Extension to the Quantum Langevin Equation in the Incoherent Hopping Regime.

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An extension to the quantum Langevin equation is derived, that is valid in the incoherent hopping regime, and which allows one to incorporate quantum tunneling events. This is achieved by the inclusion of additional stochastic variables in the Langevin equation representing the tunneling events. A systematic derivation of this extension and of its regime of validity is presented. The study is motivated by efforts to determine the error in reading the state of a super-conducting quantum bit.

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The quantum Langevin equation[1, 2] provides a physically appealing and numerically simple description of the dynamics of a system coupled to a heat bath. It describes the system's non-linear semiclasical dynamics and the effects of coupling to quantum and thermal fluctuations in the heat bath. It does not, however, describe quantum tunneling of the system. Instanton approaches[3, 4, 5] provide a powerful framework in which to describe these latter effects. Here, we synthesize these two methods within an extended quantum Langevin equation that includes quantum tunneling. We focus upon two effects; quantum tunneling through or reflection from an energy barrier. These may be incorporated into the Langevin equation by the inclusion of additional stochastic variables, representing the tunneling and reflection events. This is valid in the regime of incoherent hopping.

Specifically, we concentrate upon the case of the Josephson junction. Quantum Langevin equations have been used extensively in the study of such systems. Recent experiments[6, 7] have probed Josephson junctions in regimes where current analytical tools do not provide a full description. In the experiments of Refs.[6, 7], a Josephson junction was used to read out the state of a charge/phase quantum bit. The most recent[7] made novel use of the *non-linear*, semi-classical dynamics of the junction through its vicinity to a classical bifurcation instability. Readout incurred errors due to quantum effects (tunneling between phase-space trajectories[8]) and thermal and quantum fluctuations in the transmission line. Here, we consider an experimentally realisable alternative scheme where the junction absorbs energy from a chirped microwave pulse with frequency modulated to match the response of the junction (whose frequency falls as the amplitude of its response increases). Depending upon the state of the qubit, the junction will either absorb enough energy to surmount the barrier— leading to a π phase-shift in the reflected signal— or not. The readout incurs errors due to the effect of the bath and due to quantum tunneling/reflection at the barrier.

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In order to fully understand such systems one must describe the non-linear semi-classical dynamics and quantum tunneling in concert with coupling to thermal and quantum fluctuations in the bath. One approach is to follow the evolution of the density matrix through its master equation. This is numerically extremely intensive when the Josephson junction contains more than a few levels. An extension of the Langevin equation is, therefore, highly desirable[9]. We first give a heuristic justification for such an extension, before turning to a derivation within a Keldysh field theory. We describe how this extended Langevin equation may be used to estimate errors in the chirped pulse readout scheme.

Consider a Josephson junction coupled by a transmission lead of impedance Z to measurement apparatus. The quantum Langevin equation is given by[3]

$$\left(\frac{\hbar}{2e}\right) C_J \ddot{\phi} + I_J \sin\phi(t) + \frac{1}{Z}\left(\frac{\hbar}{2e}\right)\dot{\phi}(t) = I_N(t) + I_D(t)$$
$$\langle I_N(\omega) I_N(-\omega)\rangle = 2\hbar\omega \frac{1}{Z}\coth[\hbar\omega/2T], \quad (1)$$

$\phi(t)$ is the phase difference of the superconducting order parameter across the junction, C_J is the junction capacitance and I_J is the Josephson current ($I_J = (2e/\hbar)E_J$, where E_J is the Josephson energy). Fluctuations in the transmission line produce a current noise $I_N(t)$. $I_D(t)$ is a drive current produced by the microwave source.

It is useful to explicitly introduce the charge, $n(t)$, on the junction and re-write the quantum Langevin equation (1) as a pair of coupled equations;

$$\left(\frac{\hbar}{2e}\right)\dot{\phi} - \frac{n}{C_J} = 0$$
$$\dot{n} - \left(\frac{\hbar}{2e}\right)\frac{\dot{\phi}}{Z} + \dot{q} + I_J \sin(\phi) = I_D(t)$$
$$\langle q(\omega) q(-\omega)\rangle = \frac{2\hbar}{\omega Z}\coth(\hbar\omega/2T) \quad (2)$$

The noise is now given in terms of fluctuations in the charge on the transmission lead, $q(t)$. Eliminating n from Eqs.(2) and substituting $\dot{q} = I_N$ recovers Eq.(1).

The dynamics of the Josephson junction is equivalent to that of a rigid pendulum; the superconducting phase difference plays the role of the angle of the pendulum and the Josephson potential the role of the gravitational potential. If the pendulum does not quite have enough energy to perform a complete revolution, classically, it will momentarily stop at some angle short of the vertical and then reverse its motion. Quantum mechanics allows the pendulum to tunnel through the remaining potential barrier. If the pendulum does have sufficient energy to pass through the vertical, the pendulum may be quantum mechanically reflected from the barrier and its motion reversed. These two processes can be represented by boundary conditions for the phase of the junction; $\phi \to -\phi$ at $t(\dot{\phi} = 0)$ and $\dot{\phi} \to -\dot{\phi}$ at $t(\phi = \pm\pi)$ or, re-expressing these using the first of Eqs. (2)

$$\begin{aligned} \phi &\to -\phi \qquad \text{at} \quad t(n = 0) \\ n &\to -n \qquad \text{at} \quad t(\phi = \pm\pi) \end{aligned} \tag{3}$$

At each juncture where the junction/pendulum is momentarily stationary short of the vertical or passing through the upwards vertical, with some probability, ϕ and n are modified by quantum processes according to Eqs. (3). We may heuristically modify the Langevin equation in order to incorporate these effects by the addition of suitable δ-functions as follows:

$$\left(\frac{\hbar}{2e}\right)\dot{\phi} - \frac{n}{C} = -2\left(\frac{\hbar}{2e}\right)\sum_a \eta_a \phi(t_a)\delta(t - t_a)$$

$$\dot{n} - \left(\frac{\hbar}{2e}\right)\frac{\dot{\phi}}{Z} + \dot{q} + I_J \sin\phi$$

$$= -2\sum_b \eta_b n(t_b)\delta(t - t_b) + I_D(t)$$

$$\langle q(\omega)q(-\omega)\rangle = \frac{2\hbar}{\omega Z}\coth(\omega/2T). \tag{4}$$

t_a are times such that $n(t_a) = 0$ and t_b such that $\phi(t_b) = \pm\pi$. η_a and η_b are additional stochastic variables accounting for the probability of quantum tunneling/reflection. They take the values $\eta = 0$ or 1 with a probability $P(\eta)$ that is a function of the energy of the junction at the stationary point, $E = E_J(1 + \cos\phi(t)) + n^2/2C$. Without a bath, $P(\eta = 1) = 1/(e^{2\pi E/\Omega} + 1)$, where $\Omega = (2e/\hbar)\sqrt{E_J/C}$ is the curvature at the top of the junction potential. Coupling to the bath renormalizes the potential[3] giving $\Omega = (2e/\hbar)\sqrt{E_J/C}\left[1 - (2e/\hbar)\sqrt{E_J/Z^2C^3}\right]$. Further corrections occur due to the finite drive[4, 5] and may be incorporated *via* additional modifications to $P(\eta)$. In the case of the chirped drive, the potential is zero at the stationary points and these corrections are not required.

In a chirped readout, the junction will gradually absorb energy from the microwave drive and go through a number of stationary points at which it approaches within an (decreasing) energy E of the top of the junction potential. Coupling to fluctuations in the transmission line leads to an energy uncertainty $\Delta E = T$ at high temperatures; this may be seen by linearizing Eq.(4) around the classical, zero-noise solution with a chirped drive. The error probability at each stationary point is given by the convolution of the distribution of arrival energy with the tunneling probability. The total error probability is given by $\sum_{n=1}^{n=n_{max}} [\prod_{i=1}^{n-1}(1-p_i)]p_n$, where p_n is the error probability at the nth stationary point. When the chirped drive takes only a few cycles to bring the junction to the top of its potential, only the error probability $p_{n_{max}}$ will be significant. In this case, analytic approximations to the error probability may be made. In the more general case, numerical integration of Eq.(4) provides an elegant way of calculating the cumulative effect of errors.

Next, we derive the modified Langevin Eq.(4) from a Keldysh field theory. The kernel for propagation of the density matrix may be expressed as a Schwinger-Keldysh field theory[11, 12, 13, 14]. In essence, the Keldysh field theory expresses the propagation of the right and left projections of the density matrix in terms of fields which propagate forwards and backwards in time[14]. It is useful to make a change of basis to the sums and differences of these fields. Since classical field configurations take the same value for both forwards and backwards propagation in time, the sum is known as the classical component (denoted below with a subscript c) and the difference is known as the quantum component (denoted with a subscript q). In certain circumstances (discussed below) the effective theory of the classical components can be expressed as a quantum Langevin equation[1].

The Keldysh Lagrangian for the Josephson junction is

$$\begin{aligned} & \mathcal{L}(n, \phi, Q, V) \\ = \; & \frac{\hbar}{2e} n\sigma_x^{qc}\dot{\phi} - \frac{n\sigma_x^{qc} n}{2C_J} + E_J\left(\cos(\phi_c + \phi_q) - \cos(\phi_c - \phi_q)\right) \\ & + Q\sigma_x^{qc}\left(\frac{\hbar}{2e}\dot{\phi} - V\right) + \frac{1}{2}V(t)\int_{-\infty}^{\infty} dt' \mathbf{D}^{-1}(t,t')V(t') \end{aligned} \tag{5}$$

The fields n, ϕ, Q and V are vectors in the Keldysh (quantum/classical) space, *e.g* $\phi \equiv (\phi_c(t), \phi_q(t))$, except where the indices q or c are given explicitly. Q is a Lagrange multiplier that imposes the Josephson relation $V = \hbar\dot{\phi}/2e$ and V is the voltage across the junction. The first term expresses the fact that ϕ and n are conjugate, the second term gives the charging energy and the third term the Josephson energy (or non-linear inductance energy). The final term describes voltage fluctuations at the end of the transmission line. The correlation matrix is given, in the Keldysh basis, by

$$\mathbf{D}(t_1, t_2) = -i\langle V_\alpha(t_1)V_\beta(t_2)\rangle = \begin{pmatrix} D_K(t_{12}) & D_R(t_{12}) \\ D_A(t_{12}) & 0 \end{pmatrix}.$$

where the subscripts K, R and A refer to Keldysh, retarded and advanced correlators, respectively. These are calculated for a transmission lead in thermal equilibrium;

$$\begin{aligned} D_R(t_{12}) &= D_A(t_{21}) = -\frac{i}{2}\theta(t_1 - t_2)\langle[V(t_1), V(t_2)]\rangle \\ D_K(t_{12}) &= -\frac{i}{2}\langle\{V(t_1), V(t_2)\}\rangle \end{aligned}$$

Their Fourier transforms are $D_R(\omega) = i(\omega - i\delta)Z$ and $D_K(\omega) = 2i\omega Z \coth(\omega/2T)$. The quantum Langevin equation (2) can be derived from Eq. (5) as follows[1, 2]: After integrating over Q, V is replaced by $\hbar\dot{\phi}/2e$ in the final term. The Josephson potential term is linearized in ϕ_q, reducing it to $2\phi_q E_J \sin\phi_c$. This assumes that the quantum mechanical spread of the phase difference is small[15]. The term quadratic in ϕ_q is decoupled *via* a Hubbard-Stratonovich transformation with a field $\dot{q}$. The resulting theory is linear in ϕ_q and n_q. Integrating over these fields leads to δ-functionals that impose Eqs.(2). The remaining quadratic Lagrangian for $q(t)$ determines its correlation function; $\langle q(\omega)q(-\omega)\rangle = D_K(\omega)/[D_R(\omega)D_A(\omega)]$. After these manipulations, the Keldysh partition function reduces to

$$
\begin{aligned}
\mathcal{Z} &= \int D\phi_c Dn_c \delta\left[\left(\frac{\hbar}{2e}\right)\dot{\phi} - \frac{n}{C}\right] \\
&\times \delta\left[\dot{n} - \left(\frac{\hbar}{2e}\right)\frac{\dot{\phi}}{Z} + \dot{q} + 2I_J\sin(\phi)\right] \\
&\times \exp\left[-\frac{\hbar}{\omega Z}\coth(\hbar\omega/2T)q(\omega)q(-\omega)\right] \qquad (6)
\end{aligned}
$$

which is equivalent to Eqs.(2).

This derivation ignores instantons; imaginary-time diversions of the Keldysh contour. These describe the quantum tunneling and reflection discussed in our heuristic derivation of the extended Langevin Eq.(4). Instantons occur on both the outgoing and return parts of the Keldysh contour, as shown in Fig.1. Each dot corresponds to an imaginary time excursion in the evolution of the fields in the path integral. During the imaginary-time evolution, the potential is inverted and the equations of motion are such that the particle can travel between minima of the potential in a classically forbidden way[16].

Consider the effect of a single instanton at time t_0 on the upper part of the Keldysh contour that takes the forward propagating ϕ_+ to $-\phi_+$. This instanton leads to boundary conditions $\phi_+(t_0 - 0^+) = -\phi_+(t_0 + 0^+)$ in the path integral for the real-time evolution of the fields $\phi(t)$ and $n(t)$. The probability of this instanton is given by the exponential of its classical action[16], possibly modified by finite drive currents[4, 5]. The full path integral includes a sum over all possible configurations and numbers of instantons, weighted with the appropriate probability. In the absence of a bath, these instantons are positioned independently on the Keldysh contour each occurring at a stationary point of the classical evolution[16].

Coupling to bath fluctuations induces interactions between instantons, tending to bind them in pairs. Pairing occurs both between instantons and anti-instantons on the same part of the Keldysh contour and on opposite parts of the the Keldysh contour. Consider one instanton and one anti-instanton both on the upper contour. In the time between these two instantons, the fields on the upper and lower contour are very different and ϕ_q is large. A large cost is incurred in the action due

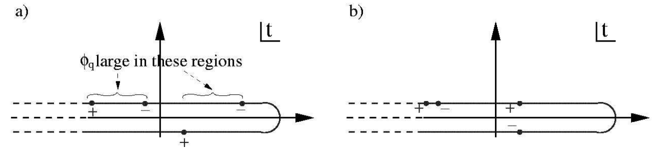

FIG. 1: **Schematic Diagram of the Real Time Integration Contour Including Instantons.** a) Shows the regime of coherent hopping where instantons are unbound. b) Shows the regime of incoherent hopping, where instantons are bound in pairs.

to the term $(\hbar/2e)^2\dot{\phi}_q(\omega)\dot{\phi}_q(-\omega)D_K(\omega)D_R^{-1}(\omega)D_A^{-1}(\omega)$, causing an attractive interaction between the instanton and anti-instanton. Similar arguments apply for an instanton/anti-instanton pair on opposite parts of the Keldysh contour. The transition between the bound and unbound phase of the instantons is the diffusion/localisation transition of Ref.[17]. A large value of ϕ_q implies that the system is in a coherent superposition of very different classical states. Coupling to a heat bath causes this coherence to decay; in a sense the heat bath *measures* the state of the system.

For an instanton/anti-instanton pair separated by a real time τ, the quantum component of the junction phase is given by $\phi_q(t) = 2\pi[\theta(t+\tau/2) - \theta(t-\tau/2)]$, so that $\phi_q(\omega) = \pi\tau\sin(\omega\tau/2)/(\omega\tau/2)$. Using a high-momentum cut-off, Λ and in the limit $T \to 0$, $D_K/(D_A D_R) = 2|\omega|(1 + 2e^{-\hbar|\omega|/kT})/Z$ and the dissipative contribution to the action is given by $\mathcal{S}_{Diss} = i(h/2e^2 Z)[\ln(\Lambda\tau) + (kT\tau/\hbar)^2]$. We interpret $e^{i\mathcal{S}_{Diss}/\hbar}$ as a distribution function for τ. At zero temperature, one finds that for $Z < h/2e^2$ the instantons are bound and tunneling is incoherent. At finite temperatures, the instantons are, strictly, always bound on a timescale of order $\tau \sim (2\pi e/k)\sqrt{2hZ}$; coherence between tunneling events is lost on timescales greater than this.

Now let us incorporate these ingredients into an extended Langevin equation. The Langevin equation is the effective theory of the *classical* part of the fields, represented as a differential equation with noise. Of course, it is not always (or even usually) possible to represent a field theory in this way. The key feature above that allowed the effective theory for the classical components to be written in Langevin form was that all terms, aside from the coupling to the bath, could be linearized in the quantum components. This required that the quantum components be small, a condition that is satisfied explicitly in the incoherent hopping regime [1, 2, 15]. In this regime, we can decouple the quadratic term in ϕ_q as before. The path integral reduces to a sum over sectors with different configurations of instanton pairs (we need only consider pairs between the upper and lower part of the Keldysh contour; those on the same contour will have no effect). Each sector is weighted in the sum by the probability of producing the instanton pairs[3, 16]. After integrating out n_q and ϕ_q the partition function reduces to

$$\mathcal{Z} = \sum_{\{t_a,t_b\}} \prod_{\{t_a,t_b\}} \int_{\substack{\phi_c(t_a-0)=-\phi_c(t_a+0)\\ n_c(t_a-0)=-n_c(t_a+0)}} D\phi_c Dn_c$$
$$\times\delta\left[\left(\frac{\hbar}{2e}\right)\dot{\phi}-\frac{n}{C}\right]\delta\left[\dot{n}-\left(\frac{\hbar}{2e}\right)\frac{\dot{\phi}}{Z}+\dot{q}+2I_J\sin(\phi)\right]$$
$$\times\exp\left[-\frac{\hbar}{\omega Z}\coth(\hbar\omega/2T)q(\omega)q(-\omega)\right]P(t_a)P(t_b). \quad (7)$$

$P(t_a)$ is the probability of producing the instanton pair corresponding to tunneling and $P(t_b)$ the probability of a pair corresponding to reflection. The path integrals over ϕ_c and n_c are carried out with the boundary conditions for the configuration of instantons in that sector. We encode these boundary conditions within the δ-functionals as follows:

$$\mathcal{Z} = \sum_{\{t_a,t_b\}} \prod_{\{t_a,t_b\}} P(t_a)P(t_b)\int D\phi_c Dn_c$$
$$\times\delta\left[\left(\frac{\hbar}{2e}\right)\dot{\phi}-\frac{n}{C}+2\left(\frac{\hbar}{2e}\right)\sum_a \phi(t_a)\delta(t-t_a)\right]$$
$$\times\delta\left[\dot{n}-\frac{\hbar\dot{\phi}}{2eZ}+\dot{q}+2I_J\sin(\phi)+2\sum_b n(t_b)\delta(t-t_b)\right]$$
$$\times\exp\left[-\frac{\hbar}{\omega Z}\coth(\hbar\omega/2T)q(\omega)q(-\omega)\right] \quad (8)$$

Eq. (8) is equivalent to the extended Langevin equation(4). The drive current $I_D(t)$ on the right-hand side of the second of Eqs.(4) arises *via* a term $I_D(t)\phi_q(t)$ in Eq.(5). The drive leads to a modification of the instanton action and probability due to the possibility of photon assisted tunneling[4]. The extended quantum Langevin equation (4) is valid in the regime of incoherent hopping provided that the constituent steps—the derivation of the quantum Langevin equation itself [1, 2, 15] and the instanton calculation [3, 4, 18]— are valid.

To conclude, we have considered an instanton expansion within the Keldysh field theory of a Josephson junction coupled to a heat bath. Using this expansion, we have developed extensions to the quantum Langevin equation, which incorporate quantum features of the junction dynamics. This extended Langevin equation represents a synthesis of established techniques for dealing with semi-classical dynamics in the presence of environmental fluctuations[1, 2] and tunneling[3, 4]. It is valid in the regime of incoherent hopping. This extended Langevin equation allows numerical simulation of the junction dynamics in response to a time-dependent drive current, including quantum and thermal effects of the bath, non-linear classical dynamics and quantum dynamics of the junction.

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