquad (2.10)$$

where S_{ν} is the specific source function as that in Eqn. (2.2).

The coefficients ζ_{ν} and ξ_{ν} are Lorentz-invariant, and their values measured in the observer's frame and in the comoving frame (i.e. the local rest frame of the medium, denoted by "co") are related by $\nu \kappa_{\nu} = \nu_{co} \kappa_{\nu,co}$ and $\epsilon_{\nu}/\nu^2 = \epsilon_{\nu,co}/\nu_{co}^2$. It follows that the Lorentz-invariant radiative transfer equation, in terms of radiation path length and the intensity and absorption and emission coefficients evaluated in the local comoving frame is

$$\frac{\mathrm{d}I_{\nu}}{\mathrm{d}s}\bigg|_{\mathrm{co}} = \left(-\kappa_{\nu} I_{\nu} + \frac{\epsilon_{\nu}}{\nu^{3}}\right)\bigg|_{\mathrm{co}},\qquad(2.11)$$

(Fuerst and Wu 2004; Younsi et al. 2012), which may also be expressed as

$$\frac{\mathrm{d}}{\mathrm{d}s} \left(\frac{I_{\nu,\mathrm{co}}}{\nu_{\mathrm{co}}^3} \right) = -\kappa_{\nu,\mathrm{co}} \left(\frac{I_{\nu,\mathrm{co}}}{\nu_{\mathrm{co}}^3} \right) + \left(\frac{\epsilon_{\nu,\mathrm{co}}}{\nu_{\mathrm{co}}^3} \right) \,. \tag{2.12}$$

2.1.3 Covariant radiative transfer formulation

In this section and the next, unless otherwise stated, the natural unit convention, with $c = G = \hbar = 1$, is adopted.

In general relativistic settings, it is more desirable that the radiative transfer equation is expressed in terms of space-time intervals instead of the optical depth or path length in the 3-space. This can be achieved by introducing an affine parameter λ_a . With this, the problem is translated into an evaluation of $ds/d\lambda_a$ (i.e. the variation in the path length *s* with respect to λ_a), and the comoving 4-velocity v^{β} of a photon travelling in the medium (which is practically a fluid) that has 4-velocity u^{β} .

For photon with a 4-momentum k^{α} , the comoving 4-velocity v^{β} can be obtained by the projection of k^{α} on to the fluid frame, i.e.

$$v^{\beta} = P^{\alpha\beta}k_{\alpha} = k^{\beta} + (k_{\alpha}u^{\alpha})u^{\beta}$$
(2.13)

(Fuerst and Wu 2004), where the projection tensor $P^{\alpha\beta} = g^{\alpha\beta} + u^{\alpha}u^{\beta}$, with $g^{\alpha\beta}$ as the space-time metric tensor. The variation in *s* with respect to λ_a is therefore

$$\frac{\mathrm{d}s}{\mathrm{d}\lambda_{\mathrm{a}}} = - \left\| v^{\beta} \right\| \Big|_{\lambda_{\mathrm{a,obs}}}
= -\sqrt{g_{\alpha\beta}(k^{\beta} + (k_{\alpha}u^{\alpha})u^{\beta})(k^{\alpha} + (k_{\beta}u^{\beta})u^{\alpha})} \Big|_{\lambda_{\mathrm{a,obs}}}
= -k_{\alpha}u^{\alpha} \Big|_{\lambda_{\mathrm{a,obs}}}$$
(2.14)

(Younsi et al. 2012). Note that for a stationary observer positioned at infinity $k_{\beta}u^{\beta} = -E_{obs}$. It follows that the ratio

$$\frac{k_{\alpha}u^{\alpha}\Big|_{\lambda_{a,co}}}{k_{\beta}u^{\beta}\Big|_{\lambda_{a,obs}}} = \frac{\nu_{co}}{\nu_{obs}},$$
(2.15)

which corresponds to the relative energy shift of the photon between the observer's frame and the comoving frame. Using the Lorentz-invariant properties of I_{ν} , ζ_{ν} and ξ_{ν} yields the covariant general relativistic radiative transfer equation

$$\frac{\mathrm{d}I_{\nu}}{\mathrm{d}\lambda_{\mathrm{a}}} = -k_{\alpha}u^{\alpha}\Big|_{\lambda_{\mathrm{a,co}}}\Big(-\kappa_{\nu,\mathrm{co}}\,I_{\nu} + \frac{\epsilon_{\nu,\mathrm{co}}}{\nu_{\mathrm{co}}^{3}}\Big) \tag{2.16}$$

(Younsi et al. 2012), where all the quantities are frequency dependent and are evaluated along the path of a photon (with the comoving frame denoted by the subscript "co") as in the previous section.

2.2 Cosmological Polarised Radiative Transfer

My derivation of the covariant formulation of cosmological polarised radiative transfer (CPRT) is based on a covariant general relativistic radiative transfer (GRRT) formulation (Fuerst and Wu 2004; Younsi et al. 2012), which starts from the conservation of phase-space volume and the conservation of photon number. I assume a flat geometry of the Universe in my derivation as this geometrical property is consistent with the recent observations (see Planck Collaboration XIII 2016). I adopt a flat Friedmann–Robertson–Walker (FRW) metric with diagonal elements $(-1, a^2, a^2, a^2)$, where a = 1/(1 + z) is the cosmological scale factor for the expansion of the universe, and z is the cosmological redshift.

My objective is to construct a cosmological radiative transfer formulation that correctly describes how polarisation interacts with magnetised media whose structures co-evolve with the Universe. To achieve this, the radiative transfer formulation should properly account for various local relativistic and global cosmological effects. Also, it is expressed in terms of cosmological redshift because cosmological distances and time are expressed in terms of this parameter in both theoretical and observational studies of astronomy.

With these depositions in mind, I make two generalisations from the GRRT formulation of Fuerst and Wu (2004) and Younsi et al. (2012), which (i) account for the polarisation of the radiation and (ii) can incorporate a model universe in which the radiation propagates. The former is straightforward in the sense that the PRT equation, Eqn. (2.4), takes the general form of radiative transfer, Eqn. (2.1), and that all the Stokes parameters have the same physical units. Therefore, similar to how one can obtain the Lorentz-invariant intensity by taking $I_{\nu} \equiv I_{\nu}/\nu^3$, the invariant Stokes parameters are obtained by $I_{\nu,i} = [I_{\nu}, Q_{\nu}, U_{\nu}, V_{\nu}]^{T} = [I_{\nu}, Q_{\nu}, U_{\nu}, V_{\nu}]^{T}/\nu^3$, where the tensor index *i* runs from 1 to 4, and the superscript "T" denotes the transpose. For notational simplicity we drop the subscript ν in the Stokes parameters and in the coefficients of absorption and emission hereafter. It follows that the covariant

polarised radiative transfer equation, in tensor notation, takes the form:

$$\frac{\mathrm{d}(\mathcal{I}_{i,\mathrm{co}})}{\mathrm{d}\lambda_{\mathrm{a}}} = \frac{\mathrm{d}(\mathcal{I}_{i,\mathrm{co}}/\nu_{\mathrm{co}}^{3})}{\mathrm{d}\lambda_{\mathrm{a}}} = -k_{\alpha}u^{\alpha}\Big|_{\lambda_{\mathrm{a,co}}}\left\{-\kappa_{ij,\mathrm{co}}\left(\frac{\mathcal{I}_{j}}{\nu_{\mathrm{co}}^{3}}\right) + \frac{\epsilon_{i,\mathrm{co}}}{\nu_{\mathrm{co}}^{3}}\right\},\qquad(2.17)$$

(Chan et al. 2019). Next, to make the formulation appropriate in cosmological settings and, therefore, suitable for (but not limited to) the investigation of cosmological magnetic fields, the factor $k_{\alpha}u^{\alpha}$ is to be evaluated using the space-time metric of a chosen cosmological model such that Eqn. (2.17) is evaluated in terms of a cosmological variable, e.g. the redshift *z*, instead of the affine parameter λ_a .

For simplicity, consider a photon propagating radially in a cosmological medium with 4-velocity u^{β} , i.e.

$$k^{\alpha} = \begin{bmatrix} E \\ p_r \\ p_{\theta} \\ p_{\phi} \end{bmatrix} = \nu \begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \end{bmatrix}; \qquad u^{\beta} = \gamma \begin{bmatrix} 1 \\ \beta_r \\ \beta_{\theta} \\ \beta_{\phi} \end{bmatrix}, \qquad (2.18)$$

where $p = (p_r, p_\theta, p_\phi)$ denotes the 3-velocity of the photon, $\beta = (\beta_r, \beta_\theta, \beta_\phi)$ denotes the 3-velocity of the medium, and $\gamma = 1/\sqrt{(1+\beta^2)}$ is the corresponding Lorentz factor (here, we use c = h = 1), evaluation of $k_\alpha u^\alpha$ then yields

$$k_{\alpha}u^{\alpha}\Big|_{z} = \gamma_{z}\nu_{z}(-1+a^{2}\beta_{r,z}). \qquad (2.19)$$

The ratio of $k_{\alpha}u^{\alpha}$ evaluated at an early epoch to that at the present day is given by

$$\frac{k_{\alpha}u^{\alpha}\Big|_{z}}{k_{\beta}u^{\beta}\Big|_{z_{\text{obs}}}} = \frac{\nu_{z}}{\nu_{z_{\text{obs}}}}\left(\frac{\gamma_{z}}{\gamma_{z_{\text{obs}}}}\frac{(a^{2}\beta_{r,z}-1)}{(a^{2}_{\text{obs}}\beta_{r,z_{\text{obs}}}-1)}\right).$$
(2.20)

If the motion of the medium can be neglected (i.e. $\beta=0$, $\gamma=1$), the ratio is then simplified to

$$\frac{k_{\alpha}u^{\alpha}\big|_{z}}{k_{\beta}u^{\beta}\big|_{z_{\text{obs}}}} = \frac{\nu_{z}}{\nu_{z_{\text{obs}}}},$$
(2.21)

which is the relative shift of energy (or frequency) of the photon, as one would expect from Eqn. (2.15). By defining $k^{\alpha} = (E, p) = dx^{\alpha}/d\lambda_a$, one may also obtain

$$\frac{\mathrm{d}}{\mathrm{d}\lambda_{\mathrm{a}}} = \frac{\mathrm{d}\,x^{0}}{\mathrm{d}\lambda_{\mathrm{a}}}\frac{\mathrm{d}}{\mathrm{d}\,x^{0}} = E\frac{\mathrm{d}}{\mathrm{d}s} = E\frac{\mathrm{d}z}{\mathrm{d}s}\frac{\mathrm{d}}{\mathrm{d}z},\qquad(2.22)$$

and use this to also show that the photon's energy is $E \propto a^{-1}$ and thus

$$\frac{v_z}{v_{z_{obs}}} = \frac{a_{obs}}{a} = \frac{1+z}{1+z_{obs}},$$
(2.23)

in a flat FRW universe (see e.g. Dodelson 2003). In other words, the ratio in Eqn. (2.21) corresponds to the relative energy shift of the photon due to the cosmic expansion.

Finally, by applying the chain rule given in Eqn. (2.22) to Eqn. (2.17), we obtain the CPRT equation defined in redshift space:

$$\frac{\mathrm{d}}{\mathrm{d}z} \begin{bmatrix} \mathbf{I} \\ \mathbf{Q} \\ \mathbf{\mathcal{U}} \\ \mathbf{\mathcal{V}} \end{bmatrix} = (1+z) \left\{ -\begin{bmatrix} \kappa & q & u & v \\ q & \kappa & f & -g \\ u & -f & \kappa & h \\ v & g & -h & \kappa \end{bmatrix} \begin{bmatrix} \mathbf{I} \\ \mathbf{Q} \\ \mathbf{\mathcal{U}} \\ \mathbf{\mathcal{V}} \end{bmatrix} + \begin{bmatrix} \epsilon_{I} \\ \epsilon_{Q} \\ \epsilon_{U} \\ \epsilon_{V} \end{bmatrix} \frac{1}{v^{3}} \right\} \frac{\mathrm{d}s}{\mathrm{d}z}, \quad (2.24)$$

where ds/dz in a flat FRW universe is given by

$$\frac{\mathrm{d}s}{\mathrm{d}z} = \frac{c}{H_0} \left(1+z\right)^{-1} \left[\Omega_{\mathrm{r},0}(1+z)^4 + \Omega_{\mathrm{m},0}(1+z)^3 + \Omega_{\Lambda,0}\right]^{-\frac{1}{2}}, \qquad (2.25)$$

(see e.g. Peacock 1999), where H_0 is the standard Hubble parameter, $\Omega_{r,0}$, $\Omega_{m,0}$ and $\Omega_{\Lambda,0}$ are the dimensionless energy densities of relativistic matter and radiation, non-relativistic matter, and a cosmological constant (dark energy with an equation of state of $w \equiv -1$), respectively. The subscript "0" denotes that the quantities are measured at the present epoch (i.e. z = 0).

The general covariant PRT equation, Eqn. (2.17), and the equation specific for a FRW universe, Eqn. (2.24), preserves the basic structure of the conventional polarised radiative transfer (see e.g. Sazonov and Tsytovich 1968; Sazonov 1969;

Jones and O'Dell 1977a,b; Pacholczyk 1977; Degl'innocenti and Degl'innocenti 1985), making it easy to implement for practical calculations, as I will demonstrate in the example problems and applications in Chapter 3. Note also that the CPRT formulation is general and can adopt different cosmological models with flat spacetime geometry through the $k_{\alpha}u^{\alpha}$ factor. Ray-tracing calculation for Eqn. (2.24) can then be performed for arbitrary photon geodesics. For clarity, I reiterate that a flat space-time is considered in my derivation such that straightforward parallel transport of the polarisation Stokes vector $S_{\nu,i} = [I_{\nu}, Q_{\nu}, U_{\nu}, V_{\nu}]^{T}$ of the radiation along the photon geodesics is enabled⁴. For radiation propagating in a curved space-time, the rotation of its polarisation vector measured by the observer has a contribution caused not only by the Faraday rotation but also by the curvature of the embedded manifold, i.e. angle is not preserved transporting along the line-of-sight. The flatness of space-time ensures that the angles measured in the local comoving frame would be the same everywhere along the geodesic.

The covariant nature of the CPRT formulation allows a straightforward transform of an observable between the comoving frame and the observer's frame. Computation from the invariant Stokes parameters to the observable Stokes parameters in the comoving frame requires only a scalar multiplication of the cube of the radiation frequency, i.e. $[I_{\nu}(z), Q_{\nu}(z), U_{\nu}(z), V_{\nu}(z)]^{T} = [I_{\nu}(z), Q_{\nu}(z), \mathcal{U}_{\nu}(z), \mathcal{V}_{\nu}(z)]^{T} \times$ $\nu(z)^{3}$. The results at z = 0 are then what would be measured in the observer's frame at the present time, provided that the transform of the local polarisation frame to the instrument's polarisation frame are properly handled (as is noted in Appendix A), along with the corrections of instrumental effects and foregrounds,

⁴There have been studies in polarised radiative transfer in space-time appropriate for black-hole systems (Broderick and Blandford 2003; Broderick and Blandford 2004; Shcherbakov and Huang 2011; Gammie and Leung 2012; Dexter 2016; Mościbrodzka and Gammie 2018). In general, a ray-tracing approach was adopted in these studies. It involves first solving the photon geodesic (to determine the ray), and keeping track of the local reference frame along the ray. The polarised radiative transfer is executed on a local reference frame along the ray. A reference frame on which the polarisation components are defined is connected to these local reference frame at the point of observation. This reference frame is transported along the ray as the radiation propagates. There are certain conceptual and technical issues in the standard ray-tracing approach for covariant polarised radiative transfer when a 4-Stokes parameter representation is used. They stem from the fact that the Stokes parameters are not vector, and they are rotationally invariant. A more proper formulation will require a representation in which the polarisation is expressed in terms of rotationally invariant quantities (cf. the spin-2 signals of *E*- and *B*-modes in the CMB).

such as ionospheric effects.

2.3 Line Radiative Transfer - A Phenomenological Introduction

Here I describe the basic phenomenology of line radiative transfer with a simple "stick-person" style model. In contrast to the continuum model described in the earlier section, line radiative transfer requires the opacities contributed by both the line and its underneath continuum. Thus, the radiative transfer is jointly determined by the emission and absorption coefficients of the line and the emission and absorption coefficients determined by the neighbouring continuum. In a simple phenomenological manner, the (non-polarised) radiative transfer equation in a local rest frame may take the form:

$$\frac{\mathrm{d}I_{\nu}}{\mathrm{d}s} = -(\kappa_{\mathrm{C},\nu} + \kappa_{\mathrm{L},\nu} \,\phi_{\nu,\mathrm{abs}})I_{\nu} + (\epsilon_{\mathrm{C},\nu} + \epsilon_{\mathrm{L},\nu} \,\phi_{\nu,\mathrm{emi}}) \tag{2.26}$$

(cf. Wu et al. 2001) if (i) photon scattering, (ii) energy redistribution and (iii) stimulated emission are not included. Here, the subscripts "C" denotes the continuum underneath and neighbouring to the line, "L" denotes the line centre, and "abs" associated with the line profile function ϕ_{ν} refers to line absorption line and "emi" to line emission.

In the above equation, the continuum underneath the line and at the frequencies adjacent to the line centre is assumed to be slow varying. There is no assumption of the same line profile functions for emission and absorption. In most astrophysical situations, the same line profile is applied for emission and absorption, but in a global cosmological setting, this assumption does not always hold, as the emitters and the absorbers are not co-located at the same slice of space-time. Neglecting energy redistribution simplifies the calculations greatly, as the radiative transfer equation can be solved independently, without the consideration of the couplings between the radiative transfer and the relevant physical processes, e.g. atomic transition induced by the radiation, of the line-of-sight medium.

Without losing generality, the line profile function $\phi_{\nu} = 1$ at the line-centre energy is considered. For the situation that the emission and absorption lines are centred at the same frequency, the emission and absorption coefficients for the line are therefore $\epsilon_{L,\nu} \phi_{\nu,\text{emi}} = \epsilon_{L,\nu_L}$ and $\kappa_{L,\nu} \phi_{\nu,\text{abs}} = \kappa_{L,\nu_L}$, respectively. To simplify the notation, the subscript " ν " of the frequency-dependent quantities are dropped hereafter, unless otherwise stated. With these, a qualitative description for the radiative transfer at the line-centre frequency can be derived, as well as a qualitative description for the continuum at the frequencies neighbouring to the line.

At the line-centre frequency, the radiative transfer equation is

$$\frac{\mathrm{d}I_{\mathrm{L}}}{\mathrm{d}s} = -\left(\kappa_{\mathrm{C}} + \kappa_{\mathrm{L}}\right)I_{\mathrm{L}} + \left(\epsilon_{\mathrm{C}} + \epsilon_{\mathrm{L}}\right) \tag{2.27}$$

(see Tucker 1977; Wu et al. 2001). The transfer process is contributed jointly by both the opacity of the line and the opacity of the continuum. The radiative transfer of the continuum at the line can be approximated by the radiative transfer of the continuum at the neighbouring frequencies at which the line profile function is insignificant, i.e. $\phi_{\nu} \ll 1$ when the continuum is sufficiently slow varying. This gives the continuum radiative transfer equation:

$$\frac{\mathrm{d}I_{\mathrm{C}}}{\mathrm{d}s} = -\kappa_{\mathrm{C}}I_{\mathrm{C}} + \epsilon_{\mathrm{C}} \,, \tag{2.28}$$

in which only the opacity of the continuum contributes to the transfer process.

Whether the line will appear as an emission feature or an absorption feature depends on the relative strength of $I_{\rm L}$ and $I_{\rm C}$, if the line is centrally peaked. The line will appear as emission when $I_{\rm L} > I_{\rm C}$, and in absorption when $I_{\rm L} < I_{\rm C}$. For the cosmological 21-cm line associated with the hyperfine transition in neutral hydrogen, the line is seen against the continuum CMB radiation.

For the covariant radiative transfer of line in a cosmological setting, a generalisation to account for frequency redistribution and the complexity and structure in the line profile is required. Nonetheless, with the same arguments as presented previously for the cosmological polarised continuum radiative transfer, the corresponding cosmological line radiative transfer equation is expected to be similar to the following:

$$\frac{\mathrm{d}(I_{i,\nu})}{\mathrm{d}\lambda_{\mathrm{a}}}\bigg|_{\lambda_{\mathrm{a}},\mathrm{co}} = \frac{\mathrm{d}(I_{i,\nu}/\nu^{3})}{\mathrm{d}\lambda_{\mathrm{a}}}\bigg|_{\lambda_{\mathrm{a}},\mathrm{co}} = -k_{\alpha}u^{\alpha}\bigg|_{\lambda_{\mathrm{a}},\mathrm{co}}\left\{-\kappa_{ij,\mathrm{tot},\nu}\left(\frac{I_{j,\nu}}{\nu^{3}}\right) + \frac{\epsilon_{i,\mathrm{tot},\nu}}{\nu^{3}}\right\}\bigg|_{\lambda_{\mathrm{a}},\mathrm{co}} (2.29)$$

where $\kappa_{ij,tot,\nu} = \kappa_{ij,C,\nu} + \kappa_{ij,L,\nu}$ and $\epsilon_{i,tot,\nu} = \epsilon_{i,C,\nu} + \epsilon_{i,L,\nu}$. A more comprehensive elaboration of how the covariant 21cm line radiative transfer across the cosmological time is executed in practice will be presented later in Chapter 3 of this thesis.

2.4 Wavelet Transform

In astrophysics, there are often complex systems where multiple physical processes are in simultaneous or in sequential operations. These processes could have different length scales and/or time scales, and they manifest as spatial and temporal features in the observational data. The wavelet transform is a useful tool for the analysis of such observations, as it can efficiently extract the frequency-time or scale-space information, identifying patterns in the data distributed on a real line of time (e.g. a time series) or an image, which is on a plane or a high-dimension manifold (e.g. a 2-sphere). With the simultaneous spectral and temporal (or spatial for an image) characterisation, we can separate the scale-dependent, localised features of interest within the observational data and hence identify the relevant physical processes that give rise to the corresponding observed scale-dependent temporal or spatial features. Wavelets are now a prevalent analysis technique for studying cosmology (Vielva et al. 2004; Vielva et al. 2006a; McEwen et al. 2005; Vielva et al. 2006b; Wiaux et al. 2006; McEwen et al. 2006b,c, 2007; Pietrobon et al. 2006; McEwen et al. 2008b; Wiaux et al. 2008c; Lan and Marinucci 2008; McEwen et al. 2008a; Delabrouille et al. 2009; Bobin et al. 2013; Planck Collaboration XII 2014; Planck Collaboration XXIII 2014; Planck Collaboration XXV 2014; Planck Collaboration IX 2015; Planck Collaboration XVI 2016; Planck Collaboration XVIII 2016; Rogers et al. 2016; Leistedt et al. 2017), astrophysics (e.g. Farge 1992; Frick et al. 2010; Kowal and Lazarian 2010; Juppa et al. 2012; Schmitt et al. 2012; Cornish and Littenberg 2015; Farge and Schneider 2015; Sun et al. 2015; Robitaille et al. 2017; Chatziioannou et al. 2019), planetary science (e.g. Holschneider et al. 2003; Pascal 2011; Audet 2014; Xu et al. 2019), geophysics (e.g. Foufoula-Georgiou and Kumar 1994; Schmidt et al. 2006; Simons et al. 2011; Bhardwaj et al. 2020), neuro-science (e.g. Dinov et al. 2005; Rathi et al. 2011; Hramov et al. 2015) and many disciplines in science and beyond science.

In Chapter 5, I present a new generation of spin curvelets on a sphere that I constructed. These spherical spin curvelets are specifically designed for the allsky data, and that are particularly efficient in extracting curvilinear features on spherical surfaces. Some important examples of the all-sky data are the all-sky polarisation and the all-sky 21-cm emission. These two are the core of the science themes underpinning my thesis. In the following subsections, I first introduce the concepts of the wavelet transform. I highlight the properties of wavelets and discuss the strengths of wavelet transform in the analysis of non-stationary, noisy and aperiodic (or quasi-periodic) signals, against the Fourier transform, a commonly used technique in feature characterisation. I then present the extension of the wavelet transform for Euclidean space in a plane to the wavelet transform on a sphere (i.e. in a two-dimensional spherical surface, a 2-sphere). The practical consideration in the applications are also discussed.

2.4.1 Wavelet transform versus Fourier transform

The Fourier transform decomposes a signal into a series consisting of orthogonal bases which are represented by trigonometric functions (often in terms of sines and cosines). The Fourier coefficients are variables that characterise the signal in this linear decomposition, allowing a quantitative comparison between observational/experimental signals and theoretical models or two streams of data obtained experimentally or observationally. Analogous to the Fourier transform, the wavelet transform also decomposes signals into a series consisting of a set of atomic functions, which are called wavelets, and the wavelet coefficients are variables that characterise the signals. The Fourier transform employs the trigonometric functions as the analysing functions, which, individually, are non-local as they stretch out

to infinity. In contrast, wavelets are constructed such that they are localised both temporally/spatially and spectrally.

The localisation properties of wavelets enable wavelet transforms to analyse many practical problems where the Fourier transform may be inapplicable. For instance, it is difficult for a Fourier analysis to adequately characterise a signal stream/plane with sharp discontinuities, as the Fourier transform involves an implicit averaging through the integration over the entire space or time domain, thus, only global averaged information, but not the local information, would be retained. To rectify this shortcoming, modifications of the conventional Fourier transform, such as the short-time Fourier transform (STFT), have been developed. The STFT uses a fixed-width window, which provides some degree of temporal (or spatial) resolution throughout the analysed signals. Despite the improvement, it still falls short of simultaneously capturing both the short-duration (or short-width), high-frequency and long-duration, low-frequency features for aperiodic or more general non-stationary signals.

The wavelet transform differentiates from the STFT by utilising a sliding time (or space) window of variable lengths (i.e. a frequency-dependent windowing). Thus, it allows an "arbitrarily" high resolution (limited only by the uncertainty principle, which will be discussed later) in time, or position, of the high-frequency signal components. This capability gives wavelet transform a unique ability that is not available to the STFT and methods based on the conventional Fourier transform.

In short, wavelet are mathematical functions used in representing data or other mathematical functions. Wavelets can be purposefully constructed to represent the signal of interest, picking out individual signal features by their dual localisation properties in the temporal (or spatial) and spectral domains. They satisfy the mathematical criteria of admissibility and regularity conditions, by which they obtain their name ("wave + let"). In the next subsections, I will elaborate how wavelet transform provides a multi-resolution time-frequency (or position-scale) joint representation of signals and present some of its mathematical representations.

Limit set by the uncertainty principle

The idea behind a time-frequency, or position-scale, joint representations lies in dissecting a signal into parts and the subsequent analysis (Mallat 2009b). This brings up a practical question: how to best cut the signal? The answer is, however, circumstantial. It depends on what kind of information one would aim to extract from the signals. In the techniques that involve integration of the segments of the signals, such as the wavelet transform, as well as the STFT, the cutting itself corresponds to a convolution between the signal and the cutting window. Thus, how to choose the cutting will determine how the information is extracted from the data and hence how the characterisation is presented.

Here is an elaboration. Consider that the signal of interest is a time series, and we want to determine the frequency components of the signal at a specific time. We may use a Dirac pulse to select a segment of the time series and transform it into the frequency domain. The transform will involve a convolution of the signal and the window function, the Dirac pulse in this case. Now consider that an integral transform is used. For instance, the Fourier transform of a infinitely narrow Dirac pulse is practically a white-noise spectrum. A similar integral transform of a Dirac pulse will give a spectrum consisting of all frequencies. The convolution of a Dirac pulse window will completely smear out the signals in the frequency domain under a usual Fourier transform or a similar integral transform, i.e. a perfect time localisation provides no frequency information. This outcome is precisely the opposite to that of a direct Fourier transform of the entire time series, which gives a perfect frequency resolution but at the expense of the time resolution through an integration. This shows that when an integral transform is employed, it is impossible to know at the same time the exact frequency and the exact time of occurrence of this frequency in the signal. This also implies that in time-frequency analyses, if an integral transform is used, a signal cannot be localised to a single point. Instead, its location is distributed over a region, which may be represented by a "box" of finite size (i.e. a packet of waveform, thus, wavelet). This is effectively a manifestation of the Heisenberg's uncertainty principle, derived originally for quantum mechanics.

Multi-resolution analyses

For clarity, hereafter, the notations in general signal processing applications will be adopted. The term "frequency" is reserved for Fourier transform, while the term "scale", which is the reciprocal of frequency at which we look into the signal of interest (e.g. a time series), for wavelet transform. Also, signals can be defined on domains apart from time. For instance, an image is a two-dimensional signal defined on a spatial domain. The term "scale" is thus also appropriate in this aspect.

Wavelets resolve the signal-cutting dilemma in time-frequency (or space-scale) analysis by constructing a scalable modulated window, and then shifting this window along a time series or across an image on the plane. Then, the time-scale (or spacescale) representations of the signal can be derived as follows. The scalable window (known as the mother wavelet⁵) is shifted along a signal stream, or across a signal plane, and a spectrum is computed for every location being analysed. The shifting process is repeated but with a slightly shorter or longer window (i.e. the dilated versions of the mother wavelet) for each repetition. As the entire signal is sieved through by the wavelets of varying scales, a collection of time-scale (or space-scale) representations of the signal, with different resolutions, are obtained. The original signal may be expressed in terms of a linear combination of the wavelet functions with the corresponding coefficients. With the wavelet function specified, the scale information will be retained in the wavelet coefficients. As such, operations on the signal can be performed using the wavelet coefficients. In addition, imposing an admissibility condition on the mother wavelet ensures the signal can be reconstructed from its wavelet coefficients without any loss of information (see e.g. Daubechies 1992; Mallat 2009a), resulting in an exact reconstruction. This guarantees that all the signal content is captured by the wavelet coefficients.

Sparse representation of data can be achieved if the wavelet functions are chosen to adapt to the target signals (data), or if truncation of the coefficients below a certain

⁵A mother wavelet is defined as a localised function upon which translation, dilation and rotation may be applied.

threshold is applicable. The latter is commonly practised in the applications of denoising, such as removing background white noise whose energy spreads uniformly across all scales with a flat spectrum. This sparsity is utilised in data compression, which is particularly important in practical astrophysics, as we envisaged a big data era being ushered in with the new-generation telescopes like the SKA.

2.4.2 Practical considerations

Here, several considerations for the application of the wavelet transform in practical signal/data analysis in science are highlighted. These considerations are important as they will determine the framework of wavelet transform and the selection of the wavelet functions to be used in the analysis.

Firstly, the method should accurately account for the geometrical properties of the space where the data reside. In astrophysics and cosmology, all-sky (or wide-sky) survey observations are conducted over the celestial sphere. All-sky survey data are therefore positioned on a spherical surface (often referred to as a 2D sphere). If distance (depth) information, such as the redshift, is also present, the data are residing in a solid sphere (often referred to as a 3D ball). Analyses of the data will be the most efficient and accurate if the technique is derived to accommodate the underlying spherical geometry. Thus, wavelet transforms using spherical wavelets are a natural choice for the analysis of the observed all-sky data in astrophysics and cosmology.

Secondly, the method should account for the spin information of the signals, if present. For instance, the observed all-sky polarisation is a spin-2 signal on a sphere. Such a spin signal is invariant for local rotations of $\pm \pi$. The observed all-sky 21-cm line intensity for cosmological structural evolution is a spin-0 (scalar) signal on a sphere. Spin spherical wavelet techniques are essential for the study of the all-sky radio polarisation observation and the study of all-sky 21-cm line observation.

Thirdly, the method should efficiently extract patterns and characterise structures in a complex data-set. All-sky radio polarisation and cosmological 21-cm observations produce complex data-sets, which contain information of the physical processes that modify the signal on its path of propagation from the source to the telescope, convolved together with the instrumental effects. Anisotropic signals with noticeable directional features are often embedded in the all-sky observations. An example is the Galactic polarised foreground, where oriented, elongated structures are prevalent (as those seen in Fig. 2 in Han (2017), and references therein). Removing the Galactic and extragalactic foreground signals is essential, in order to allow us to identify the features that are genuinely arisen from the large-scale magnetic fields. Similarly, the foregrounds of the 21-cm emission must be removed, so to reveal the signatures imprinted by the 21-cm hydrogen hyperfine transition occurring at the Cosmic Dawn and the EoR. In addition to Galactic and extragalactic foreground sources, ionospheric variations, human contributed Radio Frequency Interference (RFI) and instrumental effects (e.g. Labropoulos et al. 2009) can also introduce contamination in the radio all-sky observations of polarisation and of the 21 cm line. This foreground contamination must be properly accounted for in the analyses of the all-sky observations. Curvelets are an anisotropic extension to wavelets and they can efficiently extract information associated with curvilinear structures. They were first developed by Candes et al. (1999) to provide efficient representations of smooth objects with discontinuities along curves, such as edges in 2D images, or sheet-like structures in 3D space. The basis elements of curvelets obey a parabolic scaling relation with width \approx length², and they are highly anisotropic and directionally sensitive. Curvelets are capable of probing oriented, elongated structures in a complex data-set. Curvelet transforms allow us to identify and separate the anisotropic signal content at different physical scales of interest, owing to their sensitivity in the shapes and localisation properties in position, scale and orientations.

Fourthly, the method should capture all the information contained in a complex signal and process them without loss of information. In a wavelet analysis, the signals are decomposed into wavelet coefficients. In synthesis, an exact transform will ensure that there is no loss of information in the reconstruction of the signal from the wavelet coefficients. This can be achieved by appealing to sampling theorems and corresponding exact quadrature rules for the computation of integrals (McEwen

et al. 2015a; McEwen and Wiaux 2011; McEwen et al. 2018).

Finally, the method should allow an efficient computation that can handle big volumes of data obtained from observations. Thus, fast algorithms are desirable.

2.5 Wavelet Transform on a Sphere

Characterisation and analysis of data on or in a sphere are better described in a polarspherical coordinate system. A substantial amount of work have been conducted to extend wavelets from a plane to a sphere (see e.g. Torresani (1995); Dahlke and Maass (1995); Holschneider (1996); Freeden and Windheuser (1997); Antoine and Vandergheynst (1998, 1999); Antoine et al. (2002); Demanet and Vandergheynst (2003); Wiaux et al. (2005); McEwen et al. (2006a); Sanz et al. (2006) for continuous wavelet transforms on a sphere, and Schröder and Sweldens (1995); Sweldens (1996); Wiaux et al. (2005); Starck et al. (2006a,b); Wiaux et al. (2008a); Starck et al. (2009); Leistedt et al. (2013); McEwen and Price (2015); McEwen et al. (2018) for the discrete cases). The following subsections provides the mathematical preliminaries of harmonic analysis on a sphere and the rotation group representation. A particular emphasis is on how the relevant terms, that are used in this thesis, are defined. I have derived a new-generation spin curvelet transform directly on a sphere. For a review of the general spin scale-discretised wavelet framework upon which my derivation is based upon, see McEwen et al. (2015b). The details of my derivation of the generalisation of curvelet transform to a spherical manifold will be presented in Chapter 5.

2.5.1 Spin harmonic analysis

A point on a spherical surface can be marked by an angular position $\omega = (\theta, \phi) \in \mathbb{S}^2$, where $\theta \in [0, \pi]$ is the polar angle (also known as the colatitude) and $\phi \in [0, 2\pi)$ is the azimuthal angle (also known as the longitude). Generally, the polar axis is defined such that the north pole on the sphere is in the direction of the unit vector \hat{z} of a Cartesian coordinate system (x, y, z), in which the centre of the sphere is located at its origin.

Suppose that the signals of interest are square-integrable functions ${}_{s}f$, with

spin number $s \in \mathbb{Z}$, defined on a sphere, i.e. ${}_{s}f = {}_{s}f(\omega) \in L^{2}(\mathbb{S}^{2}, d\Omega)$, where $d\Omega = \sin \theta \ d\theta \ d\phi$ is the rotational invariant measure of the sphere. The signal can be expressed in terms of spin spherical harmonics ${}_{s}Y_{\ell m}(\omega) (= {}_{s}Y_{\ell m}(\theta, \phi))$, which form a complete, orthogonal basis on \mathbb{S}^{2} . The forward projection gives the coefficients corresponding to the spin harmonic components:

$${}_{s}f_{\ell m} = \langle {}_{s}f, {}_{s}Y_{\ell m} \rangle = \int_{\mathbb{S}^{2}} d\Omega(\omega) {}_{s}f(\omega) {}_{s}Y^{*}_{\ell m}(\omega) , \qquad (2.30)$$

with the orthogonal relation for the spin spherical harmonics

$$\langle {}_{s}Y_{\ell m}, {}_{s}Y_{\ell'm'} \rangle = \delta_{\ell\ell'}\delta_{mm'}, \qquad (2.31)$$

where δ_{ij} is the Kronecker delta, and the completeness relation for the spin spherical harmonics is

$$\sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} {}_{s}Y_{\ell m}(\theta,\phi) {}_{s}Y_{\ell m}^{*}(\theta',\phi') = \delta\left(\cos\theta - \cos\theta'\right)\delta\left(\phi - \phi'\right) , \qquad (2.32)$$

where $\delta(\cdot)$ is the Dirac delta function, and the asterisk * denotes a complex conjugate. This gives an expression for ${}_{s}f(\omega)$ as an expansion of the spin spherical harmonics:

$${}_{s}f(\boldsymbol{\omega}) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} {}_{s}f_{\ell m} {}_{s}Y_{\ell m}(\boldsymbol{\omega}) . \qquad (2.33)$$

The Condon-Shortley phase convention, which is adopted here, gives a conjugate symmetry relation: ${}_{s}Y^{*}_{\ell m}(\omega) = (-1)^{s+m} {}_{-s}Y_{\ell(-m)}(\omega)$. It follows that a function satisfying ${}_{s}f^{*} = {}_{-s}f$ may also be expressed as ${}_{s}f^{*}_{\ell m} = (-1)^{s+m} {}_{-s}f_{\ell(-m)}$.

Note also that ${}_{s}Y_{\ell m}$ can be constructed from scalar (spin-0) spherical harmonics $Y_{\ell m}$ through repeated action of the differential spin raising or lowering operators,

which, when applied to a spin s function, are defined as

$$\begin{cases} \eth \equiv \sin^{s} \theta \left(\frac{\partial}{\partial \theta} + \frac{i}{\sin \theta} \frac{\partial}{\partial \phi} \right) \sin^{-s} \theta \\ \bar{\eth} \equiv \sin^{-s} \theta \left(\frac{\partial}{\partial \theta} - \frac{i}{\sin \theta} \frac{\partial}{\partial \phi} \right) \sin^{s} \theta \end{cases}$$
(2.34)

(see Goldberg et al. 1967; Marinucci and Peccati 2011), respectively. Then, in terms of $Y_{\ell m}$,

$${}_{s}Y_{\ell m}(\boldsymbol{\omega}) = \begin{cases} \left[\frac{(\ell-s)!}{(\ell+s)!}\right]^{1/2} \tilde{\operatorname{O}}^{s} Y_{\ell m}(\boldsymbol{\omega}) & (0 \le s \le \ell) \\ \left[\frac{(\ell+s)!}{(\ell-s)!}\right]^{1/2} (-1)^{s} \bar{\operatorname{O}}^{(-s)} Y_{\ell m}(\boldsymbol{\omega}) & (-\ell \le s \le 0) \end{cases} .$$

$$(2.35)$$

2.5.2 The rotation group

The spherical curvelet transform probes signal content in scales, positions, and also in orientations. Rotations on the sphere, which can be specified by the Euler angles, $\rho = (\alpha, \beta, \gamma)$, with $\alpha \in [0, 2\pi)$, $\beta \in [0, \pi]$, and $\gamma \in [0, 2\pi)$, form a SO(3) group, i.e. $\rho \in$ SO(3). In this thesis, the *zyz* Euler convention is adopted, which corresponds to the rotation in a fixed coordinate system about the *z*, *y* and *z* axes (as defined in the Cartesian coordinates) in sequence by γ , β and α , respectively.

The Wigner *D*-functions $D_{mn}^{\ell} \in L^2(SO(3))$, with $\ell \in \mathbb{N}$ and $m, n \in \mathbb{Z}$ (where $|m|, |n| \leq \ell$), are matrix elements of the irreducible unitary representation of the SO(3) rotation group (Varshalovich et al. 1989). They (and their conjugate $D_{mn}^{\ell*})^6$ form a complete set of orthogonal bases in L²(SO(3)). The orthogonality relation for the Wigner *D*-functions is given by

$$\langle D_{mn}^{\ell}, D_{m'n'}^{\ell'} \rangle = \frac{8\pi^2 \delta_{\ell\ell'} \delta_{mm'} \delta_{nn'}}{(2\ell+1)} , \qquad (2.36)$$

⁶The Wigner *D*-functions satisfy the conjugate symmetry relation $D_{mn}^{\ell*}(\rho) = (-1)^{m+n} D_{-m,-n}^{\ell}(\rho)$.
and the completeness relation is given by

$$\sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \sum_{n=-\ell}^{\ell} D_{mn}^{\ell}(\alpha,\beta,\gamma) D_{mn}^{\ell*}(\alpha',\beta',\gamma')$$
$$= \delta(\alpha - \alpha')\delta(\cos\beta - \cos\beta') \delta(\gamma - \gamma')$$
(2.37)

(Varshalovich et al. 1989).

The Wigner D-functions satisfy

$$D_{mn}^{\ell}(\alpha,\beta,\gamma) = D_{nm}^{\ell_*}(-\gamma,-\beta,-\alpha) , \qquad (2.38)$$

and also

$$D_{nm}^{\ell}(\alpha,\beta,\gamma) = \sum_{k=-\ell}^{\ell} D_{mk}^{\ell}(\alpha_1,\beta_1,\gamma_1) D_{kn}^{\ell}(\alpha_2,\beta_2,\gamma_2)$$
(2.39)

(Marinucci and Peccati 2011), where $\rho = (\alpha, \beta, \gamma)$ describes the net rotation of $\rho_1 = (\alpha_1, \beta_1, \gamma_1)$ and $\rho_2 = (\alpha_2, \beta_2, \gamma_2)$, i.e. $\mathcal{R}_{\rho} = \mathcal{R}_{\rho_1} \mathcal{R}_{\rho_2}$. These Euler angles are related via

$$\cot(\alpha - \alpha_2) = \cos\beta_2 \cot(\alpha_1 + \gamma_2) + \cot\beta_1 \frac{\sin\beta_2}{\sin(\alpha_1 + \gamma_2)}, \qquad (2.40)$$

$$\cos\beta = \cos\beta_1 \cos\beta_2 - \sin\beta_1 \sin\beta_2 \cos(\alpha_1 + \gamma_2) , \qquad (2.41)$$

$$\cot(\gamma - \gamma_1) = \cos\beta_1 \cot(\alpha_1 + \gamma_2) + \cot\beta_2 \frac{\sin\beta_1}{\sin(\alpha_1 + \gamma_2)} .$$
 (2.42)

It follows that

$$\sum_{k=-\ell}^{\ell} D_{km}^{\ell_*}(\alpha_1,\beta_1,\gamma_1) D_{kn}^{\ell}(\alpha_2,\beta_2,\gamma_2) = D_{mn}^{\ell}(\alpha,\beta,\gamma)$$
(2.43)

(McEwen et al. 2018). Because of the property given in Eqn. (2.38), one can interpret ρ in Eqn. (2.43) as the Euler angles that describe the rotation formed by the inverse of the rotation by ρ_1 followed by the rotation by ρ_2 , i.e. $\mathcal{R}_{\rho} = \mathcal{R}_{\rho_1}^{-1} \mathcal{R}_{\rho_2}$.

The Wigner D-functions can be expressed in terms of the spin raised or lowered

scalar (spin-0) spherical harmonics:

$$D_{mn}^{\ell}(\alpha,\beta,\gamma) = \begin{cases} \sqrt{\frac{2\ell+1}{4\pi}} \left[\frac{(\ell-s)!}{(\ell+s)!} \right]^{1/2} \breve{\partial}^{s} Y_{\ell m}(\omega) e^{\mathbf{i}s\gamma} & (0 \le s \le \ell) \\ \sqrt{\frac{2\ell+1}{4\pi}} \left[\frac{(\ell+s)!}{(\ell-s)!} \right]^{1/2} (-1)^{s} \breve{\partial}^{-s} Y_{\ell m}(\omega) e^{\mathbf{i}s\gamma} & (-\ell \le s \le 0) \\ 0 & (\ell < |s|) \end{cases}$$

$$(2.44)$$

where the scalar spherical harmonics are

$$Y_{\ell m}(\theta,\phi) = (-1)^m \sqrt{\frac{2\ell+1}{4\pi} \frac{(\ell-m)!}{(\ell+m)!}} P_{\ell m}(\cos\theta) e^{im\phi} .$$
(2.45)

Here, the $(-1)^m$ phase factor is included following the adopted Condon-Shortley phase convention, and $P_{\ell m}(\cos \theta)$ denotes the associated Legendre polynomials:

$$P_{\ell m}(\cos \theta) = \frac{(-1)^m}{2^\ell \ell!} (1 - \cos^2 \theta)^{m/2} \frac{\mathrm{d}^{\ell+m}}{\mathrm{d}(\cos \theta)^{\ell+m}} (\cos^2 \theta - 1)^\ell , \qquad (2.46)$$

with $\theta \in [0, \pi]$, $\ell \in \mathbb{N}_0$ and $m \in \mathbb{Z}$, such that $|m| \leq \ell$. The index ℓ represents an overall frequency on the sphere and |m| represents the frequency associated with the variable of azimuthal angle ϕ .

The Wigner D-functions may, then, be related to the spin-s spherical harmonics by

$${}_{s}Y_{\ell m}(\theta,\phi) = (-1)^{s} \sqrt{\frac{2\ell+1}{4\pi}} D_{m(-s)}^{\ell *}(\phi,\theta,0)$$
(2.47)

(Goldberg et al. 1967), for $s \in \mathbb{Z}$, $\ell \in \mathbb{N}$ and $m \in \mathbb{Z}$ such that $|m| \leq \ell$, $|s| \leq \ell$. The Wigner $D_{mn}^{\ell}(\rho)$ function can be further decomposed into

$$D_{mn}^{\ell}(\alpha,\beta,\gamma) = e^{-im\alpha} d_{mn}^{\ell}(\beta) e^{-in\gamma}, \qquad (2.48)$$

where the Wigner small-d-functions may be expressed as

$$d_{mn}^{\ell}(\beta) = (-1)^{\ell-n} \sqrt{(\ell+m)!(\ell-m)!(\ell+n)!(\ell-n)!} \\ \times \sum_{k} \frac{(-1)^{k} \left(\sin\frac{\beta}{2}\right)^{2\ell-m-n-2k} \left(\cos\frac{\beta}{2}\right)^{m+n+2k}}{k!(\ell-m-k)!(\ell-n-k)!(m+n+k)!},$$
(2.49)

in which the sum is performed over all values of k such that the arguments of the factorials are non-negative. The spin harmonic in spherical coordinates is therefore

$${}_{s}Y_{\ell m}(\theta,\phi) = (-1)^{s} \sqrt{\frac{2\ell+1}{4\pi}} d^{\ell}_{m(-s)}(\theta) e^{\mathrm{i}m\phi} .$$
 (2.50)

From Eqns. (2.47), (2.38), (2.39), and (2.43), it can be shown that

$$(\mathcal{R}_{\rho \ s}Y_{\ell m})(\boldsymbol{\omega}) = \sum_{n=-\ell}^{\ell} D_{nm}^{\ell}(\rho) \ {}_{s}Y_{\ell n}(\boldsymbol{\omega}) \ .$$
(2.51)

Practical calculations often require the sphere to be sampled in grids to speed up the computation. How the data are being sampled and which sampling method to use depend on the nature of the problem to solve. For instance, HEALPix (Górski et al. 2005) is used in many CMB studies. This is an equi-area sampling method. Note that spherical harmonic transforms using the HEALPix scheme are not theoretically exact, and there are methods that allow exact spherical harmonic transforms on a sphere, enabled by the existence of a sampling theorem on equi-angular grids (e.g. Driscoll and Healy 1994; McEwen and Wiaux 2011). However, in many practical uses, the accuracy of the HEALPix scheme is often sufficient. In general, a sampling method is selected based on: (i) the number of sampling that is required to represent a band-limited signal; (ii) accuracy; (iii) the computational complexity and speed; and (iv) particular issues associated with the numerical pre-computation (or lack thereof) and the associated storage requirements.

2.5.3 Spin scale-discretised wavelet framework on a sphere

The construction of a directional spin scale-discretised wavelet transform on a sphere, ${}_{s}\psi^{(j)} \in L^{2}(\mathbb{S}^{2})$, is presented in McEwen et al. (2015b), where *j* is the discretised scale. These wavelets are designed to be well localised in scale, position and orientation, in both the spatial domain and the harmonic domain. They probe the high-frequency (i.e. large ℓ ; detailed-information) signal content. The directional wavelet coefficients are defined on $\rho \in SO(3)$ to probe directional information.

The low-frequency (rough-information) signal content that is not probed by

wavelets is probed by a scaling function ${}_{s}\Phi \in L^{2}(\mathbb{S}^{2})$. The directional structure at low ℓ is generally not of interest in real-life astrophysical applications. Therefore, an axisymmetric scaling function may be adopted, and its scaling coefficient is given by an axisymmetric convolution with the signal.

The admissibility condition for directional spin scale-discretised wavelets is

$$\frac{4\pi}{2\ell+1} |_{s} \Phi_{\ell 0}|^{2} + \frac{8\pi^{2}}{2\ell+1} \sum_{j=J_{0}}^{J} \sum_{n=-\ell}^{\ell} |_{s} \psi_{\ell n}^{(j)}|^{2} = 1 , \quad \forall \ell$$
 (2.52)

(McEwen et al. 2015b). This condition ensures that the signal $_{s}f$ can be reconstructed exactly from the wavelets and their scaling coefficients. It can also be shown that spin scale-discretised wavelets on a sphere satisfying the admissibility condition constitute a Parseval frame on the sphere (see McEwen et al. 2015b, for derivation details), thus providing a stable way of signal representation.

Chapter 3

Cosmological Polarised Radiative Transfer

This research chapter is based on J. Y. H. Chan, K. Wu, A. Y. L. On, D. J. Barnes, J. D. McEwen and T. D. Kitching, "Covariant polarised radiative transfer on cosmological scales for investigating large-scale magnetic field structures" in Monthly Notices of the Royal Astronomical Society (MNRAS), vol. 484, issue 2, pp. 1427–1455, April 2019, doi: https://doi.org/10.1093/mnras/sty3498, and A. Y. L. On, J. Y. H. Chan, K. Wu, C. J. Saxton and L. van Driel-Gesztelyi, "Polarised radiative transfer, rotation measure fluctuations and largescale magnetic fields" in Monthly Notices of the Royal Astronomical Society (MNRAS), vol. 490, issue 2, pp. 1697–1713, December 2019, doi: https://doi.org/10.1093/mnras/sty2683.

This chapter begins with a highlight of the features of the CPRT equation constructed for the FRW universe derived in Ch. 2. The construction of the all-sky CPRT algorithm, followed by some of its applications, are presented. In particular, how the CPRT formalism can (i) track the polarisation evolution of radiation travelling through an IGM-like plasma with and without a (distant or nearby) bright radio point source, (ii) generate intensity and polarisation maps of a simulated galaxy cluster by performing pencil-beam CPRT calculations, and (iii) simulate the entire polarised sky for a model magnetised universe obtained from the GCMHD+ simulations, are demonstrated. The implications on large-scale magnetic field studies are highlighted. Comparisons to the conventional methods that invoke rotation measure are discussed.

3.1 All-sky CPRT Formulation

The CPRT equation is derived from the covariant GRRT formulation as presented in Sec. 2.1.3 and Sec. 2.2. Therefore, it also implicitly satisfies the conservation of phase-space volume and conservation of photon number (see Sec. 2.1.2 for details). The CPRT equation that I derived is general (see Eqn. (2.24)), although the FRW space-time is considered in my study. I highlight some key features of my CPRT formulation before I present examples of its implementation in practical astronomical applications.

The CPRT equation for a FRW universe, Eqn. (2.24) is

$$\frac{\mathrm{d}}{\mathrm{d}z} \begin{bmatrix} \mathbf{I} \\ \mathbf{Q} \\ \mathbf{\mathcal{U}} \\ \mathbf{\mathcal{V}} \end{bmatrix} = (1+z) \left\{ -\begin{bmatrix} \kappa & q & u & v \\ q & \kappa & f & -g \\ u & -f & \kappa & h \\ v & g & -h & \kappa \end{bmatrix} \begin{bmatrix} \mathbf{I} \\ \mathbf{Q} \\ \mathbf{\mathcal{U}} \\ \mathbf{\mathcal{V}} \end{bmatrix} + \begin{bmatrix} \epsilon_{I} \\ \epsilon_{Q} \\ \epsilon_{U} \\ \epsilon_{V} \end{bmatrix} \frac{1}{v^{3}} \right\} \frac{\mathrm{d}s}{\mathrm{d}z}, \quad (3.1)$$

where ds/dz in a flat FRW universe is

$$\frac{\mathrm{d}s}{\mathrm{d}z} = \frac{c}{H_0} \left(1+z\right)^{-1} \left[\Omega_{\mathrm{r},0}(1+z)^4 + \Omega_{\mathrm{m},0}(1+z)^3 + \Omega_{\Lambda,0}\right]^{-1/2} \,. \tag{3.2}$$

The symbol definitions and the derivation of Eqn. (3.1) can be found in Sec. 2.2. The CPRT equation preserves the basic structure of the conventional polarised radiative transfer equation (see e.g. Sazonov and Tsytovich 1968; Sazonov 1969; Jones and O'Dell 1977a,b; Pacholczyk 1977; Degl'innocenti and Degl'innocenti 1985). Hence, its implementation is straightforward for practical calculations, as I will demonstrate in Sec. 3.2.

The CPRT formulation has accounted for the relativistic and cosmological effects in a self-consistent manner. The properties of the magnetic fields and electron number densities at each epoch are captured through the transfer coefficients in Eqn. (3.1), and their co-evolution with the structures in the expanding Universe are naturally accounted for since the CPRT equation is covariant. The formulation also explicitly accounts for the absorption, emission, Faraday rotation and Faraday conversion processes. The conventional rotation measure (RM) (see e.g. Rybicki and Lightman 1986) can be obtained from the CPRT equation by simply ignoring emission, absorption, Faraday conversion and the presence of non-thermal electrons in the medium (see Appendix D and On et al. (2019) for details and the generalisation of the standard RM expression to account for an isotropic distribution of non-thermal relativistic electrons with a power-law energy spectrum).

The CPRT formulation presented here is the first of its kind¹. For the study of large-scale cosmic magnetism, it provides a reliable theoretical platform to compute the polarised sky. With known input distributions of $n_e(z)$ and B(z), and the full radiative transfer processes taken into account, results obtained from the forward computation of the CPRT algorithm provide valuable data-sets that would serve as a testbed for assessing analysis tools used for large-scale magnetic field studies. Since the cosmological terms in the CPRT equation can be switched off in the numerical computation, the CPRT equation becomes a local-frame PRT equation that we can apply for the calculations of radiation of astrophysical sources, such as galaxy clusters, locally at a specific redshift, and for the modelling of the foreground contribution to the polarised sky in the cosmological studies.

3.1.1 Computational algorithm

The CPRT equation given in Eqn. (2.24) can, in principle, be either solved by direct integration via numerical methods, or by diagonalising and determining the inverse of the transfer matrix operator. I adopt the former approach and employ a ray-tracing method.

The CPRT algorithm consists of three basic components concerning (i) the interaction of radiation with the line-of-sight plasmas, (ii) the cosmological effects on radiation and the co-evolution of plasmas with the Universe's history, and (iii) nu-

¹Formulations and codes capable of computing general relativistic polarised radiative transfer (GRPRT) in the (curved) Kerr space-time metric have been extensively studied and presented (Broderick and Blandford 2003; Broderick and Blandford 2004; Shcherbakov and Huang 2011; Gammie and Leung 2012; Dexter 2016; Mościbrodzka and Gammie 2018; Pihajoki et al. 2018). Their applications primarily concern polarised emissions from magnetised accretion flows and jets around a spinning black hole.

merical computation of the CPRT equation, which is a set of four coupled differential equations evaluated in the redshift *z*-space. In the following, I discuss each of these components, starting with the numerical method. I describe the implementation of the algorithm which solves the CPRT equation for a single ray, or for multiple rays (either in a pencil-beam or an all-sky setting) wherein cosmological MHD simulation results may be incorporated to generate a set of theoretical intensity and polarisation maps. In addition, I highlight its specific designs to accommodate the inclusion of line-of-sight astrophysical sources and intervening plasmas of different properties.

Numerical method

The radiation propagation is parameterised by redshift *z* and is sampled discretely into N_{cell} number of cells. A sampling in which each *z*-interval corresponds to an approximately equal light-travel distance is adopted. The total light-travel distance s_{tot} is computed by integrating ds/dz in a flat FRW universe (Eqn. (2.25); Eqn. (3.2)), and the evaluation of the CPRT equation starts from an initial redshift (z_{init}) to the redshift of the observation (i.e. z = 0). The corresponding lower and upper boundaries of *z*-interval over which the light-travel distance is the closest to $s_{eq} = s_{tot}/N_{cell}$ are registered. The light-travel distance serves as a scaling factor in the numerical integration of the CPRT equation. The computational efficiency is optimised when its multiplications with the transfer coefficients are close to unity.

Each *z*-interval is then refined to accommodate the astrophysical structure(s) and sub-structure(s). An on/off switch for the refinement scheme is implemented in the code, and this allows appropriate adjustment when incorporating multiple structures at different redshifts when the CPRT is executed. Within the refinement zone, a uniform sampling in the $\log_{10} (1 + z)$ space is adopted. This sampling has the advantage of preserving the (polarised) intensity profile shape when multi-frequency calculations are carried out.

In algorithmic terms, at the cell of index ind^{refine} , the increment over each refined cell is given by $[\log_{10} (1 + z') - \log_{10} (1 + z)]/N_{\text{cell}}^{\text{refine}}$, where z' and z are, respectively, the upper and lower boundaries of the z-interval to be refined, and

 $N_{\rm cell}^{\rm refine}$ is the total number of refined cells.

A fourth-fifth order Runge-Kutta (RK) differential equation solver (Fehlberg 1969) is used to integrate Eqn. (2.25), and to solve Eqn. (2.24), which ultimately gives us the Stokes parameters $\{I, Q, U, V\}$ at z = 0 in the observer's frame. Parameters to be set for the solver include the total number of (coupled) differential equations to be solved N_{eqn} , the number of steps for the RK solver N_{step} ; and the error tolerance level eps. The error estimation of the solver is carried out by comparing the solution obtained with a fourth-order RK formula to that obtained with a fifth-order RK formula. If the computed error is less than eps then the calculation proceeds; otherwise the algorithm halts, reports errors of non-convergence, and returns without further computation.

The upper and lower limits of the z-variables are updated along the ray. The outputs are passed into the next computation as the inputs (i.e. as the updated initial conditions). Since the evaluation of the CPRT starts from a higher z to a lower z value until the present $z_0 = 0$ is reached, a substitution of $z \rightarrow -z$ is made in Eqn. (2.24) when that is set as the function to be evaluated by the RK solver.

Interaction of radiation with plasmas

Radiation is parameterised by frequency v(z), which has a redshift dependence of $v(z) = v_{obs}(1 + z)$, where v_{obs} is the observed frequency at the present epoch z = 0. The radiation intensity and polarisation properties change when passing through a magnetised intervening plasma(s). The strength of the radiative processes, captured through transfer coefficients in the CPRT equation, depends on the physical properties of the plasmas, in addition to the frequency of the radiation. In general, both thermal and non-thermal electrons are present in astrophysical plasmas. Parameters describing them include: the total electron number density $n_{e,tot}$, the fraction of non-thermal electrons' energy spectrum p and the electrons' low energy cut off described by the Lorentz factor γ_i . Added to this list are parameters describing the strength and orientation of magnetic fields, B, which can be decomposed into two components. One component is decomposed along the line-of-sight direction

 $|B_{\parallel}| = |B| \cos \theta$, and another component is decomposed in the plane normal to the line-of-sight $|B_{\perp}| = |B| \sin \theta$, where θ is the angle between the direction of the magnetic field and the line-of-sight.

By specifying the observed frequency of radiation v_{obs} at z = 0 and the radiation background at an initial redshift z_{init} , and given some input distributions of electron number density $n_e(z)$ and magnetic field strength |B(z)| through which light travels, solving the CPRT equation then provides the evolution of the intensity and polarisation of the radiation as a function of redshift z.

Cosmological effects

The frequency shift of the radiation due to the expansion of the Universe is given by $v(z) = v_{obs}(1 + z)$. The cosmic expansion effects on the temperatures, electron number densities, as well as the strengths of magnetic fields are given by, respectively, $T_e(z) = T_{e,0}(1+z)^2$, $n_e(z) = n_{e,0}(1+z)^3$, and $|B(z)| = |B_0|(1+z)^2$, assuming frozenin flux condition. Note that these properties, as well as the structures of magnetic fields, are also subject to local structure formation, evolution and outflows, as well as to influences by external injections, such as cosmic rays. Consequently, the interstellar medium (ISM), intra-cluster medium (ICM), and intergalactic media (IGM) all exhibit different characteristic properties.

All-sky polarisation calculation

The all-sky CPRT algorithm is designed to enable an interface between CPRT calculations and cosmological simulations, thereby generating theoretical all-sky intensity and polarisation maps that serve as model templates. The algorithm is shown in Fig. 3.1.

Fig. 3.2 illustrates the ray-tracing concept of the all-sky algorithm, in which the CPRT equation is solved in a spherical polar coordinate system (r, θ, ϕ) , where (θ, ϕ) corresponds to the celestial sky coordinates and the radial axis *r* corresponds to the redshift axis *z*. Note that outputs of the cosmological evolution of plasma properties, e.g. $n_e(z)$ and |B(z)|, from a cosmological MHD simulation can be inputted into the CPRT calculations through the transfer coefficients. Spatial fluctuations of the



Fig. 3.1: The CPRT algorithm flowchart. The program enables incorporation of cosmological MHD simulation results into the CPRT calculations to generate intensity and polarisation model templates.

plasma properties in a finite simulation volume, usually in Cartesian coordinate system (i, j, k), can also be mapped onto the spherical polar coordinate system (r, θ, ϕ) at each sampled redshift.

A more rigorous treatment that guarantees the divergence-free condition of magnetic fields to be satisfied is also possible within this all-sky framework, although this is beyond the focus of this thesis. Here, I add a remark on the sampling scheme over a sphere for efficient follow-on data analysis. Rays that are randomly positioned over the entire celestial sphere can be computed. Alternatively, one may utilise the advantages of efficient spherical sampling schemes, such as the HEALPIX sampling (Górski et al. 2005) and the sampling scheme devised by McEwen and Wiaux (2011) which affords exact numerical quadrature. In such a case, ray-tracing CPRT calculation is performed at each grid point on the sphere. Map data constructed this way allows efficient power spectrum analyses and spherical wavelet analyses (e.g. McEwen et al. 2006a; Sanz et al. 2006; Starck et al. 2006b; Geller et al. 2008; Marinucci et al. 2008; Wiaux et al. 2008b; Leistedt et al. 2013; McEwen et al. 2013, 2015b, 2018; Chan et al. 2017) to characterise the spatial fluctuations of polarisation, crucial for searching polarisation signatures imprinted by large-scale magnetic fields in observational data.

3.1.2 Polarised transfer coefficients

In this subsection I discuss the corresponding transfer coefficients in Eqn. (2.24) appropriate for the studies of cosmic plasmas and structure. The expressions of the coefficients considered in this work are explicitly specified in Appendix C.

An astrophysical plasma generally consists of both thermal electrons and nonthermal electrons. These energetic electrons can be produced by various mechanisms. For instance, non-thermal electrons may result from shock acceleration or cosmic ray interactions. In the astrophysical plasma of interest in this work, the dielectric suppression² (see e.g. Bekefi 1966; Rybicki and Lightman 1986) is

²Dielectric suppression, or known as the Razin effect or Razin-Tsytovich effect (see e.g. Ramaty 1968), is a plasma effect on synchrotron emission. Synchrotron radiation is suppressed below the Razin frequency $\omega_{\rm R} = \omega_{\rm p}^2/\omega_{\rm B}$, where $\omega_{\rm p}$ is the plasma angular frequency and $\omega_{\rm B}$ is the electron angular gyrofrequency, since the electrons can no longer maintain the phase with the emitted radiation as the wave phase velocity would



Fig. 3.2: Illustration of the concept of the all-sky algorithm based on a ray-tracing technique: the CPRT equation is solved for each light ray (indicated in red) that is parameterised by (z, θ, ϕ) . The radial direction coincides with the direction of redshift *z* while (θ, ϕ) maps onto the coordinates of the celestial sky. The observer is positioned at the centre of the circles, i.e. at *z* = 0. Note that the comoving Hubble radius is represented inside-out. The comoving Hubble sphere expands as we approach the centre (*z* = 0) due to the expansion of the Universe. This set-up is applicable for a universe that has a simple topology like ours, as is suggested by measurements of the cosmic microwave background (Planck Collaboration XXVI 2014).

insignificant (see e.g. Melrose and McPhedran 1991). As such, thermal and nonthermal electrons can be treated as separate components in the radiative transfer calculations. Thus, the total transfer coefficients are the sum of the transfer coefficients of the thermal and non-thermal populations, i.e. $\kappa_{ij} = (\kappa_{ij,th} + \kappa_{ij,nt})$ and $\epsilon_i = (\epsilon_{i,th} + \epsilon_{i,nt})$, where "th" and "nt" denote the thermal and non-thermal components of the absorption and emission coefficients respectively.

In this work, thermal bremsstrahlung and non-thermal synchrotron radiation processes are considered³. For thermal bremsstrahlung, expressions of the Faraday rotation coefficient f_{th} and Faraday conversion coefficient h_{th} , as well as the expressions of the absorption coefficients κ_{th} , q_{th} and v_{th} follow Pacholczyk (1977)⁴. The

increase to above the speed of light (see e.g. Melrose 1980).

³In addition to thermal bremsstrahlung and non-thermal synchrotron radiation processes considered in this work, we note that transfer coefficients appropriate for different astrophysical environments have been extensively studied in the literature. Accurate expressions for the coefficients of Faraday rotation and Faraday conversion in uniformly magnetised relativistic plasmas, such as those in jets and hot accretion flows around black-holes, are reported in Huang and Shcherbakov (2011). Expressions of the transfer coefficients in the case of ultra-relativistic plasma that is permeated by static uniform magnetic fields, for frequencies of high harmonic number limits, and for a number of distribution functions (isotropic, thermal, or power law) are presented in Heyvaerts et al. (2013). Emission and absorption coefficients for cyclotron process, that is important in accretion discs of compact objects, have been studied by Chanmugam et al. (1989); Vaeth and Chanmugam (1995). Careful incorporation of the above would be a useful improvement to the current CPRT implementation, expanding the range of its applications and simulate a more realistic magnetised Universe.

⁴The same expressions of κ_{th} , q_{th} and v_{th} are provided in Wickramasinghe and Meggitt (1985), although we find typographical error of an extra factor of the square of angular frequency in the denominator of v_{th} via

emission coefficients are computed via Kirchoff's law accordingly. For non-thermal synchrotron emission, relativistic electrons that have a simple power-law energy distribution is considered. The expressions of the transfer coefficients that follow Jones and O'Dell (1977a) is adopted and an isotropic distribution of relativistic electrons' momentum direction is assumed.

As detailed in Appendix B, the sign of Stokes V depends on its definition, polarisation conventions, handedness of the coordinate systems, as well as the time dependence of the electromagnetic wave (i.e. whether the exponent has $+i\omega t$ or $-i\omega t$), and the definition of the relative phase between the x and y-components of the electric field of the radiation. However, some of these information were not explicitly stated in Jones and O'Dell (1977a), and inconsistent definitions of the time dependence of the electromagnetic wave were used in Pacholczyk (1977) in deriving the radiative transfer coefficients for bremsstrahlung and synchrotron radiation processes (see their Eqn. (3.33) and Eqn. (3.93)). I therefore eliminate ambiguity in Appendix B and present a consistent set of expressions of all the transfer coefficients in Appendix C, given the geometry explicitly defined in Appendix A and the polarisation convention conforming to the IEEE/IAU standard.

3.1.3 Implementation and code verification

In this section the single-ray and multiple-ray experiments performed for code verification is presented⁵. The *z*-sampling scheme follows the recipe described in Sec. 3.1.1 (or see the related red boxes in Fig. 3.1). Polarised radiative transfer at frequencies $v_{obs} = 1.42$ GHz and 5.00 GHz is considered for illustrative purposes⁶. Properties of the intervening plasma are listed in Table 3.1, which can be IGM-like

dimensional analysis. We also note that the sign of q_{th} in Wickramasinghe and Meggitt (1985) is also different to Pacholczyk (1977), which might be due to different polarisation sign conventions or a sign error.

⁵A consistency test is also performed by comparing the results of light-travel time obtained by integrating Eqn. (2.25) using my code (then dividing by the speed of light) to those that are obtained using the publicly available cosmological calculator by Wright (2006), http://www.astro.ucla.edu/~wright/CosmoCalc. html. The results agree with each other, up to the maximum digits displayed in Wright (2006), i.e. three decimal places.

 $^{{}^{6}\}nu_{obs} = 1.4 \text{ GHz}$ is chosen since it lies within the operating range of many current and upcoming radio telescopes, such as the Arecibo radio telescope (http://www.naic.edu/), the Five hundred meter Aperture Spherical Telescope (FAST, http://fast.bao.ac.cn), the Australia Telescope Compact Array (ATCA, https://www.narrabri.atnf.csiro.au/), LOFAR, MWA, ASKAP, SKA, etc.

| | IGM-like plasma | | ICM-like plasma | |
|----------------------------------|-------------------------|-------------|-----------------------|-------------|
| Properties | A-I | A-II | B-I | B-II |
| $n_{\rm e,tot} ({\rm cm}^{-3})$ | 2.1918×10^{-7} | | 1.00×10^{-3} | |
| \mathcal{F}_{nt} (%) | 1.00 | | 1.00 | |
| $T_{\rm e,th}$ (K) | 1.875×10^{3} | | 5.00×10^{5} | |
| р | 4.00 | | 2.50 | |
| corresponds to α | 1.50 | | 0.75 | |
| $\gamma_{ m i}$ | 10.0 | | 30.0 | |
| $ \boldsymbol{B} $ (G) | 1.00×10^{-9} | | 1.00×10^{-6} | |
| $\cos \theta$ | 0.5 | [-1.0, 1.0] | 0.5 | [-1.0, 1.0] |

Table 3.1: Properties of different intervening plasma models used in this work. To test the ability of my CPRT equation solver to handle the extreme limits, the total electron number density $n_{e,tot}$ for models A is set to be equal to the mean electron number density of the Universe (see Appendix F for details); temperature of the thermal electrons in the IGM-like and ICM-like plasma models are assumed to take the lower-end values typical of the IGM and ICM. \mathcal{F}_{nt} denotes the non-thermal relativistic electron fraction, p denotes the power-law index of the energy spectrum of the non-thermal relativistic electrons, which relates to the spectral index of the synchrotron radiation $\alpha = (p - 1)/2$. γ_i is the electrons' low-energy cutoff Lorentz factor. $|\mathbf{B}|$ denotes the magnetic field strength. The magnetic field direction along the line-of-sight is described by $\cos \theta \in [-1.0, 1.0]$ which is randomised for Models A-II and B-II.

(model A) or ICM-like (model B) with magnetic field directions along the line-ofsight set at a fixed angle (models A-I and B-I) or set as oriented randomly (models A-II and B-II). Thermal bremsstrahlung and non-thermal synchrotron radiation processes are accounted for.

Single ray verification tests

To test the accuracy and precision of my CPRT integrator in handling polarised radiative transfer in scenarios investigated in this work, the two integration tests presented in Sec. 3.2 in Dexter (2016) are conducted. The numerical solutions obtained from solving the standard PRT equation (Eqn. (2.4)), which is reduced from the general CPRT equation (Eqn. (2.24)), are compared with the analytic solutions given explicitly in Appendix C of Dexter (2016) for the idealised situations with constant transfer coefficients along a ray.

Pure emission and absorption in Stokes *I* and *Q* is considered in the first test. The light ray travels through the Faraday-thin IGM-like plasma or the Faraday-thick ICM-like plasma (models A-I or B-I) over a cosmological distance from z = 6to z = 0. Detailed values of both the (thermal and non-thermal) emission and absorption transfer coefficients, as well as the optical depths used in the calculations are given in Table G.1 in Appendix G. As is seen in Fig. 3.3, the numerical solution obtained by my CPRT integrator agrees with the analytical solution up to the machine floating-point precision throughout the entire light path.

In the second test, radiation of observed frequencies $v_{obs} = 1.4$ GHz and $v_{obs} = 5.0$ GHz are considered. The radiation travels through the Faraday-thick ICM-like plasma (B-I) of a few Mpc in length scale. Only pure Faraday rotation and Faraday conversion and polarised emission in Q and V are considered (note that ϵ_U is set to zero due to the choice of coordinate systems; see Appendix A). To ease checking the oscillatory behaviour of the resulting V, the Faraday conversion effect is boosted artificially by setting its transfer coefficient to the same order magnitude as the Faraday rotation coefficient. The results of the second test is presented in Fig. 3.4. An excellent agreement between the numerical and analytic solutions is obtained in both cases of different radiation frequencies. Machine floating-point precision is maintained over the ray despite that the residuals in Q, U and V increase with each oscillation. A similar trend is also found in Fig. 4 in Dexter (2016) and Mościbrodzka and Gammie (2018).

Multi-ray verification tests

To verify the redshift-refinement scheme and the entire code, I performed multi-ray cosmological calculations of two Gaussian profiles centred at two different redshifts. The two input profiles, originating at $z_{ori} = 5.94$ and 1.00, have frequency samples assigned through the redshift-refinement scheme at that specific z_{ori} . The central frequency of the profiles is then given by $v_{central}^{in} = v_{obs}(1 + z_{central}^{refine})$, where $z_{central}^{refine}$ is the redshift value of the $N^{refine}/2$ cell, for $N^{refine} = 500$. The ray freely propagates in a vacuum, i.e. all transfer coefficients are set to zero when computing the CPRT equation. As such, frequency shift of the radiation is the only cosmological effect



Fig. 3.3: Plots of the analytic solutions (computed using Eqns. (C2) and (C3) in Dexter (2016); denoted by line) and numerical solutions (obtained from my CPRT code in Fortrar; denoted in star) to the test problem with pure emission and absorption in *I* and *Q*. Transfer coefficients are constant over the entire ray. The left-hand panels show the results using the IGM-like plasma model (A-I), where $(\epsilon_{I,tot}, \epsilon_{Q,tot}) = (2.62 \times 10^{-53}, 2.06 \times 10^{-55}) \text{ erg s}^{-1} \text{ cm}^{-3} \text{ Hz}^{-1} \text{ str}^{-1}$, $(\kappa_{tot}, q_{tot}) = (2.23 \times 10^{-38}, 7.07 \times 10^{-52}) \text{ cm}^{-1}$. The right-hand panels show the results using the ICM-like plasma model (B-I), where $(\epsilon_{I,tot}, \epsilon_{Q,tot}) = (1.25 \times 10^{-38}, 9.05 \times 10^{-39}) \text{ erg s}^{-1} \text{ cm}^{-3} \text{ Hz}^{-1} \text{ str}^{-1}$, $\kappa_{tot}, q_{tot} = (9.34 \times 10^{-34}, 5.49 \times 10^{-34}) \text{ cm}^{-1}$. The other transfer coefficients are set to zero. Note that the resulting *I* and *Q* have a very small order of magnitude, and thus their residuals $res_x = x_{emp} - x_{ana}$ too, with $x = \{I, Q\}$; dividing res_x by the order of magnitude of quantity *x* gives the machine floating-point precision. Note that such a precision is attained over the entire light path in both models.



Fig. 3.4: Plots of the analytic solutions (computed using Eqns. (C6), (C7), and (C8) in Dexter (2016); denoted by line) and numerical solutions (obtained from my CPRT code in Fortran; denoted in star) to the test problem with pure constant Faraday rotation, Faraday conversion and emission in Q and V. ICM-like plasma parameters (model B-I) are used to compute the coefficients f, ϵ_Q , and ϵ_V while h is set to be of the same order of magnitude as f to make the oscillatory behaviour in V apparent. The left- and right-hand panels show the results using $v_{obs} = 1.4$ GHz and $v_{obs} = 5.0$ GHz, respectively. At $v_{obs} = 1.4$ GHz, the non-zero transfer coefficients are $(f_{tot}, h_{tot}) = (1.16 \times 10^{-23}, 1.00 \times 10^{-23}) \text{ cm}^{-1}$, $(\epsilon_{Q,tot}, \epsilon_{V,tot}) = (9.05 \times 10^{-39}, 5.51 \times 10^{-43}) \text{ erg s}^{-1} \text{ cm}^{-3} \text{ Hz}^{-1} \text{ str}^{-1}$. At $v_{obs} = 5.0$ GHz, the non-zero transfer coefficients are $(f_{tot}, h_{tot}) = (9.37 \times 10^{-25}, 1.00 \times 10^{-25}) \text{ cm}^{-1}$, $(\epsilon_{Q,tot}, \epsilon_{V,tot}) = (3.52 \times 10^{-39}, 1.14 \times 10^{-43}) \text{ erg s}^{-1} \text{ cm}^{-3} \text{ Hz}^{-1} \text{ str}^{-1}$. Residuals grow with each oscillation, yet machine floating-point precision is attained (with residual divided by the order of magnitude of the corresponding Stokes parameters) over the entire light path in both cases.

which modifies the radiation properties in its transport. The values of four quantities obtained from the CPRT calculations are compared against their theoretical expected values. These quantities are (i) the frequency at which the resulting profile peaks, $v_{\text{peak},0}$, (ii) the standard deviation of the resulting profile, σ_0 , (iii) the empirical ratio of the output to the input peak intensity $r_I^{\text{emp}} = I_{\text{peak}}^{\text{in}}/I_{\text{peak},0}$, for each Gaussian profile, and (iv) the power-law index of the ratio of the output peak intensities of the two profiles, m^{emp} . Analytically, the resulting profile obtained from the CPRT of each case (i.e. emission at $z_{\text{ori}} = 5.94$ or at $z_{\text{ori}} = 1.00$) should remain Gaussian and peak at the frequency of $v_{\text{obs}} \times (1 + z_{\text{central}}^{\text{refine}})/(1 + z_{\text{ori}})$ with $v_{\text{obs}} = 1.42$ GHz. The standard deviation of the normalised input and the output Gaussian profiles should also remain the same. The ratio of the peak intensity of the output emission profile to that of the input profile is $r_I^{\text{ana}} = 1/(1 + z_{\text{ori}})^3$. Furthermore, comparing the outputs of the two cases, the ratio of the peak intensity at zero redshift follows a power law of $[(1 + z'_{\text{ori}})/(1 + z'_{\text{ori}})]^3$, where z'' denotes the higher redshift, i.e. the power-law index $m^{\text{ana}} = 3.0$.

The results are summarised in Table 3.2, from which one can see that the empirical results are consistent with the theoretical expectations up to machine floating-point precision. Furthermore, consistent results are obtained using the OpenMP parallelised code as those obtained by the serial execution.

3.2 Applications

Here a set of CPRT calculations that demonstrates the ability of the algorithm in tracking the change of polarisation on astrophysical and cosmological scales is presented. Changes in polarisation features caused by the frequency shift of the radiation or those caused by the evolution of intervening cosmic plasmas can be separately investigated; direct studies of their combined effects can also be carried out.

I start with a set of single-ray calculations, with and without a bright lineof-sight point source. I then demonstrate how to incorporate cosmological MHD simulation results into CPRT calculations to make polarisation maps. I compute

| | | Profile I | Profile II | |
|--|--|-------------------------------------|--------------------------------------|--|
| | Zori | 5.93623409775142 | 1.00082825012323 | |
| | zrefine Zcentral | 5.90499449730497 | 0.9992434724235666 | |
| Peak | Input $v_{\text{central}}^{\text{in}}$ (GHz) | 1.41400848881021 | 1.41928070323115 | |
| frequency | Output $v_{\text{peak},0}$ (GHz) | 1.41400848881021 | 1.41928070323115 | |
| | Fractional difference $(v_{\text{peak},0} - v_{\text{central}}^{\text{in}})/v_{\text{central}}^{\text{in}}$ | $-8.99280649946616 \times 10^{-15}$ | $-1.110223037256493 \times 10^{-16}$ | |
| Dispersion | Input σ^{in} | 0.000866648853601 | -0.000123250853536 | |
| | Output σ_0 | 0.000866648853601 | -0.000123250853536 | |
| | Fractional difference $(\sigma_0 - \sigma^{in})/\sigma^{in}$ | $1.59377719355 \times 10^{-17}$ | $5.66495635124 \times 10^{-18}$ | |
| Peak | Analytical r _I ^{ana} | 0.00299659998884 | 0.12484483163785 | |
| intensity | Empirical r_I^{emp} | 0.00299659998884 | 0.12484483163785 | |
| $\begin{pmatrix} \text{ratio} \\ I_{\text{peak},0}^{z_{\text{ori}}=5.94} \\ I_{\text{peak},0}^{z_{\text{ori}}=1.00} \end{pmatrix}$ | Fractional difference $(r_I^{\text{emp}} - r_I^{\text{ana}})/r_I^{\text{ana}}$ | $4.34172933267 \times 10^{-16}$ | $1.06713879307 \times 10^{-14}$ | |
| Power-law | Analytical m ^{ana} | 3.0000 | | |
| index of | Empirical m ^{emp} | 3.000000000099 | | |
| $\left(\frac{I_{\text{peak},0}^{z_{\text{ori}}=5.94}}{I_{\text{peak},0}^{z_{\text{ori}}=1.00}}\right)$ | Fractional difference $(m^{\text{emp}} - m^{\text{ana}})/m^{\text{ana}}$ | $-3.29218134236 \times 10^{-13}$ | | |

Table 3.2: Results of the multi-ray code verification test where two Gaussian profiles, originating at $z_{ori} = 5.94$ and at $z_{ori} = 1.00$ respectively, are cosmologically transported in a vacuum in an expanding flat space-time. Four parameters are compared against their theoretical values; the empirical results are found to be consistent with the expected values up to machine floating-point precision.

the polarisation of a simulated galaxy cluster. I also compute the entire polarised sky using a model magnetised universe. Polarisation maps generated in such a way, i.e. by CPRT calculations interfaced with simulation results, encapsulate theoretical predictions. They are crucial to aid our interpretation of observational data. Model templates of the entire sky are particularly important for comparison with future observational data, such as those from all-sky surveys of polarised emission with the SKA.

3.2.1 Cosmological evolution of polarisation

The polarised radiative transfer calculations were conducted using a ray tracing approach, for the observed frequency $v_{obs} = v_0 = 1.42$ GHz. The radiation propagates from z = 6.0 through the magneto-ionic media along the line-of-sight, with the electron number distribution given by $n_e(z)$ and |B(z)| (see more detailed description below). The *z*-sampling scheme is described in Sec. 3.1.1.

Point-source emissions

Bright polarised emitters such as quasars and radio galaxies may lie along the line-of-sight acting as back-light illuminating the foreground. Here, I calculate how the polarisation and intensity of a fiducial quasar-like point source changes over a cosmological distance. Emissions of such a point source at *z* observed at 1.42 GHz is given by $[I, Q, U, V]|_z = [I, Q, U, V]|_{z=0}(1 + z)^3$, where $[I, Q, U, V]|_{z=0} = [2.54 \times 10^{-16}, -1.32 \times 10^{-18}, 7.50 \times 10^{-18}, 1.27 \times 10^{-19}]$ erg s⁻¹ cm⁻² Hz⁻¹ str⁻¹. The degree of linear polarisation is assumed to be 3.00% (Jagers et al. 1982), the degree of circular polarisation to be 0.05% (Conway et al. 1971), and the polarisation angle is randomly selected as $\varphi = 0.87$ rad. For demonstrative purposes, a simple interpolation of from $[I, Q, U, V]|_{z=0}$ to $[I, Q, U, V]|_z$ is adopted, focusing on polarisation effects caused by the input plasma of known properties.

Three cases are investigated, including where (i) the control experiment where there is no bright point source lying along the line-of-sight, no radiation background, but the intervening medium is a self-emitting, absorbing, Faraday-rotating and

| | (i) | | (iii) |
|---|--|--|--|
| | Without point source | Point source at | Point source at |
| | | z = 6.0 | z = 0.206 |
| $\begin{bmatrix} I \end{bmatrix}$ | [0.0000] | $\left[8.7096 \times 10^{-14} \right]$ | [0.0000] |
| Q | 0.0000 | -4.5372×10^{-16} | 0.0000 |
| | 0.0000 | 2.5731×10^{-15} | 0.0000 |
| $\begin{bmatrix} V \end{bmatrix}_{7=6,0}$ | 0.0000 | $\begin{bmatrix} 4.3548 \times 10^{-17} \end{bmatrix}$ | 0.0000 |
| $\begin{bmatrix} I \end{bmatrix}^{\sim}$ | $\begin{bmatrix} 1.0438 \times 10^{-23} \end{bmatrix}$ | $\begin{bmatrix} 2.5392 \times 10^{-16} \end{bmatrix}$ | $\begin{bmatrix} 2.5392 \times 10^{-16} \end{bmatrix}$ |
| final Q | 6.7617×10^{-25} | -2.8095×10^{-18} | -1.3221×10^{-18} |
| | 5.1681×10^{-26} | 7.0807×10^{-18} | 7.5021×10^{-18} |
| $\begin{bmatrix} V \end{bmatrix}_{z=0.0}$ | $\left[-1.7613 \times 10^{-32} \right]$ | $\left[1.2696 \times 10^{-19} \right]$ | $\left[1.2696 \times 10^{-19} \right]$ |
| initial $\varphi(z = 6.0)$ | 0.0000 | 0.8727 | 0.0000 |
| final $\varphi(z = 0.0)$ | 3.8142×10^{-2} | 0.9731 | 0.8726 |
| initial $\Pi_l(z = 6.0)$ | 0.0000 | 3.0000 | 0.0000 |
| final $\Pi_l(z=0.0)$ | 6.4969 | 3.0000 | 3.0000 |
| initial $\Pi_{\rm c}(z=6.0)$ | 0.0000 | 5.0000×10^{-2} | 0.0000 |
| final $\Pi_{\rm c}(z=0.0)$ | 1.6874×10^{-7} | 5.0000×10^{-2} | 5.0000×10^{-2} |
| initial $\Pi_{\text{tot}}(z = 6.0)$ | 0.0000 | 3.0004 | 0.0000 |
| final $\Pi_{\text{tot}}(z = 0.0)$ | 6.4969 | 3.0004 | 3.0004 |

Table 3.3: Numerical results of the CPRT calculations for the demonstrative cases where a bright point source is (i) absent, (ii) located at z = 6.0 or (iii) located at z = 0.206. Magnetic fields have unbiased random orientations along the line-of-sight (see Sec. 3.2.1). The Stokes parameters are in units of erg s⁻¹ cm⁻² Hz⁻¹ str⁻¹, φ is measured in radian, and Π_1 , Π_c , and Π_{tot} are expressed in percentages. Note that for case (i) the resulting *I* has an order of magnitude 10^{-23} , which is much smaller than the specific intensity of the cosmic microwave background of 10^{-18} erg s⁻¹ cm⁻² Hz⁻¹ str⁻¹ at the same observed frequency. This suggests that emission and polarisation signals would be overwhelmed by the CMB background in real observations.



Fig. 3.5: Cosmological evolution of the *invariant* Stokes parameters (in units of erg s⁻¹ cm⁻² Hz⁻⁴ str⁻¹) for $v_{obs} = 1.42$ GHz for the cases where the radio bright point source is (i) absent, (ii) located at z = 6.0, and (iii) located at z = 0.206.



cases where the radio bright point source is (i) absent, (ii) located at z = 6.0, and (iii) located at z = 0.206.



Fig. 3.7: Cosmological evolution of $\Delta \varphi$ (in radian), Π_l , Π_c and Π_{tot} (in percent) for the cases where the radio bright point source is (i) absent, (ii) located at z = 6.0, and (iii) located at z = 0.206. Note that the change of polarisation angle is sensitive to the randomness of the magnetic field angle along the line-of-sight.

Faraday-converting medium, (ii) the fiducial point source is placed at $z = z_{init} = 6.0$, serving as a bright distant radio back-light, and (iii) the fiducial point source is located much nearer, at z = 0.206 (cf.Jagers et al. 1982). The prescription of the intervening plasma at z = 0 follows model A-II described in Table 3.1; simple cosmological evolution of $n_e(z)$, $T_e(z)$ and |B(z)| described in Sec. 3.1.1 are now accounted for while the fraction of non-thermal relativistic electrons \mathcal{F}_{nt} , their energy spectral index p and the Lorentz factor of low-energy electron cutoff γ_i are assumed to be constant over all redshifts. The results of the three different scenarios are displayed alongside in Fig. 3.5 – Fig. 3.7 for comparison purposes. Numerical results are summarised in Table 3.3.

Differences in the results of the three cases indicate that on a cosmological scale, polarised radiative transfer of light travelling through a foreground cosmologically-evolving IGM-like plasma, with or without a bright point source, can impart unique polarisation features. Also, it can be readily seen from Fig. 3.5 and Fig. 3.6 that both the total emission and the polarised emission from the fiducial point source dominate over the contributions from the foreground plasma, as expected. The invariant intensity I of the radiation stays by and large constant from where the bright point source is positioned with a very small increase over increasing *z* due to the emission of the line-of-sight plasma, which is calculated in case (i). Fluctuations in Stokes parameters are induced by random magnetic field orientations along the line-of-sight.

The observed change of polarisation angle $\Delta \varphi$, which is a measure of the amount of Faraday rotation and is sensitive to the magnetic field directions along the line-of-sight, depends on the *z*-position of the point-source, as is seen in Fig. 3.7 and Table 3.3. In all three cases, $\Delta \varphi < \pi$. This indicates that the effect of Faraday rotation is weak, as is expected for a line-of-sight plasma that is threaded with a weak magnetic field of nG and has a low electron number density. Insignificant Faraday conversion is also observed in case (i), for which there is only the plasma but no bright sources lying along the line-of-sight. Note that Π_c is much weaker than Π_l by 10^5 . For case (ii), Π_l and Π_c are dominated by the contributions of the bright point

source over the foreground plasmas. For case (iii), the sudden drops in Π_{l} and Π_{tot} and the large rises in $\Delta \varphi$ and Π_{c} shows the effects of having a foreground (nearby) source. Understanding the foregrounds, particularly any bright line-of-sight sources and their locations, is crucial for the correct inference of magnetic fields and their evolution.

In addition, a depolarisation effect is observed: there is a net drop in Π_{tot} as *z* decreases (i.e. as path length increases). By the experimental set up, this is mainly due to differential Faraday rotation (i.e. emission at different *z* is rotated by different amounts due to their magneto-ionised foreground, thus reducing the net polarisation). Random magnetic fields, in the context that the total magnetic fields are decomposed into a regular (large-scale average) component, \overline{B} , and a random (small-scale fluctuation) component b_{random} , i.e. $B = \overline{B} + b_{random}$, have also been identified as another cause of depolarisation in the literature (see e.g. Burn 1966; Sokoloff et al. 1998; Horellou and Fletcher 2014). Investigating the effects of such random fields is beyond the scope of this demonstration, but the results here illustrate how the effects on polarisation can be quantified by performing a full cosmological polarised radiative transfer.

3.2.2 Single galaxy cluster

Here pencil-beam CPRT calculations are conducted, demonstrating the ability of the CPRT formulation to interface with cosmological MHD simulation results (via a post-processing treatment) and generate intensity and polarisation maps of an astrophysical object. Each pixel of the maps corresponds to a solution obtained by the radiative transfer calculation.

Polarisation of a simulated galaxy cluster obtained from the "cleaned" implementation of a higher resolution GCMHD+ simulation (see Sec. 4 in Barnes et al. 2018) is computed. The GCMHD+ simulations, designed to focus on the evolution of the magnetic fields due to structure formation without the additional physics, are adiabatic, i.e. no radiative cooling, reionisation, star formation and feedback from supernovae and Active Galactic Nuclei (AGN). The cluster obtained at z = 0 from the simulation has a virial radius of $R_{\rm vir} = 1.44$ Mpc, and a gas mass of $m_{\rm gas} \sim 10^{13}$ M_{\odot}. It is assumed that non-thermal electrons have energy density that amounts to 1% of the thermal energy density (see Barnes et al. 2018). Properties of the cluster are summarised in Table 3.4. The central slices of the data cube viewed along the *z*-direction are shown in Fig. 3.8, illustrating the input structures of electron number density, magnetic field strength and orientation for the CPRT calculation.

Radiative transfer of a total number of $256^2 = 65536$ rays is computed from z = 6.0 to z = 0.0 through the galaxy cluster centred at $z_{cluster}$. Without loss of generality, $z_{cluster} = 0.5$ (i.e. placed between z = 0.500645 and z = 0.499355, corresponding to a length scale of 2.89 Mpc $\approx 2R_{vir}$) is chosen. In order to study the intrinsic polarisation emission of the cluster, no materials fill the line-of-sight outside of the cluster and there is zero initial radiation background. Emission, absorption, Faraday rotation, and Faraday conversion by thermal bremsstrahlung and non-thermal synchrotron radiation processes are taken into account.

Fig. 3.9 shows the resulting intensity and polarisation maps obtained at z = 0; statistics of those maps are summarised in Table 3.4. The simulated cluster is intrinsically polarised at $v_{obs} = 1.42$ GHz with a mean degree of total polarisation of ~ 68.57 %, dominated by linear polarisation. Emission is the highest in the cluster's central region, where the magnetic field strength and the electron number density are the highest (see Fig. 3.8). Faraday rotation is also strong in the central region, leading to a bigger change of polarisation angle, as is seen in the map of $\Delta \varphi$ shown in Fig. 3.9. At the same time, depolarisation in that region is also the most significant, where the degree of polarisation and the effect of random field orientations along the line-of-sight are the causes of depolarisation in this demonstration. These results agree with the observational trends of smaller degree of polarisation for sources close to the cluster centre (e.g. Bonafede et al. 2011; Feretti et al. 2012).

The CPRT calculation provides a rich set of data products, enables quantitative measures of polarisation and intensity, and its algorithm allows interfacing with simulation results. While here the calculation for a simulated cluster at a fixed

| | Mean | Standard Deviation | Minimum | Maximum |
|-------------------|---------------------------|--------------------------|----------------------------|--------------------------|
| Input | | | | |
| $n_{\rm e, tot}$ | 6.3561×10^{-5} | 2.7001×10^{-4} | 6.3577×10^{-7} | 2.6508×10^{-2} |
| B | 1.5585×10^{-8} | 5.0621×10^{-8} | 2.5227×10^{-14} | 2.5175×10^{-6} |
| $\cos \theta$ | -5.9235×10^{-3} | 5.7434×10^{-8} | -1.0000 | 1.0000 |
| Output | | | | |
| Ι | 7.0217×10^{-18} | 4.4204×10^{-18} | 2.2564×10^{-27} | 1.3000×10^{-16} |
| Q | 1.6270×10^{-19} | 1.0358×10^{-18} | -2.96286×10^{-19} | 3.3099×10^{-17} |
| U | -2.3702×10^{-21} | 9.3950×10^{-19} | -2.9899×10^{-17} | 3.2602×10^{-17} |
| V | -2.6325×10^{-25} | 4.2232×10^{-23} | -1.5752×10^{-21} | 1.9561×10^{-21} |
| $\Delta arphi$ | 1.1957×10^{-3} | 0.2543 | -3.1240 | 3.1401 |
| Π_{l} | 68.5725 | 8.0302 | 1.1191 | 70.5876 |
| Π_{c} | 2.3278×10^{-4} | 2.8580×10^{-4} | 6.4526×10^{-10} | 4.2846×10^{-3} |
| Π_{tot} | 68.5725 | 8.0302 | 1.1191 | 70.5876 |

Table 3.4: Statistics of the input and output parameters at z = 0 of the demonstrative pencilbeam CPRT calculation using the simulated galaxy cluster obtained from the GCMHD+ cosmological MHD simulation; see Sec. 3.2.2. $n_{e, \text{ tot}}$ is in units of cm⁻³, while $|\mathbf{B}|$ is in G. The Stokes parameters are in units of erg s⁻¹ cm⁻² Hz⁻¹ str⁻¹, $\Delta \varphi$ is in radian, and Π_{l} , Π_{c} , Π_{tot} are in percent. All values are corrected to four decimal places for compactness.

redshift is demonstrated and only the intensity and polarisation maps at z = 0 are presented, the CPRT algorithm can generate maps at any sampled redshifts. Comparisons of the statistics of maps generated at different redshifts may provide a useful means to study the cosmological evolution of magnetic fields, as well as giving insights into tomographic studies of large-scale magnetic fields in real data. Mock data-sets obtained from CPRT calculations can also be used to test analysis tools used for magnetic field structure inference.

3.2.3 All-sky calculation

Here an all-sky CPRT calculation is performed to compute theoretical radio polarised sky maps, matching the sky coverage and the frequency that are covered by current and upcoming radio surveys. The demonstrative application uses a model magnetised universe obtained from a cosmological MHD simulation with the GCMHD+ code (Barnes et al. 2012, 2018) as an input structure.

Ray-tracing CPRT calculations are carried out for a total number of $N_{ray} = 12 \times 64^2 = 49152$ rays distributed on *z*-spheres according to the HEALPix sampling scheme (Górski et al. 2005). Radiation frequency is chosen to be $v_{obs} = 1.42$ GHz.



Fig. 3.8: The line-of-sight view of the central slices of a simulated galaxy cluster from the GCMHD+ simulation, showing the structure of electron number density (top), magnetic field strength (middle) and magnetic field orientations along the line-of-sight as defined by $\cos \theta$ (bottom). The whole galaxy cluster data of dimension $256 \times 256 \times 256$ are used for the demonstrative pencil-beam calculation (see Sec. 3.2.2).



Fig. 3.9: The resulting maps at z = 0 of $\log I$, $\log |V|$, $\log |Q|$, and $\log |U|$ in units of erg s⁻¹ cm⁻² Hz⁻¹ str⁻¹, $\Delta \varphi$ in radian, and the maps of Π_1 , Π_c , Π_{tot} in percent, obtained from the demonstrative CPRT calculation for the simulated galaxy cluster (see Sec. 3.2.2).

The redshifted CMB background radiation and its influences are neglected, and radio polarisation is attributed to sources consisting both thermal and non-thermal electrons distributed across the entire universe in the post-reionisation epoch⁷ (i.e. $z \le 6.0$). Both thermal bremsstrahlung and non-thermal synchrotron radiation processes are taken into account. To highlight the polarisation signatures imparted by magnetic structures, electron number density $n_{e,tot}(z, \theta, \phi)$ is assumed to be uniform across the entire sky at each z; its cosmological evolution over zunderwent a dilution in an expanding universe, i.e. $n_{e,tot}(z) = n_{e,tot,0}(1 + z)^3$, where $n_{e,tot,0} = 2.1918 \times 10^{-7}$ cm⁻³ (see Appendix F for details). Non-thermal relativistic electrons are assumed to amount to 1% of the total electron number density. Their energy spectrum follows a power law with a spectral index of p = 4.0 (i.e. the nonthermal electrons have aged, steepening the spectrum), corresponding to a radiation power-law spectrum with index $\alpha = (p-1)/2 = 1.5$. The low cutoff of the electron energy is set to $\gamma_i = 10.0$, and the high cutoff is set to infinity.

The GCMHD+ cosmological MHD simulation (Barnes et al. 2012, 2018) is used to determine the evolution of the large-scale magnetic field as structures in the universe assemble. A cubic region of comoving volume (40 Mpc)³ was taken from a comoving (100 Mpc)³ volume in the simulation, which started at z = 47.4as determined by the initial condition generator GRAFIC++. The magnetic field was assumed to be generated at some early epoch via a method that filled the volume of the simulation. It has a configuration of $B = (10^{-11}, 0, 0)$ G. The output of $B_{\parallel}(z)$ obtained from the GCMHD+ simulation is fitted analytically by the piece-wise

⁷The non-linear growth in magnitudes and structures of electron number density during the reionisation epoch would have imparted observational signatures to the travelling radiation, varying statistics such as the polarisation power spectrum. However, for demonstrative purpose I do not consider such an effect in this work.

function:

$$\log_{10}\left(\frac{B_{\parallel}^{2}(z)}{8\pi}\right) = \begin{cases} 8.1737 \, x^{4} - 40.352 \, x^{3} + 73.647 \, x^{2} - 55.264 \, x - 12.16 & (0.64 < x < 1.70) \\ 0.67 \, \tanh(-x/0.18 + 2.72) - 26.14 & (0.15 \le x \le 0.64) \\ -\tanh(x/0.52 + 0.28) - 24.91 & (-2.00 \le x < 0.15) \end{cases}$$
(3.3)

with $x = \log_{10} z$. This fit, plotted in Fig. 3.10, is smoothed by interpolation using twenty-one-point averages to model the input of $B_{\parallel}(z)$ for the CPRT calculation. A log-normal spatial distribution of $B_{\parallel}(z, \theta, \phi)$ is assumed over each *z*-sphere, where the mean value is calculated from Eqn. (3.3) multiplied by a factor of 10^3 to match the expected observed field strength of 1.0 nG typical of filaments (see e.g. Araya-Melo et al. 2012). The log-normal distribution ensures the magnetic field strength to be all positive. Directions of the magnetic fields, which are defined by the $\cos \theta$, are assumed to have random orientations along the line-of-sight.

Results and discussion

(I) Along a randomly selected ray

Fig. 3.11 shows the resulting cosmological evolution of both the invariant and comoving Stokes parameters, as well as the cosmological evolution of $\Delta \varphi$, Π_{l} , Π_{c} and Π_{tot} of a randomly selected ray. Notably, one can see that the fluctuations in Q, U and V increase significantly during the later period, i.e. when the structure formation and evolution processes (such as the assembly of galaxy clusters) in the cosmological simulation become prominent and the magnetic fields become significantly amplified during these processes, hence imposing a Faraday screen (i.e. strong Faraday-rotating component). In addition, highly volatile behaviour is observed in the change of polarisation angle over all z. Volatility in the evolution of polarisation angle increases the difficulty to distinguish between different Faraday depth components, limiting the usage of the standard approach to infer magnetic field properties using RM synthesis (see e.g. Brentjens and de Bruyn 2005) in some



Fig. 3.10: Plots of the cosmological evolution of the electron number density $n_{e, tot}$ (upper panel) and the logarithmic of magnetic energy density $U_{\rm B} = |\mathbf{B}|^2/8\pi$ (lower panel) outputted from the GCMHD+ cosmological simulation. The solid red line in the bottom diagram shows the piece-wise function that fits to the data, ignoring the anomalous bump caused by instantaneous infall and outflow of the simulation box. Note that smoothing via the 21-point averaging method is applied to obtain $B_{\parallel}(z)$ for the CPRT calculation. Note also that I consider only the post-reionisation epoch, i.e. $6.0 \ge z \ge 0.0$, in the calculation. Note that the anomalous bump in the evolution of magnetic energy density at $\log z = -0.5$ is caused by the instantaneous infall and outflow of the simulation box. This structure does not appear in the other four simulations that ran with different initial conditions, and is therefore neglected.



Fig. 3.11: Cosmological evolution of the invariant Stokes parameters, the comoving Stokes parameters, $\Delta \varphi$, Π_{l} , Π_{c} and Π_{tot} over the redshifts $6.0 \ge z \ge 0.0$ obtained from the CPRT calculation using a model magnetised universe obtained from the GCMHD+ simulation as the input structure; see Sec. 3.2.3.

| | Mean | Standard Deviation | Minimum | Maximum |
|-------------------|---------------------------|--------------------------|---------------------------|--------------------------|
| Input | | | | |
| $n_{\rm e, tot}$ | 2.1918×10^{-7} | 0.0000 | 2.1918×10^{-7} | 2.1918×10^{-7} |
| B | 5.2855×10^{-9} | 6.8763×10^{-9} | 4.5734×10^{-11} | 1.9587×10^{-7} |
| $\cos \theta$ | -1.8850×10^{-3} | 0.5769 | -1.0000 | 0.9999 |
| Output | | | | |
| Ι | 9.6274×10^{-24} | 3.3006×10^{-26} | 9.5894×10^{-24} | 1.1695×10^{-23} |
| Q | 4.7385×10^{-26} | 2.6055×10^{-26} | 1.7357×10^{-26} | 1.6790×10^{-24} |
| U | 2.9300×10^{-31} | 3.5445×10^{-28} | -2.7505×10^{-26} | 1.0346×10^{-26} |
| V | -1.0209×10^{-33} | 2.0177×10^{-30} | -2.1578×10^{-28} | 8.4035×10^{-29} |
| $\Delta arphi$ | 1.1597×10^{-5} | 4.7925×10^{-1} | -3.0689×10^{-1} | 3.4868×10^{-1} |
| Π_{l} | 4.9131×10^{-3} | 2.5886×10^{-3} | 1.8100×10^{-3} | 1.4359×10^{-1} |
| Π_{c} | 5.4946×10^{-8} | 1.8629×10^{-7} | 1.5424×10^{-12} | 1.8452×10^{-5} |
| Π_{tot} | 4.9131×10^{-3} | 2.5886×10^{-3} | 1.8100×10^{-3} | 1.4359×10^{-1} |

Table 3.5: Statistics of the input and output parameters at z = 0 of the demonstrative allsky CPRT calculation using a model magnetised universe obtained from the cosmological GCMHD+ simulation; see Section 3.2.3. $n_{e, tot}$ is in units of cm⁻³, while |B| is in G. The Stokes parameters are in units of erg s⁻¹ cm⁻² Hz⁻¹ str⁻¹, $\Delta \varphi$ is in radian, and Π_{l} , Π_{c} , Π_{tot} are in percent. All values are corrected to four decimal places for compactness.

cases. Similar trends in polarisation evolution are observed in all the other randomly selected rays.

(II) All-sky maps

Theoretical all-sky polarisation maps of I, Q, U, and V can be generated at any chosen redshift. Fig. 3.12 shows the Stokes maps obtained at z = 0. Their statistics are summarised in Table 3.5. As pointed out from the previous discussion about the single-ray results, the evolution of the change of polarisation angle, which serves as a probe of the Faraday rotation effect, is highly volatile and complex. Thus, covariant CPRT calculations and advanced statistical analysis techniques are essential for proper science extraction from map data.

3.3 Implications on the Study of Large-scale Magnetic Fields

The results of the demonstrative calculations shown above have two major implications to the study of large-scale magnetic fields, firstly on the power spectrum analyses, and secondly on the validity of the current methodologies to investigate large-scale magnetic fields.


Fig. 3.12: All-sky maps of the Stokes parameters I, Q, U, V at z = 0 obtained from the demonstrative CPRT calculation in which cosmological GCMHD+ simulation results of the cosmological evolution of magnetic field strength is incorporated, log-normal distribution of the field strength over the redshift spheres are assumed, and the electron number density is diluted by $1/(1 + z)^3$ due to the expansion of the universe; see Sec. 3.2.3. The scale of the colorbar is adopted to make the fluctuations in the Stokes maps apparent. The full dynamical range of the data is given in Table 3.5.

A dominating complex Faraday component can be introduced when cosmological structure formation and evolution processes become prominent, as is seen in Fig. 3.11, where significant polarisation fluctuations happened during the later period when galaxy clusters started to assemble in the simulation, boosting the mean magnetic field strength. This finding means that cosmological contributions from line-of-sight IGM-like media will likely be screened (or shielded) by fluctuations sourced from astrophysical structures like a galaxy cluster (i.e. ionised systems with relatively high magnetic field strengths and electron number density). This further implies that the power spectrum of an all-sky polarisation map will be dominated by high frequency (small-scale) signals. At the same time, it is worth noting that the morphology of ionised bubbles during the Epoch of Reionisation, which has not been investigated in this work, may imprint observable signatures onto the polarisation maps, contributing to the power in low frequency (large-scale) in polarisation power spectrum as those ionised regions overlapped.

Moreover, the highly volatile cosmological evolution of the Stokes parameters reveals the need of a more sophisticated approach to extract information about the properties of cosmological magnetic fields from polarisation data. Conventional analyses using RM and its fluctuations, RMF, would be inadequate in such a situation. This is because RM/RMF are derived from a restrictive form of polarised radiative transfer and their associated methods typically consider simplified models, thus limiting their applicability. See On et al. (2019) for detailed discussion and important assessments of the validity of RMF analyses in different astrophysical conditions; see Appendices D and E in this thesis for a concise summary. Here, emphasis is put on the studies of the situations where Faraday rotation is not the sole important radiative process in operation and effects from cosmological evolution are nonnegligible. Unambiguous predictions of polarisation signals from covariant CPRT calculations are crucial for meaningful comparison with observations, as well as providing insights to properly interpret the polarised sky and correctly determine how large-scale magnetic fields have evolved and where they came from.

3.4 Concluding Remarks

In this chapter, an all-sky algorithm for covariant cosmological polarised radiative transfer is presented. The space-time metric of the FRW cosmological model, which has a flat geometry, is considered. The CPRT formulation is constructed from a covariant GRRT formulation, derived from the first principles of conservation of phase-space volume and photon number. The (all-sky) CPRT algorithm allows the results from cosmological MHD simulations to be incorporated and a straightforward generation of theoretical intensity and polarisation maps. Since the algorithm is constructed based on a self-consistent fully-covariant CPRT formulation, it provides a reliable means to study the propagation of polarised radiation, henceforth the cosmic magneto-ionic properties (through the Faraday effects and synchrotron intensity) throughout the evolutionary history of the universe or from a specific redshift of an astrophysical system of interest. Moreover, all radiation processes (emission, absorption, Faraday rotation and Faraday conversion) are treated explicitly in the CPRT formalism. Therefore its applicability is broad and general, and not restricted to the special cases wherein all radiative processes except Faraday rotation is absent/insignificant, the condition from which the standard RM formulae is derived.

The CPRT algorithm is able to produce polarised radio maps with sky coverage ranges from a point, to a patch, up to the entire celestial sky. Not only can it be applied to study the polarised signatures/emissions of cosmic plasmas against/ambient to bright radio point sources, such as pulsars, quasars and fast radio bursts (FRBs), it can also calculate the polarisation of extended cosmological structure, such as emitting filaments of the cosmic web. The feature of the CPRT formalism to handle complex spatial structure(s) along each line of sight and in the mapmaking processes, not offered by conventional RMF analyses (see Appendix E), is demonstrated in Sec. 3.2.2 and Sec. 3.2.3. Furthermore, the maps generated from CPRT calculations contain unambiguous intensity and polarisation predictions of the models of a magnetised structure (e.g. a magnetic universe as a whole, or the

complex structure(s) within it). These maps serve as model templates to provide physical insights that aid observational interpretations. Together with the application of advanced statistical analyses which characterise structural features in the map data, complex theoretical models can then be meaningfully compared with observational data, such as those to be collected by the forthcoming SKA, as well as from spectro-polarimetric observations by SKA's precursors (ASKAP, MeerKAT, MWA) and pathfinders (in particular, LOFAR, CHIME, and FAST), which are operating currently.

Two sets of CPRT numerical tests have been conducted to validate the code implementation in single/multiple ray settings. Three sets of CPRT calculations have been performed to demonstrate its application for practical astrophysical studies, including the study of the propagation of polarised radiation against a bright radio point-source (or not), in a stimulated galaxy cluster, and in a stimulated magnetised universe that underwent cosmological structural evolution. I summarise below the data products of the CPRT algorithm, the scientific information that they contain, as well as the astrophysical implications of the findings of the demonstrative calculations.

Solving the CPRT equation yields the evolution of the Stokes parameters of radiation as a function of redshift z. This enables quantitative tracking of the changes in the radiation intensity and polarisation over its path and studies of the impacts by local radiation processes (thermal bremsstrahlung and non-thermal synchrotron radiation processes in this work) in a cosmologically evolving universe.

The set of single-ray proof-of-concept calculations, which is presented in Sec. 3.2.1, considered the cases in which a bright radio point source is absent or present. In all cases, unbiased randomly-oriented magnetic fields are distributed along the line-of-sight, and the field strength evolved adiabatically (frozen-in condition). As expected, the evolution of the radiation's properties along the line-of-sight are completely different in cases with or without a bright radio backlight, with significant differences seen in the evolution of the degrees of linear, circular and total polarisation. In the presence of a strong backlight, the case wherein the source is

positioned at a high redshift also different clearly to the case in which the source is nearby. The former situation allows studies of the foreground weakly magnetised IGM-like plasmas, while the latter have the past evolution shielded by the bright nearby sources. A key take-away message is the ability of the CPRT calcaultions to directly track the cosmological evolution of the 4-Stokes parameters, the change of polarisation angle, and the degrees of all types of polarisation. Not only does it naturally resolve the issue of $n\pi$ -ambiguity, which concerns the number of 180° rotations of the polarisation angle unknown to an observer, it also enables further investigation of depolarisation and repolarisation of radiation caused by Faraday effects along a ray path.

Carrying out multiple-ray CPRT calculations generates maps of the 4-Stokes parameters, the change of polarisation angles, and the degree of linear, circular and total polarisation, at the oberver's frame (or at any arbitrary redshifts). In the demonstrative calculations, polarisation of the simulated galaxy cluster obtained from a GCMHD+ simulation is calculated, taking into account the three-dimensional spatial variations of electron number density and magnetic fields inside the cluster. The galaxy cluster acts as a 3D Faraday block of magnetised plasma (in contrast to the Faraday screen approximation commonly used in the studies of foreground Faraday rotation), exhibiting more substantial Faraday effects than those in the intergalactic space, which is explained by the much higher electron number density and magnetic field strengths in an intra-cluster environment. At the same time, significant depolarisation effects due to differential Faraday rotation occurred in the central region of the galaxy cluster, agreeing with the trends seen in several observational studies. The galaxy-cluster calculations have demonstrated the ability of the CPRT calculations to deal with a complex spatial structure, whose electron number density and magnetic field strength are inhomogeneous, exhibit different configurations, and display structural features on varying spatial scales.

Conducting CPRT calculations over the entire sky in full cosmological settings results in spherical maps of the observables. In the demonstrative application, all-sky CPRT calculation are conducted using a model magnetised universe obtained from the cosmological GCMHD+ simulation, accounting for the cosmological evolution of the magneto-ionic properties of the universe after the epoch of reionisation. The cosmological evolution of the polarisation components of propagating radiation is found to be highly volatile, implying that full covariant CPRT consideration is essential for accurate inter-galactic magnetic field studies. Another implication concerns the polarisation power spectra from all-sky observations. Those spectra are likely to be dominated by the high-frequency (small-scale) signals caused by strong Faraday-rotating components, such as galaxy clusters. Emissions from the medium and the embedded sources along the line-of-sight also boost power in the fluctuation on the small scales, which should be differentiated from the signals truly arising from magnetic field structures (see Appendix E for the discussion about issues relating to magnetic field inference from the polarisation data).

Finally, since the variations of the observable quantities along the ray propagation and those across the sky plane are determined by the convolution of the spatial variations of the magneto-ionic plasma properties at different epochs over the ray path and the temporal variations of the magneto-ionic plasma properties over cosmological evolution, ionised structures arisen during the EoR also impart polarisation fluctuations. Investigations of the imprints on the polarisation signals due to the morphology of cosmological reionisation, which are not addressed in this thesis but are important research problems, can be achieved by utilising the CPRT formalism.

Chapter 4

Cosmological 21-cm Line Radiative Transfer

This chapter presents my derivation of a covariant formulation for cosmological 21-cm line radiative transfer (C21cmLRT). The formulation is the first of its kind. It takes full account of (i) global effects, in particular, cosmic expansion and the changes in the ionisation state of hydrogen along the line-of-sight as the cosmological reionisation proceeds, and (ii) local effects, such as bulk motions of the medium in the scales of galaxies and galaxy clusters, and the microscopic kinetic movements and turbulence. Demonstrations of its applications in astrophysical settings are also presented.

4.1 Hyperfine 21-cm Line of Neutral Hydrogen

4.1.1 Spin-coupling and hyperfine splitting

The 21-cm line (in the GHz radio waveband) observed in astrophysical sources is attributed to the emission due to the hyperfine transition in the electronic ground state of neutral atomic hydrogen (H I gas). The hyperfine splitting is induced by the interaction of the magnetic moment (spin) of the electron with the magnetic field generated by the magnetic moment (spin) of the proton at the hydrogen nucleus. The orbital of the electron in the hydrogen atom is spherically symmetric in the ground state. This symmetry makes all except one term in the interaction Hamiltonian vanish. The surviving term corresponds to a direct spin-spin coupling (interaction) between the electron and the proton. This spin-spin coupling has two energy states, with the spins of the electron and the proton either in parallel or in anti-parallel, which breaks the degeneracy of the $1S_{1/2}$ state of the hydrogen atom, and reveals a triplet state and a singlet state of different energy levels. The triplet state, corresponding to the electron and proton spins in parallel, has a higher energy and is referred to as the

upper hyperfine level. On the other hand, the singlet state, corresponding to spins in anti-parallel, has a lower energy and is referred to as the lower hyperfine level. Hereafter, the triplet and the singlet states are denoted as "u" and "l", respectively.

The energy shift of the triplet and the singlet states of the hyperfine splitting are asymmetrical, in contrary to the energy shifts in Zeeman splitting in the electronic ground state of hydrogen, although both are essentially caused by the interaction of an electron spin with a magnetic field "exterior" to the electron. The hyperfine interaction causes a perturbation in the Hamiltonian, and in hydrogen, it gives rise to a perturbed Hamiltonian operator, which can be decomposed into two separated terms:

$$\Delta H_1 \propto (\hat{\boldsymbol{r}} \cdot \boldsymbol{\mu}_{\rm e})(\hat{\boldsymbol{r}} \cdot \boldsymbol{\mu}_{\rm p}); \qquad (4.1)$$

$$\Delta H_2 \propto (\boldsymbol{\mu}_{\rm e} \cdot \boldsymbol{\mu}_{\rm p}) , \qquad (4.2)$$

where μ_e and μ_p are the magnetic moments of the electron and the proton, respectively. The spherical symmetry of the unperturbed electronic wave-function of hydrogen implies that the expected value of ΔH_1 is zero, as

$$\langle \Delta H_1 \rangle \propto 2\pi \int_0^\pi \mathrm{d}\,\tilde{\theta}\,\sin\tilde{\theta}\,(\cos\tilde{\theta}) = 0\,,$$
(4.3)

where $\tilde{\theta} = \cos^{-1}(\hat{r} \cdot \mu_e / |\mu_e|)$. It leaves the non-vanishing perturbation arisen from the spin-spin coupling, i.e.

$$\langle \Delta H_2 \rangle \propto \langle (\boldsymbol{\mu}_{\mathrm{e}} \cdot \boldsymbol{\mu}_{\mathrm{p}}) \rangle \propto \langle (\hat{\boldsymbol{s}}_{\mathrm{e}} \cdot \hat{\boldsymbol{s}}_{\mathrm{p}}) \rangle .$$
 (4.4)

Electron and proton are both spin-1/2 fermions, i.e. $s_e = 1/2$ and $s_p = 1/2$, and hence, the spin of an electron-proton pair, *F*, is either 1 (parallel configuration) or 0 (anti-parallel configuration). The spin-1 (*F* = 1, parallel) state is a triplet, as its projection can take values of 1, 0, or -1. The spin-0 (*F* = 0, anti-parallel) state is a singlet, as its projection can only take a value of 0. It follows that

$$\langle (\hat{s}_{\mathrm{e}} \cdot \hat{s}_{\mathrm{p}}) \rangle = \frac{1}{2} \left\langle \left((\hat{s}_{\mathrm{e}} + \hat{s}_{\mathrm{p}})^2 - \hat{s}_{\mathrm{e}}^2 - \hat{s}_{\mathrm{p}}^2 \right) \right\rangle$$
(4.5)

$$= \frac{1}{2} \left(F(F+1) - s_{\rm e}(s_{\rm e}+1) - s_{\rm p}(s_{\rm p}+1) \right) \, [\hbar^2] \,. \tag{4.6}$$

For the triplet state, $s_e = s_p = 1/2$ and F = 1, which gives $\langle (\hat{s}_e \cdot \hat{s}_p) / [\hbar^2] = +1/4$; for the singlet state, $s_e = s_p = 1/2$ and F = 0, which gives $\langle (\hat{s}_e \cdot \hat{s}_p) / [\hbar^2] = -3/4$. The downshift-energy of the singlet state is, therefore, 3 times the upshift-energy of the triplet state.

Hyperfine splitting can also occur in the excited states. For instance, if the electron is in one of the 2P orbitals, then, $\langle \Delta H_1 \rangle$ will be non-zero. This results in a more complex network of state transitions, especially when the transition is also coupled with an external radiation field.

The transition between the hyperfine triplet state and singlet state of neutral hydrogen in a ground state involves a spin-flip of the electron, and the transition is a magnetic dipole transition. The transition is mediated by an emission or absorption of a photon of an energy difference between the two hyperfine levels, i.e. $\Delta E_{ul} = 5.87 \times 10^{-6}$ eV, corresponding to a frequency of 1.42 GHz and a wavelength of 21.1 cm. This 21-cm hyperfine line has long been predicted (van de Hulst 1945) and observed (Ewen and Purcell 1951; Muller and Oort 1951; Pawsey 1951), and its rest-frame frequency is one of the most precisely measured physical quantities¹. The precision in its frequency measurement and the abundance of hydrogen in the Universe make the neutral hydrogen 21-cm hyperfine line a useful means for the

$$v_{\rm ul} = \frac{8}{3} g_{\rm I} \left(\frac{m_{\rm e}}{m_{\rm p}}\right) \alpha^2 \left(R_{\rm H}c\right) \approx 1420.405751 \text{MHz}$$
 (4.7)

¹The frequency of the hyperfine transition in HI in the ground state has been measured at a high precision with 1420405751.7667 ± 0.001 Hz (Essen et al. 1971) and 1420405751.768 ± 0.002 Hz (Hellwig et al. 1970), through maser experiments. The experimental uncertainty does not exceed 1 part in 10¹² in these studies. The highly-precise measurement of the 21-cm line frequency enables the searches for the variations, if any, in the fundamental physical constants over cosmological time. One example is the fine structure constant α ($\equiv e^2/\hbar c \approx 1/137.036$), which relates to the rest-frame frequency of the 21-cm line as

⁽see e.g. Condon and Ransom 2016), where $g_{\rm I} \approx 5.58569$ is the nuclear *g*-factor of proton. The hydrogen Rydberg constant is $R_{\rm H} = R_{\infty} \left[1 + (m_{\rm e}/m_{\rm p}) \right]^{-1}$, where $R_{\infty} (= \alpha^2 m_{\rm e} c/4\pi\hbar)$ is the Rydberg constant. This gives a hydrogen Rydberg frequency $R_{\rm H}c = 3.28805 \times 10^{15}$ Hz.

investigation of various dynamical and physical processes in the diffuse medium on galactic and cosmological scales.

4.1.2 Hyperfine 21-cm line in galactic astrophysics

The first study using the 21-cm emission to probe the properties of galaxies dates back to the time when radio astronomy just emerged. Radio emission at the GHz frequencies does not suffer much dust extinction. The 21-cm hyperfine emission line from neutral hydrogen is, therefore, transparent across the Galactic plane, allowing us to derive useful information regarding the kinematics, dynamics and structure of the Galactic disk (see e.g. Sofue and Rubin 2001). Muller and Oort (1951) used the Doppler broadening of the 21-cm line to deduce the rotational speed of the Galaxy (Milky Way). Since then, the 21-cm hyperfine emission line has been used to construct the Galactic rotation curves (e.g. van de Hulst et al. 1957; Clemens 1985; Sofue and Rubin 2001; Sofue 2016a,b) and also map the spiral structures (e.g. van de Hulst et al. 1954; Sofue 2013).

The interstellar 21-cm emission line is now established as a standard kinematic tracer for galaxies. In addition to the Milky Way galaxy, the rotation curves (see Huchtmeier 1975; Sofue 2016a,b, and references therein) and the spiral structures (e.g. Bosma 1981) of the external spiral galaxies have been determined using the 21-cm observations. The observed 21-cm emission provides a two-dimensional velocity map (see e.g. Bosma 1981), from which not only the rotation curve of a galaxy can be constructed, but also the deviations from the circular rotation velocity can be measured. This precision measurement of the velocity field (e.g. Sanna et al. 2017; Wenger et al. 2018), would reveal galactic structures such as spiral arms, and bars, if they are also present (e.g. Crosthwaite et al. 2000). The rotation curve is a marker of the gravitational potential, and hence, the mass distribution of the galaxy (e.g. Sofue 2013, 2016a). The flattening of the rotation curve out to tens of kpc from their galactic centre universally observed in the spiral galaxies (e.g. Rubin and Ford 1970; Rubin and Graham 1987) are one of the key evidences to establish the presence of an invisible, non-baryonic matter component, which is referred to as

dark matter, on the galactic scale and above (e.g. Ostriker and Peebles 1973; Ostriker et al. 1974; Einasto et al. 1974).

The centre frequency of the 21-cm emission line, which is accurately determined in the laboratory (e.g. Peters et al. 1965), is a good reference of the local rest frame. Thus, it provides a means to determine the radial velocities of external galaxies from the measurement of the 21-cm lines. The radial velocities can, in turn, be used to estimate the Hubble distances to the galaxies, if the peculiar velocities associated with them are insignificant.

The strength of the 21-cm emission indicates the column density along the line-of-sight, and hence, it can be used to map the amount of HI gas in the Milky Way and the external galaxies (e.g. Dickey 1990; Dickey and Lockman 1990). Note that HI gas can also be present outside of galaxies, and it has a detectable 21-cm emission. Observations have shown that the interactions of galaxies could leave long streamers and tails of atomic hydrogen gas (e.g. Cottrell 1977). The dynamics of the galactic interactions can, therefore, be inferred from mapping the velocity structures and density distributions of these cold galactic debris, which would otherwise not be detected in the optical and X-ray observations.

The 21-cm line can appear in absorption in the presence of H I between a bright GHz radio source and the observer. In fact, the 21-line absorption spectra have been used to constrain the distances of hydrogen clouds in the Milky Way using the bright radio emission from a background source, e.g. a pulsar (see Gordon and Gordon 1973), or even a warm background continuum (Wienen et al. 2015).

4.1.3 Epoch of Reionisation and 21-cm tomography

The ability of the 21-cm line to trace the content and the distribution of neutral hydrogen in the early Universe makes it an important probe of the cosmological reionisation process (see e.g. Furlanetto et al. 2006; Pritchard and Loeb 2012, for reviews). Hydrogen filling the early Universe went through three major transitions in its ionisation state. It went from being fully ionised in the hot nucleosynthesis era to becoming neutral and atomic, as the Universe cooled when it expanded. It then

became ionised again when the first structures, such as stars and galaxies, emerged, producing X-rays and UV radiation, and perhaps energetic particles, that drove the global reionisation process. The unique spectral properties of the 21-cm line, which is optically thin to the mostly-ionised intergalactic media (see e.g. Madau et al. 1997), and the abundance of neutral hydrogen in the Universe, have made it an important probe to the evolutionary history of the Universe, starting from the end of the Cosmic Dark Ages and the beginning of the Cosmic Dawn through the entire era of reionisation to the present (see Furlanetto et al. 2006; Morales and Wyithe 2010; Pritchard and Loeb 2012).

The 21-cm line originating from different cosmological epochs is identified by the amount of redshifts in its frequency. Thus, the line spectrum is a tomographic measurement of the structures of the Universe as it evolves, (see e.g. Madau et al. 1997; Loeb and Zaldarriaga 2004; Furlanetto and Briggs 2004; Mellema et al. 2015). The angular variations of the line intensity across the sky maps the spatial structures in the Universe at the particular epochs associated with the redshifts of the line. It gives important information of the Universe even before the first galactic structures had formed² (Loeb and Zaldarriaga 2004; Barkana and Loeb 2005), as well as the progression of cosmological reionisation (see e.g. Furlanetto et al. 2006; Morales and Wyithe 2010; Pritchard and Loeb 2012; Mellema et al. 2015).

4.2 Radiative Transfer of the 21-cm Line

The generic line transfer equation at the local rest frame, accounting for the line and continuum opacities, takes the form:

$$\frac{\mathrm{d}I_{\nu}}{\mathrm{d}s} = -\left(\kappa_{\mathrm{C},\nu} + \kappa_{\mathrm{L},\nu}^{\mathrm{abs}} \,\phi_{\nu,\mathrm{abs}} - \kappa_{\mathrm{L},\nu}^{\mathrm{sti}} \,\phi_{\nu,\mathrm{sti}}\right) I_{\nu} + \left(\epsilon_{\mathrm{C},\nu} + \epsilon_{\mathrm{L},\nu} \,\phi_{\nu,\mathrm{emi}}\right) \,, \qquad (4.8)$$

where the subscripts "L" and "C" denote the line, and the continuum underneath and adjacent to the line, respectively. (The line transfer equation has assumed that the emission is not polarised and also energy distribution is unimportant.) The

²In addition to the redshift information offered by the spectral nature of the 21-cm line, the 21-cm line does not suffer from Silk damping that suppresses the CMB fluctuations on small scales, enabling it to probe the small-scale (linear) density fluctuations prior to the first structure formation (Loeb et al. 2008).

absorption coefficient has three components, contributed by the absorption of the line and the continuum and the stimulated emission (which can be considered as a negative absorption) of the line; the emission coefficient has two components, contributed by the emission of the line and the continuum.

The line profile functions $\phi_{\nu,x} \equiv \phi_x(\nu - \nu_{21cm})$, with $x \in \{abs, emi, sti\}$ corresponding to absorption, spontaneous emission and stimulated emission respectively, are defined with respect to the rest-frame frequency of the 21-cm line, ν_{21cm} . They are normalised, i.e.

$$\int_0^\infty d\nu \ \phi_{\nu,x} = \int_0^\infty d\nu \ \phi_x(\nu - \nu_{21cm}) = 1 \ . \tag{4.9}$$

This gives the strength of the 21-cm line, in the context of absorption, spontaneous emission and stimulated emission. In terms of the total effective line intensity, it can be expressed as

$$I_{21\rm cm} = \int_0^\infty d\nu \ I_\nu \phi_{\rm x} (\nu - \nu_{21\rm cm}) \ . \tag{4.10}$$

Equivalently, the expressions for the effective absorption, the spontaneous emission and the stimulated emission coefficients of the 21-cm line are

$$\kappa_{21\rm cm}^{\rm abs} = \int_0^\infty d\nu \; \kappa_{21\rm cm,\nu}^{\rm abs} \, \phi_{\rm abs}(\nu - \nu_{21\rm cm}) \;, \tag{4.11}$$

$$\epsilon_{21\rm cm} = \int_0^\infty d\nu \; \epsilon_{21\rm cm,\nu} \, \phi_{\rm emi}(\nu - \nu_{21\rm cm}) \;, \tag{4.12}$$

$$\kappa_{21\rm cm}^{\rm sti} = \int_0^\infty d\nu \; \kappa_{21\rm cm,\nu}^{\rm sti} \, \phi_{\rm sti}(\nu - \nu_{21\rm cm}) \; . \tag{4.13}$$

If the radiative processes for the continuum are unimportant, the line radiative transfer equation can be simplified to

$$\frac{\mathrm{d}I_{\nu}}{\mathrm{d}s} = -\left(\kappa_{\mathrm{L},\nu}^{\mathrm{abs}}\,\phi_{\nu,\mathrm{abs}} - \kappa_{\mathrm{L},\nu}^{\mathrm{sti}}\,\phi_{\nu,\mathrm{sti}}\right)I_{\nu} + \left(\epsilon_{\mathrm{L},\nu}\,\phi_{\nu,\mathrm{emi}}\right) \,. \tag{4.14}$$



Fig. 4.1: The Grotrian diagram of the 2P and 1S levels of the hyperfine structure and the associated transitions of neutral hydrogen. The transitions relevant for the Wouthuysen–Field effect are represented by the solid blue lines, and the other allowed transitions, but not contributing to electron spin-flips, are represented by the dashed blue lines. The hyperfine transitions, represented by the red lines, are characterised by the corresponding Einstein coefficients. Figure adapted from Pritchard and Furlanetto (2006).

4.2.1 Einstein coefficients, line emission and absorption

The coefficients in the radiative transfer equations, Eqns. (4.8) and (4.14), are macroscopic variables. They are, however, governed by microscopic processes. For the radiative transfer of the 21-cm line associated with the cosmological reionisation, the line absorption and emission are determined by the probability of transition between the hyperfine states due to the spin-flip of the ground state electron in the neutral hydrogen. The absorption and emission in the continuum at frequencies of the line and adjacent to the line are less relevant, although electron scattering could cause a certain degree of extinction when the line photons traverse the ionised matter along the line-of-sight.

Fig. 4.1 shows the Grotrian diagram of the hyperfine transitions between the two spin states ("u" for the higher-energy triplet $1_1S_{1/2}$ state) and "l" for the lower-energy $1_0S_{1/2}$ singlet state) of neutral hydrogen. The energy $\Delta E_{ul} = hv_{ul}$ (= hv_{21cm}).

The transition probabilities of the absorption, spontaneous emission and stimulated emission of a photon with ΔE_{ul} are specified by the Einstein coefficients B_{lu} , A_{ul} and B_{ul} , respectively. Consider an ensemble of neutral hydrogen atoms in the 1S ground state, with the populations of electrons in its triplet and singlet spin states specified by the number densities n_u and n_l , respectively. Thus, the effective emission coefficient of the 21-cm line may be expressed as

$$\epsilon_{21\text{cm}} = \epsilon_{\text{ul}} = \frac{h\nu_{\text{ul}}}{4\pi} n_{\text{u}}A_{\text{ul}} \int_{0}^{\infty} d\nu \ \phi_{\nu,\text{emi}} ; \qquad (4.15)$$

Similarly, the expression for the effective absorption coefficient of the 21-cm line is

$$\kappa_{\rm L} = \kappa_{21\rm cm}^{\rm abs} - \kappa_{21\rm cm}^{\rm sti}$$
$$= \kappa_{\rm ul}^{\rm abs} - \kappa_{\rm ul}^{\rm sti}$$
$$= \frac{h\nu_{\rm ul}}{4\pi} \left[n_{\rm l}B_{\rm lu} \int_0^\infty d\nu \ \phi_{\nu,\rm abs} - n_{\rm u}B_{\rm ul} \int_0^\infty d\nu \ \phi_{\nu,\rm sti} \right] . \tag{4.16}$$

It follows that the specific emission and absorption coefficients are

$$\epsilon_{\mathrm{L},\nu} = \frac{h\nu_{\mathrm{ul}}}{4\pi} n_{\mathrm{u}} A_{\mathrm{ul}} \phi_{\nu,\mathrm{emi}} ; \qquad (4.17)$$

$$\kappa_{\mathrm{L},\nu} = \frac{h\nu_{\mathrm{ul}}}{4\pi} \left[n_{\mathrm{l}}B_{\mathrm{lu}} \phi_{\nu,\mathrm{abs}} - n_{\mathrm{u}}B_{\mathrm{ul}} \phi_{\nu,\mathrm{sti}} \right]$$
(4.18)

(cf. Eqns. (4.11), (4.12) and (4.13)).

The Einstein coefficients are not independent. The ratio of B_{lu} and B_{ul} is determined by the multiplicity (degeneracy) of the upper and lower energy states:

$$\left(\frac{B_{\rm lu}}{B_{\rm ul}}\right) = \frac{g_{\rm u}}{g_{\rm l}} , \qquad (4.19)$$

Also, A_{ul} and B_{ul} are related via

$$\left(\frac{A_{\rm ul}}{B_{\rm ul}}\right) = \frac{2h\nu^3}{c^2}\Big|_{\nu=\nu_{\rm ul}}$$
(4.20)

(Einstein 1916, 1917). The Einstein coefficients are derived in terms of the atomic parameters. They have no explicit dependence on the external conditions. Thus, the relations in Eqn. (4.19) and Eqn. (4.20) hold universally, regardless of whether or not the medium is in a local thermal equilibrium with itself and with the radiation.

For a two-level system in thermal equilibrium, characterised by a thermal tem-

$$\frac{n_{\rm b}}{n_{\rm a}} = \frac{g_{\rm b}}{g_{\rm a}} \exp\left(-\frac{\Delta E_{\rm ba}}{k_{\rm B}T}\right) \,. \tag{4.21}$$

Analogous to the expression for the thermal system, the relative population of the upper and lower hyperfine states of the 21-cm line may be expressed in a term of a temperature, T_s , known as the spin temperature:

$$\frac{1}{3}\left(\frac{n_{\rm u}}{n_{\rm l}}\right) = \exp\left(-\frac{\Delta E_{\rm ul}}{k_{\rm B}T_{\rm s}}\right) = \exp\left(-\frac{T_{\star}}{T_{\rm s}}\right) , \qquad (4.22)$$

with $g_u = 3g_1$ (for neutral hydrogen in the 1S ground state) and $T_{\star} \equiv hv_{21cm}/k_B = \Delta E_{ul}/k_B = 0.0682$ K. Note that when $T_s \gg T_{\star}$, three of four atoms will be in the upper hyperfine level. However, there are mechanisms, which will be discussed later, that can cause violation of this population partition.

It is now clear that the emission and absorption coefficients of the radiative transfer of the hyperfine 21-cm line of neutral hydrogen can be computed from the Einstein coefficient A_{ul} , for spontaneous emission, if the number density of neutral hydrogen (which is $n_u + n_l$) and the ratio of n_u/n_l (given by the spin temperature T_s) are known, and the line profile functions $\phi_{v,x}$, where $x \in \{abs, emi, sti\}$, are specified. $A_{ul} \approx 2.87 \times 10^{-15} \text{ s}^{-1}$ for the hyperfine transition of an electron in a ground-state hydrogen atom (see e.g. Condon and Ransom 2016). The lifetime of an electron in the upper hyperfine triplet state is therefore $\Delta t_{21cm} = 1/A_{ul} \approx 3.5 \times 10^{14} \text{ s} (11 \text{ Myr})$. This implies a negligibly narrow intrinsic width, $(\Delta v_{21cm})^{\text{intrinsic}} = (2\pi \Delta t_{21cm})^{-1} \ll v_{21cm} (\approx 1.4 \text{ GHz})$, for the 21-cm line³.

$$\phi(v - v_{21cm}) = \frac{\Gamma_{rad}/4\pi^2}{(v - v_{21cm})^2 + (\Gamma_{rad}/4\pi)^2}$$

(see e.g. Rutten 2003), where the damping parameter $\Gamma_{rad} = (\Delta t_{21cm})^{-1} = A_{ul}$, corresponding to an intrinsic frequency broadening $(\Delta v_{21cm})^{intrinsic} = \Gamma_{rad}/2\pi$. More details on the profile of the 21-cm line and the possible

³An emission line would have a Lorentzian profile if the broadening is due to radiative damping, specified by a damping parameter Γ_{rad} . If there is only radiative-damping induced broadening, the profile of the hyperfine 21-cm line, centred at v_{21cm} , is

The spontaneous emission of 21-cm photons is forbidden in the electric dipole transition and rarely occurs. Thus, electrons would reside in the upper hyperfine triplet state for more than 10 Myr, unless they are disturbed by an external process, e.g. de-excitation caused by atomic collisions or stimulated de-excitation by a radiation field. However, it is evident that the 21-cm hyperfine lines are observed in astrophysical systems, e.g. the Milky Way galaxy and many external galaxies. The 21-cm hyperfine transition could happen frequent enough for it to be detectable, when taking into account of the amount of neutral hydrogen for a sufficiently large astrophysical system, such as a spiral galaxy. Because of the abundance of neutral hydrogen throughout the entire Universe⁴, especially before the Universe was completely reionised, the 21-cm hyperfine transition would be the major source of line emission, from an atomic process, before the formation of luminous objects such as stars and galaxies.

4.2.2 Radiative transfer equation for the 21-cm line

Without loss of generality, consider only the line absorption and the emission opacity and ignore the continuum and its opacity for the time being. Then, the radiative transfer equation is simply

$$\frac{dI_{\nu}}{ds} = -\kappa_{L,\nu}I_{\nu} + \epsilon_{L,\nu} = -\kappa_{L,\nu}\left(I_{\nu} - S_{L,\nu}\right)$$
(4.23)

in the local rest frame, where $S_{L,\nu} = \epsilon_{L,\nu}/\kappa_{L,\nu}$ is the source function of the line. (This can be justified if the free-free processes, which usually contribute to the continuum emission and absorption, are insignificant, i.e. $\kappa_{C,\nu} \ll \kappa_{L,\nu}$ and $\epsilon_{C,\nu} \ll \epsilon_{L,\nu}$.) In terms of the Einstein coefficients, the radiative transfer equation for the 21-cm line, therefore, is

$$\frac{\mathrm{d}I_{\nu}}{\mathrm{d}s} = -\frac{h\nu_{\mathrm{ul}}}{4\pi} \left[\left(n_{\mathrm{l}}B_{\mathrm{lu}} \,\phi_{\nu,\mathrm{abs}} - n_{\mathrm{u}}B_{\mathrm{ul}} \,\phi_{\nu,\mathrm{sti}} \right) \,I_{\nu} - n_{\mathrm{u}}A_{\mathrm{ul}}\phi_{\nu,\mathrm{emi}} \right], \tag{4.24}$$

broadening processes in astrophysical systems are discussed in Sec. 4.2.5.

⁴H I amounts to about 75% of baryonic matter (by mass) and over ~ 90% of all of the atoms (by number) in the Universe (Los Alamos National Lab: https://periodic.lanl.gov/1.shtml).

where $v_{ul} = v_{21cm}$, and the source function is

$$S_{L,\nu} = \frac{n_{u}A_{ul} \phi_{\nu,emi}}{n_{l}B_{lu} \phi_{\nu,abs} - n_{u}B_{ul} \phi_{\nu,sti}} = \left(\frac{A_{ul}}{B_{ul}}\right) \frac{(\phi_{\nu,emi}/\phi_{\nu,abs})}{(n_{l}B_{lu}/n_{u}B_{ul}) - (\phi_{\nu,sti}/\phi_{\nu,abs})} = \left(\frac{2h\nu_{ul}^{3}}{c^{2}}\right) \frac{(\phi_{\nu,emi}/\phi_{\nu,abs})}{(n_{l}g_{u}/n_{u}g_{l}) - (\phi_{\nu,sti}/\phi_{\nu,abs})} .$$
(4.25)

The derivation of the source function here has not assumed a thermal equilibrium. If local thermal equilibrium is imposed, the source function will become the Planck function, recovering the Kirchhoff's Law⁵.

The line transfer equation can be further simplified using the relations between the Einstein coefficients in the absorption coefficient. This gives

$$\kappa_{\mathrm{L},\nu} = \frac{h\nu_{\mathrm{ul}}}{4\pi} \left(n_{\mathrm{l}}B_{\mathrm{lu}} \phi_{\nu,\mathrm{abs}} - n_{\mathrm{u}}B_{\mathrm{ul}} \phi_{\nu,\mathrm{sti}} \right)$$
$$= \kappa_{\mathrm{L},\nu}^{\mathrm{abs}} \phi_{\nu,\mathrm{abs}} \left(1 - \Xi \right) , \qquad (4.26)$$

where the normalised absorption coefficient is

$$\kappa_{\mathrm{L},\nu}^{\mathrm{abs}} = \frac{h\nu_{\mathrm{ul}}}{4\pi} n_{\mathrm{l}} B_{\mathrm{lu}}$$
$$= \frac{1}{8\pi} \left(\frac{c}{\nu_{\mathrm{ul}}}\right)^2 \left(\frac{g_{\mathrm{u}}}{g_{\mathrm{l}}}\right) n_{\mathrm{l}} A_{\mathrm{ul}} , \qquad (4.27)$$

⁵In a local frame, $\phi_{\nu,abs} = \phi_{\nu,emi} = \phi_{\nu,sti}$. If local thermal equilibrium (LTE) between the radiation and the medium holds, then

$$\frac{n_{\rm u}}{n_{\rm l}} = \frac{g_{\rm u}}{g_{\rm l}} \exp\left(-\frac{h\nu_{\rm ul}}{k_{\rm B}T}\right) ,$$

and the source function in Eqn. (4.25) becomes

$$S_{\mathrm{L},\nu} = \left(\frac{2h\nu_{\mathrm{ul}}^{3}}{c^{2}}\right) \left[\exp\left(\frac{h\nu_{\mathrm{ul}}}{k_{\mathrm{B}}T}\right) - 1\right]^{-1} = B_{\nu}(T) \; .$$

The condition for a LTE between the radiation and the medium is not always satisfied, especially when the transition is coupled with an external radiative process. In this situation,

$$\frac{n_{\rm u}}{n_{\rm l}} \neq \frac{g_{\rm u}}{g_{\rm l}} \exp\left(-\frac{h\nu_{\rm ul}}{k_{\rm B}T}\right) ,$$

and the source function cannot be represented by the Planck function, i.e. the radiation is non-thermal, although the relevant radiative processes involved could be thermal processes themselves.

and the factor for the stimulated emission is

$$\Xi = \frac{n_{\rm u}}{n_{\rm l}} \frac{g_{\rm l}}{g_{\rm u}} \frac{\phi_{\nu,\rm sti}}{\phi_{\nu,\rm abs}} . \tag{4.28}$$

The factor Ξ can exceed unity if the upper hyperfine level is sufficiently populated, i.e. when $(n_u/n_1) > (g_u/g_1) = 3$ for $\phi_{\nu,sti} = \phi_{\nu,abs}$. This could occur during the Epoch of Reionisation where a strong radiation field can be created by the first quasars, first stars, or first galaxies.

Generally, there is no guarantee that the line profile functions $\phi_{\nu,\text{emi}}$, $\phi_{\nu,\text{abs}}$, and $\phi_{\nu,\text{sti}}$ are the same. However, the intrinsic width of the 21-cm hyperfine line is insignificant in comparison to the broadening of the line due to other processes. In the local rest frame, all atoms are subject to the same external line broadening processes. Thus, $\phi_{\nu,\text{emi}} = \phi_{\nu,\text{abs}} = \phi_{\nu,\text{sti}}$ can be adopted in the radiative transfer equation. It follows that, by including the factor accounting also for the stimulated emission $[1 - \Xi]$, the radiative transfer equation becomes

$$\frac{dI_{\nu}}{ds} = -(\kappa_{L,\nu}^{abs} \phi_{\nu} [1 - \Xi]) I_{\nu} + \epsilon_{L,\nu} \phi_{\nu} , \qquad (4.29)$$

where ϕ_{ν} is the line profile function (for absorption, spontaneous emission and stimulated emission). The continuum and line absorption and emission coefficients are additive, if there is no correlation between the continuum and the line opacities. Hence, the radiative transfer equation is

$$\frac{dI_{\nu}}{ds} = -(\kappa_{C,\nu} + \kappa_{L,\nu}^{abs} \phi_{\nu} [1 - \Xi]) I_{\nu} + (\epsilon_{C,\nu} + \epsilon_{L,\nu} \phi_{\nu}) . \qquad (4.30)$$

4.2.3 Excitation and de-excitation of electrons

The line emission coefficient $\epsilon_{L,\nu}$ depends on the population of electrons (in number density) in the upper hyperfine level, n_u , while the total effective line absorption coefficient $\kappa_{L,\nu}$ is determined by the relative population of electrons in the two hyperfine states, i.e. (n_u/n_l) . The total populations of electrons in the two levels combined is given by the population (in number density) of neutral hydrogen atoms,

i.e. $n_1 + n_u = n_{HI}$.

The concentration of HI (neutral hydrogen) gas, $n_{\rm HI}$, and hence, $n_{\rm u}$ and $n_{\rm l}$, changes as the Universe evolves. First of all, they are diluted as the Universe expands: the overall amount of HI gas per unit volume scales as $n_{\rm HI}(z) = n_{\rm HI,0}(1+z)^3$. Secondly, HI had been converted into HII during cosmological reionisation, which resulted in an overall reduction of $n_{\rm HI}$ as the reionisation process proceeded. The survival of neutral hydrogen depends on several factors, and the most important two are (i) the degree of shielding from the ionised radiation, and (ii) the efficiency of recombination to compete with ionisation. Pockets of HI can survive in overdense regions, where they are self-shielded from irradiation. The high density also enhances the recombination rate (see e.g. Sobacchi and Mesinger 2014), counteracting ionisation, especially when there is already a sufficiently high ratio of the HI number density to the photon number density. Recombination is particularly efficient in the cool regions, where the gas is not strongly heated and so maintains a temperature well below ~ 10^4 K such that collisional ionisation of hydrogen is insignificant.

The relative population of the neutral hydrogen atoms in the two hyperfine states can be altered by processes that can induce the spin-flip (excitation and deexcitation) of the electrons. Obviously, the absorption of a 21-cm photon would excite the electron from the lower hyperfine (singlet) state to the upper (triplet) state, and the reverse process (de-excitation) would be induced by the emission of a 21-cm photon. An electronic spin-flip can also occur when a hydrogen atom collides with a free electron, a proton or another hydrogen atom. In the presence of a strong UV radiation field, an electronic spin-flip is made possible, facilitated by an intermediate excited state, and an example is the resonant scattering of the Ly α photons (i.e. the Wouthuysen-Field effect; Wouthuysen 1952; Field 1958), which were present during the EoR, presumably produced by the massive stars and/or by the accretion into massive black holes (i.e. quasars).

Radiative excitation and de-excitation

High-frequency radio background radiation at a high z can be redshifted into the frequency of the 21-cm line, causing absorption or inducing stimulated emission.

The background radio sources can be the diffuse ambient CMB, but can also be strong radio emitters, such as quasars. An absorption will excite the electrons from the lower-energy to the higher-energy hyperfine level, and the stimulated emission will induce the de-excitation of the electrons from the higher-energy to the low-energy hyperfine level.

Collisional excitation and de-excitation

Spin-flips of the electron can be induced by collisions between two hydrogen atoms (H-H) (Allison and Dalgarno 1969; Zygelman 2005), between a hydrogen atom and an electron (e-H) (Hirata and Sigurdson 2007) or between a hydrogen atom and a proton (p-H) (Furlanetto and Furlanetto 2007). In the absence of an external radiation field, collisional excitation is important in establishing the population of electrons in the upper (triplet) hyperfine state. The collision rate between particles generally increases with the square of particle number densities. Collisional excitation and de-excitation are, therefore, particularly important in high-density environments. Collisions could be the dominant process for the hyperfine transitions during the Dark Ages. However, they would give way to the radiative processes, when the first luminous objects began to appear.

Wouthuysen-Field effect (Ly α scattering)

Resonant scattering of Ly α photons can induce a spin-flip. In Fig. 4.1, the hyperfine structure of the hydrogen 1S and 2P levels, together with the transitions relevant to the Wouthuysen-Field effect, are shown. The absorption of a Ly α photon will excite an electron from the 1S lower hyperfine level into either of the central 2P hyperfine levels. The subsequent spontaneous emission of a Ly α photon will send the electron to one of the two 1S hyperfine levels. The absorption and re-emission of a Ly α photon thus cause a spin-flip of the electron, and hence, alter the relative populations between the two 1S hyperfine levels. This Ly α pumping is important to populate the upper hyperfine (triplet) state, breaking the thermal equilibrium between the 1S hyperfine transitions of neutral hydrogen and the CMB. It is this process that allows the 21-cm line from the reionisation era to be seen in emission.

4.2.4 Spin temperature and its coupling

A HI gas will be in a stationary state for the hyperfine transition when an equilibrium between excitation and de-excitation, determined jointly by the collisional and radiative processes, is set up. This implies that the rate of electrons entering a hyperfine level equals to the rate of electrons leaving the level, i.e.

$$n_{\rm l} \left(C_{\rm lu} + P_{\rm lu} + B_{\rm lu} I_{\nu} \right) = n_{\rm u} \left(C_{\rm ul} + P_{\rm ul} + A_{\rm ul} + B_{\rm ul} I_{\nu} \right) \tag{4.31}$$

(see Furlanetto et al. 2006). Here, C_{lu} and C_{ul} are the rates for collisional excitation and de-excitation, respectively. P_{lu} and P_{ul} are the rates for radiative excitation and de-excitation, respectively, due to $Ly\alpha$ scattering. $B_{lu}I_{\nu}$ is the rate of excitation caused by photon absorption, $B_{ul}I_{\nu}$ is the rate of de-excitation caused by stimulated photon emission, and A_{ul} is the rate of de-excitation caused by spontaneous photon emission. In the low-frequency limit, which is appropriate for the radio emission due to the hyperfine transition in H I gas, the Rayleigh-limit approximation is applicable, and the intensity,

$$I_{\nu} = 2(k_{\rm B}T_{\rm r}) \,\frac{\nu^2}{c^2} \,, \tag{4.32}$$

is characterised by a brightness temperature T_r .

Suppose that the ratio of the rates of excitation to de-excitation due to particle collisions can be represented by a temperature T_k , and also, the ratio of the rates of excitation to de-excitation due to Ly α scattering by a temperature T_{α} . Then, Eqn. (4.31) gives the spin temperature:

$$T_{\rm s} = \left[\frac{T_{\rm r}^{-1} + x_{\alpha}T_{\alpha}^{-1} + x_{\rm c}T_{\rm k}^{-1}}{1 + x_{\alpha} + x_{\rm c}}\right]^{-1}$$
(4.33)

(Field 1958, 1959; Pritchard and Loeb 2012). Here, the coupling coefficients x_c and x_{α} indicate the strengths of collisions and Ly α scattering, respectively, in determining the excitation and de-excitation processes, relative to the ambient radiation field (that

is characterised by the brightness temperature T_r).

For cosmological reionisation, the ambient radiation field in the GHz radio frequencies is provided mainly by the CMB. Hence, $T_r = T_{CMB}(z)$. Collisions are determined by the kinetics of the particles involved. The temperature relevant for the efficiency of particle collisions is, therefore, the thermal temperature, which is referred to as T_k here. If only collisions are present, the populations of the electrons in the two hyperfine levels for a H I gas in a thermal equilibrium will depend only on T_k , and the transition rates satisfy

$$\left(\frac{C_{\rm lu}}{C_{\rm ul}}\right)\left(\frac{g_{\rm l}}{g_{\rm u}}\right) = \exp\left(-\frac{T_{\star}}{T_{\rm k}}\right) . \tag{4.34}$$

For $T_k \gg T_{\star} (= h \nu_{\rm ul} / k_{\rm B} = 0.0682 \text{ K})$, $\exp(-T_{\star} / T_k) \approx (1 - T_{\star} / T_k)$. Hence,

$$\frac{1}{T_{\rm k}} \approx \frac{1}{T_{\star}} \left[1 - \left(\frac{C_{\rm lu}}{C_{\rm ul}}\right) \left(\frac{g_{\rm l}}{g_{\rm u}}\right) \right] \,. \tag{4.35}$$

Analogous to the collisional excitation and de-excitation, an effective temperature T_{α} may be defined for the excitation and de-excitation caused by Ly α scattering:

$$\left(\frac{P_{\rm lu}}{P_{\rm ul}}\right)\left(\frac{g_{\rm l}}{g_{\rm u}}\right) \equiv \exp\left(-\frac{T_{\star}}{T_{\alpha}}\right) , \qquad (4.36)$$

where T_{α} is referred to as the colour temperature of the Ly α radiation field (see e.g. Field 1958; Madau et al. 1997; Pritchard and Furlanetto 2006; Furlanetto and Pritchard 2006). It follows that

$$\frac{1}{T_{\alpha}} \approx \frac{1}{T_{\star}} \left[1 - \left(\frac{P_{\rm lu}}{P_{\rm ul}}\right) \left(\frac{g_{\rm l}}{g_{\rm u}}\right) \right]$$
(4.37)

as $T_{\alpha} \gg T_{\star}$.

The spin temperature T_s , as expressed in Eqn. (4.33), is a weighted harmonic mean of the three effective temperatures, T_r , T_k and T_α , corresponding to the three main mechanisms driving the electron excitation and de-excitation. When collision and Ly α scattering are unimportant, i.e. $x_c + x_\alpha \ll 1$, the relative population of the electrons in the two hyperfine levels is determined by the ambient radiation field, and hence, $T_s \approx T_r$. If collision and Ly α scattering are not negligible, i.e. $x_{\alpha} + x_c \gtrsim 1$, then $T_s \sim [(x_c/T_k) + (x_{\alpha}/T_{\alpha})]^{-1} \sim T_k$.

The spin temperature T_s is a useful parameter in the radiative transfer equation of the 21-cm line. Provided that $T_s(z)$ and $n_{HI}(z)$ are known, the emission and absorption coefficients along the line-of-sight can be computed. Theoretical models of the evolution of T_s over cosmological time has been conducted, using semi-analytic or numerical methods (e.g. Nusser 2005; Furlanetto et al. 2006; Pritchard and Loeb 2008; Thomas and Zaroubi 2011; Mesinger et al. 2011).

4.2.5 Shaping the profile of the 21-cm line

Line frequency shifting

When an emitting medium and the observer are not co-located and do not co-move, the frequency of the emitted radiation will appear to be shifted as seen by the observer. For the hyperfine 21-cm line from distant astrophysical systems, the shift of the line can be caused by (i) cosmic expansion, and (ii) the relative velocity between the sources and the observer.

The former is a global effect. It leads to a red-shift of the frequency of the radiation, and it can be manifested in the shift of centre frequency of the hyperfine 21-cm line to a lower frequency at the observer's reference frame. Quantitatively, the relative frequency shift at two cosmological location/epoch z and z' is given by

$$\frac{\nu(z')}{(1+z')} = \frac{\nu(z)}{(1+z)} . \tag{4.38}$$

In the context of radiative transfer and spectral evolution, the frequency red-shift of radiation caused by cosmic expansion is essential to a flow of photons from the high frequencies to the low frequencies at a constant rate if evaluated in terms of the cosmological redshift z.

The latter is associated with the local movement of the emitter with respect to the observer. The frequency shift is simply a Doppler effect. In the non-relativistic limit, the frequency of the centre of the observed 21-cm line v' is

$$v'_{21cm} = v_{21cm} \left(1 \pm v_{\parallel} / c \right),$$
 (4.39)

where v_{\parallel} is the relative line-of-sight velocity of the HI gas with respect to the observer. v_{\parallel} can be positive or negative. The 21-cm line will be shifted to higher frequencies if the emitting HI gas is approaching, and to lower frequencies if the emitting HI gas is receding.

Line broadening

Spectral lines can be broadened by various mechanisms. The astrophysical 21-cm hyperfine line is broadened by radiative damping, particle collision, thermal motion and turbulence. The first two are intrinsic to individual emitters, and they can be explained in terms of damped oscillations in models for line emission. The last two are essentially a manifestation of Doppler effects, caused by the incoherent movements of a collection of H I gas particles with respect to the observer.

The damped oscillations⁶ associated with the emission process will lead to broadening of the 21-cm hyperfine line, resulting in a Lorentzian profile (see e.g. Rutten 2003):

$$\phi(\nu - \nu_{21cm}) = \frac{1}{\pi} \left[\frac{(\Gamma_{all}/4\pi)}{(\nu - \nu_{21cm})^2 + (\Gamma_{all}/4\pi)^2} \right], \qquad (4.40)$$

where Γ_{all} is the sum of the damping parameters (i.e. reciprocals of the damping timescales) of all the uncorrelated damping processes.

The spontaneous emission of a photon for the spin-flip of the electrons from

$$f(\nu - \nu_0) = \frac{1}{\pi} \left[\frac{(\Gamma_{\rm all}/4\pi)}{(\nu - \nu_0)^2 + (\Gamma_{\rm all}/4\pi)^2} \right] \,,$$

$$\ddot{\xi} + \left(\sum_{i} \Gamma_{i}\right) \dot{\xi} + (2\pi\nu_{0})^{2} \xi = 0$$

where ξ is the oscillating variable.

⁶The frequency response of damped oscillations has the functional form:

where v_0 is the normal-mode frequency. The damping parameter Γ_{all} is the linear sum of the damping parameters Γ_i (which have the dimension of 1/time) of all uncorrelated damping processes, as those described in the differential equation:

the triplet hyperfine state to singlet hyperfine state is essentially a radiative damping process, where energy is released as a result of the state transition. The radiative lifetime, which equals to $1/A_{ul}$, gives the characteristic damping timescale, and hence, a damping parameter Γ_{rad} . Collisions will cause a perturbation of the electron spins, and the restoration of the system from perturbation will involve energy dissipation, i.e. a damping process, leading to line broadening. A consequence of the collision is the reduction of the effective lifetime of an electron at the upper hyperfine state (see Padmanabhan 2000a), and the effective timescale for spin-flips induced by the collision process gives the damping parameter Γ_{coll} , and hence, the broadened width of the 21-cm line. Spontaneous emission and collision-induced emission are independent processes, and hence, their combined broadening will be specified by a total damping parameter: $\Gamma_{all} = \Gamma_{rad} + \Gamma_{coll} \propto 1/t_{rad,spon} + 1/t_{rad,coll}$, where $t_{rad,spon}$ $(= 1/A_{ul})$ and $t_{rad,coll}$ are the timescales for the spontaneous emission and for the collision-induced emission, respectively. During the Epoch of Reionisation, the Universe was sufficiently dense such that the timescale of collisional de-excitation was significantly shorter than the timescale for spontaneous emission⁷, implying that $\Gamma_{coll} \gg \Gamma_{rad}$. The total broadening of the two processes combined is, therefore, $\Gamma_{all} \approx \Gamma_{coll}$, corresponding to a full-width-half-maximum (FWHM) in frequency, FWHM_{ν}, of ($\Gamma_{coll}/2\pi$) in the Lorentzian line profile.

The thermal motion and turbulent motion of the gas particles will give rise to Doppler shifts in the radiation that they emit. The incoherent Doppler shifts of the 21-cm line emitted from an ensemble of H I gas particles with different line-of-sight velocities would make the line appear to be broadened. When the H I gas particles have a Gaussian velocity distribution, the line will have a Gaussian profile.

The thermal velocities of an ensemble of particles is characterised by a kinetic temperature. Suppose that the particles are identical and each has a mass m, then

⁷The collisional timescale is inversely proportional to the density of the gas. The relative importance of collisional damping and radiative damping is, therefore, environment dependent in the 21-cm hyperfine transition. While collisional damping dominated in H I gas suffusing the early Universe, it is less important in the present-day IGM.

their velocities have a Maxwellian distribution:

$$f(\boldsymbol{v}) \,\mathrm{d}^3 \boldsymbol{v} = \left(\frac{m}{2\pi k_\mathrm{B} T_\mathrm{k}}\right)^{3/2} \exp\left(-\frac{m v^2}{2k_\mathrm{B} T_\mathrm{k}}\right) \mathrm{d}^3 \boldsymbol{v} \,, \tag{4.41}$$

where T_k is the kinetic (thermal) temperature. For isotropic velocities, $d^3v = 4\pi v^2 dv$, and hence,

$$f(v) d^{3}v = \sqrt{\frac{2}{\pi}} \left(\frac{m}{k_{\rm B}T_{\rm k}}\right)^{3/2} \exp\left(-\frac{mv^{2}}{2k_{\rm B}T_{\rm k}}\right) v^{2} dv . \qquad (4.42)$$

However, Doppler shift is caused by the line-of-sight motions (denoted as v_{\parallel} , hereafter) of the emitters only. Note that $v^2 = v_{\parallel}^2 + v_{\perp}^2$, and an isotropic velocity distribution would ensure that the equi-partition of energy between the three degrees of freedom in the velocities. Hence, the distribution of the line-of-sight velocity is

$$\tilde{f}(v_{\parallel}) dv_{\parallel} = \left[\int d^2 \boldsymbol{v}_{\perp} f(\boldsymbol{v}) \right] dv_{\parallel}$$
$$= \left(\frac{m}{2\pi k_{\rm B} T_{\rm k}} \right)^{1/2} \exp\left(-\frac{m v_{\parallel}^2}{2k_{\rm B} T_{\rm k}} \right) dv_{\parallel} . \tag{4.43}$$

The velocity-induced Doppler shift of the 21-cm line is given by

$$\frac{\nu - \nu_{21cm}}{\nu_{21cm}} = \frac{\nu_{\parallel}}{c} .$$
 (4.44)

The normalised profile function of the 21-cm line subject to thermal broadening should, therefore, satisfy

$$\phi(\nu - \nu_{21\text{cm}}) \,\mathrm{d}\nu \propto \tilde{f}(\nu_{\parallel}) \left(\frac{\mathrm{d}\nu_{\parallel}}{\mathrm{d}\nu}\right) \mathrm{d}\nu \,, \tag{4.45}$$

where $v_{\parallel} \in (-\infty, \infty)$ and $(v - v_{21cm}) \in [-v_{21cm}, \infty)$. However, if the frequency broadening Δv is sufficiently small such that $(v_{21cm} - \Delta v) \gg 0$, then the line profile

function effectively becomes a simple Gaussian:

$$\phi(\nu - \nu_{21\text{cm}}) = \frac{1}{\sqrt{\pi} \Delta \nu_{\text{D}}} \exp\left[-\left(\frac{\nu - \nu_{21\text{cm}}}{\Delta \nu_{\text{D}}}\right)^2\right], \qquad (4.46)$$

and the width of the Doppler broadening, Δv_D , is simply

$$\Delta \nu_{\rm D} = \nu_{21\rm cm} \left(\frac{v_{\parallel}}{c}\right) = \nu_{21\rm cm} \sqrt{\frac{2k_{\rm B}T_{\rm k}}{mc^2}} . \tag{4.47}$$

An expression for the turbulence-induced broadening can be obtained from a similar argument as in the thermal broadening. Suppose that the turbulent motion in a HI gas has a well-defined characteristic mean-square velocity, v_{turb}^2 . Then, a velocity dispersion can be assigned for the HI gas particles, analogous to the thermal velocity dispersion, and from it, a Maxwellian velocity distribution can be constructed. As thermal motion and turbulence motion are independent, their velocity dispersions are additive. In terms of the Doppler parameter b_D , the effective width of the broadened line is

$$\Delta v_{\rm D} \equiv v_{21\rm cm} \left(\frac{b_{\rm D}}{c}\right) = v_{21\rm cm} \sqrt{\frac{2k_{\rm B}T_{\rm k}}{mc^2} + \left(\frac{v_{\rm turb}}{c}\right)^2}, \qquad (4.48)$$

with a Doppler parameter

$$b_{\rm D} = \sqrt{\frac{2k_{\rm B}T_{\rm k}}{m} + v_{\rm turb}^2} .$$
 (4.49)

The broadened line has a FWHM_v = $2\sqrt{\ln 2} b_D$ in velocity, for a Gaussian profile function. The corresponding FWHM_v, in frequency, is

$$FWHM_{\nu} = 2\sqrt{\ln 2} \left(\nu_{21cm}\right) \left(\frac{b_{\rm D}}{c}\right)$$
$$= 2\sqrt{\ln 2} \left(\nu_{21cm}\right) \sqrt{\frac{2k_{\rm B}T_{\rm k}}{mc^2} + \left(\frac{v_{\rm turb}}{c}\right)^2} . \tag{4.50}$$

Convolved line profile

While the damping-induced line broadening is associated with the internal action and response of the emitters, the velocity-induced line broadening is associated with the kinetics of the emitters. These two broadening mechanisms are different by nature, but their effects are not additive, despite that damping and velocity induced broadening are independent. If the processes of both mechanisms are present, the resulting broadening will be determined by the convolution of the two mechanisms to which the processes belong. The convolution of a Lorentzian line profile and a Gaussian line profile is a Voigt line profile. Voigt profiles have no simple analytic form in terms of elementary functions (see e.g. Schreier 1992; Boyer and Lynas-Gray 2014; Mohankumar and Sen 2019; AlOmar 2020). However, the normalised Voigt profile for the 21-cm hyperfine line can be expressed as

$$\phi(v - v_{21cm}) = \frac{H(q, x(v))}{\sqrt{\pi} \Delta v_{D}} \bigg|_{v_{21cm}}$$
 (4.51)

(see e.g. Rutten 2003). It is an implicit function of frequency ν , and is specified by three parameters: the line frequency centre, ν_{21cm} , the damping parameter, Γ_{all} , and velocity induced width, $\Delta \nu_D$, within the Voigt parameter q and the Voigt function $H(q, x(\nu))$. The Voigt parameter,

$$q = \frac{\Gamma_{\rm all}}{4\pi \,\Delta\nu_{\rm D}}\,,\tag{4.52}$$

is a measure of the relative strength of the damping and the kinetic effects. The Voigt function,

$$H(q, x(\nu)) = \frac{q}{\pi} \int_{-\infty}^{+\infty} dy \, \frac{\exp(-y^2)}{[x(\nu) - y]^2 + q^2} \,, \tag{4.53}$$

is the convolution of the Lorentzian and the Gaussian functions in a dimensionless form. The variable x specifies the frequency spread from the line centre frequency

normalised to the velocity-induced width:

$$x(\nu) = \frac{\nu - \nu_{21cm}}{\Delta \nu_{\rm D}}$$
 (4.54)

The variable *y* is a dimensionless measure of the line-of-sight velocity, over which the weighted effects of its induced Doppler shift are summed. It is given by

$$y = \frac{v_{\parallel}}{b_{\rm D}} = \frac{v_{21\rm cm}}{\Delta v_{\rm D}} \left(\frac{v_{\parallel}}{c}\right) . \tag{4.55}$$

For $\Delta v_D \gg (\Gamma_{all}/4\pi)$, $q \ll 1$, and the velocity-induced broadening dominates over the damping-induced broadening, Note that $H(q, x) \approx (e^{-x^2} + q/x^2\sqrt{\pi})$ for $q \ll 1$, and hence, the line profile function becomes

$$\phi \left(\nu - \nu_{21 \text{cm}} \right) \approx \frac{1}{\sqrt{\pi} \,\Delta \nu_{\text{D}}} \left(e^{-x^2} + \frac{q}{\sqrt{\pi} \,x^2} \right) \tag{4.56}$$

(see Padmanabhan 2000b; Rutten 2003). In the case where velocity-induced Doppler broadening is significant, then setting q = 0 in Eqn. (4.56) will give a pure Gaussian line profile. In the astrophysical environments of cosmological reionisation, damping-induced broadening is unimportant when compared with velocity-induced broadening. Thus, a Gaussian line profile is adopted in the radiative transfer calculations presented in the following sections of this chapter.

4.2.6 21-cm forests

A line is seen as emission when it has a higher brightness temperature than its neighbouring continuum. It is seen as absorption when it has a brightness temperature lower than its neighbouring continuum. The 21-cm line will appear as absorption when it is observed against a continuum background of a bright source, e.g. a radio-loud quasar⁸. The radio continuum emission of a quasar is generally non-thermal

⁸Distant quasars have been identified as candidate sources for the detection of 21-cm forests. Several quasars have already been found at z > 6 (during the Epoch of Reionisation). The most distant radio-loud quasar known to date is QSO J1427+3312, at z = 6.12 (Momjian et al. 2008). The most distant quasar known is ULAS J1342+0928, at z = 7.54 (Bañados et al. 2018). Note that, other candidate bright point sources would be hypernovae. They show gamma-ray burst, with radio afterglows, and some could be fast radio burst sources. However, little is known about the number distribution of hypernovae and evolution at very high redshifts, such as $z \sim 6$ or higher.

synchrotron radiation from relativistic electrons, and it tends to have a very high brightness temperature (e.g. Jagers et al. 1982; Kellermann and Verschuur 1988; Willott et al. 1998; Vernstrom et al. 2018). In comparison, the T_s associated with the 21-cm emission is negligible. The 21-cm line is, therefore, always in absorption against the emission from a background quasar.

The presence of cold H I gas at different redshifts along the line-of-sight in front of a bright radio source, presumably a radio quasar, leads to a "forest" of absorption lines (Carilli et al. 2002; Furlanetto and Loeb 2002; Furlanetto 2006; Xu et al. 2009; Mack and Wyithe 2012; Ciardi et al. 2015). The 21-cm forests can be considered as direct analogues to the Ly α forests. Here, photons emitted at frequencies $\nu > \nu_{ul}$ by the bright background radio quasar at redshift z_{emi} are absorbed by the diffuse neutral hydrogen gas along the line-of-sight at redshift $z = [\nu_{ul}(1 + z_{emi})/\nu - 1]$.

The detectability of the 21-cm forest depends on the strength of the absorption, which, in turn, depends on the optical depth of the absorbing line-of-sight diffuse H I gas. Dense gas with a high $n_{\rm HI}$ and a low $T_{\rm s}$ would have a large optical depth in the 21-cm line, hence, giving observable signatures. The 21-cm forest is expected to be stronger at the redshifts where the gas is cold and mostly neutral, i.e. before reionisation and the associated heating have already substantially proceeded. The 21-cm forest, if it is detected, will complement the Ly α forests, which probes the properties of the IGM at intermediate and low redshifts ($z \leq 6$), for providing important information of the diffuse media in the Universe crossing over the cosmic time when the Universe was barely ionised to become almost completely ionised.

The 21-cm line is relatively optically thin to the diffuse gas suffusing the entire Universe ($\tau_{21cm} < 1$) and would not saturate even at high redshifts. The 21-cm forests, therefore, preserve the detailed information about the progression of the cosmological reionisation. For example, the emergence of ionised bubbles will appear in the 21-cm forest as an increasing number of transparent windows. The 21-cm forest may also be a diagnostic of the dense structures in the line-of-sight IGM in the post-reionisation structural formation era. Absorption systems that contribute to the 21-cm forest could be of different scales, ranging from mini-halos, dwarf galaxies, galaxies, large-scale neutral/ionised regions to the cosmic web. In particular, mini-halos tend to have a high overdensity and low virial temperatures ($< 10^4$ K), and therefore, they would show 21-cm absorption features (see Furlanetto and Loeb 2002). The number density of these mini-halos is sensitively dependent on the thermal properties of IGM (by varying the Jeans mass upon the degree of heating, with the collapse of the halos prevented by strong heating). Thus, the 21-cm forest can, in principle, be used to probe the early halo formation, and hence, the thermal state of their ambient IGM.

The presence and the amount of the 21-cm absorption have important implications to the statistical properties of the 21-cm line measurements over the sky, in particular, the power spectra. Even when the ionisation fraction and spin temperature are fixed for each neutral gas cloud, which is unlikely, fluctuations in the 21-cm hyperfine line across the redshift space and across the sky would not vanish.

4.3 Cosmological Radiative Transfer of the 21-cm Line

4.3.1 Covariant formulation and representation

The cosmological radiative transfer of an emission line is described by the covariant radiative transfer equation:

$$\frac{\mathrm{d}}{\mathrm{d}\lambda_{\mathrm{a}}} \left(\frac{I_{\nu}}{\nu^{3}} \right) = -k_{\alpha} u^{\alpha} \Big|_{\lambda_{\mathrm{a}},\mathrm{co}} \left\{ -\kappa_{\mathrm{tot},\nu} \left(\frac{I_{\nu}}{\nu^{3}} \right) + \frac{\epsilon_{\mathrm{tot},\nu}}{\nu^{3}} \right\}$$
(4.57)

(see Sec. 2.3). For the radiative transfer of the 21-cm hyperfine line of neutral hydrogen, the processes that give rise to the opacity of the line and the continuum are independent. The absorption and emission coefficients can, therefore, be expressed as the sum of the contributions of the relevant processes, i.e. $\kappa_{tot,\nu} = \kappa_{C,\nu} + \kappa_{L,\nu}$ and $\epsilon_{tot,\nu} = \epsilon_{C,\nu} + \epsilon_{L,\nu}$. In the covariant radiative transfer equation, Eqn. (4.57), the emission and absorption coefficients are evaluated in a local reference frame, specified by the redshift *z*. The covariant line radiative transfer equation for a flat

Friedmann-Robertson-Walker (FRW) Universe (see Sec. 2.2) is therefore

$$\frac{\mathrm{d}}{\mathrm{d}z} \left(\frac{I_{\nu}}{\nu^3} \right) = (1+z) \left[-\left(\kappa_{\mathrm{C},\nu} + \tilde{\kappa}_{\mathrm{L},\nu} \right) \left(\frac{I_{\nu}}{\nu^3} \right) + \frac{(\epsilon_{\mathrm{C},\nu} + \tilde{\epsilon}_{\mathrm{L},\nu})}{\nu^3} \right] \frac{\mathrm{d}s}{\mathrm{d}z} \,. \tag{4.58}$$

The line profile functions depend only on the properties of the emitting and absorbing gas. Thus, when z is fixed, the line profile functions $\phi_{\nu,\text{emi}} = \phi_{\nu,\text{abs}} = \phi_{\nu,\text{sti}}$, and they can be represented by a single line profile function ϕ_{ν} . Here, the line emission coefficient is $\tilde{\epsilon}_{\text{L},\nu} = (h\nu_{\text{ul}}/4\pi) n_{\text{u}}A_{\text{ul}} \phi_{\nu}$ (see Eqn. (4.17)), and the line absorption coefficient is $\tilde{\kappa}_{\text{L},\nu} = (h\nu_{\text{ul}}/4\pi) n_{\text{l}}B_{\text{lu}} \phi_{\nu} [1 - \Xi]$ (see Eqns. (4.26) and (4.27)), where $\Xi = (n_{\text{u}}/n_{\text{l}})(g_{\text{l}}/g_{\text{u}})$ (see Eqn. (4.28)). The increment of path length with respect to the change in redshift is

$$\frac{\mathrm{d}s}{\mathrm{d}z} = \frac{c}{H_0} \left(1+z\right)^{-1} \left[\Omega_{\mathrm{r},0}(1+z)^4 + \Omega_{\mathrm{m},0}(1+z)^3 + \Omega_{\Lambda,0}\right]^{-1/2}.$$
(4.59)

4.3.2 Computational algorithm and numerical implementation

The cosmological 21-cm line radiative transfer (C21LRT) calculations consist of three key elements: (i) a ray-tracing algorithm accounting for the transport of radiation from the past to the observer in an expanding Universe, (ii) a computational component to determine the interaction between the incoming background radiation and the local medium and to evaluate the absorption of the incoming background radiation radiation and emission in the local medium, and (iii) a numerical solver of the C21LRT equation, Eqn. (4.58), along with the ray-tracing calculations.

Ray tracing: redshift and frequency sampling

Solving the line radiative transfer equation, Eqn. (4.57), requires the determination of the continuum and the line transfer coefficients over a frequency range fully covering the line and the relevant underlying continuum, in the local rest frame. The propagation of the radiation is parameterised by the redshift z (as in the CPRT calculations presented in Sec. 3.1.1), which is divided into N_z discrete cells along each ray. In addition to the discretisation along the ray, another sampling in frequency on each z-grid is constructed to account for the changes in the line profile and the



Fig. 4.2: An illustration of a two-dimensional C21LRT square computational grid. The grid runs through the indices "k" (for redshift) and "j" (for frequency). Equal uniform samplings in log(1 + z), through the index "k", and in log v, through the index "j" are adopted. The propagation of a ray is a diagonal shift in the computational grid coordinates (j, k). The C21LRT calculations are performed along the rays as those indicated by the red dotted lines.

continuum along the ray. The sampling scheme is constructed also to optimise the efficiency in the line radiative transfer calculations.

For a discretisation of ray-tracing in the logarithmic representation, Eqn. (4.38) becomes

$$\log v_{z'} - \log v_z = \log (1 + z') - \log (1 + z) . \tag{4.60}$$

The interval in $\log v$ is $\Delta_{\log v} \equiv \log v_{z'} - \log v_z$, and the interval in $\log (1 + z)$ is $\Delta_{\log (1+z)} \equiv \log (1 + z') - \log (1 + z)$. Thus, Eqn. (4.60) can be re-expressed as

$$\Delta_{\log \nu} = \Delta_{\log (1+z)} . \tag{4.61}$$

In the computation, the grid is specified by the coordinates (j, k) with the index "k" running through the redshift, and the index "j" through the frequency of the radiation. For a uniform sampling in $\log(1 + z)$, through the index "k", and in $\log v$, through the index "j", the interval $\Delta_{\log v} = \Delta_{\log(1+z)} = C$, where C is a positive constant. This gives a square (j, k) lattice, and the tracing of a ray over cosmic time, stamped by $z = 10^{\log_{10} \Delta_{1+z}} - 1$, is simply a diagonal shift in the (j, k) lattice, as illustrated in Fig. 4.2. The sampling scheme with $\Delta_{\log v} = \Delta_{\log(1+z)} = C$



Fig. 4.3: An illustration of the two-dimensional C21LRT rectangular computational grid (top panel), where frequency can be "reallocated" to each grid point (shown in the bottom panel). A uniform sampling is adopted in both log(1 + z) and log v. The propagation of rays over cosmological redshift, represented by the red dotted lines in the top panel, corresponds to the tracing of the rays through the index "*k*" with fixed "*j*" in the lattice in the bottom panel.

is straightforward, but it requires a high density sampling across the redshift to simultaneously resolve the line. The variations in the physical conditions associated with redshift are generally on a rate slower than the rate of the variations in the line profile when the radiation is transported in a ray through the computation lattice defined above. While an appropriate sampling in the frequency is chosen, a less dense sampling in the redshift would be sufficient in most practical situations. A rectangular grid is, therefore, preferred for achieving a higher computational efficiency.

An optimal scheme with $\Delta_{\log(1+z)} = C_1$ in the redshift sampling and $\Delta_{\log v} = C_2$

in the frequency sampling, where C_1 and C_2 are positive constants, and their ratio C_1/C_2 is set to be a fixed positive integer *S*, is adopted in the ray-tracing for the C21LRT calculations. Fig. 4.3 illustrates the ray tracing in the rectangular grid.

In the covariant formulation constructed for the C21LRT calculations here, the emission and absorption processes are evaluated in a local rest frame. This allows the physical variables, and hence, the emission and absorption coefficients and their changes along a ray, to be parameterised by the cosmological redshift only. The computational grids for the C21LRT calculations can then be constructed such that a ray is traced along the same *j* over a descending *k* (from a high redshift z_k to $z_0 = 0$ at k = 0). Each grid point (j, k) along the ray is assigned with a redshift *z*, according to $z_k = 10^{k \Delta_{\log 1+z}} - 1$, where $\Delta_{\log (1+z)} = C_1 = [\log (1 + z_{\max}) - \log (1 + z_0)]/N_z$. Also, a specific frequency is assigned to the grid point, satisfying the rectangular grid specification as described above.

At k = 0, the redshift $z_0 = z_{obs} = 0$, and the frequency v(j, 0) is specified by the frequency from v_{max} to v_{min} with the frequency interval (resolution) $\tilde{\Delta}_{\log(v)}|_{z_0} = [\log v_{max} - \log v_{min})/N_j|_{z_0} = C_2$. The radiation frequencies at higher redshifts are assigned by $v(j, k)|_{z_k} = v(j, 0) \times (1 + z_k)$, satisfying Eqn. (4.60). The frequency interval at each k is different, and it scales by $(1 + z_k)$ with respect to that at $z_0 = 0$, with a coarser frequency interval at a higher z_k . A sufficient frequency sampling around v_{21cm} at the maximum sample redshift z_{max} would be sufficient for a detailed tomographic study of the changes in the line shape at all z_k . Fig. 4.3 illustrates the assignment of the frequency and the redshift to the computational grids. The constant integer ratio $[\Delta_{\log(1+z)}/\Delta_{\log v}] = C_1/C_2 = S$ governs a constant shift in the *j* index of where v_{21cm} lies (denoted by ind_{21cm}) at each z_k . If at k = 0, $ind_{21cm} = 0$ by a choice (i.e. $v(0, 0) = v_{21cm}$), then, for $k \ge 1$, $ind_{21cm}|_{z_k} = -kS$. Local 21-cm emission and absorption at all redshifts can, therefore, be tracked.

The algorithm can be optimised to increase computational efficiency. For instance, in certain post-reionisation epochs, where foreground effects are insignificant (i.e. absence of significant foreground absorption, emission, and line-continuum interaction), the radiative transfer of the 21-cm line can be performed simply by passing
on the invariant specific intensity along the same j index as the index k descends to zero in the computational lattice. The local comoving specific intensity in the observer frame is calculated directly from invariant specific intensity.

The computational efficiency can further be boosted by an OpenMP parallelisation of the C21LRT code, when evaluating the frequency range (over the index j) at each redshift (at a given k). Consistent results are obtained using the OpenMP parallelised code as those obtained by the serial execution in all code verification tests, which are presented in the subsequent section.

Emission, absorption, and background radiation

The line transfer coefficients (Eqn. (4.17) and Eqn. (4.18)) can be computed when the line profile function ϕ_v and the number densities of H I atoms in the two hyperfine states n_1 and n_u at each location along the ray are known. The population of atoms in the upper (or lower) hyperfine state can be re-expressed using the relation $n_u = n_{\text{HIs}} - n_1$, where n_{HIs} is the number density of H I atoms in the (1S) ground state. At the temperature of interest here, practically all H I atoms are in the ground state, and hence, $n_{\text{HIs}} = n_{\text{HI}}$. Hereafter, n_{HI} is used without distinguishing from n_{HIs} for simplicity of notation.

Modelling of either n_1 or n_u and $n_{\rm HI}$ in astrophysical environments involves detailed investigations of the spin-flip mechanisms at play (see Sec. 4.2.3) and is beyond the scopes of this work. Here, a post-processing approach is adopted for which given an input model of these parameters, the line transfer coefficients can be computed and the (cosmological) 21-cm line radiative transfer calculations can be conducted to predict the observed spectra at individual lines-of-sight. For calculations in the cosmological context, the upper limit of $n_{\rm HI}$ is constrained by the baryonic number density and can be further combined with a spin temperature model $T_s(z)$ to calculate n_1 or $n_{\rm u}$.

The omnipresence of the CMB photons provide the radiation background that must be accounted for when looking at the cosmological 21-cm line. The CMB's spectra at different redshifts are well described by the Planck function at its characteristic temperature $T_{\text{CMB}}(z) = T_{\text{CMB},0}(1 + z)$, with $T_{\text{CMB},0} = 2.73$ K. In addition to the CMB, continuum radiation can arise from free-free processes and synchrotron radiation. The continuum absorption and emission coefficients for the thermal free-free process and the non-thermal synchrotron radiation have been discussed in Sec. 3.1.2 and presented in Appendix C. To isolate the 21-cm line emission and absorption, which is the focus of this work, the continuum emission and absorption are assumed to be zeros.

Numerical method

The radiative transfer equation can be directly integrated. A fourth-fifth order Runge-Kutta (RK) differential equation solver (Fehlberg 1969) is used to solve Eqn. (4.58) and also Eqn. (4.59). The description of the implementation of the RK solver can be found in Sec. 3.1.1. Different to the CPRT calculations, which involve simultaneously solving four coupled differential equations in the radiative transfer, the C21LRT calculations have only one differential equation. Therefore, N_{eqn} is set to be 1 in the RK solver. Also, N_{step} (the number steps) is set to be 1000 over each *z* interval, and eps (the error tolerance level) is set to be 10^{-5} .

4.4 Code Verification

A number of numerical tests are conducted to verify the implementation of the algorithm and the execution of the code for C21LRT calculations. Here shows the example tests that verify the ability of the code to account for the cosmological evolution effects and for the local effects on the line shift and broadening on the line-continuum interaction in the ray-tracing.

4.4.1 Code verification I: Generic continuum and line

Case IA: Radiative transfer of the CMB

This test, referred to as Case 1A, is to verify that the C21LRT code properly accounts for the sole effect of cosmic expansion, i.e. in the absence of emission and absorption. The CMB is chosen as the radiation to be transferred, as the evolution of its properties with the Universe can be determined to great precision. It is a continuum, with a blackbody spectrum, specified by the Planck function that only has one parameter:



Fig. 4.4: The observational frequencies covered by the low frequency array (SKA-low) and the mid frequency array (SKA-mid) of the SKA. The redshifted 21-cm lines originating from different cosmological epochs are shown, as vertical dotted lines, at z = 30 (corresponding the end of the Dark Ages), z = 15 and z = 6 (corresponding to the start and the end of the Epoch of Reionisation, respectively), z = 2 (corresponding to the epoch that star-forming activity peaked), and z = 0 (present time). The spectra of the CMB, representing the continuum background, at z = 0 (with T = 2.73 K) and at z = 15 (with T = 43.6 K) are also shown as a reference.



Fig. 4.5: The transfer of the CMB spectrum, in a log-log representation, from high redshifts to the present epoch. The hyperfine 21-cm transition of the neutral hydrogen in the local rest frame, with $v = v_{21cm}$, is indicated by the vertical dotted line.



Fig. 4.6: Numerical output of the computed CMB spectrum I_{ν} at z = 0 (purple solid line), is plotted along with the Planck function B_{ν} at T = 2.73 K (black dotted line) in the top panel. The corresponding residuals, $res_{\log I_{\nu}} = [\log I_{\nu}/\log B_{\nu}(T = 2.73 \text{ K})]|_{z=0.0} - 1.0$, are shown in the bottom panel. The residuals do not exceed 7.5×10^{-15} , indicating that the numerical outputs of the C21LRT calculations agree with the theoretical values up to the machine floating-point precision. The pattern in the residual plot is due to the over-sampling of the continuum spectrum in the frequency space, which will be the case for the study of the 21-cm line profile.

the thermal temperature.

The computation is assigned to trace a ray from $z (= z_{\text{max}}) = 38.8$ to z = 0, with the initial specific intensity $I_v|_{z_{\text{max}}} = B_v(T_{\text{CMB}}|_{z_{\text{max}}})$. Without absorption and emission along the ray, the evolution of the CMB spectrum is determined by the cosmic expansion only, and hence, the redshift. In a FRW universe, the thermal temperature of the CMB scales with the redshift as $T_{\text{CMB}}(z)/(1 + z) = T_{\text{CMB},0}$ (see Fig. 4.4), where $T_{\text{CMB},0} = 2.73$ K at the current epoch (e.g. Spergel et al. 2003; Planck Collaboration XVI 2014). The C21LRT code will be validated if the computed CMB spectrum at z = 0 is a blackbody of a thermal temperature T = 2.73 K. Fig. 4.5 shows the CMB spectra at different cosmological epochs, and Fig. 4.6 shows the results of Case IA, demonstrating that the computed CMB spectra deviate from the Planck functions at the expected temperatures in smaller than 1 part in 10^{14} .

Case IB: Radiative transfer of a line in an expanding universe

This test, referred to as Case 1B, is to verify correct shifting, broadening and intensity reduction of a generic 21-cm line when it is transported in an expanding Universe, in the absence of absorption, emission, and external radiation, in the ray-tracing using the C21LRT code. As in Case 1A for the CMB, the 21-cm line is assigned also to originate from $z_{emi} = 38.8$, and it propagates along a ray towards z = 0. The frequency shift of the line is determined by the $\left[\frac{1+z}{1+z_{emi}}\right]$ factor (see Eqn. (4.38)). Moreover, in a FRW universe, the line profile should exhibit the following properties along its propagation: (i) the invariant intensity I_{ν} remains constant along the ray, implying that the comoving intensity I_{ν} will be suppressed by a factor of $[(1 + z)/(1 + z_{emi})]^3$, (ii) the line width in frequency will be squeezed (as opposed to the stretch in wavelength) by a factor of $[(1 + z)/(1 + z_{emi})]$. The line width in terms of velocity will, however, stay constant, in the absence of local physical processes that can broaden the line. Also, the shape of the line will be preserved when it is expressed in the $\log v$ representation instead of in the v representation. In the calculations, the line is assumed to have a Gaussian profile initially, in the local rest frame at $z_{emi} = 38.8$. It is centred at $v_{21cm} = 1.42$ GHz. The line width is specified by Δv_D , which is set to be 4.738 MHz. This corresponds to a velocity dispersion⁹ of $\Delta v = 1000 \text{ km s}^{-1}$.

Fig. 4.7 shows the profiles of the 21-cm line, in terms of the specific intensity I_{ν} and frequency ν , at the selected redshifts. The three panels, from top to bottom,

⁹Velocity dispersions $\Delta v \approx 1000 \text{ km s}^{-1}$ have been observed in galaxies inside massive galaxy clusters, e.g. the Coma cluster (see Struble and Rood 1999), where the thermal and turbulent motions are substantial. A large value of $\Delta v (= 1000 \text{ km s}^{-1})$ is selected in the tests here for the verification that the C21LRT code is capable to handle the extreme situations of line broadening. The velocity dispersion caused by the differential motions within a galaxy is generally in the range $\Delta v \sim 100 - 400 \text{ km s}^{-1}$ (see e.g. Bezanson and Franx 2012), which gives rise to a frequency spread of $\Delta v_{\rm D} = 0.474 - 1.89 \text{ MHz}$.



Fig. 4.7: The computed frequency shift and the intensity change of a 21-cm line propagating from $z_{emi} = 38.8$ to $z_{obs} = 0$ in an expanding universe, in the absence of line-of-sight absorption, emission and external radiation. For an illustrative purpose, the specific intensity of the 21-cm line in the local rest frame is arbitrarily scaled up such that its peak is $1.0 \text{ erg s}^{-1} \text{ cm}^{-2} \text{ Hz}^{-1} \text{ str}^{-1}$ at z = 38.8. The redshift range is sub-divided into three regimes, shown in the three panels: (i) (top panel) before the completion of cosmological reionisation, at $z \gtrsim 6$; (ii) (middle panel) between the end of reionisation and the period of peak star formation and quasar activities peaked, at $z \sim (2 - 3)$, galaxy clusters assembled, and the cosmic web underwent virialisation, at $z \lesssim 3$. The comoving intensity of the line against the comoving (i.e. cosmological redshifted) frequency at different redshifts are indicated by different colours as labelled in the legends.



Fig. 4.8: The computed invariant line intensity I_{ν} (first panel) and line intensity I_{ν} (second panel) against ν in log-log scales, in an expanding universe without a line-of-sight medium and an external radiation field. The arbitrary scaling of the specific intensity I_{ν} in Fig. 4.7 is also adopted here. The results show that I_{ν} remains constant over redshift z, I_{ν} scales with $[(1 + z)/(1 + z_{emi})]^3$, and the line shape is preserved in the log ν space, all agreeing with the predictions of the analytical calculations. The log-linear plot of I_{ν} against ν shows an apparent reduction in the frequency spread of the line (third panel), and the linear-linear plot of I_{ν} against ν shows the decrease of the comoving intensity as z approaches zero (fourth panel).



Fig. 4.9: The peak intensity for each output redshift (from $z_{emi} = 38.8$ to $z_{obs} = 0$) is plotted against the frequency of the shifted line centre (top panel). This plot corresponds to the tilted straight line in the second panel of Fig. 4.8. The residuals of I_v (middle panel) and the residuals of v (bottom panel) are calculated by subtracting the ratio of the computed value to the analytical value by one. The plots show agreements between the computation and analytical calculation to the machine floating-point precision.



Fig. 4.10: The line profiles, characterised by the full-width-half-maximum of the line in frequency, FWHM_ν, at $z_{emi} = 38.8$ (top panel) and $z_{obs} = 0.0$ (bottom panel). The arbitrary scaling of the specific intensity I_{ν} in Fig. 4.7 is also adopted here. Note that the *x*- and *y*-axes in the two panels are in different scales. Frequencies at which I_{ν} attains its half maximum value, $(I_{peak}|_z)/2$, at the specific redshift are labelled by $v_L|_z$ and $v_R|_z$, with $v_R|_z > v_L|_z$. The FWHM in frequency is then calculated by FWHM_ν $|_z = v_R|_z - v_L|_z$. FWHM_ν $|_{z=38.8} = 11.15$ MHz while FWHM_ν $|_{z=0.0} = 0.2801$ MHz, showing a reduction in the line width, in the frequency space, as expected from cosmic expansion. The fractional difference between the computed value and the theoretical value at FWHM_ν $|_{z=0.0}$ is -2.14×10^{-13} .



Fig. 4.11: (Top panel): The full-width-half-maximum of the line in frequency (FWHM_{ν}) at each output redshift against the frequency of the shifted line centre. The slope of the FWHM_{ν} with the line frequency is equal to 1.0, as predicted by the theoretical scaling that both FWHM_{ν} and ν decrease following $[(1 + z)/(1 + z_{emi})]$ as z decreases. (Bottom panel): The corresponding normalised full-width-half-maximum of the line in the velocity (FWHM_{ν}/FWHM_{ν} – 1) against the frequency of the shifted line centre, where FWHM_{ν} = $(\sum_k FWHM_{\nu}|_{z_k})/N_{z_{output}} = 2353.8939150709657 km s⁻¹, with <math>N_{z_{output}} = 11$. The velocity dispersion, which depends only on the line broadening mechanisms (absent here) in a local frame, should not vary. The fluctuations at the level of 10^{-13} indicate that the computed and the theoretical values are in excellent agreement.

in the figure correspond, respectively, to the three epochs: (i) before the completion of cosmological reionisation ($z \gtrsim 6$), (ii) in between the end of the Epoch of Reionisation and before the period of peak star formation and quasar activities ($6 \gtrsim z \gtrsim 3$), and (iii) in the epochs when star formation (Hopkins and Beacom 2006; Lacaille et al. 2019) and quasar activities (Friaca and Terlevich 1998; Mújica and Maiolino 2004) peaked ($z \sim 2 - 3$), galaxy clusters assembled, and the vast cosmic web underwent virialisation ($z \lesssim 3$). Fig. 4.8 shows the invariant specific intensity and the comoving specific intensity of the 21-cm line at the frequencies of the corresponding eleven redshifts.

The frequency of the 21-cm line decreases and the specific intensity is suppressed as the line is transferred from high to low redshifts (see Fig. 4.7). The decrease of the specific intensity with the line propagation (which is stamped by the redshift z) follows a trend as indicated by the dashed straight line in the second panel of Fig. 4.8. The shape of the line is preserved in $\log -\nu$ (top two panels, Fig. 4.8), and the invariant specific intensity remains constant (first panel, Fig. 4.8). The line width in frequency, however, decreases in the transfer from high to low redshifts (bottom two panels, Fig. 4.8). All of these findings agree with the theoretical predictions. Quantitative assessment of the computed line profile with respect to the analytical counterparts are presented in Fig. 4.9, for the line peak intensity and centre frequency, and in Figs. 4.10 and 4.11, for the line width. The residuals of I_{ν} and ν , which are calculated by subtracting the ratio of the computed values to their corresponding analytical values by unity, attain a level below 10^{-14} , reaching machine floating-point precision. The variations of the line frequency, characterised by FWHM_{ν}, in frequency, and FWHM_{ν}, in velocity, also agree with their analytical values at a level of 10^{-13} .

Note that the reduction of the line width, in terms of frequency, can become significant in the cosmological evolutionary context. For instance, a FWHM_{ν}|_{z=38.8} = 11.2 MHz when the line was emitted near the end of the Dark Ages would be reduced to a FWHM_{ν}|_{z=0} = 11.2 MHz/(1+38.8) = 0.28 MHz when it is observed at the present. This width reduction is caused by the expansion of the Universe, and the line width is scaled by $[(1 + z)/(1 + z_{emi})]$, which is the same as the scaling factor¹⁰ of the radiation frequency. This scaling will be cancelled out if $\Delta v/v$ (where Δv is the line width) is used in an observational analysis. Interpretation of data using a theoretical model is an inverse process. Therefore, caution must be taken when using the line width in interpreting spectroscopic results associated with distant sources, and, in particular, the subtleties on cosmological expansion effects and on local physical processes that lead to the change in the line profile must be properly accounted for.

4.4.2 Code verification II: Galactic rotation

This test, referred to as Case 2, is to verify the ability of the C21LRT code in (i) handling the differential structures of HI gas along the ray, (ii) accounting for the effects on the line spectrum arising locally from the movement of the HI gas with respect to a distant stationary observer but at the same redshift, and (iii) giving a correct combination of the line spectra of multiple rays. Mock galaxies are constructed such that the radiative transfer calculations are conducted for rays propagating through the galaxy in the \tilde{x} - \tilde{y} plane.

Geometry

Standard spherical (r, θ, ϕ) and Cartesian $(\tilde{x}, \tilde{y}, \tilde{z})$ coordinate systems are adopted in the calculations, and the geometrical set up of the system is shown in Fig. 4.12.

$$(1 + z_{\text{emi}}) \equiv \frac{\lambda_{\text{obs}}}{\lambda_{\text{emi}}} = \frac{\nu_{\text{emi}}}{\nu_{\text{obs}}}$$

with a rest-frame observer at $z_{obs} = 0$. This gives

$$(1 + z_{\text{emi}}) = \frac{\nu_{\text{emi}} + \delta \nu_{\text{emi}}}{\nu_{\text{obs}} + \delta \nu_{\text{obs}}} = \frac{\nu_{\text{emi}}}{\nu_{\text{obs}}} \left[\frac{1 + (\delta \nu_{\text{emi}} / \nu_{\text{emi}})}{1 + (\delta \nu_{\text{obs}} / \nu_{\text{obs}})} \right]$$

where δv_{emi} is a frequency displacement from v_{emi} , and δv_{obs} is the corresponding frequency displacement from v_{obs} measured by the observer. It follows from the two expressions that

$$\frac{\delta v_{\rm emi}}{v_{\rm emi}} = \frac{\delta v_{\rm obs}}{v_{\rm obs}} ,$$

which implies that

$$\frac{\delta v_{\rm obs}}{\delta v_{\rm emi}} = \frac{v_{\rm obs}}{v_{\rm emi}} = \frac{1}{(1 + z_{\rm emi})}$$

If δv_{emi} is the marker of the width of a line, centred at v_{emi} , emitted from z_{emi} , the width of the line will reduce when measured by the observer in its local reference frame (for $z_{emi} > z_{obs} = 0$ in an expanding Universe).

¹⁰Cosmological redshift z is defined as



Fig. 4.12: Geometry of the galactic rotation example problems.

The galactic disk is geometrically thin, with a negligible thickness. It is centred at the origin $((\tilde{x}, \tilde{y}, \tilde{z}) = (0, 0, 0))$ and lies in the $(\tilde{x}-\tilde{y})$ plane, i.e. $\theta = \pi/2$. The HI emitting gas located at $(R, \pi/2, \phi)$ in the disk is specified by a vector

$$\begin{bmatrix} \tilde{x} & \tilde{y} & \tilde{z} \end{bmatrix} = R \begin{bmatrix} \cos \phi & \sin \phi & 0 \end{bmatrix}$$
(4.62)

in the Cartesian coordinate. The disk rotates clockwise with a speed $v_{rot}(R)$. The rotational velocity of the HI emitting gas at $(R, \pi/2, \phi)$ in the disk is therefore

$$\boldsymbol{v}_{\text{rot}} = \begin{bmatrix} v_{\tilde{x}} & v_{\tilde{y}} & v_{\tilde{z}} \end{bmatrix} = v_{\text{rot}}(R) \begin{bmatrix} \sin \phi & -\cos \phi & 0 \end{bmatrix} .$$
(4.63)

The disk is viewed at an inclination angle, *i*, by a distant observer in the \tilde{y} - \tilde{z} half-plane containing the $-\tilde{y}$ axis. Thus, the emission that reaches the observer propagates in the direction specified by the unit vector

$$\hat{k} = \begin{bmatrix} k_{\tilde{x}} & k_{\tilde{y}} & k_{\tilde{z}} \end{bmatrix} = \begin{bmatrix} 0 & -\sin i & \cos i \end{bmatrix} .$$
(4.64)

This gives the pitch angle of the emission (i.e. the angle between the propagation unit vector of the emission and the rotation velocity of the HI emitting gas)

$$\varrho = \cos^{-1}\left(\frac{\hat{k} \cdot v_{\text{rot}}}{|v_{\text{rot}}|}\right) = \sin i \cos \phi , \qquad (4.65)$$

and the magnitude of the projected line-of-sight velocity of the HI emitting gas

$$v_{\parallel} = \hat{k} \cdot v_{\text{rot}} = v_{\text{rot}}(R) \sin i \cos \phi . \qquad (4.66)$$

Galactic structure

Three model galaxies are first constructed: model galaxy (i) has a disk with no spiral arms, model galaxy (ii-a) a disk with two loosely-winded spiral arms, and model galaxy (iii-a) a disk with two winded clumpy spiral arms. Two controls, with respect to model galaxies (ii-a) and (iii-a) are also constructed: model galaxy (ii-b) has two loosely-winded spiral arms without a disk, and (iii-b) a disk with two winded non-clumpy spiral arms. The galaxies have a radius of R = 17 kpc, and their disks, if present, have a uniform H I number density $n_{\rm HI} = 0.5$ cm⁻³. The spiral arms have an enhanced H I number density $n_{\rm HI} = 30.0$ cm⁻³. The clumps in model galaxy (ii-a) are randomly positioned¹¹ across the disk. The number density of the H I gas of the five model galaxies are shown in Fig. 4.13.

A cold-phase HI gas with a uniform $T_k = 100$ K across the entire galactic structure is assumed¹². At this temperature, all neutral hydrogen atoms are practically in the (1S) ground state. In the absence of Ly α pumping (assumed here), as $T_k > T_{\text{CMB}} \gg T_{\star}$ the relative populations of the electrons in the two hyperfine levels

¹¹The Mersenne Twister pseudo-random number generator (Tada 2005) is used to select twenty-three (ind_x, ind_y). The clumpy arms are then produced by resetting $n_{\text{HI, arm}} = 30.0 \text{ cm}^{-3}$ to $n_{\text{HI, disk}} = 0.5 \text{ cm}^{-3}$ at the randomly selected coordinates and their adjacent eight cells (two cells up, down, left, right to the selected cell). The H I gas density is zero for radial distances > R = 17 kpc from the galactic centre.

¹²The interstellar medium (ISM) in galaxies is multi-phase (see Sec. 1.3). Two distinct phases of atomic neutral hydrogen gas can co-exist in the ISM: (i) a denser cold neutral medium (CNM; $T_k \sim 100$ K, $n_{\rm HI} \sim 30$ cm⁻³), and (ii) a warm neutral medium (WNM ; $T_k \sim 5000$ K, $n_{\rm HI} \sim 0.5$ cm⁻³) (see e.g. Draine 2011). The CNM is thought to predominant at high interstellar pressure, while the WNM should dominant at low pressure (Braun 1997). In a WNM, collisional excitation of the 21-cm hyperfine transition alone is not strong enough to establish the thermal equilibrium equilibrium $T_s = T_k$, but requiring the resonant scattering of the Ly α photons (Liszt 2001). Calculation of the spin temperature in the WNM involves knowledge about the ionisation state, phase structure and spatial distribution of the ISM (see Liszt 2001).















Fig. 4.13: The H I distribution, in $n_{\rm HI}$, of model galaxies (i) with no spiral arms (top panels), (ii-a) with two loosely winded arms (middle panels), and (iii-a) with two winded clumpy arms (bottom panels). The disks of the galaxies have a uniform $n_{\rm HI} = 0.5 \text{ cm}^{-3}$. The arms have an enhanced density $n_{\rm HI} = 30 \text{ cm}^{-3}$. The H I distribution $n_{\rm HI} (\theta, \phi)$ in the polar coordinate are shown in the left panels. The rays for radiative transfer in each galaxy are shown in the corresponding right panel. The vertical red lines indicate the rays for the calculations of the 21-cm line spectra in the later figures.





Fig. 4.14: The H I distribution, in $n_{\rm HI}$, of model galaxies (ii-b) with two loosely-winded arms and no disk (top panels), and (iii-b) with two winded non-clumpy arms and a disk (bottom panels). These two galaxies serve as the controls to model galaxies (ii-a) and (iii-a), respectively.



Fig. 4.15: The distribution of v_{rot} (left) and v_{\parallel} (right) of the H I gas in a model galaxy with a rotation curve similar to that of the Milky Way. The + \tilde{x} -axis corresponds to $\phi = 0^{\circ}$, and + \tilde{y} -axis corresponds to $\phi = 90^{\circ}$ ($\pi/2$) (see Fig. 4.12). The markers (5, 10, 15, 20) on the radial axis indicate the radial distances in kpc from the galactic centre, which is at (0,0). The galaxy is observed edge-on, in the $-\tilde{y}$ -direction, from afar. All rays are in parallel with each other on the disk plane and are traced in a direction from positive to negative \tilde{y} in the radiative transfer calculations.

is $n_u/n_l = 3$. The number density of HI in the upper (triplet) and lower (singlet) hyperfine states is

$$n_{\rm u}(\theta,\phi) = 3n_{\rm l}(\theta,\phi) = \frac{3}{4}n_{\rm HI}(\theta,\phi)$$
 (4.67)

The stimulated emission factor Ξ (in Eqn. (4.28)) is equal to 1 when $n_u/n_l = 3$. This corresponds to a balance between stimulated emission and absorption (see Eqn. (4.26)). The redistribution of electrons in the two hyperfine levels is, therefore, caused only by the spontaneous emission. The incoming radiation background is provided solely by the CMB.

Velocity induced line frequency shift and broadening

The galaxy is assumed to be at rest with respect to the observer and at a redshift z = 0. Without losing generality, an edge-on disk (i.e. $i = \pi/2$) is adopted in the calculations, as the viewing inclination simply introduces a scaling factor sin *i* that is uniformly applied to the projected line-of-sight velocities of all the H I emitting gas in the disk. The galaxy has a rotation curve similar to that of the Milky Way galaxy,

which can be described by an analytical fit-model¹³ as that in Clemens (1985), for the IAU standard parameters of $R_{\odot} = 8.5$ kpc for the distance of the Sun to the Galactic centre and $v_{rot_{\odot}} = 220$ km s⁻¹ for the rotation speed of the Sun. The rotational speed profile of the galaxy and its projected line-of-sight value for the viewing geometry adopted for the calculations are shown in Fig. 4.15. These bulk differential motions of the H I emitting gas in the galactic disk leads to the differential frequency shifts in the 21-cm emission. A uniform temperature of $T_{\rm k} = 100$ K and a uniform turbulent velocity $v_{\rm turb} = 10$ km s⁻¹ (Agertz et al. 2009) are adopted for the H I gas in the entire galactic disk. The thermal and turbulent motion broadens the line, resulting in a Gaussian line profile, which is as described in Eqn. (4.48).

Results and Discussion

The spectra of the 21-cm line from a galaxy is determined jointly by bulk rotation of the galaxy and turbulence and microscopic thermal motion of the H I gas within. Along each line-of-sight the spread of a line seen by an observer is caused not only by the turbulence and the microscopic motion but also by the differential frequency shift due to the projected speed of the galactic rotation velocity, which varies with the radial distance from the galactic centre. The differential smearing of the 21-cm line along the line-of-sight propagation of the radiation will introduce radiative transfer effects, because of the interactions between the line and its underlying continuum. This effect is present except in the ray along the line-of-sight passing through the galactic centre, as $v_{\parallel} = 0$ throughout.

The 21-cm line spectra over the ray path along different lines-of-sight symmetrical to the galactic centre (see 4.14) for the five model galaxies are shown in Figs. 4.16 - 4.20. As expected, the 21-cm lines are red-shifted for the rays along the lines-ofsight on the left-hand side of the galactic centre but are blue-shifted for the rays along the lines-of-sight on the right-hand side in the spectra (cf. the velocity map in the right panel, Fig. 4.13). In the absence of spiral arms, i.e. in model galaxy (i), there would be a left-right symmetry in the line spectra of the line-of-sights, which is as

¹³See Eqn. (6) and Table 3 in Clemens (1985) for the polynomial fit and the associated coefficient values, respectively.



Fig. 4.16: The 21-cm line spectrum of model galaxy (i), which has a uniform H I disk but no spiral arms. Panels from top to bottom show the spectra for the lines-of-sight as labelled in Fig. 4.13i. Different coloured lines (from blue to red) represent the spectra at different light travel distances, showing the progressive changes of the spectra (in every four steps in ind_y). The red line corresponds to the spectrum seen by the distant observer.



Fig. 4.17: The 21-cm line spectra of model galaxy (ii-a), which has a pair of loosely-winded spiral arms in addition to a uniform HI disk. Panels from top to bottom show the spectra for the lines-of-sight as labelled in Fig. 4.13ii-a. Different coloured lines (from blue to red) represent the spectra at different light travel distances, showing the progressive changes of the spectra (in every four steps in ind_y). The red line corresponds to the spectrum seen by the distant observer.



Fig. 4.18: The 21-cm line spectra of model galaxy (ii-b), which has only a pair of loosely winded spiral arms (i.e. the H I disk is absent). Panels from top to bottom show the spectra for the lines-of-sight as labelled in Fig. 4.14ii-b. Different coloured lines (from blue to red) represent the spectra at different light travel distances, showing the progressive changes of the spectra (in every four steps in ind_y). The red line corresponds to the spectrum seen by the distant observer.



Fig. 4.19: The 21-cm line spectra of model galaxy (iii-a), which has a uniform H I disk and a pair of clumpy spiral arms. Panels from top to bottom show the spectra for the lines-of-sight as labelled in Fig. 4.13iii-a. Different coloured lines (from blue to red) represent the spectra at different light travel distances, showing the progressive changes of the spectra (in every four steps in ind_y). The red line corresponds to the spectrum seen by the distant observer.



Fig. 4.20: The 21-cm line spectra of model galaxy (iii-b), which has a uniform HI disk and a pair of non-clumpy spiral arms. Panels from top to bottom show the spectra for the lines-of-sight as labelled in Fig. 4.14iii-b. Different coloured lines (from blue to red) represent the spectra at different light travel distances, showing the progressive changes of the spectra (in every four steps in ind_y). The red line corresponds to the spectrum seen by the distant observer.



Fig. 4.21: I_{max} (maximum I_{ν} at each pixel) of the 21-cm emissions from the model galaxies. The maximum values of I_{max} are 9.909×10^{-16} for model galaxy (i), 1.095×10^{-14} for model galaxy (ii-a), 1.083×10^{-14} for model galaxy (ii-b), 1.508×10^{-14} for model galaxy (iii-a), and 1.776×10^{-14} for model galaxy (iii-b). The minimum value of I_{max} is 1.673×10^{-18} , which is the CMB continuum intensity, for all the model galaxies.

shown in Fig. 4.16. The left-right symmetry in the frequency shift and broadening will be broken if arms are present (see the line spectra of model galaxies (ii-a), (ii-b),



Fig. 4.22: Same as Fig. 4.21 but for $\log I_{\text{max}}$ (the logarithm of the maximum I_{ν} at each pixel) of the 21-cm emissions from the model galaxies. The colour-bars for model galaxies (ii-a) (ii-b) (iii-a) and (iii-b) are plotted on the same scales for comparison purposes.

(iii-a) and (iii-b) in Figs. 4.17 – 4.20, respectively). The asymmetry can be seen, for example, by comparing the line spectra of the pair of lines-of-sight at $ind_x = 16$ and 76 in model galaxies (ii-a) and (ii-b), in Figs. 4.17 and 4.18, respectively. This asymmetry in the red-shifted line and its corresponding blue-shifted line is due to the difference in the order of encounter of H I gas with the same kinetic and thermal

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Fig. 4.23: (Top panel): 2D intensity-position-velocity diagram of model galaxy (i), which has a uniform HI gas but no spiral arms. v_{\parallel} is the line-of-sight projection of the rotational velocity and Δr is the displacements of lines-of-sight from the line-of-sight passing through the centre of the galaxy. The diagram shows the rotation curve of the galaxy and the velocity dispersion in the galaxy. (Bottom panel): 3D surface plot with I_{max} on a plane spanned by Δr and v_{\parallel} . I_{max} is indicated by height in a linear scale and by colour in a logarithmic scale.

properties along a line-of-sight on the left-hand side with respect to the galactic centre and its counterpart on the right-hand side. For instance, the resulting line spectra to be observed by a distant observer, indicated by the red lines in the Figures, have different peak intensities, because of the different radiative transfer effects and the different contributions by the H I gas along different lines-of-sight. The subtle evolution of the line profile when the 21-cm line is transported progressively along the lines-of-sight to the observer can be seen in the intermediate spectra, marked by the rainbow colours (with blue colour denoting the farthest from the observer), in Figs. 4.17 and 4.18. The radiative transfer effects are more significant for the model galaxies (iii-a) and (iii-b), which have greater arm sweeps than model galaxies (ii-a) and (ii-b). The effects are manifested in the more obvious difference in the line profiles of each pair of lines-of-sights mirrored left-right with respect to the galactic centre. The clumpiness of the spiral arms, as those in model galaxy (iii-a), further enhances the effects, leading to an increasing asymmetry in the spectral profile of the 21-cm lines of the mirror pair of the lines-of-sight. This left-right (a)symmetry in the line spectra of the corresponding pair rays can also be seen in the polar plots of the maximum specific intensity of each pixel, I_{max} , in the rays propagating in the galactic plane to the observer (see Figs. 4.21 and 4.22).

The outputs of the C21LRT calculations are (2+1)D cuboids each containing the information of their individual spatial location and line profile, in term of the specific intensity evaluated at the local rest frame. This information allows a construction of an intensity-position-velocity diagrams¹⁴ for the model galaxies. Figs. 4.23 – 4.26 show the 2D projections and 3D visualisations of I_{max} with respect to δr , the displacement from the galactic centre and v_{\parallel} , the local projected line-of-sight velocity. These diagrams also serve as a self-consistency check of the code in properly handling the modification of the frequency and specific intensity of the 21-cm line in a system with both velocity and density structures. The plots show that the galactic bulk velocity, v_{\parallel} , at the galactic centre, $\delta r = 0$, is zero in all model galaxies, as required. The galactic rotation curve is also fully recovered when tracing

¹⁴The intensity-position-velocity diagrams shown in this C21LRT test are distinct from those commonly used in observational galactic studies. Here, a forward modelling approach is adopted for which the galactic rotation curve and the distribution of $n_{\rm HI}$ are the inputs. This differs from the conventional observational construction of the intensity-position-velocity diagrams, which are used for deducing the rotation curve of a galaxy from the spatial-spectral data and the intensity are an overlay in those plots. Instead, the intensity-position-velocity diagrams here show the 21-cm emissions at a given horizontal displacement from the galactic centre, δr , and at the line-of-sight velocity allowed at that position v_{\parallel} .

along the maximum v_{\parallel} values in the right-hand-side of each diagram¹⁵ of the model galaxies. The spread in v_{\parallel} at a fixed δr reveals the range of the allowed v_{\parallel} given the geometric structure and the rotation curve of the model galaxy. (Note that $v_{\parallel} = 0$ is seen across all δr due to the line-of-sight components outside the galactic disk, except that at $\delta r = 0$, v_{\parallel} has its a true physical meaning of the velocity of the entire galaxy.)

¹⁵The left-hand-side of each diagram shows the galactic structure receding from the observer, and has a shape mirrored (about both the y- and x-axes) to the shape in the left-hand-side of the diagram, which shows the galactic structure towards the observer.



Fig. 4.24: The 2D intensity-position-velocity diagrams for the model galaxies with spiral arms, with model galaxies (ii-a) and (ii-b) in the top left and right panels, respectively, and model galaxies (iii-a) and (iii-b) in the bottom left and right panels, respectively. In each panel, the colour-bar indicates I_{max} .



 10^{-14} 10^{-16} 10^{-17}

Fig. 4.25: The 3D intensity-position-velocity diagrams for the galaxy (ii-a), which has both a H I disk and two spiral arms, and model galaxy (ii-b), which has only two spiral arms and no H I disk.





Fig. 4.26: The 3D intensity-position-velocity diagrams for model galaxy (iii-a), which has clumpy spiral arms, and model galaxy (iii-b), which has smooth spiral arms.

4.5 Demonstrative Study: Cosmological Radiative Transfer

The cosmological 21-cm line radiative transfer (C21LRT) calculations can be performed for the entire sky using a ray-tracing scheme as those in the cosmological polarised radiative transfer (see Fig. 3.2). The C21LRT equation is solved along rays specified in a spherical polar coordinate system $(r(z), \theta, \phi)$, with (θ, ϕ) being the celestial sky coordinates. Here, the C21LRT equation is solved along a single ray as a conceptual demonstration that the convolution of cosmological and radiative transfer effects are properly accounted for. The rays reaching the observer at the present epoch are specified by (θ, ϕ) , and are independent of each other in an isotropic universe, in the absence of significant photon scattering along the lineof-sight. Thus, the radiative transfer calculations of 21-cm line in the rays of the entire sky just follow the same procedures as the calculation of the ray shown in this demonstrative study.

4.5.1 Evolution of neutral hydrogen density and populations of the hyperfine states

The diffuse gas suffusing the Universe (hereafter, referred to as the intergalactic medium, IGM, after the appearances of the first luminous structures) consist of two phases: (i) ionised (hereafter, referred to as H II, without losing generality) gas in bubbles embedded with luminous sources which provide the ionising photons, (ii) largely neutral IGM in regions outside the H II bubbles. Gas inside the H II bubbles with a strong radiation field is practically fully ionised, as recombination cannot keep up with ionisation. Gas in regions far outside the bubbles would remain neutral. Ionised gas and neutral gas can co-exist in a transition region between the H II bubble and the ambient neutral medium. The ionisation state of the gas in these three regions can be described in terms of a parameter, the ionisation fraction x_i , with $x_i = 0$ for neutral gas and and $x_i = 1$ for fully ionised gas.

In this demonstrative study, the detailed structures and the cosmological evolution of these three regions are not considered. Instead, the cosmological evolution of the ionisation state of the line-of-sight medium is parameterised by a volumeaveraged value for the ionisation fraction, i.e. $x_i(z)$. In other words, the transfer of 21-cm line photons in the H II bubble, the neutral medium and the transition regions are not explicitly distinguished. Without losing generality, the values of $x_i(z)$ are adopted directly from model C given in Pritchard and Loeb (2008). Fig. 4.27 shows the ionisation fraction $x_i(z)$, the mean neutral hydrogen number density $\overline{n}_{HI}(z)$ and the spin temperature $T_s(z)^{16}$ in the adopted evolution model.

With $x_i(z)$ specified, the amount of H I gas and the relative population of neutral hydrogen atoms in the two hyperfine states can be computed from a cosmological model, with the procedures described as follows. The density of hydrogen is approximately 75% of the baryon density by mass, i.e. $\rho_H = 3\rho_b/4$, and the remaining 25% is mainly contributed by helium, especially before the mass production of metals in stars. Assuming a two-species (H-He) description of the baryonic content, the cosmological number density of hydrogen is then

$$\overline{n}_{\rm H}(z) = \left(\Omega_{\rm b}(z)/m_{\rm p}\right)\rho_{\rm crit}\left(1 - Y_{\rm He}\right)$$
$$\approx \left(\Omega_{\rm b,0}/m_{\rm p}\right)\left(1 + z\right)^{3}\rho_{\rm crit}\left(1 - Y_{\rm He}\right)$$
$$= \overline{n}_{\rm H,0}(1 + z)^{3}. \tag{4.68}$$

In the calculations, the mass fraction of helium is set to be $Y_{\text{He}} = 1/4$. The present baryonic density $\rho_{b,0} = 4.18977 \times 10^{-31} \text{ g cm}^{-3}$, deduced from $\Omega_{b,0} = \rho_{b,0}/\rho_{\text{crit}}$, where $\Omega_{b,0}h^2 = 0.02230$ (Planck Collaboration XIII 2016), $\rho_{\text{crit}} = 3H_0/(8\pi G) =$

¹⁶The spin temperature was first equal to the CMB temperature, i.e. $T_s = T_r = T_{CMB}$, during the Dark Ages $(z \gtrsim 210)$ after recombination, because of strong thermal couplings between the hyperfine state transition and the CMB. This thermal coupling became less effective as the Universe expanded. The gas kinetic, and hence, the hyperfine transition, eventually decoupled. A faster adiabatic cooling of the gas compared to the radiation led to $T_k < T_{CMB}$. This occurred during the redshifts $210 \gtrsim z > 40$, which was before the first luminous sources began to appear. When the gas pressure was sufficiently high, collisional coupling would set $T_s \approx T_k$. The expansion of Universe lowered the rate of collisions and hence, weakened the collisional coupling. The competition between radiative coupling with the CMB and the collisional coupling leads to $T_{CMB} \gtrsim T_s > T_k$. This state continued to proceed until the appearance of the first luminous sources. These sources released UV radiation and X-rays, which caused ionisation and heating of the H I gas. More importantly, the UV radiation would give rise to Ly α pumping process, and the hyperfine states of the H I gas were no longer determined solely by the thermal and collision coupling processes. The Ly α radiation and X-rays of the H I gas resulted in $T_k > T_r$. The ionisation and the heating of the H I gas by the emergence of the luminous sources also ushered the Universe into the cosmological reionisation epoch.



Fig. 4.27: Panels from top to bottom show the plots of the cosmological evolution of $T_s(z)$ (along with $T_{\text{CMB}}(z)$ in dark red dashed line), $x_i(z)$ and $\overline{n}_{\text{HI}}(z)$ against (1 + z). Models of $T_s(z)$ and $x_i(z)$ (in blue dots) are constructed by extrapolating the model C of Pritchard and Loeb (2008) (in orange dotted line). For $z \gtrsim 210$ (rightward to the vertical brown dotted line), when a strong coupling between the gas temperature and the CMB temperature is established by Compton scattering, it is assumed that $T_s = T_{\text{CMB}} = T_k$. The ionisation fraction underwent major transition from z = 18.8 to z = 11.7 (in vertical green dotted lines), marking the beginning and the end of cosmological reionisation, respectively.

 $1.87882 \times 10^{-29} h^2$ g cm⁻³ (with h = 0.6774), and hence, the present hydrogen number density $\overline{n}_{\rm H,0} = 1.87745 \times 10^{-7}$ cm⁻³. It follows that

$$\overline{n}_{\mathrm{HI}}(z) = \overline{n}_{\mathrm{H}}(z) \, x_{\mathrm{HI}}(z) = \overline{n}_{\mathrm{H}}(z) \left(1 - x_{\mathrm{i}}(z)\right) \,. \tag{4.69}$$

Note that a major neutral-ionisation phase transition occurred from z = 18.8 to z = 11.7, as indicated in the ionisation fraction against redshift plot in Fig. 4.27. After the completion of the cosmological reionisation, only the self-shielded surviving dense clumps of neutral hydrogen would contribute to the cosmological 21-cm line signals. The observational imprints caused by convolution of these dense neutral hydrogen structures in the post-reionisation era and the ionised bubbles developed in the Epoch of Reionisation have not been thoroughly investigated. Although these complex issues would not be addressed in this demonstrative calculation, they can been studied explicitly and their observational consequences can be quantified using the C21LRT formulation presented in this chapter.

Each ray is marked by a celestial coordinate (θ, ϕ) , and the propagation of the radiation along the ray is stamped by the redshift *z*. The number density of the H I atoms in the lower (singlet) hyperfine state along a ray is given by

$$n_{I}(z) \Big|_{(\theta,\phi)} = \frac{n_{\rm HI}(z)}{1 + 3\exp(-T_{\star}/T_{\rm s}(z))} \Big|_{(\theta,\phi)}$$

$$\approx \frac{n_{\rm HI}(z)}{4 - 3(T_{\star}/T_{\rm s}(z))} \Big|_{(\theta,\phi)}$$

$$= \frac{\overline{n}_{\rm H}(z)x_{\rm HI}(z)(1 + \delta_{\rm b}(z))}{4 - 3T_{\star}/T_{\rm s}(z)} \Big|_{(\theta,\phi)}, \qquad (4.70)$$

for $T_s \gg T_{\star}$, where the baryonic matter overdensity is $\delta_b \equiv (\rho_b/\overline{\rho}_b - 1)$, with $\overline{\rho}_b$ being the mean density. The corresponding number density of the H I atoms in the upper (triplet) hyperfine state is given by $n_u(z) = n_{\text{HI}}(z) - n_1(z)$. Therefore,

$$n_{\rm u}(z) \Big|_{(\theta,\phi)} \approx \frac{3\,\bar{n}_{\rm H}(z)x_{\rm HI}(z)\,(1+\delta_{\rm b}(z))\,(1-T_{\star}/T_{\rm s}(z))}{4-3\,T_{\star}/T_{\rm s}(z)} \Big|_{(\theta,\phi)} \,. \tag{4.71}$$

The above parameterisation of the relative population of HI atoms in the two

hyperfine states, (n_u/n_l) , using the spin temperature T_s has imposed a constant 3 : 1 (= g_u : g_l) ratio for the relative populations. This parameterisation will be invalid, if there is a strong UV radiation field. The Ly α pumping will allow a higher number of HI atoms in the upper hyperfine state through the Wouthuysen-Field mechanism. In this situation, an additional local radiative transfer calculation will be required so to determine n_u and n_l .

The spread of the 21-cm line is caused by the velocity dispersion of the H I atoms, whose velocities have a Maxwellian distribution, due to turbulence and thermal motion. This gives a Gaussian profile function of the 21-cm line for the local emission and absorption coefficients. Without losing generality, line broadening caused by thermal motion is assumed to be insignificant in this demonstrative study. The line broadening is, therefore, caused only by turbulent motion characterised by a root-mean-square velocity $(v_{turb}^2)^{1/2}$. Furthermore, the root-mean-square velocity is uniform along the line-of-sight, whose value is set to be either 1000 km s⁻¹ or 100 km s⁻¹. The effective width of the broadened line is specified by a Doppler parameter, which is now given by $b_D = v_{turb}$.

4.5.2 Continuum radiation field

The CMB photons provides a radiation background and causes local line-continuum interaction. Its presence and evolution is determined self-consistently as in the calculations shown in Sec. 4.4.1. Without further complicating the 21-cm emission and absorption, other continuum radiative processes, such as thermal and non-thermal free-free process and synchrotron radiation, are ignored, although the C21LRT algorithm can easily account for their contribution if they are present (see Sec. 4.3.2).

4.5.3 **Results and discussion**

The strength of the 21-cm line signal at a given redshift z' observed at the present epoch (z = 0) is determined by the integrated optical depth of the line from the present z = 0 to the redshift z = z'. At a given z, the variation of the transfer coefficients across the line frequency ν follows the line profile function ϕ_{ν} . Thus, the broadening of the line will modify the transfer coefficients and hence, the line


Fig. 4.28: (Top two panels): The absorption and emission coefficients of the H I hyperfine line at the line-centre frequency $v = v_{21cm}$ evaluated in the comoving frame at *z* for the case with $b_D = 1000 \text{ km s}^{-1}$. (Bottom two panels): The absorption and emission coefficients of the cases with $b_D = 100 \text{ km s}^{-1}$ and $b_D = 1 \text{ km s}^{-1}$ normalised by the respective coefficients of the case with $b_D = 1000 \text{ km s}^{-1}$. The top auxiliary *x*-axes indicate the redshifted frequency that would be observed at z = 0 (given by $v_{obs} = v_{21cm}/(1+z)$).

optical depth. For a Gaussian line profile, this will lead to a reduction of the optical depth at the line centre frequency, hence, suppressing the line signal with respect to the neighbouring continuum. Fig. 4.28 shows the transfer coefficients of the HI hyperfine line (without a continuum) at the line-centre frequency, evaluated in the comoving *z* frames for the case with $b_D = v_{turb} = 1000 \text{ km s}^{-1}$ and the comparison with the cases with 100 km s^{-1} and 1 km s^{-1} . The narrower the line width, the larger the transfer coefficient at the line centre. The values of the transfer coefficients scale with $(b_D \sqrt{\pi})^{-1}$, which is a consequence of the assumed Gaussian form of the line profile function. It follows that the suppression of the 21-cm line signal would be subject to the same scaling factor, if other frequency modification processes (e.g. cosmological redshifting) are insignificant or absent.

This study demonstrates the radiative transfer of the 21-cm hyperfine line from $z = z_{decouple} = 210$ (the redshift at and above which $T_s = T_{CMB} = T_k$) to $z = z_0 = 0$ (the present epoch) using a ray-tracing approach for two values of line broadening: $b_D = 1000 \text{ km s}^{-1}$ and 100 km s⁻¹. Figs. 4.29 and 4.30 show the comoving 21-cm spectra at different redshifts obtained from the C21LRT calculations for the two cases of line broadening, respectively. The spectra in both cases are characterised by two absorption troughs and an emission crest which is located at a lower redshift. These structures are the consequences of the cosmological evolution of the spin temperature of the electrons in the H I gas and the ionisation fraction of hydrogen. These features will remain in the 21-cm line spectra when observed at z = 0, although their relative strengths will be modified because of the cosmological redshifting in the line frequencies and the suppression of the line intensities. This effect can be seen in the line spectra at z = 0 for the two cases, shown in Fig. 4.31, with the first and third panels in terms of the specific intensity $(I_{L,v} - I_{C,v})$, and the second and fourth panels in terms of the differential brightness temperature δT_b , respectively.

For an optically thin emission, the specific intensity is the product of the specific optical depth and the source function, i.e. $I_{\nu} \propto \tau_{\nu} S_{\nu}$, where the source function S_{ν} of a thermal process is the Planck function, B_{ν} , which is uniquely determined and is specified by a thermal temperature when the system is in a local thermal equilibrium.



Fig. 4.29: Spectra of the 21-cm line in the comoving frames obtained from the C21LRT calculations for redshifts from z = 25.2 to z = 9 for the case with $b_D = v_{turb} = 1000$ km s⁻¹. In each spectrum, the local CMB continuum is subtracted. The redshift range has covered the cosmic dawn and the epoch of reionisation.



Fig. 4.30: Spectra of the 21-cm line in the comoving frames obtained from the C21LRT calculations for redshifts from z = 25.2 to z = 0.9 for the case with $b_D = v_{turb} = 100 \text{ km s}^{-1}$. In each spectrum, the local CMB continuum is subtracted. The redshift range has covered the cosmic dawn and the epoch of reionisation.



Fig. 4.31: Spectra of the 21-cm line observed at z = 0 obtained from the C21LRT calculations. Spectra in the top two and the bottom two panels correspond to the cases with $b_D = 1000 \text{ km s}^{-1}$ and 100 km s^{-1} , respectively. In each case, the spectra are shown in terms of specific intensity $(I_{L,\nu} - I_{C,\nu})$ and differential brightness temperature $\delta T_b (= (I_{L,\nu} - I_{C,\nu})(c/\nu)^2/(2k_B))$. The top auxiliary *x*-axes indicates a cosmological redshift z' given by $v_{obs} = v_{21cm}/(1 + z')$. The brown dotted line indicates the frequency corresponding to the decoupling redshift $z_{dec} = 210$; and the two green dotted lines mark the frequencies corresponding to the beginning and the end of the epoch of reionisation.



Fig. 4.32: Spectra showing the effect of line broadening convolved with cosmological radiative transfer. The local broadening of the 21-cm line is assumed to be caused by turbulence, which gives $b_D = v_{turb} = 1000 \text{ km s}^{-1}$. The redshift-frequency grids in the very high redshift, with $T_s < T_{CMB}$, are shown for an illustrative purpose (i.e. not the true physical condition at $z > z_{dec}$). The spectra in the comoving frames are shown in the top panel, and the corresponding spectra to be observed at z = 0 are shown in the bottom panel. As shown, the redshifted intensity contributions and the local intensity contribution superposed, which gives a series of absorption troughs. The grey dash lines indicate where the local 21-cm absorption and emission begin to contribute. In all cases, there is a small emission bump at the low frequency wing of the line, making the line appear to have a P Cygni profile, as those seen in the line from an expanding stellar atmosphere.

Thus, we may expect that $I_{L,\nu} \propto \tau_{L,\nu} B_{\nu} \propto \kappa_{L,\nu} B_{\nu}$ at a given *z* would roughly hold in the 21-cm line calculations as the HI gas is not in a state far from a thermal equilibrium. As shown in Fig. 4.28, the values of the transfer coefficients at the line peak scale with b_D^{-1} , implying that $\tau_{L,\nu}$ at the line peak also scales with b_D^{-1} . This scaling is indeed manifested in the 21-cm line spectra at z = 0 (in terms of either $(I_{L,\nu} - I_{C,\nu})$ or δT_b), as the strength of the first absorption trough located at the low frequencies, of the case with $b_D = 1000 \text{ km s}^{-1}$ is 10 times weaker that the strength of the tough of the case with $b_D = 1000 \text{ km s}^{-1}$ (see Fig. 4.31).

The scaling implies that the strength of the low-frequency trough for $b_D = 1 \text{ km s}^{-1}$ would be about 1000 times stronger than that for $b_D = 1000 \text{ km s}^{-1}$. This gives an amplitude of $\delta T_b \approx 36 \text{ mK}$ at z = 0, a value consistent with those obtained in the previous work (see e.g. Fig.1, third panel, in Pritchard and Loeb (2008), which showed the 21-cm signal, in δT_b , across the cosmological redshift, in (1 + z)). However, the scaling factor of 10 is not uniform across all redshifts. Comparing between the spectra of the two cases with different amounts of line broadening in Fig. 4.31, the scaling factor is about 5 for the amplitude of the second absorption trough that is associated with the cosmic dawn, and the scaling factor is about 6 for the amplitude of the emission bump that is formed at the epoch of reionisation.

The differences among the scaling factors for the three prominent features in the 21-cm line spectra are due to a number of factors. Among them is the convolution of the radiative transfer of the 21-cm line and the continuum with the differential frequency shifts of the radiation when the Universe expands. This factor is more effective at lower redshifts. Thus, the high-frequency trough and the emission crest are expected to be more affected than the low-frequency trough. This phenomenon is counter-intuitive, but it can be understood in a qualitative manner with the following consideration. The variation of the specific optical depth τ_{ν} over ν may be expressed as

$$\frac{\mathrm{d}\tau_{\nu}}{\mathrm{d}\nu} = \frac{\partial\tau_{\nu}}{\partial\nu} + \frac{\partial\tau_{\nu}}{\partial\nu_{*}} \left(\frac{\mathrm{d}\nu}{\mathrm{d}\nu_{*}}\right)^{-1} + \frac{\partial\tau_{\nu}}{\partial z} \left(\frac{\mathrm{d}\nu}{\mathrm{d}z}\right)^{-1} \,. \tag{4.72}$$

Here, v_* is the velocity spread among of gas/particles that contribute to the opacity, (and hence, participate in the radiative transfer process). At a fixed *z*, the first two terms, which correspond to the spectral variation in the local absorption coefficient and to the local velocity-induced frequency spread, respectively, are not explicit functions of the redshift *z*. The third term, in contrast, depends on *z* explicitly. As $d\tau_v = \kappa_v ds$, where ds is the distance increment of the radiation propagation,

$$\left. \frac{\partial \tau_{\nu}}{\partial z} \right|_{z} = \kappa_{\nu} \left(\frac{\mathrm{d}s}{\mathrm{d}z} \right) \left|_{z} = \frac{c \kappa_{\nu}}{(1+z) H_{0}} \left[\Omega_{\mathrm{r},0} (1+z)^{4} + \Omega_{\mathrm{m},0} (1+z)^{3} + \Omega_{\Lambda,0} \right]^{-\frac{1}{2}} \quad (4.73)$$

for the FRW cosmology adopted in this study. Note that $(\partial v/\partial z)$ is independent of z, since $v/v_0 = (1+z)/(1+z_0)$. Note also that here $(\partial \tau_v/\partial z)|_z \neq (d\tau_v/dz)|_v$, where the former specifies the contribution to the variation of τ_v across the frequency v at a specific redshift z whereas the latter denotes the change in the specific optical depth τ_v at a given frequency v over a distance scale, in terms of the cosmological redshift z.

At the centre of the 21-cm line, where the opacity is the largest, the first term in the right side of Eqn. (4.72) vanishes, because of the symmetry of the line profile function (in frequency) about the line centre. The variations in the optical depth τ_{ν} is, therefore, contributed by the second term, which specifies how the line opacity changes when the line is broadened, and by the third term, which concerns the cosmological effects on the local spectral variation. As the significance of the third term increases when z decreases, which is indicated in Eqn. (4.73), the scaling relation that holds for the first absorption trough formed at high redshifts before the onset of reionisation would eventually break down in the later epochs.

There is a subtlety in the cosmological radiative transfer, which also contributes to the distortion in the scaling of the amplitude of spectral feature with $(b_D \sqrt{\pi})^{-1}$ across the line spectra. The non-uniformity of the scaling of the features with the reciprocal of the local line broadening is caused by the interplay between absorption and emission of the line and the continuum when the radiation propagates from high z to low z in an expanding Universe. Fig. 4.32 illustrates the convolution of radiative transfer and line broadening in the presence of a continuum for the 21-cm line originating at redshifts ranging from z = 995 to z = 975. The CMB temperature is set to be higher than the spin temperature of the electrons in the HI atom, thus the 21-cm line is expected to be predominantly in absorption. However, there is a small emission bump at all redshifts (top panel, Fig. 4.32), making the 21-cm line profile as a P Cygni profile, as those seen in the line originating from an expanding stellar atmosphere with the negative temperature gradient in a radially outward direction. This structure in the 21-cm line is a consequence of the relative recession velocities between HI gas at different redshifts in the presence of a continuum emission. When the radiation propagates from a high z to a low z, it encounters a negative temperature gradient in the CMB, a situation analogous to thermal structure of an expanding stellar envelope that gives rise to the P Cygni type lines. Although the P Cygni lines in stars are in general emission in nature, the cosmological 21cm hyperfine line considered here in this illustration is absorption in nature. The successive presence of a small emission red bump in the line along the propagation of the ray from high z to low z will reduce the amplitude of the 21-cm trough in the observed line spectrum at the present epoch (bottom panel, Fig. 4.32).

The C21LRT formulation presented here has properly accounted for (i) the relevant radiation processes, in particular, the absorption and emission of the hyperfine 21-cm line arising from the spin flip of electrons in the HI gas, (ii) the effect of line broadening, due to various kinetic and dynamical processes on the line opacity, and (iii) the subtle convolution of the 21-cm line radiative transfer (in the presence of a continuum) with the cosmological effects in the expanding Universe. All-sky 21-cm line spectra can be computed by solving C21LRT equation along rays across the sky, as in the all-sky cosmological polarised radiative transfer calculations (see Sec. 3.2.3). These spectra contain tomographic signals across redshift z, crucial for our understanding of how the Universe underwent a transition from a neutral gaseous atomic phase to an ionised plasma phase.

4.6 Conclusions and Remarks

In this chapter, an all-sky cosmological 21-cm line radiative transfer (C21LRT) formalism appropriate for the studies of cosmological reionisation is devised, implemented, and verified.

The C21LRT formulation is derived, from a general relativistic radiative transfer formulation that stems from the first principles of conservation of phase-space volume and photon number. It is fully covariant and explicitly treats local radiation processes (via the absorption and emission coefficients of the line and the continuum radiation) and line broadening (via the line profile function in the line transfer coefficients) along a ray transported in a cosmologically evolving universe. The C21LRT formulation provides a solid theoretical foundation upon which 21-cm line signals arising from both the local and distant Universe can be calculated from first principles, with the relevant radiation processes, the relativistic and the cosmological effects self-consistently accounted for. Without loss of generality, the covariant cosmological 21-cm line radiative transfer equation suitable for the FRW universe is derived (Eqn. (4.58)). An efficient computational algorithm that adopts a ray-tracing method and solves the C21LRT equation is constructed (Sec. 4.3.2).

The abilities of the C21LRT algorithm and its code implementation in dealing with (i) the cosmological evolution effects, and (ii) the local effects on the line shifting and broadening and on the line-continuum interaction, are verified by a number of numerical experiments presented in Sec. 4.4. The calculations of the cosmological transfer of the CMB continuum radiation and the transfer of a generic 21-cm line radiation give correct evolution of the radiative properties. The galactic rotation experiment yields a correct combination of the line spectra of multiple rays and validates the code in handling the effects on the line spectrum arising locally from an astrophysical system with differential velocity and density structures, in the presence of the CMB continuum radiation.

The validated C21LRT code is then applied to calculate the cosmological evolution of the redshifted 21-cm signals (Sec. 4.5), demonstrating the ability of direct, quantitative tracking of the development of spectral features in the 21-cm line spectra. C21LRT calculations are conducted in two cases with different amounts of line broadening; comparisons with the previous work are drawn. It is shown that the strength of the absorption trough located at the low observed frequencies (originating from the dark ages) is subject to the scaling of the reciprocal of the local line broadening b_D^{-1} , and the result in previous work (e.g. in Pritchard and Loeb (2008)) can be recovered when $b_D = 1 \text{ km s}^{-1}$. At the same time, different scaling factors for the strengths of the high-frequency absorption trough (originating from the cosmic dawn) and the emission crest (originating from the epoch of reionisation) are obtained. These differences signify the importance of a proper account for (i) the convolution of the radiative transfer of the 21-cm line and the continuum with the differential frequency shifts of the radiation, and (ii) the interplay between absorption and emission of the line and the continuum when the radiation travels from high to low *z* in an expanding Universe.

Using ray-tracing C21LRT calculations all-sky 21-cm line spectra can be computed, thus providing a reliable means to predict the theoretical signals for the 21-cm tomographic study of cosmological reionisation.

Chapter 5

Curvelets on a Sphere

This chapter is based on J. Y. H. Chan, B. Leistedt, T. D. Kitching and J. D. McEwen, "Second-Generation curvelets on the sphere" in IEEE Transactions on Signal Processing, vol. 65, no. 1, pp. 5-14, Jan 2017, doi: https://doi.org/10.1109/TSP.2016.2600506[©]IEEE 2016.

In this chapter, a new-generation of curvelets on a sphere that I developed is presented. These curvelets are constructed directly on a sphere. They can simultaneously extract the position-scale-orientation information in images, and provide an efficient representation of the curvilinear features within signals. They also exhibit a variety of desirable properties, well-suited for the inference purposes in sciences as listed in Sec. 2.4.2 and for applications in a range of other disciplines (see examples in Cai et al. 2020, and related papers).

5.1 Introduction

Spherical wavelets (e.g. Antoine and Vandergheynst 1998, 1999; Wiaux et al. 2005; McEwen et al. 2006a; Narcowich et al. 2006; Sanz et al. 2006; Starck et al. 2006b; Wiaux et al. 2008b; Geller et al. 2008; Marinucci et al. 2008; McEwen and Scaife 2008; Baldi et al. 2009; Geller and Marinucci 2010, 2011; Michailovich and Rathi 2010; McEwen et al. 2011; Leistedt et al. 2013; McEwen et al. 2013, 2015b; McEwen and Price 2015; McEwen et al. 2018) are capable of extracting both spectral and spatial (or temporal) information simultaneously, thus making them a natural and powerful tool for the analyses of spherical systems with multiple spatial scales and complex structures. In addition to scale-dependent and localised characteristics, signals often contain directional and geometrical features, such as linear or curvi-

linear structures in 2D images (e.g. edges), or sheet-like and filamentary structures in 3D space. Extraction of these features can, in turn, provide insightful information about the origin of signals or play crucial roles in diagnostic uses. Traditional wavelets, however, fall short of capturing this signal content effectively, which has motivated the development of a variety of directional or geometric wavelets.

Ridgelet (e.g. Candès and Donoho 1999) and curvelet (e.g. Candes et al. 1999; Candès and Donoho 2004, 2005a,b) transforms are of substantial interest since they provide efficient representations of line-type structures and exploit the anisotropic content of signals. Among the two, ridgelets are limited to applications to signals with global straight-line features only. In order to analyse local linear or curvilinear structures, which are dominant in nature, a block ridgelet-based transform, namely the first-generation curvelet transform, has been proposed. In Euclidean space, such a curvelet transform consists of applying an isotropic wavelet transform, followed by a special partitioning of the image and the application of the ridgelet transform to local overlapping blocks (Candes et al. 1999). The overlapping blocks, which are used to mitigate blocking artefacts, increase the redundancy, hence, increasing the computational storage and timing costs. The same authors proposed secondgeneration Euclidean curvelets, rectifying these issues, where the discrete frequency domain is tiled and a ridgelet transform is no longer required (Candès and Donoho 2004, 2005a,b). The second-generation curvelet construction is conceptually more natural and enables faster algorithms, thus opening up a wider and more successful applicability of curvelets, particularly in the fields of image processing, seismic image recovery and scientific computing (for reviews of the planar ridgelet and curvelet transforms, see Ma and Plonka 2010; Fadili and Starck 2012).

Recently, a new generation of ridgelets on the sphere was constructed in McEwen and Price (2019), which is applicable to study antipodal signals on the sphere and is capable to handle both scalar and spin signals. First-generation curvelets have also been constructed on the sphere (Starck et al. 2006a), where the HEALPix (Górski et al. 2005) scheme of partitioning of the sphere is employed and a discrete planar ridgelet transform is performed on each block indepen-

dently. First-generation spherical curvelets are, therefore, not defined natively on the sphere (but rather by stitching together planar patches). Furthermore, unlike the approach of the first-generation planar curvelets, the twelve base-resolution faces of the HEALPix pixelisation do not overlap. This unavoidably leads to blocking artefacts (Starck et al. 2006a,b). In addition, in this framework, curvelets larger than the scale of the base-resolution face cannot be constructed and firstgeneration spherical curvelets only satisfy the typical curvelet parabolic scaling relation (i.e. width \approx length²) in the Euclidean limit.

In this work, a second-generation curvelet transform is constructed, which is not built on a ridgelet transform, following a similar motivation to the development of the second-generation planar curvelets. Second-generation curvelets live natively on a sphere (i.e. are not reliant on a specific pixelisation such as HEALPix), are free from any blocking artefacts, satisfy the typical curvelet parabolic scaling relation, and support the exact synthesis of a band-limited signal from its curvelet coefficients (i.e. capture all of the information content of the signal of interest without loss).

It is possible to construct spherical curvelets through the inverse stereographic projection of planar wavelets (Antoine and Vandergheynst 1998, 1999; Wiaux et al. 2005), but the continuous scales required for the continuous analysis prevents exact reconstruction of the signals in practice. Scale-discretised curvelets are therefore constructed using the general spin scale-discretised wavelet framework presented in McEwen et al. (2015b), where the dilations of the curvelets are directly defined in harmonic space and exact synthesis can be performed in practice. This framework also enables a straightforward generalisation of the curvelet transform to spin signals, where the spin value of the curvelets is a free parameter. Depending on the desired applications, different spin values can be chosen: spin-0 for analysing scalar signals, spin-1 for vector fields and spin-2 for polarisation studies, for example. Furthermore, it can be shown explicitly how the parabolic scaling relation is rendered in (spin) spherical polar coordinates by setting the absolute value of the azimuthal frequency index. Curvelets constructed in this manner exhibit many desirable properties, as listed

earlier, which are lacking in alternative constructions (e.g. Starck et al. 2006a).

Having constructed scale-discretised curvelets applicable to transform signals of arbitrary spin on the sphere, a fast algorithm to compute the curvelet transform exactly and efficiently is then presented. Optimisation is achieved by working in a rotated coordinate system that renders the harmonic representation of many curvelets coefficients zero; only a relatively small number of non-zero terms need then be computed. This fast algorithm leverages novel sampling theorems on the sphere (Driscoll and Healy 1994; McEwen and Wiaux 2011) and on the rotation group (McEwen et al. 2015a), where the latter is further optimised for curvelets. These curvelet algorithms are implemented in the existing s2LET code¹ (Leistedt et al. 2013) – an implementation of the scale-discretised wavelet transform on the sphere – and are publicly available.

The remainder of this chapter is organised as follows. In Section 5.2, curvelets that live natively on a sphere are constructed. The properties of curvelets and their differences to axisymmetric and directional wavelets on the sphere are highlighted. In Section 5.3, the exact and efficient algorithms for the numerical implementation of the curvelet transform are derived. Numerical accuracy and computational-time scaling for a complete forward and inverse transform are evaluated. In Section 5.4, an illustrative application is presented, where a spherical image of a natural scene is analysed and the performance of curvelets and directional wavelets is compared. Section 5.5 outlines the possible applications of the spherical curvelet transform and the future extensions of this work.

5.2 Scale-Discretised Curvelets on a Sphere

In this section, curvelets that are defined on a sphere are constructed. They exhibit the standard curvelet parabolic scaling relation, are well-localised in both spatial and harmonic domains, and support the exact analysis and synthesis of both scalar and spin signals. The construction follows closely to that of spin scale-discretised wavelets (McEwen et al. 2015b), and their analogous scalar forms (Wiaux et al.

¹www.s2let.org

2008b; Leistedt et al. 2013; McEwen et al. 2013, 2018), except that the directionality component of curvelets is designed differently. For further details of the scale-discretised wavelet framework, including a review of harmonic analysis of (spin) functions on the sphere, interested readers are referred to Sec. 2.5 or the aforementioned papers. This section is concluded by noting some properties of curvelets, comparing them to axisymmetric and directional wavelets.

All the transforms throughout this work are formulated for the general spin setting, where the scalar setting can be simply rendered by setting the spin value $s \in \mathbb{Z}$ to zero. Also, signals on the sphere band-limited at *L* are considered throughout, i.e. ${}_{s}f_{\ell m} = 0$, $\forall \ell \ge L$, where ${}_{s}f_{\ell m}$, with integer $\ell, m \in \mathbb{Z}$, $|m| \le \ell$, are the spin spherical harmonic coefficients of a spin signal of interest ${}_{s}f \in L^{2}(\mathbb{S}^{2})$, and are given by the usual projection onto each spin spherical harmonic (basis) function ${}_{s}Y_{\ell m} \in L^{2}(\mathbb{S}^{2})$: ${}_{s}f_{\ell m} = \langle {}_{s}f, {}_{s}Y_{\ell m} \rangle$.

5.2.1 Curvelet construction

Scale-discretised curvelets ${}_{s}\psi^{(j)} \in L^{2}(\mathbb{S}^{2})$ are constructed in harmonic space in factorised form

$${}_{s}\psi_{\ell m}^{(j)} \equiv \sqrt{\frac{2\ell+1}{8\pi^{2}}} \,\kappa^{(j)}(\ell) \,{}_{s}s_{\ell m} \,, \tag{5.1}$$

where ${}_{s}\psi_{\ell m}^{(j)} = \langle {}_{s}\psi^{(j)}, {}_{s}Y_{\ell m} \rangle$ are the spin spherical harmonic coefficients of the curvelets with ${}_{s}Y_{\ell m} \in L^{2}(\mathbb{S}^{2})$ denoting the spin spherical harmonic functions, for $s \in \mathbb{Z}, \ell \in \mathbb{N}$ and $m \in \mathbb{Z}$ such that $|m| \leq \ell, |s| \leq \ell$. The angular localisation of the *j*-th scale curvelet is characterised by the kernel $\kappa^{(j)} \in L^{2}(\mathbb{R}^{+})$ whose construction follows exactly the same as that of the spin directional scale-discretised wavelets given in McEwen et al. (2015b). On the other hand, the directional localisation of curvelets is controlled by the directional component ${}_{s}s$, with harmonic components ${}_{s}s_{\ell m} = \langle {}_{s}s, {}_{s}Y_{\ell m} \rangle$. It is this directional component that is defined in such a way that the parabolic scaling relation typical of curvelets is satisfied.

The standard curvelet parabolic scaling relation can be rendered in spherical coordinates by considering spin spherical harmonics with the absolute value of the azimuthal frequency index equal to the angular frequency index, i.e. $|m| = \ell$.

Specifically, the full-width-half-maximum (FWHM) of the colatitude $\theta \in [0, \pi]$ part of ${}_{s}Y_{\ell\ell}$ is shown to be approximately the square of that of the longitude $\phi \in [0, 2\pi)$ part. Such a parabolic scaling also applies to curvelets since their harmonic coefficients are constucted from a windowed sum of spherical harmonics, with a central dominant angular frequency.

The FWHM, which characterises the width about the peak of a function, is defined as the difference between θ (or ϕ) at which the real or imaginary part of the function ${}_{s}Y_{\ell\ell}$ is equal to half of its maximum value. It is then straightforward to show that

FWHM_{$$\phi$$} = $2\phi_0 = \frac{2}{\ell} \cos^{-1}\left(\frac{1}{2}\right) = \frac{2\pi}{3\ell}$, (5.2)

where ϕ_0 is the angle at the half maximum of the ϕ -part of ${}_{s}Y_{\ell\ell}$ (i.e. real or imaginary part of $e^{i\ell\phi}$) within the interval $0 < \phi_0 < \pi/2$. The θ -dependence of ${}_{s}Y_{\ell\ell}$ is determined by the Wigner small-*d*-function

$$d_{\ell(-s)}^{\ell}(\theta) = (-1)^{\ell+s} \sqrt{\frac{(2\ell)!}{(\ell-s)!(\ell+s)!}} \sin^{\ell+s} \frac{\theta}{2} \cos^{\ell-s} \frac{\theta}{2}, \qquad (5.3)$$

which attains its maximum at

$$\theta_{\max} = \cos^{-1}\left(\frac{-s}{\ell}\right),$$
(5.4)

for $|s| \leq \ell$. As *s* varies from 0 to ℓ , θ_{max} takes the value from $\pi/2$ to π (indicating a change of the colatitude position at which spin-curvelets are centred, as will become explicit in the complete curvelet construction that follows). Furthermore, note that for the scalar setting s = 0 and also for $s \ll \ell$, Eqn. (5.3) reduces to the form of $A_{\ell} \sin^{\ell} \theta$, where A_{ℓ} is a function of ℓ contributing to the overall magnitude of ${}_{s}Y_{\ell\ell}$ only (and thus can be ignored in the evaluation of FWHM_{θ}). It follows that

FWHM_{$$\theta$$} = $2\left(\frac{\pi}{2} - \theta_0\right) = \pi - 2\sin^{-1}\left(\frac{1}{2^{1/\ell}}\right),$ (5.5)

where θ_0 is the angle at the half maximum of the θ -part of ${}_sY_{\ell\ell}$ within the interval of $0 < \theta_0 < \pi/2$. Eqn. (5.5) can be further rearranged to

$$\sin\left(\frac{\pi - \text{FWHM}_{\theta}}{2}\right) = 2^{-u} , \qquad (5.6)$$

where $u = 1/\ell$. In the limit $\ell \to \infty$, *u* and FWHM_{θ} both approach to zero. Hence, by taking Taylor's expansion at both sides of Eqn. (5.6), one obtains

$$1 - \frac{1}{8} \text{FWHM}_{\theta}^2 \approx 1 - (\ln 2) \frac{1}{\ell},$$
 (5.7)

which implies the important curvelet parabolic scaling relation

$$\mathrm{FWHM}_{\theta}^{2} \approx \mathrm{FWHM}_{\phi} \,. \tag{5.8}$$

The cases of spin value s = 0 or $s \ll \ell$, for which the parabolic scaling relation has been shown to hold, are common in real-life applications since physical signals are often scalar or have a low spin value. Furthermore, low- ℓ information is often not probed by curvelets but rather by a scaling function, which will be discussed subsequently. Nevertheless, for completeness and clarity, In the extreme cases when $s = \ell$, the approximate parabolic scaling relation still holds, with the value of FWHM²_{θ} double that in the scalar setting. Note that the parabolic scaling relation may start to deteriorate as $s \rightarrow (\ell - 1)$ due to the asymmetry of $d^{\ell}_{\ell-s}(\theta)$ about θ_{max} . However, for at least $s \simeq \lfloor \ell/2 \rfloor$ (a very conservative limit), empirical numerical findings show that any deviation from the scalar setting is insignificant, so the parabolic scaling relation remains to hold. (Here and hereafter, $\lfloor \cdot \rfloor$ and $\lceil \cdot \rceil$ denote the floor and ceiling functions respectively.) Readers are referred to Appendix I for further details.

Apart from setting $|m| = \ell$, the directionality component of curvelets ${}_{s}s_{\ell m}$, without loss of generality, is defined to satisfy the condition

$$\sum_{m=-\ell}^{\ell} |{}_{s}s_{\ell m}|^{2} = 1 , \qquad (5.9)$$

for all values of ℓ for which ${}_{s}s_{\ell m}$ are non-zero for at least one value of m. Consequently, the directionality component reads

$${}_{s}\widetilde{s}_{\ell m} = \frac{1}{\sqrt{2}} \begin{cases} (-1)^{m} \,\delta_{\ell m}, & m < 0\\ \delta_{\ell m}, & m \ge 0 \end{cases}$$

$$(5.10)$$

for all ℓ of interest (with largest possible domain $0 < \ell < L$) and |m| < L. Here, δ denotes the Kronecker delta, and the symbol $\tilde{}$ denotes that the quantity is associated to unrotated curvelets offset from the North pole (see Eqn. (5.4)). It is desirable to centre curvelets on the North pole, so that the Euler angles parameterising curvelet coefficients have their standard interpretation, and their directionality components are given by the harmonic rotation

$${}_{s}s_{\ell m} = \sum_{n=-\ell}^{\ell} D_{mn}^{\ell}(\rho^{\star})_{s}\widetilde{s}_{\ell n}, \qquad (5.11)$$

where ρ^{\star} is the Euler angle describing the rotation to the North pole and is specified subsequently.

As in McEwen et al. (2015b), Wiaux et al. (2008b), Leistedt et al. (2013), McEwen et al. (2013), and McEwen et al. (2018), the scale-discretised curvelet kernel for scale j is constructed by

$$\kappa^{(j)}(\ell) \equiv \kappa_{\lambda}(\lambda^{-j}\ell) . \tag{5.12}$$

The curvelet kernel reaches a peak of unity at $\ell = \lambda^j$ and has a compact support on $\ell \in [\lfloor \lambda^{j-1} \rfloor, \lceil \lambda^{j+1} \rceil]$. It is generated from $\kappa_{\lambda}(t) \equiv \sqrt{k_{\lambda}(\lambda^{-1}t) - k_{\lambda}(t)}$. The function k_{λ} is defined as

$$k_{\lambda}(t) \equiv \frac{\int_{t}^{1} \frac{dt'}{t'} s_{\lambda}^{2}(t')}{\int_{\lambda^{-1}}^{1} \frac{dt'}{t'} s_{\lambda}^{2}(t')},$$
(5.13)

which is unity for $t < \lambda^{-1}$, zero for t > 1, and smoothly decreasing from unity to zero for $t \in [\lambda^{-1}, 1]$. It is defined through the infinitely differentiable Schwartz

function

$$s_{\lambda}(t) \equiv s\left(\frac{2\lambda}{\lambda-1}(t-\lambda^{-1})-1\right),\tag{5.14}$$

where

$$s(t) \equiv \begin{cases} e^{-(1-t^2)^{-1}} & t \in [-1,1] \\ 0 & t \notin [-1,1] \end{cases},$$
(5.15)

which has compact support $t \in [\lambda^{-1}, 1]$, for dilation parameter $\lambda \in \mathbb{R}^+_*$, $\lambda > 1$. Note that $\lambda = 2$ corresponds to a common dyadic transform (i.e. the mother curvelet is dilated by powers of two).

As noted earlier, without applying any rotation the constructed spin-*s* curvelets ${}_{s}\widetilde{\psi}_{\ell m}^{(j)}$ are not centred on the North pole but at colatitude

$$\vartheta^j = \cos^{-1}\left(\frac{-s}{\lambda^j}\right),$$
(5.16)

cf. Eqn. (5.4), which lies in the range $[\pi/2, \pi]$. Explicitly, spin-0 curvelets are centred along the equator (-x-axis), and for higher-*s* curvelets up to $s = \ell$, curvelets effectively move down to be centred around the South pole. Curvelets are, therefore, rotated to the North pole by a rotation with Euler angle $\rho^* = (0, \vartheta^j, 0)$.

Scaling functions ${}_{s}\Phi \in L^{2}(\mathbb{S}^{2})$, which are required to probe the low-frequency content (approximation-information) of the signal not probed by curvelets, are defined explicitly in McEwen et al. (2015b); Leistedt et al. (2013); McEwen et al. (2013, 2018). They are chosen to be axisymmetric since directional structure of the approximation-information of signal is typically not of interest. Their definition is repeated here for completeness:

$${}_{s}\Phi_{\ell m} \equiv \sqrt{\frac{2\ell+1}{4\pi}} \sqrt{k_{\lambda}(\lambda^{-J_{0}}\ell)} \,\delta_{m0} \,, \qquad (5.17)$$

where J_0 is the minimum scale to be probed by curvelets.

5.2.2 Curvelet tiling and properties

Examples of spin-0 (scalar) and spin-2 curvelets rotated to the North pole of the sphere are plotted in Fig. 5.1 and Fig. 5.2, respectively. Note that the spin value is a

free parameter, allowing easy construction of curvelets of any spin $s \in \mathbb{Z}$. Note also that as the scale *j* increases, curvelets become increasingly elongated and exhibit increasingly higher directional sensitivity and anisotropic features (for spin curvelets, notice their absolute value is directional). This feature, which is warranted by the satisfaction of the parabolic scaling relation, is absent in directional scale-discretised wavelets.



Fig. 5.1: Scalar scale-discretised curvelets on the sphere $(L = 256, \lambda = 2)$. Cuvelets are rotated to be centred on the North pole. Notice that the characteristic curvelet parabolic scaling (i.e. width \approx length²) makes them highly anisotropic and directionally sensitive.

The harmonic tiling of scale-discretised curvelets is schematically depicted in the right-most panel of Fig. 5.3, along with the tilings of the axisymmetric scale-discretised wavelets (Leistedt et al. 2013) (left-most panel) and the directional scale-discretised wavelets (McEwen et al. 2015b, 2013, 2018) (middle panel) for comparison purposes. Axisymmetric wavelets probe signals in scale and position, but not in orientation, by tiling the line m = 0 only. Directional wavelets are capable of probing the directional features of signals, but do not exploit the geometric properties of structures in signals. Tiling therefore occurs up to a low azimuthal band-limit N < L (typically only even or odd m are non-zero to enforce various azimuthal



Fig. 5.2: Spin-2 scale-discretised curvelets on the sphere ($L = 256, \lambda = 2$). Cuvelets are rotated to be centred on the North pole. Notice that the absolute value of the spin-curvelet is directional and the characteristic curvelet parabolic scaling (i.e. width \approx length²) makes them highly anisotropic and directionally sensitive.

symmetries). In contrast to axisymmetric and directional wavelets, curvelets probe not only spatial and spectral information, but also both directional and geometric contents of a signal. Such an ability is afforded by their specific design to render the parabolic scaling relation. This standard curvelet scaling relation is imposed by the tiling of curvelets along the corresponding lines.

5.2.3 Curvelet transform

The curvelet transform is built upon the spin scale-discretised wavelet framework presented in McEwen et al. (2015b). The discrete nature of the analysis scales (i.e. $j \in \mathbb{N}_0$) allows the exact reconstruction of band-limited signals from their curvelet coefficients. This is ensured by the satisfaction of the admissibility condition

$$\frac{4\pi}{2\ell+1} |_{s} \Phi_{\ell 0}|^{2} + \frac{8\pi^{2}}{2\ell+1} \sum_{j=J_{0}}^{J} \sum_{n=-\ell}^{\ell} |_{s} \psi_{\ell n}^{(j)}|^{2} = 1, \qquad \forall \ell$$
(5.18)



Fig. 5.3: Tiling of different types of wavelets. Notice in particular that by tiling curvelets along the diagonal, an approximate parabolic scaling relationship is imposed.

(McEwen et al. 2015b, and reference therein). Curvelet analysis and synthesis operations (i.e. forward and inverse transform) are defined subsequently. Curvelets are rotated to the North pole in the following description.

Curvelet analysis

The scale-discretised curvelet transform of a function ${}_{s}f \in L^{2}(\mathbb{S}^{2})$ is defined by its directional convolution with the curvelets ${}_{s}\psi^{(j)} \in L^{2}(\mathbb{S}^{2})$, where the curvelet coefficients are given by

$$W^{s\psi^{(j)}}(\rho) \equiv \langle sf, \mathcal{R}_{\rho s}\psi^{(j)} \rangle$$

=
$$\int_{\mathbb{S}^2} d\Omega(\omega) sf(\omega) (\mathcal{R}_{\rho s}\psi^{(j)})^*(\omega) . \qquad (5.19)$$

The rotation operator \mathcal{R}_{ρ} is parameterised by the Euler angles $\rho = (\alpha, \beta, \gamma) \in SO(3)$, with $\alpha \in [0, 2\pi), \beta \in [0, \pi]$ and $\gamma \in [0, 2\pi)$. Eqn. (5.19) may also be re-written as

$$W^{s\psi^{(j)}}(\rho) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \sum_{n=-\ell}^{\ell} {}^{s} f_{\ell m} {}^{s} \psi^{(j)*}_{\ell n} D^{\ell*}_{mn}(\rho) , \qquad (5.20)$$

where ${}_{s}f_{\ell m} = \langle {}_{s}f, {}_{s}Y_{\ell m} \rangle$ and ${}_{s}\psi_{\ell m}^{(j)} = \langle {}_{s}\psi^{(j)}, {}_{s}Y_{\ell m} \rangle$ are the spin spherical harmonic coefficients of the function of interest and of the curvelets, respectively.

The Wigner coefficients of the wavelet coefficients defined on SO(3) are given

by $(W^{s\psi^{(j)}})_{mn}^{\ell} = \langle W^{s\psi^{(j)}}, D_{mn}^{\ell*} \rangle$, which can be reduced to

$$\left(W^{s\psi^{(j)}}\right)_{mn}^{\ell} = \frac{8\pi^2}{2\ell+1} \, {}_{s}f_{\ell m} \, {}_{s}\psi^{(j)*}_{\ell n} \,. \tag{5.21}$$

As such, the forward curvelet transform may be computed via an inverse Wigner transform.

The low-frequency content of the signal is captured by the scaling coefficients ${}_{s}\Phi \in L^{2}(\mathbb{S}^{2})$, which are given by the axisymmetric convolution

$$W^{s\Phi}(\omega) \equiv \langle sf, \mathcal{R}_{\omega s}\Phi \rangle$$

= $\int_{\mathbb{S}^2} d\Omega(\omega') sf(\omega') (\mathcal{R}_{\omega s}\Phi)^*(\omega'),$ (5.22)

where $\mathcal{R}_{\omega} = \mathcal{R}_{(\phi,\theta,0)}$. Since the scaling function is, by design, axisymmetric, its harmonic coefficients are non-zero for m = 0 only: ${}_{s}\Phi_{\ell 0}\delta_{m0} = \langle {}_{s}\Phi, {}_{s}Y_{\ell m} \rangle$. Decomposing the scaling coefficients into their harmonic expansion yields

$$W^{s\Phi}(\omega) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \sqrt{\frac{4\pi}{2\ell+1}} \, {}_{s}f_{\ell m \ s} \Phi^{*}_{\ell 0 \ 0} Y_{\ell m}(\omega) , \qquad (5.23)$$

whose spherical harmonic coefficient is simply given by

$$(W^{s\Phi})_{\ell m} = \langle W^{s\Phi}, {}_{0}Y_{\ell m} \rangle = \sqrt{\frac{4\pi}{2\ell+1}} {}_{s}f_{\ell m \ s}\Phi^{*}_{\ell 0} .$$
(5.24)

Curvelet synthesis

Provided that the admissibility condition in Eqn. (5.18) is satisfied, the signal $_{s}f$ can be reconstructed exactly from its curvelet and scaling coefficients by

$${}_{s}f(\omega) = \int_{\mathbb{S}^{2}} \mathrm{d}\Omega(\omega') W^{s\Phi}(\omega') (\mathcal{R}_{\omega' s}\Phi)(\omega)$$

+
$$\sum_{j=J_{0}}^{J} \int_{\mathrm{SO}(3)} \mathrm{d}\varrho(\rho) W^{s\psi^{j}}(\rho) (\mathcal{R}_{\rho s}\psi^{j})(\omega), \qquad (5.25)$$

where the invariant measure on SO(3) is $d\rho(\rho) = \sin\beta \, d\alpha \, d\beta \, d\gamma$, and J_0 and J are, respectively, the minimum and maximum analysis depths considered, i.e. $J_0 \le j \le J$. Eqn. (5.25) may be re-written as

$${}_{s}f(\omega) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \left[\sqrt{\frac{4\pi}{2\ell+1}} \left(W^{s\Phi} \right)_{\ell m} {}_{s}\Phi_{\ell 0} + \sum_{j=J_{0}}^{J} \sum_{n=-\ell}^{\ell} \left(W^{s\psi^{(j)}} \right)_{mn}^{\ell} {}_{s}\psi^{(j)}_{\ell n} \right]_{s} Y_{\ell m}(\omega) ,$$
(5.26)

(McEwen et al. 2015b). As such, the inverse curvelet transform of Eqn. (5.25) may be computed via a forward Wigner transform.

5.3 Exact and Efficient Computation

In this section, a fast algorithm is devised to compute the curvelet transform, which is theoretically exact by appealing to sampling theorems on the sphere (McEwen and Wiaux 2011) and rotation group (McEwen et al. 2015a). The computational complexity of the algorithm attains $O(L^3 \log_2 L)$, compared to a naive scaling of $O(L^5)$. I then discuss the implementation of this algorithm and evaluate its performance in terms of both numerical accuracy and computation time via simulations of random test signals on the sphere.

5.3.1 Fast algorithm

Wigner transforms can be computed efficiently using the fast algorithm of McEwen et al. (2015a) which reduces the complexity from $O(L^6)$ to $O(L^4)$. For (steerable) directional wavelet transforms, for which the wavelets have an azimuthal band-limit N, the complexity is reduced to $O(NL^3)$ and since typically $N \ll L$, the overall complexity of $O(L^3)$ is recovered. However, there is no azimuthal band-limit for curvelets so fast Wigner transforms can only yield $O(L^4)$. Here, an algorithm that attains $O(L^3 \log_2 L)$ is developed. This is achieved by first rotating the Wigner coefficients of curvelet coefficients (rather than the curvelets themselves) and by optimising the fast Wigner transform for curvelets. I present these algorithmic details next, followed by a description of additional optimisation that are exploited to further speed up the code implementation.

Rotating Wigner coefficients

As highlighted in Sec. 5.2.3, curvelets are centred on the North pole in the constructed scale-discretised curvelet transform so that the Euler angles parameterising curvelet coefficients have their standard interpretation. However, the directly constructed curvelet $_{s}\tilde{\psi}$ is naturally centred at a different position. A rotation is, therefore, needed: either by rotating the curvelets directly or by rotating the Wigner coefficients of the curvelet coefficients. By exploiting the unrotated curvelet's property that $_{s}\tilde{\psi}_{\ell n} = _{s}\tilde{\psi}_{\ell \ell}\delta_{\ell n}$, and hence,

$$\left(\widetilde{W}^{s\widetilde{\psi}^{(j)}}\right)_{mn}^{\ell} = \left(\widetilde{W}^{s\widetilde{\psi}^{(j)}}\right)_{mn}^{\ell} \delta_{|n|\ell} , \qquad (5.27)$$

i.e. unrotated Wigner coefficients are non-zero for $|n| = \ell$ only. In the following, an additional optimisation achieved by rotating Wigner coefficients (rather than curvelets) is shown.

The rotation of the Wigner coefficients for the forward transform proceeds as follows. The Wigner coefficients of unrotated curvelets (offset from the North pole) can be computed by $\widetilde{W}^{s\widetilde{\psi}^{(j)}}(\rho) \equiv \langle sf, \mathcal{R}_{\rho \ s}\widetilde{\psi}^{(j)} \rangle$, but we require

$$W^{s\psi^{(j)}}(\rho) \equiv \langle sf, \mathcal{R}_{\rho s}\psi^{(j)}\rangle = \langle sf, \mathcal{R}_{\rho}\mathcal{R}_{\rho^{\star}}\widetilde{\psi}^{(j)}\rangle, \qquad (5.28)$$

where ${}_{s}\psi^{(j)}(\rho) = \mathcal{R}_{\rho^{\star}s}\widetilde{\psi}^{(j)}(\rho)$ denotes curvelets centred on the North pole, and $\rho^{\star} = (0, \vartheta^{j}, 0)$ is the Euler angle defining rotation to the North pole. It follows that

$$W^{s\psi^{(j)}}(\rho) = \widetilde{W}^{s\widetilde{\psi}^{(j)}}(\rho'), \qquad (5.29)$$

where ρ' describes the rotation formed by compositing the rotations described by ρ and ρ^{\star} , i.e. $\mathcal{R}_{\rho'} = \mathcal{R}_{\rho} \mathcal{R}_{\rho^{\star}}$. Eqn. (5.29) then can be computed by

$$\left(W^{s\psi^{(j)}}\right)_{mk}^{\ell} = \sum_{n} \left(\widetilde{W}^{s\widetilde{\psi}^{(j)}}\right)_{mn}^{\ell} D_{kn}^{\ell}^{*}(\rho^{\star})$$
(5.30)

$$= \left(\widetilde{W}^{s\widetilde{\psi}^{(j)}}\right)_{m\ell}^{\ell} D_{k\ell}^{\ell *}(\rho^{\star}) + \left(\widetilde{W}^{s\widetilde{\psi}^{(j)}}\right)_{m(-\ell)}^{\ell} D_{k(-\ell)}^{\ell *}(\rho^{\star}), \qquad (5.31)$$

where the additive property of the Wigner *D*-functions and Eqn. (5.27) have been exploited; see Appendix H for full details.

For the inverse transform, unrotated Wigner coefficients, which are non-zero for $|k| = \ell$ only, are computed by

$$\left(\widetilde{W}^{s\psi^{(j)}}\right)_{mk}^{\ell} = \sum_{n=-\ell}^{\ell} \left(W^{s\psi^{(j)}}\right)_{mn}^{\ell} D_{kn}^{\ell}^{*}(\rho^{\star'}), \qquad (5.32)$$

where inverse rotation described by the Euler angle $\rho^{\star'} = (0, -\vartheta^j, 0)$ is performed, i.e. $\mathcal{R}_{\rho^{\star'}} = \mathcal{R}_{\rho^{\star}}^{-1}$.

Notice from Eqn. (5.30) and Eqn. (5.32) that the computational complexity of the rotation is $O(L^3)$ only. In contrast, if one chooses to rotate curvelets directly, non-zero rotated curvelet coefficients would span across the domain of n < L, prohibiting additional optimisation enabled by computing only the non-zero coefficients.

Optimising Wigner transform

It is not possible to directly optimise the fast algorithm to compute the Wigner transform presented in McEwen et al. (2015a), where fast spin spherical harmonic transforms are used for intermediate calculations, even with minor modifications, since the order of summations needs to be altered. Instead, this approach is adapted by interchanging the order of summations and performing all computations explicitly.

An equi-angular sampling of the rotation group is adopted, and the sample positions are given by

$$\alpha_a = \frac{2\pi a}{2M - 1} \quad (a \in \{0, 1, \dots, 2M - 2\}), \tag{5.33}$$

$$\beta_b = \frac{\pi(2b+1)}{2L-1} \quad (b \in \{0, 1, \dots, L-1\}), \tag{5.34}$$

and

$$\gamma_g = \frac{2\pi g}{2N - 1} \quad (g \in \{0, 1, \dots, 2N - 2\}) \tag{5.35}$$

(McEwen et al. 2015a). The forward Wigner transform, optimised for curvelets, proceeds as follows. First, a Fourier transform is performed over Euler angles α

and γ :

$$\mathcal{X}_{mn}(\beta_b) = \sum_{a=-(M-1)}^{M-1} \sum_{g=-(N-1)}^{N-1} \frac{\widetilde{W}^{s\psi^{(j)}}(\alpha_a, \beta_b, \gamma_g)}{(2M-1)(2N-1)} e^{-i(m\alpha_a + n\gamma_g)}$$
(5.36)

for $b \in \{0, ..., L - 1\}$, $|m|, |n| \le \ell$. The computational demand can then be reduced from $O(L^5)$ to $O(L^3 \log_2 L)$ using a fast Fourier transform (FFT), where O(L) = O(M) = O(N). Next, a trick considered in McEwen and Wiaux (2011); McEwen et al. (2015a) is employed, which extends $X_{mn}(\beta_b)$ to the domain $[0, 2\pi)$ through the construction of

$$\overline{\mathcal{X}}_{mn}(\beta_b) = \begin{cases} (-1)^{m+n} \mathcal{X}_{mn}(-\beta_b) & (b \in \{L, ... 2L - 2\}) \\ \mathcal{X}_{mn}(\beta_b) & (b \in \{0, ... L - 1\}) \end{cases}$$
(5.37)

The computational complexity to calculate $\overline{X}_{mn}(\beta_b)$ for all the arguments and indices is $O(L^3)$. The Fourier transform of $\overline{X}_{mn}(\beta_b)$ in β is

$$\mathcal{X}_{mnm'} = \frac{1}{(2L-1)} \sum_{b=-(L-1)}^{L-1} \overline{\mathcal{X}}_{mn}(\beta_b) e^{-im'\beta_b} .$$
(5.38)

Calculations of $X_{mnm'}$ for all indices using FFTs have a computational complexity in $O(L^3 \log_2 L)$. Then, an exact quadrature for integration over β follows as

$$\mathcal{Y}_{mnm'} = (2\pi)^2 \sum_{m''=-(L-1)}^{L-1} \mathcal{X}_{mnm''} w(m''-m') , \qquad (5.39)$$

where the weights are given by $w(m') = \int_0^{\pi} d\beta \sin\beta e^{im'\beta}$, which can be evaluated analytically (McEwen and Wiaux 2011). Eqn. (5.39) can be computed directly at $O(L^4)$ or through its dual Fourier representation at $O(L^3 \log_2 L)$, noting that it is essentially a discrete convolution (see McEwen and Wiaux 2011). With these and the relation in Eqn. (5.27), the Wigner coefficients are readily computed, which gives

$$\left(\widetilde{W}^{s\psi^{(j)}}\right)_{m\ell}^{\ell} = \mathbf{i}^{m-\ell} \sum_{m'=-(L-1)}^{L-1} \Delta_{m'm}^{\ell} \Delta_{m'\ell}^{\ell} \,\mathcal{Y}_{m\ell m'} \tag{5.40}$$

(at $O(L^3)$), where $\Delta_{mn}^{\ell} \equiv d_{mn}^{\ell}(\pi/2)$ for $|m|, |n| \leq \ell$. The computation of the forward transform is dominated by those associated with Eqn. (5.36) or Eqn. (5.38). Thus, the overall efficiency in the computation scales as $O(L^3 \log_2 L)$.

The inverse Wigner transform, optimised for curvelets, proceeds as follows. First, the Fourier coefficients of the Wigner coefficients are computed by

$$\mathcal{X}_{mnm'} = \mathbf{i}^{n-m} \, \frac{2|n|+1}{8\pi^2} \, \Delta_{m'm}^{|n|} \, \Delta_{m'n}^{|n|} \left(\widetilde{W}_s^{\psi^{(j)}} \right)_{mn}^{|n|}, \tag{5.41}$$

at $O(L^3)$, where Eqn. (5.27) have been exploited. Then, the curvelet coefficients are computed from the Fourier representation of their Wigner representation by

$$\widetilde{W}^{s\psi^{(j)}}(\alpha_{a},\beta_{b},\gamma_{g}) = \sum_{m=-(M-1)}^{M-1} \sum_{n=-(N-1)}^{N-1} \sum_{m'=-(L-1)}^{L-1} X_{mnm'} \times e^{i(m\alpha_{a}+m'\beta_{b}+n\gamma_{g})}$$
(5.42)

for which the computation can be reduced from $O(L^6)$ to $O(L^3 \log_2 L)$ by FFTs. The samples of $\widetilde{W}^{s\psi^{(j)}}$ computed over $\beta \in (\pi, 2\pi)$ are discarded. The overall inverse transform is dominated by the computation of Eqn. (5.42) and thus scales as $O(L^3 \log_2 L)$.

Additional optimisations

A multi-resolution algorithm is constructed, exploiting the reduced band-limit $L_j = \lambda^{j+1}$ of the curvelets for scales j < J - 1 such that the minimal number of samples on the sphere is used to reconstruct curvelet coefficients for each scale (see also Leistedt et al. 2013; McEwen et al. 2015b). Consequently, only the finest curvelet scales at the largest $j \in \{J - 1, J\}$ are computed at maximal resolution (corresponding to the band-limit of the signal) and thereby dominating the computation. The overall complexity of computing both forward and inverse wavelet transforms,

including all scales, is thus $O(L^3 \log_2 L)$. In addition, for real signals, I exploit their conjugate symmetry which leads to a further reduction of computational and memory requirements by a factor of two.

5.3.2 Implementation

I have implemented the spherical curvelet transform in the existing s2LET code². The s2LET package, which currently supports scale-discretised scalar and spin axisymmetric wavelet (Leistedt et al. 2013), directional wavelet (McEwen et al. 2013, 2018, 2015b) and ridgelet (McEwen and Price 2015) transforms, relies on the ssHT code³ (McEwen and Wiaux 2011) to compute spherical harmonic transforms, the so3 code (McEwen et al. 2015a)⁴ to compute Wigner transforms (optimised for curvelets), and the FFTw code⁵ (Frigo and Johnson 2005) to compute fast Fourier transforms. Its core algorithms are implemented in C, with also Matlab, Python, IDL and JAVA interfaces provided, and HEALPix maps are also supported.

5.3.3 Numerical experiments

The numerical accuracy and computation time of the scale-discretised curvelet transform implemented in the s2LET code are evaluated as follows. First, random band-limited test signals are simulated on the sphere through the inverse spherical harmonic transform of their spherical harmonic coefficients ${}_{s}f_{\ell m}$ with real and imaginary parts uniformly distributed in the interval [-1, 1]. A forward curvelet transform is then performed, followed by an inverse transform to reconstruct the original signals from their curvelet coefficients. Three repeats of the complete transform are conducted for each *L*, where $L = \{4, 8, 16, 32, 64, 128\}$. All numerical experiments are carried out on a workstation with 2×12 core 1.8 GHz Intel(R) Xeon(R) processors and 256 GB of RAM (but parallelisation of the code has not been performed to fully exploit the multi-core architecture).

²http://www.s2let.org

³http://www.spinsht.org

⁴http://www.sothree.org

⁵http://www.fftw.org



Fig. 5.4: Numerical accuracy and computation time of the spherical curvelet transform, averaged over three round-trip transforms of random test signals. Numerical accuracy attains close to machine precision and is found empirically (shown by the dashed green line) to scale as $O(L^2)$ (shown by the solid red line). Computation time is found empirically to scale closely to the theoretical prediction of $O(L^3 \log_2 L)$. Plots showing the empirical results for spherical axisymmetric and directional wavelets can be found in Leistedt et al. (2013); McEwen et al. (2015b) respectively.

Numerical accuracy

Numerical accuracy of a round-trip curvelet transform is measured by the maximum absolute error between the spherical harmonic coefficients of the original test signal ${}_{s}f^{o}_{\ell m}$ and the recomputed values ${}_{s}f^{r}_{\ell m}$, i.e. $\epsilon = \max_{\ell,m} |{}_{s}f^{r}_{\ell m} - {}_{s}f^{o}_{\ell m}|$. Results of the numerical accuracy tests, averaged over three random test signals, are plotted in Fig. 5.4i. Results for a scalar signal are presented, although the accuracy for spin signals is identical since the spin number is simply a parameter of the transform. The numerical accuracy of the round-trip transform is close to machine precision and found empirically to scale as $O(L^2)$.

Computation time

Computation time is measured by the round-trip computation time taken to perform a forward and inverse curvelet transform. Results of the computation time tests, averaged over three random test signals, are plotted in Fig. 5.4ii. Results for a scalar signal are presented, although the computation time for signals of different spin numbers is identical. The computational complexity of the curvelet transform is found empirically to scale closely to the theoretical prediction of $O(L^3 \log_2 L)$.

5.4 Illustration

In this section, I present a simple application and analyse a spherical image of a natural scene with scale-discretised curvelets. It is shown that the spherical curvelet decomposition is sparse, with few large curvelet coefficients and many small coefficients. The ability of curvelets to represent natural spherical images efficiently is demonstrated using the light probe image of the Uffizi Gallery in Florence (Debevec 1998)⁶, which contains substantial line and curvilinear structures. For simple illustrative purposes, the image is band-limited to L = 256 and the image intensity is clipped and rescaled before the curvelet transform is performed. Plots of the scaling coefficients and curvelet coefficients are shown in Fig. 5.5. These plots show clearly that curvelets extract oriented, spatially localised, scale-dependent features in the image and are highly sensitive to edge-like features.

⁶http://www.pauldebevec.com/Probes/



Fig. 5.5: Plots of the scaling coefficients and the curvelet coefficients at various scales and orientations obtained from analysing the light probe image of the Uffizi Gallery. Notice the ability of curvelets to extract oriented, spatially localised, scale-dependent features in the light probe images and their very high sensitivity to line and curvilinear structures.



Fig. 5.6: Histogram showing the probability of the coefficients of directional wavelets (in blue) and curvelets (in red) obtained from analysing the light probe image plotted in Fig. 5.5 for scale j = 6 against the normalised coefficient magnitudes. The vertical axis shows the number of the wavelet or curvelet coefficients at each magnitude interval divided by the total count of the coefficients. The horizontal axis is normalised to unity by the maximum binned magnitude of the coefficients for comparison purposes. Curvelets yield a sparser representation than directional wavelets: there are many small curvelet coefficients and only few large coefficients.

To compare the performance of curvelets and directional wavelets, both transforms are applied with the same parameters and the directional wavelets have azimuthal limit set to N = L for fair comparison with curvelets. The histogram of curvelet and directional wavelet coefficients for scale j = 6 of the Uffizi image are shown in Fig. 5.6. It is apparent that curvelets yield a sparser representation than directional wavelets, where not only are there many small curvelet coefficients and few large coefficients, but the decay in number of coefficients is much faster than that of directional wavelets. This sparseness of curvelet representations of natural spherical image can be exploited in practical applications such as denoising, inpainting, and data compression, for example.

5.5 Summary

The second-generation curvelet transform that lives natively on the sphere is constructed. This curvelet transform exhibits the typical curvelet parabolic scaling relation for efficient representation of highly anisotropic signal content. It does not exhibit blocking artefacts due to special partitioning, does not rely on ridgelet transforms, and admits exact inversion for signals defined on the sphere. Scale-discretised curvelets are constructed based on a general spin scale-discretised wavelet framework, which supports both scalar and spin settings. Fast algorithms to compute the exact forward and inverse curvelet transform are devised and are implemented in the existing s2LET code package, which leverages a novel sampling theorem on the rotation group whose implementation is further optimised for curvelets. Through simulations, it is demonstrated that the numerical accuracy of curvelet transforms is close to machine precision and the computational speed scales as $O(L^3 \log_2 L)$, compared to a naive scaling of $O(L^5)$. The implementation of the curvelet transform is made publicly available.

The effectiveness of spherical curvelets for decomposing images with substantial line and curvilinear structures are illustrated using an example natural spherical image. The curvelet decomposition is found to be sparser than the directional wavelet analysis in this case. This sparseness can be exploited in applications to data compression and signal processing (e.g. to mitigate noise or handle incomplete data-sets). More generally, the curvelets developed in this work may find wide applications to transform scalar or spin signals acquired on the sphere where anisotropic and geometric structures in the signal content are of interest. For example, curvelets could be applied to identify and characterise (granules and) sunspots of the Sun and to study all-sky polarisation signals, which are crucial in understanding the structures of large-scale cosmic magnetic fields.

In addition, for data-sets where different signal characteristics are targeted at different scales, a hybrid use of curvelets and the other type of wavelets, where curvelets are tiled at some scales and the axisymmetric or directional wavelets are tiled at others, can be considered. Applications of this hybrid transform to segment spherical images are presented in Cai et al. (2020), which I have co-authored. Furthermore, this hybrid transform, or the curvelet transform, may also be extended to the three-dimensional ball, i.e. solid sphere formed by augmenting the sphere with radial line (Leistedt and McEwen 2012; McEwen and Leistedt 2013).

Such tools could be used to study a diverse range of data-sets defined on the ball, such as cosmological 21-cm tomographic data-sets, which is an important probe to understand what happened when the first stars and first black holes formed and how the Universe transformed from almost featureless to a structure-filled state as seen today. They are also important for weak gravitational lensing studies, in which the signal is a spin-2 field on the ball, which can be used to test the nature of dark energy and dark matter.
Chapter 6

Conclusions

The overarching theme of this thesis is to probe cosmic magnetism and cosmological reionisation of hydrogen gas in the Universe on the largest possible scales. These two thematic sciences have a close tie to the structure formation and evolution in the cosmos. They are also deeply linked to the fundamental questions of why the present Universe is filled with brightly-lit ionised plasma threaded by well-organised, large-scale magnetic fields. Substantial observational efforts targeting the two sciences are underway, where the current (e.g. LOFAR, GMRT, MWA, HERA, ASKAP and MeerKAT) and next-generation (e.g. SKA) radio telescopes would collect a wealth of wide-sky (up to all-sky) polarisation and cosmological 21-cm line data. These data have an underlying spherical geometry on the celestial sphere and contain complex physical signals imparted by multiple processes over the cosmological transport of the radio wave. Extracting the sciences from these data is a frontier challenge.

This thesis contributed to addressing this challenge in two main aspects. It has developed solid theoretical formalisms and appropriate all-sky methodologies that enable (i) unambiguous predictions of polarisation and cosmological 21-cm signals from complex physical models using the cosmological transport of electromagnetic radiation, and (ii) efficient characterisation of directional, structural features within all-sky data using a curvelet transform on the sphere. These developments are threefold, and as follows.

(1) An all-sky cosmological polarised radiative transfer (CPRT) formalism and numerical implementation have been constructed.

The CPRT formulation provides a reliable theoretical framework that accounts for the development of magnetic fields over cosmic history, the relevant radiation processes, and the cosmological effects self-consistently. Its code implementation calculates, from first principles, the polarisation of the continuum radio emission associated with magnetic fields (and electron number density distribution) co-evolving with the structure formation and evolution of the Universe. This fills the existing gaps between theoretical and observational studies of cosmic magnetism. Up to now, the former has been mostly focused on weak, large-scale magnetic fields generated in the early Universe, whereas the latter on strong, small-scale magnetic fields in the late Universe. To this end, the all-sky CPRT framework can be applied to investigate both.

A collection of demonstrative calculations with applications in different physical scenarios has been performed, including (i) the tracing of an individual ray that is influenced by the presence of a radio-bright point source or not, (ii) the pencil-beam calculations for a bundle of rays that traverses through a simulated galaxy cluster, and (iii) the computation of an entire polarised sky of a magnetised universe. It has been shown that the changes of polarisation along the radiation propagation can be directly tracked. This has an advantage of naturally resolving the $n\pi$ -ambiguity issue that concerns the number of 180° rotations of the polarisation angle unknown to an observer. It also enables detailed investigations of depolarisation and repolarisation of radiation caused by Faraday effects along the radiation path. Furthermore, the multiple-ray calculations have demonstrated the viability to account for post-processed cosmological MHD simulation results in CPRT calculations, thereby generating maps of the observables (e.g. the 4-Stokes parameters, polarisation angles, and degree of polarisation) at any arbitrary redshift. Statistical properties of the observables in these maps can then be determined for drawing physical interpretations of observations. The data products of CPRT calculations can also be used as testbeds for assessing the robustness of existing methods, such as rotation measure fluctuation analyses for probing the structure of large-scale magnetic fields. Such work has been presented in On et al. (2019) and summarised in Appendices D and E. The all-sky CPRT calculations have demonstrated the computation of unambiguous point-to-point theoretical predictions of the polarisation, in both the direction along the ray and across the sky plane, with the frequency range

and sky coverage matching to observations. This is critical to meet the science goals of current and next-generation radio observations of cosmic magnetism.

(2) A covariant formulation for cosmological 21-cm line radiative transfer (C21LRT) has been derived and a ray-tracing numerical scheme to compute the line signals (in intensity and line shape) has been developed.

The C21LRT formulation derived in Chapter 4 shares the same root as the CPRT formulation: both are constructed from a covariant general relativistic radiative transfer (GRRT) formulation derived from the first principles of conservation of phase-space volume and photon number. It takes full account of (i) the relevant radiation processes, in particular, the absorption and emission of the hyperfine 21-cm line arising from the spin flip of electrons in HI gas, (ii) the effect of line broadening caused by various kinetic and dynamical processes, (iii) the general-relativistic effects, and (iv) the cosmological effects, along a ray in an expanding and evolving Universe. As such, the C21LRT formulation provides a solid theoretical framework to compute the 21-cm line signals arising from both early and late Universe.

An all-sky C21LRT algorithm that adopts a ray-tracing method and solves the C21LRT equation along the ray has been devised and implemented. The ability of the C21LRT code to properly account for various cosmological and astrophysical effects has been validated by a collection of numerical experiments. The calculations of the cosmological transfer of the CMB continuum radiation and the transfer of a generic 21-cm line radiation have shown correct evolution of the radiative properties (i.e. thermal temperature for the former and the line shifting, broadening and intensity reduction for the latter). The galactic rotation experiment has given a correct combination of the line spectra of multiple rays and validated the power of the C21LRT code in properly handling the line-continuum interaction and the effects on the line spectrum arising locally from a system with differential velocity and density structures.

In the demonstrative study, the validated C21LRT code is applied to compute the cosmological 21-cm spectra with different amounts of line broadening, specified by a Doppler parameter b_D . Two cases with $b_D = 100 \text{ km s}^{-1}$ and $b_D = 1000 \text{ km s}^{-1}$ are considered. It has shown that comoving line spectra at any arbitrary redshift can be directly generated from C21LRT calculation and the development of spectral signatures can be directly tracked. Moreover, the resulting 21-cm spectra are characterised by two absorption troughs and an emission crest, which is consistent with the previous work (e.g. Pritchard and Loeb 2008). Comparison between the spectra of the two cases with different amounts of line broadening have shown nonuniform scaling of the signal strength across the three prominent spectral features arising from different redshifts (thus located at different observed frequencies). The strength of the low-frequency absorption trough scales with the reciprocal of the local line broadening, i.e. $(b_D \sqrt{\pi})^{-1}$. This is a consequence of the effect of line broadening on the line opacity, and hence, the amplitude of the line peak. Using such a scaling, the strength of the low-frequency trough in the previous work (e.g. Pritchard and Loeb 2008) can be recovered with $b_D = 1 \text{ km s}^{-1}$. The strengths of the high-frequency absorption trough and the emission crest are found to be scaled by factors smaller than $(b_D \sqrt{\pi})^{-1}$. This is due to the effects of (i) the convolution of the radiative transfer of the 21-cm line (in the presence of a continuum) with the differential frequency shifts when the Universe expands, and (ii) the interplay between absorption and emission of the line and the continuum when the radiation propagates down the redshift in an expanding Universe. The C21LRT formulation has properly accounted for these effects, thus providing a reliable means to compute the theoretical predictions of the tomographic 21-cm line spectra.

(3) A second-generation spin curvelet transform on a sphere has been built.

The newly constructed curvelets are defined natively on the sphere, and do not suffer from blocking artefacts that the first-generation spherical curvelets had. They allow for efficient representation of oriented, elongated structures in the data defined on a sphere, applicable (but not restricted) to the all-sky and wide-sky observational survey data that may carry spin information (e.g. polarisation). The curvelet transform is theoretically exact, meaning that the total information content of signals can be fully captured in analyses and reconstruction. Its algorithm is also optimised, making it computationally efficient to handle large data sets. The efficacy of the curvelet transform to characterise signal contents in positions, scales, and orientations, and to extract structural information encoded in the data, has been demonstrated using a natural spherical light-probe image. This also illustrates the wide applications of the tool outside of astrophysics and cosmology.

With the culmination of observational data and the advent of the world's most powerful radio telescope, the SKA, our understanding of the two largely uncharted fields of cosmic magnetism and cosmological reionisation are set be revolutionised. Some fundamental questions on the first magnetic fields, and on the first luminous structures and their impacts on the reionisation of gas, which previously could not be studied (due to insufficient sensitivities and resolutions), can finally be addressed, if scientific information encoded in the data can be accurately extracted and correctly understood. The covariant cosmological radiative transfer and spin spherical curvelet formalisms presented in this thesis establish a solid theoretical platform upon which theories and models of cosmic magnetism or cosmological reionisation can intersect and be meaningfully compared with observations. Much exciting research can be built upon and branched out from these developments for the physical interpretation of astrophysical and cosmological observations to study fundamental physics and beyond.

This thesis research represents one of the many research efforts aiming to uncover the astrophysical and cosmological information accessible to us from observing the Universe, in particular, using "light" (electromagnetic radiation) to probe the invisible magnetic fields and the impact of the first lights of the Universe (the first stars, the first galaxies, and the first quasars) on their surroundings. As a final remark, which echos the preface of this thesis, two questions are posed. To what extent will our missing knowledge about the evolution of magnetic fields and the proceeding of the cosmological reionisation change our views of the Universe? Are we closing in on the answers of our cosmic origins, or are we opening up more unexplored new territories? These are still open questions, but knowledge gathered in our cosmic exploration will illuminate the way.

Appendix A

Adopted Coordinate Systems

A right-handed coordinate system is adopted, as depicted in Fig. A.1, in this work, following Huang and Shcherbakov (2011). The magnetic field B is directed along the \tilde{z} -axis, making an angle θ clockwise to the direction of the propagation of the radiation k. An orthonormal (x, y, z) basis is defined such that $z \parallel k$, and $x = C(B \times k)$, where C is a scalar that can be positive or negative, and $x \parallel \tilde{x}$, and $y = (k \times x)$. Here x is perpendicular to the plane of (B, k), and B, k, and y are coplanar. The electric field of an electromagnetic wave propagating in the direction $k \parallel z$ oscillates in the (x, y)-plane. By such a choice of configuration (or by the choice of $y \parallel \tilde{y}$ in the systems defined in Sazonov (1969); Pacholczyk (1977)), the absorption coefficient u_{ν} , conversion coefficient g_{ν} and emission coefficient $\epsilon_{U,\nu}$ are zeros.

The transfer matrices are often derived by adopting the "magnetic-field" system, i.e. first in the $(\tilde{x}, \tilde{y}, \tilde{z})$ basis, and then projecting them onto (x, y) for $k \parallel z$, and $\cos \theta = (\mathbf{k} \cdot \mathbf{B})/(|\mathbf{k}||\mathbf{B}|)$ (see e.g. Sazonov 1969; Pacholczyk 1970, 1977; Jones and



Fig. A.1: The coordinate systems and the geometry of the magnetic field adopted in this work.

O'Dell 1977a; Huang and Shcherbakov 2011). The transformation between the coordinate systems $\tilde{e}_i = (\tilde{x}, \tilde{y}, \tilde{z})$ and $e_j = (x, y, z)$ is given by $e_j = \tilde{e}_i M_{ij}$, where

$$M_{ij} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & \sin\theta \\ 0 & -\sin\theta & \cos\theta \end{pmatrix},$$
(A.1)

i.e.

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \theta & -\sin \theta \\ 0 & \sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} \tilde{x} \\ \tilde{y} \\ \tilde{z} \end{pmatrix}.$$
 (A.2)

It follows that the rotation of vectors is given by $A_i = (M^T)_{ij}\tilde{A}_j$, and the rotation of tensors is given by $\sigma_{ij} = (M^T)_{ik}\tilde{\sigma}_{km}(M)_{mj}$ (Huang and Shcherbakov 2011). In future studies where observational data are confronted with theoretical predictions obtained by CPRT calculations, it is also useful to introduce the "observer's" (or polarimeter's) system (a, b), which is defined by rotating the (x, y)-plane about the *k*-direction. The transformation is between the local system (given by the local projection of the magnetic field) in the comoving frame and the frame in which polarimetric data are measured. It invokes the use of rotational matrix $\mathcal{R}(\chi)$, which follows the definition given in Eqns. (50) and (51) in Huang and Shcherbakov (2011), where the angle χ relates *a* and *b* to the magnetic field components perpendicular to *k*, i.e. $B_{\perp} = B - k(k \cdot B)/k^2$, by $\sin \chi = (a \cdot B_{\perp})/|B_{\perp}|$ and $\cos \chi = -(b \cdot B_{\perp})/|B_{\perp}|$ respectively.

Appendix B

Polarisation and Magnetic Field Conventions

Stokes parameters I_{ν} , Q_{ν} , and U_{ν} are defined unambiguously once the (x, y) coordinate system is specified. The different definitions of polarisation angle adopted in the cosmic microwave background community and the International Astronomical Union (IAU) can be reconciled by a sign change of U_{ν} . However, interpretation of the sign of V_{ν} (and consequently the signs for the corresponding transfer coefficients $\epsilon_{V,\nu}$, v_{ν} and h_{ν}) in the literature is often ambiguous. This is because the sign of V_{ν} depends not only on the definition of the senses of circular polarisation (which also depends on the handedness of the coordinate systems used) and the definition of V_{ν} , but also on the choice of sign in the time-dependent description of the electromagnetic wave, as well as the definition of the relative phase between the *x* and *y*-components of the electric vector of the wave. Much variation in these dependences exist in the literature, or sometimes this information is inexplicitly assumed or left unstated. Another source of variation comes from the choice of the attachment of the sense of circular polarisation to the helicity of the photon. Any confusion and ambiguity can easily cause a slip in the interpretation of V_{ν} .

Here, the circular polarisation sense defined by the Institute of Electrical and Electronics Engineers (IEEE) (IEEE 1998) is first described. Such a convention is commonly adopted by radio astronomers (but opposite to classical physicists and optical astronomers' common practice¹), and the International Astronomical Union (IAU) convention of Stokes V_{ν} (Reid 2007). Then, the intricacies to test the conformity to the IEEE/IAU polarisation convention are discussed. Finally, I remark on the magnetic field direction of the system and state explicitly the Stokes

¹The right-handed circular polarisation convention by the IEEE corresponds to the left-handed circular polarisation convention in the classical sense, i.e. IEEE-RCP = classical-LCP.



Fig. B.1: A right-handed circularly polarised wave, as defined by the IEEE, in the adopted right-handed coordinate system (cf. Fig. 1 in van Straten et al. (2010) with the angle and electric field notations made consistent to the notations used in this work). The electric vector rotates counter-clockwise as seen by the observer, i.e. at a fixed position as time advances (note that at fixed time, the electric vector along the line-of-sight rotates clockwise i.e. forms a left-handed screw in space).

V convention used in this thesis.

B.1 IEEE/IAU polarisation Convention

The exact quote of the IEEE (1998)'s definition² of a right-handed polarised wave reads "a circularly or an elliptically polarised electromagnetic wave for which the electric field vector, when viewed with the wave approaching the observer, rotates counter-clockwise in space". As pointed out by Hamaker and Bregman (1996), such a definition stipulates that the position angle φ of the electric vector of the wave at any point *increases* with time, implying that the *y*-component of the field, E_y , to *lag behind* the *x*-component, E_x . In other words, the electric field traces out a counter-clockwise helix (right-hand screw) in time at a fixed position, whereas in space at any instant in time, it forms a clock-wise helix (left-hand screw) (see e.g. Rochford 2001). The IAU endorses the sense of circular polarisation defined by IEEE and defines $V_v = (\text{RCP} - \text{LCP})$, i.e. V_v is positive for RCP (Reid 2007). The *x*- and *y*- axes of a right-hand triad align with the North and astronomical East, and the *z*- axis points towards the observer following the standard IAU convention.

²The same definition was first introduced in 1942 when the IEEE was still known as the Institute of Radio Engineers (IRE).

B.2 Conformity to the IEEE/IAU Convention

It is important to note that even when the Stokes parameters are uniquely defined when combined the IEEE/IAU definition with the standard formulae for $I_v = \langle |E_x|^2 + |E_y|^2 \rangle$, $Q_v = \langle |E_x|^2 - |E_y|^2 \rangle$, and $U_v = 2\langle |E_x| |E_y| \cos \delta \rangle$, two similar but distinct mathematical representations are allowed for the same physics of the problem, as is shown by Hamaker and Bregman (1996). One can choose³ of the sign of the time dependence of the electromagnetic wave, i.e. $e^{+i\omega t}$ or $e^{-i\omega t}$, for $\omega > 0$. Both choices are equally valid, but once the sign is chosen for

$$\boldsymbol{E}(z,t) = \boldsymbol{E}_0 e^{\pm i(\omega t - kz)} = \begin{pmatrix} E_x(z,t) \\ E_y(z,t) \end{pmatrix} = \begin{pmatrix} E_{x0} e^{\pm i(\omega t - kz + \phi_x)} \\ E_{y0} e^{\pm i(\omega t - kz + \phi_y)} \end{pmatrix}, \quad (B.1)$$

the following quantities must have the sign adjustments such that E_y lags behind E_x for a (unit amplitude) RCP wave:

$$\boldsymbol{E}^{\text{RCP}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\ \pm i \end{pmatrix}, \qquad (B.2)$$

and

$$V_{\nu} = 2 \langle |E_x| |E_{\nu}| \sin \delta \rangle \tag{B.4}$$

$$= \mp i \left\langle E_x E_y^* - E_y E_x^* \right\rangle \tag{B.5}$$

Hamaker and Bregman (1996). This ensures a positive *V* for the RCP, i.e. IEEE/IAU compliant. The sign adjustment in Eqn. (B.5) is equivalent to defining the sign of $\delta = \pm (\phi_y - \phi_x)$ in Eqn. (B.4) for $\delta \in (0, \pi)$, where time delays correspond to negative (positive) values of the phases ϕ_x and ϕ_y for $e^{\pm i(\omega t - kz)}$ according to Eqn. (B.1). It is

³Another choice is related to the attachment of the RCP and LCP to positive and negative helicity (see also Appendix III in Simmons and Guttmann (1970) for a complete table of different conventions of RCP, including those that do not comply to the IEEE/IAU convention).

apparent that a differing convention in any of the above would lead to a sign reversal. An unambiguous interpretation of the circular polarisation from V_{ν} will require a clear specification of the handedness of the coordinate systems, the convention of circular polarisation, and the definition of Stokes V_{ν} , as well as a properly chosen mathematical representation of the travelling wave (radiation).

B.3 Remark on the B-field Convention

Given the coordinate systems and the geometry of the problem presented in Fig. A.1, let's consider a simple case where a uniform magnetic field B aligns with k such that $\theta = 0$. An electron would then precess about B in the (\tilde{x}, \tilde{y}) -plane, moving counterclockwise as viewed along $k \parallel B$. The electric vector of the electromagnetic wave follows the electron motion, thus also rotating counter-clockwise as viewed by the observer. This results in IEEE-RCP, and according to the IAU convention, $V_{y} > 0$.

In this work, I adopt the conventions conforming to the IEEE/IAU standard and stick to the magnetic field convention where the magnetic field is positive when pointing towards the observer⁴. The same coordinate systems as in Huang and Shcherbakov (2011) is adopted and used, as the main reference paper, to check against the signs of the Stokes parameters and their corresponding transfer coefficients. The transfer coefficients, therefore, all have positive signs in their expressions.

⁴This is opposite to the astronomical convention that traditionally defines magnetic field direction as positive when pointing away from the observer (i.e. $\theta = 0$ corresponds to a negative field while $\theta = \pi$ corresponds to a positive field).

Appendix C

Transfer Coefficients

In this Appendix, the transfer coefficients for both thermal bremsstrahlung and nonthermal synchrotron radiation processes are presented. The non-thermal relativistic electrons gyrating around magnetic field lines have a power-law energy spectrum. The expressions given in Pacholczyk (1977) and Jones and O'Dell (1977a) are adopted respectively, but the sign of the circular polarisation described by Stokes V are made to be consistent and compliant to the IEEE/IAU convention, given the coordinate system explicitly shown in Appendix A. The emission coefficients have units of erg s⁻¹ cm⁻³ Hz⁻¹ str⁻¹ and the absorption and Faraday coefficients have units of cm⁻¹.

C.1 Thermal Bremsstrahlung Radiation

Transfer coefficients of thermal bremsstrahlung have been presented in Pacholczyk (1977); Meggitt and Wickramasinghe (1982); Wickramasinghe and Meggitt (1985); Rybicki and Lightman (1986). In this work, I adopt the expressions given in Pacholczyk (1977) and make certain changes such that the set of coefficients would follow the same conventions of polarisation that have been specified in Sec. 1.5 and Appendix B.

For a magnetised thermal plasma, the coefficients of Faraday rotation and Faraday conversion are respectively,

$$f_{\rm th} = \frac{\left(\omega_{\rm p}^2/c\,\omega_{\rm B}\right)\cos\theta}{\left(\omega^2/\omega_{\rm B}^2\right) - 1}; \qquad (C.1)$$

$$h_{\rm th} = \frac{\left(\omega_{\rm p}^2/c\,\omega_{\rm B}\right)\sin^2\theta}{2\left(\omega^3/\omega_{\rm B}^3 - \omega/\omega_{\rm B}\right)} \tag{C.2}$$

(Pacholczyk 1977), where $\omega (= 2\pi v)$ is the angular frequency of the radiation, $\omega_{\rm p} = (4\pi n_{\rm e,th} e^2/m_{\rm e})^{1/2}$ is the plasma frequency, $\omega_{\rm B} = (eB/m_{\rm e}c)$ is the electron gyrofrequency, and θ is the angle between the radiation propagation direction and the magnetic field vector. The absorption coefficients of the thermal bremsstrahlung component are given by

$$\kappa_{\rm th} = \frac{\omega_{\rm p}^2 \left(2\omega^4 + 2\omega^2 \omega_{\rm B}^2 - 3\omega^2 \omega_{\rm B}^2 \sin^2 \theta + \omega_{\rm B}^4 \sin^2 \theta\right)}{2 c \, \omega^2 \left(\omega^2 - \omega_{\rm B}^2\right)^2} \, v_{\rm c} \, ; \qquad (C.3)$$

$$q_{\rm th} = \frac{\omega_{\rm p}^2 \,\omega_{\rm B}^2 \sin^2 \theta \, \left(3\omega^2 - \omega_{\rm B}^2\right)}{2 \, c \, \omega^2 \left(\omega^2 - \omega_{\rm B}^2\right)^2} \, \nu_{\rm c} \, ; \qquad (C.4)$$

$$v_{\rm th} = \frac{2\,\omega_{\rm p}^2\,\omega\,\omega_{\rm B}\cos\theta}{c\,\left(\omega^2 - \omega_{\rm B}^2\right)^2}\,v_{\rm c} \tag{C.5}$$

(Pacholczyk 1977), with the collisional frequency

$$\nu_{\rm c} = \frac{4\sqrt{2\pi}e^4 n_{\rm e}}{3\sqrt{m_{\rm e}} (k_{\rm B}T_{\rm e})^{3/2}} \ln \Lambda \approx 3.64 \, n_{\rm e} \, T_{\rm e}^{-3/2} \ln \Lambda \,. \tag{C.6}$$

Here, $k_{\rm B}$ is the Boltzmann constant and $T_{\rm e}$ is the temperature of the electrons in thermal equilibrium, and the Coulomb logarithm factor is given by

$$\Lambda = \begin{cases} \left(\frac{2}{1.781}\right)^{5/2} \left(\frac{k_{\rm B}T_{\rm e}}{m_{\rm e}}\right)^{1/2} \left(\frac{k_{\rm B}T_{\rm e}}{e^2\omega}\right) & (T_{\rm e} \le 3.16 \times 10^5 \text{ K}) \\ \frac{8\pi k_{\rm B}T_{\rm e}}{1.781h\omega} & (T_{\rm e} > 3.16 \times 10^5 \text{ K}) \end{cases}, \quad (C.7)$$

for $\omega \gg \omega_p$ (see e.g. Lang 1974). The emission coefficients in *I*, *Q* and *V* can be computed via the Kirchoff's law:

$$\epsilon_{I,\text{th}} = \kappa_{\text{th}} B_{\omega}, \quad \epsilon_{Q,\text{th}} = q_{\text{th}} B_{\omega}, \text{ and } \epsilon_{V,\text{th}} = v_{\text{th}} B_{\omega}, \quad (C.8)$$

where the Planck function at the low frequencies is the Rayleigh-Jeans intensity, i.e. $B_{\omega} = k_{\rm B}T_{\rm e}\omega^2/(2\pi^2c^2)$.

It is interesting to note that both the frequency dependence and the dependence on the magnetic field are different for Faraday rotation and Faraday conversion. The strength of the Faraday rotation effect is proportional to $v^{-2} n_{e,th} |B_{\parallel}| \delta s$, and the strength of Faraday conversion is proportional to $v^{-3} n_{e,th} |B_{\perp}|^2 \delta s$, where $|B_{\parallel}| = |B| \cos \theta$, $|B_{\perp}| = |B| \sin \theta$, and δs is the photon propagation length.

Another remark concerns the use of rotation measure (RM) in the literature for quantifying the strength of Faraday rotation. RM is defined as $\mathcal{R} \equiv \Delta \varphi c^2 / v^2$, where $\varphi = 0.5 \arctan(U/Q)$, and the formula

$$\mathcal{R}(s) = 0.812 \int_{s_0}^{s} \frac{\mathrm{d}s'}{\mathrm{pc}} \frac{n_e(s')}{\mathrm{cm}^{-3}} \frac{|\mathbf{B}_{\parallel}(s')|}{\mu \mathrm{G}} \, \mathrm{rad} \, \mathrm{m}^{-2} \tag{C.9}$$

is widely used in RM analyses. This formula can be derived directly from the polarised radiative transfer equation (Eqn. 2.4), under the assumptions that the effects of emission, absorption, Faraday conversion and contribution from non-thermal electrons are negligible, see Appendix D and On et al. (2019) for details. In a realistic situation, however, these assumptions do not hold. The magnitudes of Q and U of the observed polarised light are not solely dictated by Faraday rotation process. An accurate inference of magnetic field properties from the polarisation signatures of observed light, therefore, demands a full polarised radiative transfer treatment.

C.2 Non-thermal Synchrotron Radiation

The expressions of the transfer coefficients for cosmic synchrotron sources from Jones and O'Dell (1977a) are adopted, where sign changes for the transfer coefficients at V_{ν} are appropriately adopted to keep a self-consistent polarisation convention defined explicitly in this thesis. For relativistic electrons following a power-law energy distribution with an index p,

$$dn = [n_{\gamma}\gamma^{p}]\gamma^{-p}\Theta(\gamma - \gamma_{i})g(\Psi) d\gamma d\Omega_{\Psi}, \qquad (C.10)$$

where $\Theta(\gamma - \gamma_i)$ is the step function, γ_i is the low-energy cutoff of electrons, and $g(\Psi)$ is the pitch-angle distribution, normalised to $\int d\Omega_{\Psi} g(\Psi) = 1$. The corresponding

electron number density is

$$n_{\gamma} = \int_{\gamma_i}^{\infty} \mathrm{d}\gamma \, [n_{\gamma}\gamma^p] \gamma^{-p} = \frac{[n_{\gamma}\gamma^p] \gamma_i^{-(p-1)}}{p-1} \qquad (\text{for } p > 1) \;. \tag{C.11}$$

The normalisation factor $[n_{\gamma}\gamma^{p}]$ and the index *p* are related to the spectral index of the radiation by $\alpha = (p-1)/2$. The transfer coefficients for non-thermal synchrotron radiation are

$$f_{\rm nt} = f_{\alpha} \kappa_{\perp} \left(\frac{\omega_{B_{\perp}}}{\omega}\right)^2 (\ln \gamma_i) \gamma_i^{-2(\alpha+1)} \cot \theta \\ \times \left[1 + \frac{\alpha+2}{2\alpha+3} \frac{d (\ln g(\theta))}{d (\ln (\sin \theta))}\right]; \qquad (C.12)$$

$$h_{\rm nt} = h_{\alpha} \kappa_{\perp} \left(\frac{\omega_{B_{\perp}}}{\omega}\right)^3 \gamma_i^{-(2\alpha-1)} \left[\frac{1 - (\omega_i/\omega)^{\alpha-1/2}}{\alpha - 1/2}\right] ; \qquad (C.13)$$

$$\kappa_{\rm nt} = \kappa_{\alpha} \kappa_{\perp} \left(\frac{\omega_{B_{\perp}}}{\omega}\right)^{\alpha+5/2} ; \qquad (C.14)$$

$$q_{\rm nt} = q_{\alpha} \kappa_{\perp} \left(\frac{\omega_{B_{\perp}}}{\omega}\right)^{\alpha+5/2};$$
 (C.15)

$$v_{\rm nt} = v_{\alpha} \kappa_{\perp} \left(\frac{\omega_{B_{\perp}}}{\omega}\right)^{\alpha+3} \cot \theta \left[1 + \frac{1}{2\alpha+3} \frac{d \left(\ln g(\theta)\right)}{d \left(\ln \left(\sin \theta\right)\right)}\right]; \qquad (C.16)$$

$$\epsilon_{I,\text{nt}} = \epsilon_{\alpha}^{I} \epsilon_{\perp} \left(\frac{\omega_{B_{\perp}}}{\omega}\right)^{\alpha}; \qquad (C.17)$$

$$\epsilon_{Q,\text{nt}} = \epsilon_{\alpha}^{Q} \epsilon_{\perp} \left(\frac{\omega_{B_{\perp}}}{\omega}\right)^{\alpha} ; \qquad (C.18)$$

$$\epsilon_{V,\text{nt}} = \epsilon_{\alpha}^{V} \epsilon_{\perp} \left(\frac{\omega_{B_{\perp}}}{\omega}\right)^{\alpha+1/2} \cot \theta \left[1 + \frac{1}{2\alpha+3} \frac{d\left(\ln g(\theta)\right)}{d\left(\ln\left(\sin\theta\right)\right)}\right], \quad (C.19)$$

for $\alpha > 1/2$ (Jones and O'Dell 1977a), where $\kappa_{\perp} = (2\pi r_e c) \omega_{B_{\perp}}^{-1} [4\pi g(\theta)] [n_{\gamma} \gamma^p]$, $\epsilon_{\perp} = (m_e c^2) (r_e/2\pi c) \omega_{B_{\perp}} [4\pi g(\theta)] [n_{\gamma} \gamma^p]$, $r_e = e^2/m_e c^2$, $\omega_{B_{\perp}} = \omega_B \sin \theta$, and $\omega_i = \gamma_i^2 \omega_{B_{\perp}}$ (which is the fiducial frequency). The dimensionless functions in the transfer coefficients are

$$f_{\alpha} = 2 \frac{(\alpha + 3/2)}{\alpha + 1};$$
 (C.20)

$$h_{\alpha} = 1; \qquad (C.21)$$

$$\kappa_{\alpha} = \frac{3^{\alpha+1}}{2} \Gamma\left(\frac{\alpha}{2} + \frac{25}{2}\right) \Gamma\left(\frac{\alpha}{2} + \frac{5}{2}\right); \qquad (C.22)$$

$$\kappa_{\alpha} = \frac{3}{4} \Gamma\left(\frac{\alpha}{2} + \frac{23}{12}\right) \Gamma\left(\frac{\alpha}{2} + \frac{3}{12}\right); \qquad (C.22)$$

$$q_{\alpha} = \frac{(\alpha + 3/2)}{(\alpha + 13/6)} \kappa_{\alpha}; \qquad (C.23)$$

$$v_{\alpha} = \frac{3^{\alpha+1/2}}{2} \frac{(\alpha+2)}{(\alpha+1)} \left(\alpha + \frac{3}{2}\right) \Gamma\left(\frac{\alpha}{2} + \frac{7}{6}\right) \Gamma\left(\frac{\alpha}{2} + \frac{5}{6}\right) ; \qquad (C.24)$$

$$\epsilon_{\alpha}^{I} = \frac{3^{\alpha+1/2}}{4(\alpha+1)} \Gamma\left(\frac{\alpha}{2} + \frac{11}{6}\right) \Gamma\left(\frac{\alpha}{2} + \frac{1}{6}\right) ; \qquad (C.25)$$

$$\epsilon_{\alpha}^{Q} = \frac{(\alpha+1)}{(\alpha+5/3)} \epsilon_{\alpha}^{I}; \qquad (C.26)$$

$$\epsilon_{\alpha}^{V} = \frac{3^{\alpha}}{2} \frac{(\alpha + 3/2)}{(\alpha + 1/2)} \Gamma\left(\frac{\alpha}{2} + \frac{11}{12}\right) \Gamma\left(\frac{\alpha}{2} + \frac{7}{12}\right) .$$
(C.27)

The transfer coefficients are derived from a nearly isotropic dielectric tensor, appropriate for an astrophysical plasma with low electron number densities and weak magnetic fields, for which $\omega > \omega_i$ and both ω and ω_i are above the gyro-frequency $\omega_{\rm B}$. The condition $\gamma_i^2 > \cot^2 \theta$ also has to be satisfied. In addition, dielectric suppression is assumed to be negligible. This assumption generally holds for astrophysical media (see Jones et al. 1974; Melrose and McPhedran 1991, for details). In this work, isotropic electron distribution is assumed, so $g(\theta) = 1/4\pi$. Comparing to the expression for the thermal bremsstrahlung process in the high-frequency limit ($\omega \gg \omega_{\rm B}$), the non-thermal synchrotron Faraday rotation coefficient has an extra factor

$$\zeta(p,\gamma_i) = \frac{(p-1)(p+2)}{(p+1)} \left(\frac{\ln \gamma_i}{\gamma_i^2}\right),$$
 (C.28)

implying that Faraday rotation weakens with increasing electron energy (see Melrose 1997; Huang and Shcherbakov 2011).

Appendix D

Derivation of Rotation Measure Formula from CPRT

This Appendix shows how the the widely-used formula in RM analysis of magnetised astrophysical media can be derived from the general covariant CPRT equation. The derivation can also be found in On et al. (2019).

In a local frame, the covariant CPRT equation in Eqn. (2.24) reduces to the standard polarised radiative transfer (PRT) equation, Eqn. (2.4):

$$\frac{\mathrm{d}}{\mathrm{d}s} \begin{bmatrix} I \\ Q \\ U \\ V \end{bmatrix} = -\begin{bmatrix} \kappa & q & u & v \\ q & \kappa & f & -g \\ u & -f & \kappa & h \\ v & g & -h & \kappa \end{bmatrix} \begin{bmatrix} I \\ Q \\ U \\ V \end{bmatrix} + \begin{bmatrix} \epsilon_I \\ \epsilon_Q \\ \epsilon_U \\ \epsilon_V \end{bmatrix}.$$
(D.1)

In the situations where

1. absorption and emission are absent

i.e. ($\kappa = q = u = v = 0$) and ([$\epsilon_I, \epsilon_Q, \epsilon_U, \epsilon_V$] = 0), which imposes dI/ds = 0 and

$$\frac{\mathrm{d}}{\mathrm{d}s} \begin{bmatrix} Q\\ U\\ V \end{bmatrix} = -\begin{bmatrix} 0 & f & -g\\ -f & 0 & h\\ g & -h & 0 \end{bmatrix} \begin{bmatrix} Q\\ U\\ V \end{bmatrix}, \qquad (D.2)$$

- 2. circular polarisation is insignificant ($V \rightarrow 0$), and
- 3. inter-conversion between linear and circular polarisation is negligible $(g \rightarrow 0, h \rightarrow 0)$,

one may consider only the two linearly polarised Stokes components (Q and U) in the PRT calculation. In that case, the PRT equation is simplified to

$$\frac{\mathrm{d}}{\mathrm{d}s} \begin{bmatrix} Q\\ U \end{bmatrix} = -\begin{bmatrix} 0 & f\\ -f & 0 \end{bmatrix} \begin{bmatrix} Q\\ U \end{bmatrix}, \qquad (D.3)$$

leaving the Faraday rotation coefficient f as the sole parameter. It follows that the change in the linear polarisation angle along the line-of-sight is

$$\frac{\mathrm{d}\varphi}{\mathrm{d}s} = \frac{1}{2} \left(\frac{1}{U^2 + Q^2} \right) \left(Q \, \frac{\mathrm{d}U}{\mathrm{d}s} - U \, \frac{\mathrm{d}Q}{\mathrm{d}s} \right) = \frac{f}{2} \,. \tag{D.4}$$

An astrophysical plasma may contain both thermal and non-thermal electrons. The expressions for Faraday rotation due to thermal electrons and non-thermal electrons are given in Eqn. (C.1) and Eqn. (C.13) in Appendix C, respectively. Note that the polarised radiative transfer equations (D.1), (D.2) and (D.3) are linear, thus the contributions to the Faraday rotation coefficient by a collection of thermal and non-thermal electrons are additive: i.e. $f = f_{th} + f_{nt}$.

In the high-frequency limit (i.e. $\omega \gg \omega_{\rm B}$), the thermal Faraday rotation coefficient, Eqn. (C.1), can be expressed as,

$$f_{\rm th} = \frac{1}{\pi} \left(\frac{e^3}{m_{\rm e}^2 c^4} \right) n_{\rm e,th} B_{\parallel} \lambda^2 ,$$
 (D.5)

and the corresponding expression for non-thermal Faraday rotation, Eqn. (C.13), is

$$f_{\rm nt} = \frac{1}{\pi} \left(\frac{e^3}{m_{\rm e}^2 c^4} \right) \zeta(p, \gamma_{\rm i}) \, n_{\rm e,nt} \, B_{\parallel} \, \lambda^2 \,, \tag{D.6}$$

assuming an isotropic distribution of non-thermal electrons with a power-law energy spectrum of index p (Jones and O'Dell 1977a). Provided that neither $n_{e,nt}$ nor $n_{e,th}$ correlates or anti-correlates significantly with B_{\parallel} , the relative strength of their

contributions to the Faraday rotation is¹.

$$\frac{f_{\rm nt}}{f_{\rm th}} \approx \zeta(p, \gamma_{\rm i}) \left(\frac{n_{\rm e,nt}}{n_{\rm e,th}}\right) , \qquad ({\rm D.7})$$

where the factor

$$\zeta(p,\gamma_{\rm i}) = \frac{(p-1)(p+2)}{(p+1)} \left(\frac{\ln \gamma_{\rm i}}{\gamma_{\rm i}^2}\right) \qquad (\text{for } p > 1) \;. \tag{D.8}$$

In a plasma consisting of *only thermal electrons in a sufficiently weak magnetic field*, where $\omega_B \ll \omega$, a direct integration of equation (D.4) with $f = f_{th}$ yields

$$\varphi(s) = \varphi_0 + \frac{2\pi e^3}{m_e^2 (c\,\omega)^2} \int_{s_0}^s ds' \, n_{e,\text{th}}(s') \, B_{\parallel}(s') \; . \tag{D.9}$$

Recall that rotation measure (RM) is defined as

$$\mathcal{R} = (\Delta \varphi) \lambda^{-2} = (\varphi - \varphi_0) \lambda^{-2} . \tag{D.10}$$

Hence, for a magnetised plasma consisting of both thermal and non-thermal electron populations, the RM for radiation traversing through such a medium between an interval s_0 and s is

$$\mathcal{R}(s) = \frac{e^3}{2\pi m_e^2 c^4} \int_{s_0}^{s} ds' \, n_{e,\text{tot}}(s') \,\Theta(s') \,B_{\parallel}(s') \,, \tag{D.11}$$

where $n_{e,tot}$ is the total electron number density, and $\Theta(s) = 1 - \mathcal{F}_{nt}(s) [1 - \zeta(p, \gamma_i)]|_s$ is the weighting factor of $n_{e,tot}$ contributing to the total Faraday rotation effect, with $\mathcal{F}_{nt}(s)$ the local fraction of non-thermal electrons.

If only thermal electrons are present, $\mathcal{F}_{nt}(s) = 0$ such that $\Theta(s) = 1$. Eqn. (D.11)

¹A similar relation was given in Jones and O'Dell (1977a) for the relative contributions of relativistic and thermal electrons to the Faraday rotation. Their relation is expressed in terms of the spectral index α of the optically thin power-law synchrotron spectrum. The relation (D.7) here is expressed in terms of the power-law index p of the electron energy distribution, which is intrinsic to the magneto-ionic medium. Note that $\alpha = (p-1)/2$.

then reduces to

$$\mathcal{R}(s) = 0.812 \int_{s_0}^{s} \frac{ds'}{pc} \left(\frac{n_{e,th}(s')}{cm^{-3}}\right) \left(\frac{B_{\parallel}(s')}{\mu G}\right) rad m^{-2}, \qquad (D.12)$$

hence recovering the widely-used formula in RM analysis of magnetised astrophysical media (see e.g. Carilli and Taylor 2002).

Appendix E

Main Findings of On et al. (2019)

On et al. (2019) conducted a study on the radiative transfer theory behind the analysis of large-scale magnetic field using rotation measures (RM) and its fluctuations (RMF) in the observed polarised radio emissions, testing the validity of the RM/RMF analysis in various astrophysical situations. Here, three main aspects of their findings are summarised.

E.1 Theoretical Foundation of RMF Analysis as a Diagnostics of the Structure of Large-scale Magnetic Fields

Characteristic length-scales for the variation of large-scale magnetic fields in diffuse astrophysical media are often inferred from the statistical properties of polarised radiation. One particular technique is using the correlation lengths of the observed RM. In most of the observational and numerical studies, the correlation length of the magnetic fields inferred from the standard deviation of RM, σ_R , use the following expression (see e.g. Sokoloff et al. 1998; Blasi et al. 1999; Govoni and Feretti 2004; Subramanian et al. 2006; Cho and Ryu 2009; Dolag et al. 2011; Sur 2019):

$$\sigma_{\mathcal{R}} = \frac{e^3}{2\pi m_{\rm e}^2 c^4} \sqrt{\frac{L}{\Delta s}} \,\overline{\Delta s} \,\overline{n_{\rm e,tot} \,\Theta} \left[\left\langle B_{\parallel}^2 \right\rangle_s \right]^{1/2} \,, \tag{E.1}$$

where $\overline{\Delta s}$ is the propagation path interval segments of equal length, and $\overline{n_e \Theta}$ is the mean value of $(n_{e,tot} \Theta)$. The other symbols have the same meanings as given in

Appendix D. The alternative expression used in some of the studies is

$$\sigma_{\mathcal{R}} = \frac{e^3}{2\pi m_e^2 c^4} \sqrt{\frac{L}{\Delta s}} \,\overline{\Delta s} \,\overline{n}_{e,\text{th}} B_{\parallel\text{rms}}$$
$$= 0.812 \,\sqrt{\frac{L}{\Delta s}} \left(\frac{\overline{\Delta s}}{\text{pc}}\right) \left(\frac{\overline{n}_{e,\text{th}}}{\text{cm}^{-3}}\right) \left(\frac{B_{\parallel\text{rms}}}{\mu\text{G}}\right) \,\text{rad m}^{-2} \,. \tag{E.2}$$

The two expressions above can be derived from radiative transfer theory, assuming the change in the magnetic field and the plasma density along the line-of-sight can be modelled by an unbiased random walk process. On et al. (2019) have shown that there are additional conditions that have to be satisfied in order to validate the above expressions for the analysis of large-scale magnetic fields in astrophysical systems. These conditions are: (i) Faraday rotation is caused by the variations in the magnetic fields with field strength distributions (e.g. uniform or Gaussian distributed strengths, where the first moment of their statistics are well defined); (ii) the magnetic fields have unbiased random orientations such that B_{\parallel} have a symmetric probability distribution, i.e. $Pr(B_{\parallel}) = Pr(-B_{\parallel})$; (iii) there exists a characteristic electron number density with a well-defined mean value; and (iv) there is no correlation between the electron number density and the magnetic fields locally or globally. Eqn. (E.2) further assumes the presence of only thermal electrons and an electron contribution weighting factor $\Theta = 1$.

Condition (iii) breaks down for astrophysical environments with electron number densities that have a fractal or a log-normal spatial distribution. In reality, electron number density and magnetic field strength are often related. Hence, condition (iv) does not usually hold.

Note that the fluctuations of polarisation properties along individual rays are not directly observable. Observations map the polarised sky over the celestial sphere, but the polarisation signatures that are obtained are the collection of the end-point results of the path-integrated polarised rays. This is compounded by the fact that the spatial correlations of electron number density or magnetic fields are not the same in the line-of-sight longitudinal direction and in the directions across sky plane.

This can be understood as follows. Without losing generality, consider that the observable, $x \in \{Q, U, V, \Delta \varphi, \text{ or } \mathcal{R}\}$, has two independent orthogonal components, whose fluctuations are designated by $\sigma_x|_{\perp}$ and $\sigma_x|_{\parallel}$, corresponding to perpendicular and parallel with respect to to the line-of-sight (which is specified by the radiation propagation unit vector \hat{k}). Obviously, there is no guarantee that $\sigma_x|_{\perp} = \sigma_x|_{\parallel}$, in a general situation. Thus, we cannot simply take the value $\sigma_{\mathcal{R}}|_{\perp}$ derived from the polarisation data on the sky-plane to infer the structure of cosmic magnetic fields, without clarifying the physical contexts of the model and its assumptions.

The polarisation observed at a location on the sky plane is an outcome of a radiative transfer process operating along the line-of-sight. It is determined by the magneto-ionic properties of the line-of-sight plasmas and the astrophysical systems. It is also determined by the large-scale (\geq Mpc) magnetic fields, which evolve with the cosmological structures (see e.g. Ryu et al. 2008; Cho and Ryu 2009; Ryu et al. 2012; Barnes et al. 2012, 2018; Marinacci et al. 2015; Katz et al. 2019). For cosmological-scale structures, the transfer of radiation is not only a propagation in space but also a propagation from a distant past to the present.

The statistical properties of the observed polarisation signatures across a skyplane, therefore, depend on the spatial variations of the magneto-ionic plasma properties at different cosmological epochs over the transport of radiation, and the temporal variations of the magneto-ionic plasma properties over cosmological evolution. The convolution of these two factors determines (i) the variations of the observable variables along the ray as it propagates (i.e. in the direction along \hat{k} , denoted by ||) and (ii) the variations of the observable variables among the collection of rays reaching the sky plane (i.e. in directions \perp to \hat{k}). There is no guarantee that the fluctuations in (i) and in (ii) are statistically identical.

In the astrophysical settings where cosmological effects can be neglected, the time evolution of the magnetic field is insignificant. However, there are also complex and subtle issues in the interpretation of what RMF means for the observed astrophysical systems. The fluctuations in the the local polarisation along a ray are

jointly determined by the fluctuations in the energy distribution as well as number density of the electrons, and the fluctuations of the parallel magnetic field component, i.e. $|B_{\parallel}| = |B| \cos(\hat{k} \cdot B)$, where the exact magnitude and orientation of the magnetic field is actually undetermined in observation. If the rays reaching the celestial sky are independent, the variations in the polarisation that we observe, such as the RM fluctuations, are due to the convolution of the fluctuations in $|B_{\parallel}|$ and $n_{\rm e}$. Even if the electron number density and its energy spectrum are uniform in the entire astrophysical system of interest, there are ambiguities when inferring the structure of the magnetic field in the system. These ambiguities arise from the degeneracy in the fluctuations in the field strength and the field orientation, because of the vectorial nature of the local magnetic field *B*.

Furthermore, even without degeneracy between the signals from density and field fluctuations, radiative processes such as absorption, emission, and Faraday conversion may confuse and ambiguate the interpretation of the observed RM. Moreover, in addition to the thermal electrons, non-thermal electrons can also contribute to the Faraday rotation and conversion processes.

E.2 Quantitative Assessment of the Robustness of the RMF Methods in Determining the Magnetic-field Correlation Lengths

Numerical experiments are conducted to assess when (and the degree to which) the widely-used formula Eqn. (E.2) is valid, and when cautions are needed in the interpretations of the resulting $\sigma_{\mathcal{R}}$ statistics. RM maps are generated from the simulated cubes of Mpc side-length with thermal electron number density (d) and magnetic field strength (b) following either a uniform (U), Gaussian (G), fractal (F) and log-normal (L) distribution. Another set of calculations are performed in a fractal medium with two density phases, mimicking the typical environment in the ICM/ISM (referred to as cloudy models). RMF statistics (using standard deviation in RM) are then calculated in longitudinal direction (\parallel -direction), $\sigma_{\mathcal{R}}$, by performing PRT calculations under

the restrictive conditions that match to the underlying assumptions of Eqn. (E.2). As PRT calculations account for all the geometrical and transfer effects, they provide accurate results against which the sky-transverse standard deviations obtained from Eqn. (E.2) can be compared.

The main results of the numerical experiments are summarised as follows: (1) $\sigma_{\mathcal{R}}$ depend on both the electron number density and magnetic field fluctuations. It is difficult to disentangle the signals from these two types of fluctuations based on the value of $\sigma_{\mathcal{R}}$ itself.

(2) $\sigma_{\mathcal{R}}$ cannot distinguish between a range of different clumpy (or smooth) configurations of density and magnetic fields and are unable to tell the cloudy features apart. Density fluctuations could, therefore, confuse the correlation length of the magnetic fields inferred from the conventional RMF analyses.

(3) $\sigma_{\Re} < \varsigma_{\Re}$, by tens of percents or by factors of a few (if there is unrecognised cloudiness). Hence, different statistical indicators can potentially mislead the physical interpretations.

(4) The σ_{\Re} statistics obtained from the widely-used RMF formula would be inadequate for the interpretation of the magnetic field properties when one or some of the following criteria is not met: (i) cosmic medium with an ill-defined characteristic density, e.g. in cases of log-normal distributed and fractal-like density structures, (ii) magnetic field orientation are not random along the line-of-sight, (iii) magnetic field strengths follows a non-uniform or non-Gaussian distribution (i.e. losing the symmetry in its probability distribution), (iv) the field is non-isotropic, and (v) the density and the magnetic field are correlated.

E.3 Some Guidelines for Magnetic Field Inference from the Polarisation Observations

There are separate correlation lengths, ℓ_{\parallel} and ℓ_{\perp} , for each plasma quantity, e.g. the electron number density, $n_{\rm e}$, and the magnetic field, B, when a ray (line-of-sight) is specified. Inference of ℓ_{\parallel} of the magneto-ionic properties of a medium (or media) along the line-of-sight from the observed polarisation signatures in the traverse

sky-plane requires proper radiative transfer considerations.

It is important to distinguish between the Faraday rotation, as well as Faraday conversion, contributed by multiple sources along the line-of-sight. It is also important to take into consideration of the propagation effects in multi-phase media along the line-of-sight. To properly interpret the observed polarised sky (or RM/RMF statistics) and to identify the polarisation signatures of large-scale magnetic fields which co-evolved with the cosmological structures, it is also essential to account for all the magneto-ionic plasma effects throughout the evolutionary history of the Universe. For the analysis of cosmological-scale magnetic fields, the effects due to cosmic expansion, such as shifting of wavelength and stretching of wavebands, in addition to the astrophysical effects, such as structural evolution of the Universe, must be properly and simultaneously accounted for. RM/RMF analysis is generally inadequate for an accurate extraction of information from the observed polarisation signals imprinted by the large-scale cosmological magnetic fields. In this situation, a proper treatment with covariant cosmological polarised radiative transfer becomes essential.

A polarised radiative transfer treatment is also essential in situations where depolarisation effects are not negligible. Depolarisation due to differential Faraday rotation (see e.g. Sokoloff et al. 1998; Beck 1999; Shukurov and Berkhuijsen 2003; Fletcher and Shukurov 2006) in an emissive, Faraday-rotating medium is particularly important for very extended sources. An example of such sources is the emitting filaments in the cosmic web. Obviously, models using a simple Faraday screen with a bright source behind a (non-emitting) Faraday-rotating medium are unable to capture the essence of magnetism of an extended system. For the analysis of cosmological scale structures, such as the cosmic web filaments, a proper covariant polarised radiative transfer calculation is necessary to determine the line-of-sight depolarisation effects from all processes operating at different redshifts.

The power spectrum of the observed polarised intensity may be contaminated by emissions from the medium and the embedded sources along the line-of-sight. This will cause an apparent higher power in the fluctuations at the small scales. Special attention is required so to discern the signals due to spatially separated sources from those truly imprinted by the structures of magnetic fields. The observed power spectrum is the sum of the contributions from all redshifts. While the local power spectrum at a particular redshift, $P(k)|_z$, generally is not contaminated by the contributions from the higher redshifts, different components at higher k can be picked up at v_{obs} observationally. When interpreting the observed power spectrum, one must keep in mind the possible complications caused by the convolution of the contributions from different cosmological redshifts. A proper covariant polarised radiative transfer treatment will provide a means to resolve some of this complex and subtle issues.

Appendix F

Calculation of the Total Electron Number Density at the Present Epoch

The Universe is neutral as a whole and the most common atoms in it are hydrogen and helium. The simplification that $n_{e,tot} \approx n_{p,tot} = n_{p,He} + n_{p,H}$ is, therefore, adopted. Here, "p" stands for proton, "H" for hydrogen and "He" for helium, $n_{p,He} \approx \rho_{He}/m_{He}$, and $n_{p,H} \approx \rho_{H}/m_{H}$. By approximating the density of hydrogen taking up 75 % of the density of baryons (i.e. $\rho_{H} = 3\rho_{b}/4$), and the density of helium taking up the remainder, it gives $n_{e} = 7\rho_{b}/8m_{p}$. The value of $\rho_{b,0}$ can be calculated from $\Omega_{b,0} = \rho_{b,0}/\rho_{crit}$, with $\Omega_{b,0}h^{2} = 0.02230$ (Planck Collaboration XIII 2016), and $\rho_{crit} = 3H_{0}/(8\pi G) = 1.87882 \times 10^{-29}h^{2}$ g cm⁻³. This gives $n_{e,0} = 2.1918 \times 10^{-7}$ cm⁻³.

Appendix G

Remarks on Finding an Appropriate Scale Length

Table G.1 summarises the numerical values of the absorption, emission, Faraday rotation, and Faraday conversion coefficients used in the calculations presented in Sec. 3.1.3. The very different conditions in the cosmic media give rise to a wide range of values for the absorption, emission, Faraday rotation, and Faraday conversion coefficients. As these coefficients span many orders of magnitude, the CPRT equation is stiff. It is, therefore, essential and important to test the capability of the equation solver and the stability of the numerical solution (see Sec. 3.1.3).

Finding an appropriate scale length is crucial to overcoming the stiffness issue. In the work presented in Chapter 3, the very small order of magnitude of the transfer coefficients computed using parameters typical to an IGM and an ICM at $v_{obs} = 1.42$ GHz suggests a scale length of a few Mpc when determining the *z*-sampling scheme.

In addition, note that all the CPRT calculations for the situations discussed in this work are optically thin (i.e. $\tau \ll 1$). While the media are optically thin, they can be Faraday thick at the same time, such as in the cases of ICM-like environments. Numerical values of the optical depths and Faraday conversion coefficients obtained using the IGM-like model A-I and the ICM-like model B-I are included in Table G.1. Note also that the effect of Faraday conversion is usually much weaker than that of Faraday rotation.

| | IGM-like model A-I | ICM-like model B-I |
|--|---|---|
| $\epsilon_{I,\mathrm{tot}}$ | $\epsilon_{I,\text{th}} + \epsilon_{I,\text{nt}}$ | $\epsilon_{I,\text{th}} + \epsilon_{I,\text{nt}}$ |
| $(erg s^{-1} cm^{-3} Hz^{-1} str^{-1})$ | $= 2.59 \times 10^{-53} + 2.62 \times 10^{-55}$ | $= 6.91 \times 10^{-47} + 1.25 \times 10^{-38}$ |
| | $= 2.62 \times 10^{-53}$ | $= 1.25 \times 10^{-38}$ |
| K _{tot} | $\kappa_{\rm th} + \kappa_{\rm nt}$ | $\kappa_{\rm th} + \kappa_{\rm nt}$ |
| (cm^{-1}) | $= 2.23 \times 10^{-38} + 8.64 \times 10^{-52}$ | $= 2.23 \times 10^{-34} + 7.11 \times 10^{-34}$ |
| | $= 2.23 \times 10^{-38}$ | $= 9.34 \times 10^{-34}$ |
| $\tau = \int_{z_{\text{init}}}^{0.0} \kappa_{\text{tot}}(z) \cdot \mathrm{d}s$ | 2.72×10^{-13} | 1.14×10^{-8} |
| $f_{\rm tot}$ | $f_{\rm th} + f_{\rm nt}$ | $f_{\rm th} + f_{\rm nt}$ |
| (cm^{-1}) | $= 2.54 \times 10^{-30} + 1.52 \times 10^{-33}$ | $= 1.16 \times 10^{-23} + 8.54 \times 10^{-28}$ |
| | $= 2.54 \times 10^{-30}$ | $= 1.16 \times 10^{-23}$ |
| h _{tot} | $h_{\rm th} + h_{\rm nt}$ | $h_{\rm th} + h_{\rm nt}$ |
| (cm^{-1}) | $= 3.76 \times 10^{-42} + 8.12 \times 10^{-43}$ | $= 1.72 \times 10^{-32} + 3.01 \times 10^{-32}$ |
| | $= 4.57 \times 10^{-42}$ | $= 4.72 \times 10^{-32}$ |

Table G.1: Values of the transfer coefficients and optical depths computed using parameters of models A-I and B-I at the radiation frequency v = 1.4 GHz. The transfer coefficients have a very small order of magnitude, suggesting a scale length of a few Mpc.

Appendix H

Rotating Wigner Coefficients

Sec. 5.3.1 shows how the Wigner coefficients offset from the North pole can be rotated to be centred on the North pole. Here, I present the detailed mathematical steps, which is also general to arbitrary rotation of Wigner coefficients.

The additive property of the Wigner D-functions is given by

$$D_{nm}^{\ell}(\rho') = \sum_{k=-\ell}^{\ell} D_{mk}^{\ell}(\rho) D_{kn}^{\ell}(\rho^{\star})$$
(H.1)

Marinucci and Peccati (2011). Using this, Eqn. (5.29) can be rewritten as

$$\sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \sum_{n=-\ell}^{\ell} \frac{2\ell+1}{8\pi^2} \left(W^{s\psi^{(j)}} \right)_{mn}^{\ell} D_{mn}^{\ell^*}(\rho)$$

$$= \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \sum_{n=-\ell}^{\ell} \frac{2\ell+1}{8\pi^2} \left(\widetilde{W}^{s\widetilde{\psi}^{(j)}} \right)_{mn}^{\ell} \sum_{k=-\ell}^{\ell} D_{mk}^{\ell^*}(\rho) D_{kn}^{\ell^*}(\rho^*)$$

$$= \sum_{k=-\ell}^{\ell} \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \frac{2\ell+1}{8\pi^2} D_{mk}^{\ell^*}(\rho) \sum_{n=-\ell}^{\ell} \left(\widetilde{W}^{s\widetilde{\psi}^{(j)}} \right)_{mn}^{\ell} D_{kn}^{\ell^*}(\rho^*) .$$
(H.2)

It follows that the Wigner coefficients may be rotated by

$$(W^{s\psi^{(j)}})_{mk}^{\ell} = \sum_{n=-\ell}^{\ell} (\widetilde{W}^{s\widetilde{\psi}^{(j)}})_{mn}^{\ell} D_{kn}^{\ell}^{*}(\rho^{\star}) .$$
 (H.3)

This related is used in Eqn. (5.30).

Appendix I

Parabolic Scaling of Spin Curvelets

As noted in Sec. 5.2.1, due to the asymmetric property of $d_{\ell(-s)}^{\ell}(\theta)$ about θ_{\max} as $s \to (\ell - 1)$, the parabolic scaling relation which has been shown to hold for cases s = 0 and $s \ll \ell$ may start to break down. To investigate at which *s* the offset from parabolic scaling becomes important, the absolute percentage differences between FWHM_{θ}^{s>0} and FWHM_{θ}^{s=0} at a set of test values $\ell = 2^p$ are evaluated, where *p* runs from 1 to 8. The empirical results are plotted in Fig. I.1, from which one can see that for up to $s \simeq \ell/2$ in all test- ℓ cases, FWHM_{θ}^{s>0} (i.e. the spin setting) remains very close to FWHM_{θ}^{s=0}, with a percentage error < 0.05%. Hence, $s \simeq \lfloor \ell/2 \rfloor$ can serve as a very conservative limit for which the typical curvelet parabolic scaling relation holds to a good approximation.



Fig. I.1: Numerical accuracy (i.e. 100 minus the absolute percentage difference between FWHM_{θ}^{s>0} and FWHM_{θ}^{s=0}) against the spin value *s* of curvelets. Different curves (from left to right) correspond to different fixed $\ell = 2^p$ cases, where integer *p* runs from 1 to 8. The results show that FWHM_{θ}^{s>0} (i.e. the spin setting) remains very close to FWHM_{θ}^{s=0} (i.e. the scalar setting, for which typical curvelet parabolic scaling relation has been shown to hold). This suggests that the parabolic scaling relation should hold for at least $s \simeq \lfloor \ell/2 \rfloor$, conservatively speaking. For *s* approaching ℓ , the parabolic scaling relation still holds to a good approximation. Even in the worst case when $s = \ell - 1$, the error may be tolerable (e.g. the error is within 5% at $\ell = 256$).

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