Symmetries of cyclic work distributions for an isolated harmonic oscillator

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Abstract. We have calculated the distribution of work W done on a 1-d harmonic oscillator that is initially in canonical equilibrium at temperature T, then thermally isolated and driven by an arbitrary time-dependent cyclic spring constant $\kappa(t)$, and demonstrated that it satisfies $P(W) = \exp(\beta W)P(-W)$, where $\beta = 1/k_B T$, in both classical and quantum dynamics. This differs from the celebrated Crooks relation of nonequilibrium thermodynamics, since the latter relates distributions for forward and backward protocols of driving. We show that it is a special case of a symmetry that holds for non-cyclic work processes on the isolated oscillator, and that consideration of time reversal invariance shows it to be consistent with the Crooks relation. We have verified that the symmetry holds in both classical and quantum treatments of the dynamics, but that inherent uncertainty in the latter case leads to greater fluctuations in work performed for a given process.

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1. Introduction

The Crooks relation [1] states that the outcome of the mechanical processing of a system according to a prescribed sequence of actions is related to the outcome of a process consisting of the reversed sequence. It is a connection between the probability distributions of the amount of work W performed on the system in the course of such forward and backward processes, $P_{\rm F}(W)$ and $P_{\rm B}(W)$, respectively. A forward process might consist of the movement of a piston to compress a gas in a cylinder, while the backward process would be the opposite movement to expand the gas [2]. The validity of the Crooks relation requires that the system should start out in canonical equilibrium at the same temperature T for both processes. The system might maintain contact with a heat bath at that temperature during the processing or it could be isolated. The relation reads

$$P_{\rm F}(W) = \exp\left(\beta\left(W - \Delta F\right)\right) P_{\rm B}(-W), \qquad (1)$$

where $\beta = 1/k_B T$ and ΔF is the change in free energy of the system associated with the forward process, evaluated for example on the basis of the isothermal change in volume of the expanded gas. Equation (1) states that the probability that the forward process should require an input of work W, and the probability of requiring work $-W$ (in other words receiving work from the system) during the backward process, are related to each other, but are not in general equal. The relation has been shown to hold for a variety of choices of dynamics, though studies reveal that it is important to define carefully what is meant by work, particularly for strong coupling between a system and its environment [3, 4]. It implies [5] the Jarzynski equality $\langle \exp\left(-\beta\left(W - \Delta F\right)\right)\rangle = 1$, which in turn leads to $\langle W\rangle \geq \Delta F$ for a forward process starting in equilibrium, where the brackets indicate an average taken over the probability distribution of work done. This, of course, is a statement of the second law of thermodynamics, and the Crooks relation, Jarzynski equality and the associated fluctuation relations have received a great deal of attention as a result (see, for example [6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 3, 18]).

It has proved valuable to study the Crooks relation in the context of simple examples [19, 2, 20, 21, 22, 23, 24] in order to gain insight into its operation in more complex cases, and the 1-d harmonic oscillator has proved to be a popular system. The main purpose of this paper is to calculate work distributions for an isolated oscillator using a geometric and pictorial approach that has, we believe, some intuitive pedagogical value. In doing so, we expose a broader symmetry of the distribution of work for such a forward process, which has its origin in the simplicity of the dynamics of the harmonic oscillator, and which demonstrates the rather special character of this system with regard to its fluctuation behaviour.

Work is performed by prescribing a time-dependent spring constant $\kappa(t)$ during the process. If the spring constant varies cyclically in an interval $0 \leq t \leq \tau$ such that $\kappa(\tau) = \kappa(0)$, then $\Delta F = 0$, and moreover if the process takes place under conditions of thermal isolation, then no heat is exchanged during the cycle and $W = \Delta E$, the change in system energy. The Crooks relation reduces to $P_{\rm F}(\Delta E) = \exp(\beta \Delta E) P_{\rm B}(-\Delta E)$: a result verified, for example, by Deffner and Lutz [21, 25]. But our approach to solving the classical evolution demonstrates that a relation $P_{\rm F}(\Delta E) = \exp(\beta L \Delta E) P_{\rm F}(-\Delta E)$ also holds for a class of forward processes, with the parameter L depending on the nature of the process, and with $P_{\rm F}(\Delta E)$ taking a specified analytic form. It is quite compatible with the Crooks relation for a cyclic forward process and its backward counterpart, for which $L = 1$ and $P_{\rm F}(\Delta E) = P_{\rm B}(\Delta E)$, as we shall show. We also compare the continuous distribution of work arising from a classical treatment with the discrete distribution of work that emerges from the quantum treatment of a cyclic process to show that these properties are preserved. Fluctuations in the quantum case are broader, as a result of the wider range of possible outcomes made possible by the dynamics.

In the next section we analyse a general work process performed on a classical harmonic oscillator, represented in terms of a matrix operation on a system phasor. We evaluate the probability distribution function (pdf) of system energy change for $M \geq 1$ independent oscillators. We go on to treat the system quantum mechanically in section 3, particularly to contrast the widths of the classical and quantum pdfs for cyclic processes. Our conclusions are given in section 4.

2. Classical treatment

2.1. System phasor and process matrix

It is convenient to convert the time-dependent spring constant $\kappa(t)$ into a time-dependent natural frequency $\omega(t)$, so that the Hamiltonian at time t is

$$H(t) = p^2/2m + m\omega^2(t)x^2/2, \tag{2}$$

and the equation of motion is $\ddot{x} = -\omega^2 x$, where p and x are the momentum and position of the oscillator, and m is its mass. The response of the system may be illustrated using pictures of phase space orbits. An isolated system with constant frequency ω_0 performs clockwise circular orbits in a phase space where momentum is normalised by dividing by $m\omega_0$. The square of the radius of the orbit is proportional to the initial energy of the oscillator. If the spring constant is changed at time t_i, altering ω and the energy, then the system moves onto an elliptical orbit. A process consisting of a sequence of shifts in spring constant without contact with a heat bath can therefore be visualised as transitions to, and movement along, a set of elliptical orbits in phase space. But if the process is cyclic, characterised by a return to the original spring constant, the final orbit will be circular. Whether the energy of the system has increased or decreased as a result of the process then depends on whether the radius of the final orbit is greater than or less than the initial radius, respectively. This is illustrated in Figure 1 for a process consisting of a shift down and up in spring constant. The implication is that both upward and downward changes in energy can be generated. With the exception of some special cases, where motion on the intermediate orbit consists of one complete circuit for example, in which case $\Delta E = 0$ always, a cyclic process clearly produces a pdf that describes both positive and negative ΔE.

Let us consider a general variation in $\omega(t)$ in the interval $0 \leq t \leq \tau$, with $\omega = \omega_0 = \omega(0)$ for $t < 0$ and $\omega = \omega_N = \omega(\tau)$ for $t > \tau$. In the initial and final situations the motion will be sinusoidal, but with differing phases and amplitudes in general. We write $x(t) = A\exp(\mathrm{i}\omega_0 t) + A^* \exp(-\mathrm{i}\omega_0 t)$, where A is a complex phasor representing the phase and amplitude. The process in the interval $0 \leq t \leq \tau$ will then map an initial phasor A onto a final phasor $A' = SA$, with a matrix representation

$$\begin{pmatrix} A'_\mathrm{r} \\ A'_\mathrm{i} \end{pmatrix} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} A_\mathrm{r} \\ A_\mathrm{i} \end{pmatrix}, \tag{3}$$

where A_r and A_i are the real and imaginary parts of the phasor A. We shall call S the *process matrix.*

The energy of an oscillation with phasor A and angular frequency ω can be written as $2m\omega^2 A^T A$, so the change in energy brought about by the process is

$$\Delta E = 2m\omega_0^2 A^T \left(D^2 S^T S - I\right) A, \tag{4}$$

where $D = \omega_N/\omega_0$ and I is the unit 2×2 matrix. In terms of magnitude $\mid A \mid$ and phase $\theta = \tan^{-1}(\dot{x}(0)/\omega_0 x(0))$:

$$A = \mid A \mid \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix} \tag{5}$$

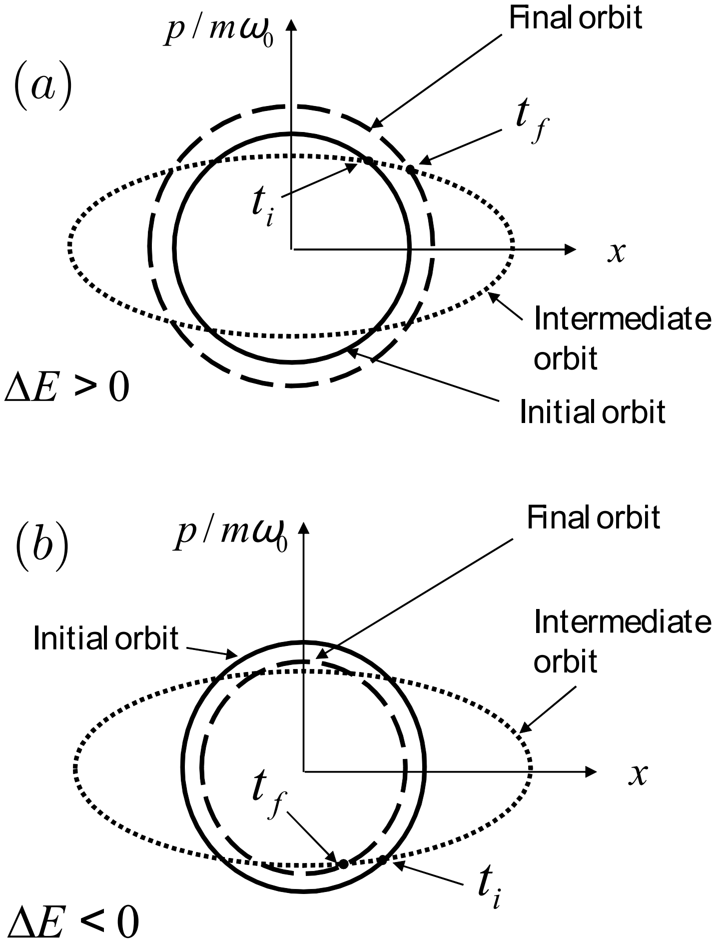

Figure 1. The system moves clockwise on a circular orbit in phase space until the spring constant changes at $t = t_i$ and it moves onto an elliptical orbit. The cycle is completed by a change in spring constant at $t = t_f$ to return the system to a circular orbit. Depending on the initial location of the system on its orbit, and the duration of the process, the radius of the final orbit could be (*a*) greater than or (*b*) less than the initial radius, illustrating how the energy change can be both positive or negative.

we find that

$$\Delta E = E\left(C_1 + C_2 \cos 2\theta + C_3 \sin 2\theta\right), \tag{6}$$

where $E = 2m\omega_0^2 |A|^2$ is the initial energy of the oscillator, and the constants C_1, C_2 and C_3 can be expressed in terms of the elements of S:

$$C_1 = \frac{D^2}{2}\left(a^2 + b^2 + c^2 + d^2\right) - 1 \tag{7}$$

$$C_2 = \frac{D^2}{2}\left(a^2 - b^2 + c^2 - d^2\right) \tag{8}$$

$$C_3 = D^2(ab + cd). \tag{9}$$

Let us consider a sequence of step changes in frequency from ω_{n-1} to ω_n at times $t_n = n\delta t$, such that in the interval $t_n \le t \le t_{n+1}$ the displacement is represented by

$$x(t) = A_n \exp\left(\mathrm{i}\omega_n\left(t - t_n\right)\right) + A_n^* \exp\left(-\mathrm{i}\omega_n\left(t - t_n\right)\right). \tag{10}$$

Imposing continuity requirements for x and $\dot{x}$ at $t=t_n$, we express A_n in terms of A_{n-1}:

$$\begin{aligned}A_n=\frac{1}{2}\Big(&A_{n-1}\exp\left(\mathrm{i}\omega_{n-1}\delta t\right)\left(1+\frac{\omega_{n-1}}{\omega_n}\right)\\&+A^*_{n-1}\exp\left(-\mathrm{i}\omega_{n-1}\delta t\right)\left(1-\frac{\omega_{n-1}}{\omega_n}\right)\Big).\end{aligned}\tag{11}$$

The *step* matrix S_n, representing the transformation from A_{n-1} to A_n through the relation $A_n=S_nA_{n-1}$, has the following structure:

$$\begin{pmatrix} c_{n-1} & -s_{n-1}\\ \frac{\omega_{n-1}}{\omega_n}s_{n-1} & \frac{\omega_{n-1}}{\omega_n}c_{n-1}\end{pmatrix}=\begin{pmatrix}1 & 0\\ 0 & \frac{\omega_{n-1}}{\omega_n}\end{pmatrix}\begin{pmatrix}c_{n-1} & -s_{n-1}\\ s_{n-1} & c_{n-1}\end{pmatrix},\tag{12}$$

where $c_{n-1}=\cos(\omega_{n-1}\delta t)$ and $s_{n-1}=\sin(\omega_{n-1}\delta t)$, corresponding to a rotation through phase angle $\omega_{n-1}\delta t$, followed by a rescaling of the imaginary part of the phasor. The process matrix S may then be constructed from the step matrices as $S=S_NS_{N-1}...S_1$. Note that $\det S_n=\omega_{n-1}/\omega_n$ so that $\det S=(\omega_{N-1}/\omega_N)\cdots(\omega_0/\omega_1)=\omega_0/\omega_N=D^{-1}=ad-bc$ and this is unity if the process is cyclic with $\omega_N=\omega_0$. By introducing small step changes in ω, we can consider processes consisting of a continuous variation in spring constant.

2.2. Construction of $P(\triangle E)$

Consideration of all possible initial conditions establishes the pdf of energy change $P(\Delta E)$ due to the process. We assume a canonical distribution over points Γ in phase space now labelled by initial energy E and phase angle θ:

$$P(\Gamma)\mathrm{d}\Gamma=P(\theta|E)P(E)\mathrm{d}E\,\mathrm{d}\theta=\frac{1}{2\pi}\beta\mathrm{e}^{-\beta E}\mathrm{d}E\,\mathrm{d}\theta,\tag{13}$$

and hence the average of ΔE is

$$\begin{aligned}\langle\Delta E\rangle&=\int_0^{2\pi}\int_0^{\infty}\frac{\beta}{2\pi}\mathrm{e}^{-\beta E}E(C_1+C_2\cos 2\theta+C_3\sin 2\theta)\mathrm{d}E\mathrm{d}\theta\\&=C_1/\beta,\end{aligned}\tag{14}$$

which, through (9), establishes a connection between $\langle\Delta E\rangle$ and the elements of the process matrix S.

Consider next the pdf Φ of energy change ΔE for an oscillator with a given initial energy E. It is straightforward to write

$$\Phi(\Delta E,E)=\sum_{j=1}^{k}P(\theta_j|E)\left|\frac{\partial\theta}{\partial\Delta E}\right|_{\theta_j},\tag{15}$$

where $\theta_1...\theta_k$ are the values of θ that satisfy (6). We employ ΔE from (6) in the following form:

$$\triangle E=E\left(C_1+\left(C_2^2+C_3^2\right)^{1/2}\cos 2(\theta+\theta_0)\right),\tag{16}$$

where $\cos 2\theta_0=C_2/\left(C_2^2+C_3^2\right)^{1/2}$. Noting that, in non-exceptional cases, $k=4$ we write:

$$\Phi(\Delta E,E)=\frac{4}{2\pi}\left|\frac{\partial\theta}{\partial\Delta E}\right|=\frac{1}{\pi\left|E\left(C_2^2+C_3^2\right)^{1/2}\sin 2\phi\right|},\tag{17}$$

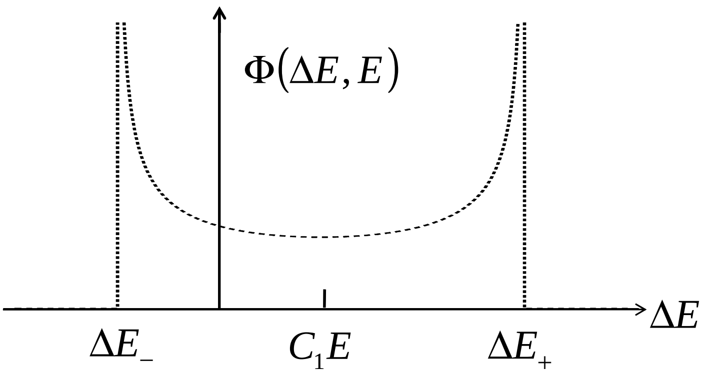

Figure 2. The pdf of energy change $\triangle E$ for an initial energy E, as specified in (18).

where $\phi = \theta + \theta_0$, and obtain

$$\begin{aligned}\Phi(\triangle E, E) &= \pi^{-1}\left(E^2(C_2^2+C_3^2) - (\triangle E - EC_1)^2\right)^{-1/2} \\ &= \frac{1}{\pi\left[(\triangle E - \Delta E_-)(\triangle E_+ - \Delta E)\right]^{1/2}}.\end{aligned} \tag{18}$$

This is valid for $\triangle E_- \leq \Delta E \leq \triangle E_+$, where $\triangle E_\pm = E\left(C_1 \pm \left(C_2^2+C_3^2\right)^{1/2}\right)$. Φ is zero outside this range, is symmetric about $\triangle E = EC_1$, and diverges at $\triangle E = \triangle E_\pm$, as illustrated in Figure 2.

Now we include the distribution of initial energies E. We write

$$P(\triangle E) \propto \int_0^\infty \Phi(\triangle E, E)\exp(-\beta E)\,\mathrm{d}E, \tag{19}$$

which for $\Delta E \geq 0$ may be cast more explicitly as

$$P(\triangle E) \propto \int_{\Delta E L_+}^\infty \Phi(\triangle E, E)\exp(-\beta E)\,\mathrm{d}E, \tag{20}$$

while for $\Delta E < 0$ we use

$$P(\triangle E) \propto \int_{\Delta E L_-}^\infty \Phi(\triangle E, E)\exp(-\beta E)\,\mathrm{d}E, \tag{21}$$

where $L_\pm = \left(C_1 \pm \left(C_2^2+C_3^2\right)^{1/2}\right)^{-1}$. We have assumed $C_2^2 + C_3^2 > C_1^2$ to ensure that both positive and negative ΔE are generated by the process: as we saw earlier this is almost always the case for a cyclic process. The integration limits are best understood by consideration of Figure 3. The lower integration limit $\Delta E L_+$ for the $\Delta E \geq 0$ case is the energy for which $\Delta E_+(E)$, the upper boundary of the range for which $\Phi(\triangle E, E)$ is non-zero, is equal to the given ΔE (shown as the dotted line). Similarly, the lower integration limit $\Delta E L_-$ for the $\Delta E < 0$ case is the energy such that $\Delta E_-(E) = -\Delta E$.

It is possible to reduce $P(\Delta E)$ to a simple analytic form for this situation. For positive ΔE we write

$$\begin{aligned}P(\Delta E) &\propto \int_0^\infty \Phi(\triangle E, E + \triangle E L_+)\mathrm{e}^{-\beta(E+\Delta E L_+)}\,\mathrm{d}E \\ &\propto \mathrm{e}^{-\beta\Delta E L_+}\int_0^\infty \frac{\exp(-\beta E)\,\mathrm{d}E}{\left((\Delta E(L_- - L_+) - E)E\right)^{1/2}} \\ &\propto \mathrm{e}^{-\beta\Delta E(L_+ + L_-)/2}K_0\left(\frac{\beta\Delta E}{2}(L_+ - L_-)\right),\end{aligned} \tag{22}$$

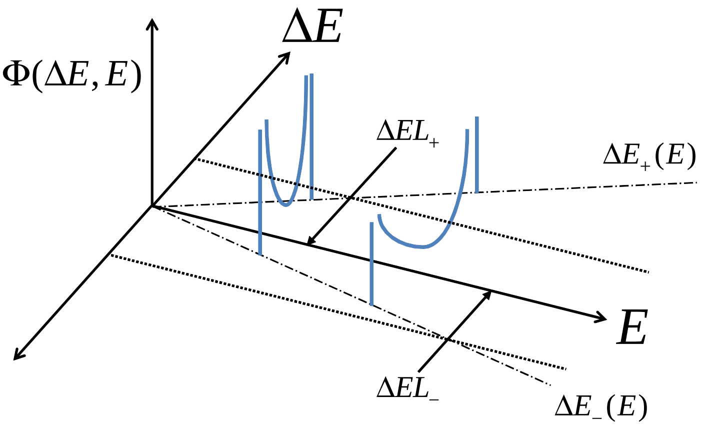

Figure 3. Indication of the domain of integration over the pdf $\Phi(\Delta E, E)$ for the case $C_1 > 0$. The function itself is sketched by curves similar to Figure 2 for two values of E.

where K_0 is a modified Bessel function of the second kind. The pdf for $\Delta E < 0$ may be constructed in a similar way:

$$\begin{aligned} P(\Delta E) &\propto \int_0^\infty \Phi(\triangle E; E + \triangle EL_-) \mathrm{e}^{-\beta(E+\Delta EL_-)} \,\mathrm{d}E \\ &\propto \mathrm{e}^{-\beta\Delta EL_-} \int_0^\infty \frac{\exp\left(-\beta E\right)\mathrm{d}E}{\left(-E\left(E - \Delta E(L_+ - L_-)\right)\right)^{1/2}} \\ &\propto \mathrm{e}^{-\beta\Delta E(L_+ + L_-)/2} K_0\left(-\frac{\beta\Delta E}{2}\left(L_+ - L_-\right)\right). \end{aligned} \tag{23}$$

We immediately notice a symmetry of the pdf of energy change:

$$P(\Delta E) = \exp(\beta L \Delta E) P(-\Delta E), \tag{24}$$

where $L = -(L_+ + L_-)$. This is reminiscent of the Crooks relation, but the distribution on both sides describes a forward process, whereas the Crooks relation concerns forward and reverse processes. A consequence is

$$\begin{aligned} \langle \exp(-\beta L \Delta E) \rangle &= \int_{-\infty}^{\infty} P(\Delta E) \exp(-\beta L \Delta E) \mathrm{d}\Delta E \\ &= \int_{-\infty}^{\infty} P(-\Delta E) \mathrm{d}\Delta E = 1, \end{aligned} \tag{25}$$

and by Jensen's inequality we deduce that $L\langle \Delta E \rangle \geq 0$.

We can express $P(\Delta E)$ in terms of process parameters C_1 and D since $C_2^2 + C_3^2 - C_1^2 = 2C_1 + 1 - D^2$ such that

$$L_+ - L_- = \frac{-2\left(C_2^2 + C_3^2\right)^{1/2}}{C_1^2 - C_2^2 - C_3^2} = \frac{2\left(C_1^2 + 2C_1 + 1 - D^2\right)^{1/2}}{2C_1 + 1 - D^2}, \tag{26}$$

and

$$L_+ + L_- = \frac{2C_1}{C_1^2 - C_2^2 - C_3^2} = -\frac{2C_1}{2C_1 + 1 - D^2}, \tag{27}$$

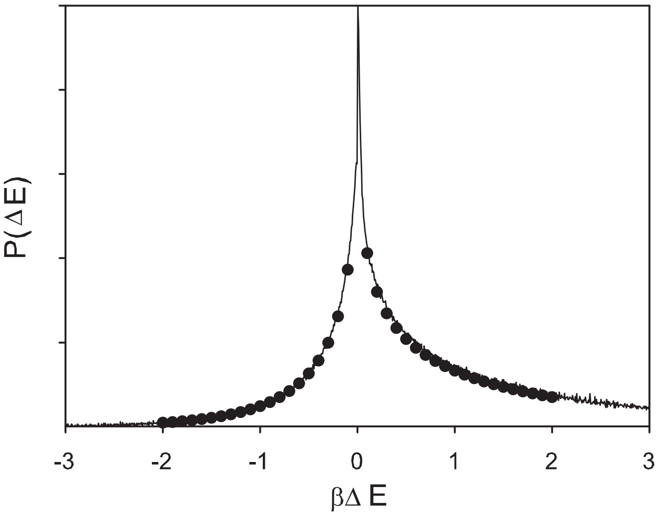

Figure 4. Distributions of energy change ΔE produced by a step up and step down in ω, generated from Monte Carlo (line) and (28) and (30) (points) with $\omega_1 = 2\omega_0$, $\omega_1\tau = \pi/2$ and $\beta = 1$.

implying that the pdf has a form that depends only on the mean energy change $\langle \Delta E\rangle = C_1/\beta$ and the ratio $D = \omega_0/\omega_N$, as long as $C_2^2 + C_3^2 - C_1^2 = 2C_1 + 1 - D^2 > 0$.

For simplicity let us now focus our attention on a cyclic process with $\omega_N = \omega_0$ and hence $D = 1$, $L = -(L_+ + L_-) = 1$ and $L_+ - L_- = (1 + 2/C_1)^{1/2}$. The earlier inequality implies that $\langle \Delta E\rangle \geq 0$ and $C_1 \geq 0$. The pdf takes the form

$$P(\Delta E) = \frac{\beta \exp\left(\beta \Delta E/2\right)}{\pi\sqrt{2\beta\langle \Delta E\rangle}} K_0\left(\frac{\beta|\Delta E|}{2}\left[1 + \frac{2}{\beta\langle \Delta E\rangle}\right]^{1/2}\right), \tag{28}$$

where a normalisation constant has been inserted. This form is consistent with $\langle \Delta E\rangle = \int_{-\infty}^{\infty} \Delta E\, P(\Delta E)\, \mathrm{d}\Delta E$. It is also consistent with the classical limit of the work distribution of a quantum harmonic oscillator for a cyclic process obtained by Deffner and Lutz [21].

2.3. Example cases

The analysis may be illustrated for a cyclic process consisting of a step change in frequency from ω_0 to ω_1 at $t = 0$, followed by another jump from ω_1 to ω_0 at $t = \tau$. The process matrix S takes the form

$$S = \begin{pmatrix} 1 & 0 \\ 0 & \frac{\omega_1}{\omega_0} \end{pmatrix} \begin{pmatrix} c_1 & -s_1 \\ s_1 & c_1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & \frac{\omega_0}{\omega_1} \end{pmatrix}, \tag{29}$$

where $c_1 = \cos\omega_1\tau$ and $s_1 = \sin\omega_1\tau$ which implies that

$$C_1 = \sin^2\omega_1\tau \left(\frac{1}{2}\left[\left(\frac{\omega_0}{\omega_1}\right)^2 + \left(\frac{\omega_1}{\omega_0}\right)^2\right] - 1\right). \tag{30}$$

The results of a Monte Carlo simulation of such a process with $\omega_1 = 2\omega_0$ and $\omega_1\tau = \pi/2$, with initial states selected from a canonical distribution with $\beta = 1$, are shown as a histogram

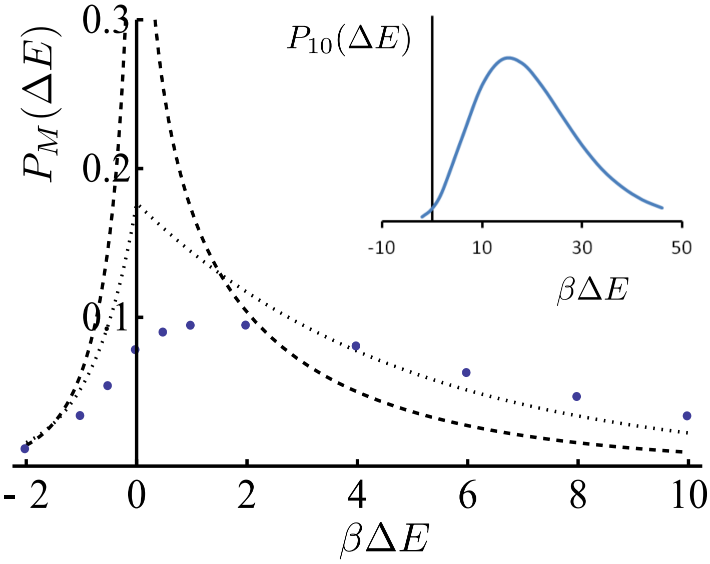

Figure 5. Probability distribution functions of energy change ΔE for ten (solid curve in inset), three (points), two (dotted) and a single oscillator (dashed), when driven by a work cycle with mean energy change $\langle \Delta E\rangle = 2/\beta$ per oscillator.

of energy changes ΔE (continuous line) in Figure 4. The points are obtained from (28) using the appropriate value $C_1 = 9/8$. The correspondence between the analytical results and the simulation is apparent.

We next calculate $P_M(\Delta E)$, the pdf of energy change for M independent oscillators undergoing a given cyclic process, using the iterated convolution operation $P_M(\Delta E) = \int_{-\infty}^{\infty} P_1(\Delta E - x)P_{M-1}(x)\mathrm{d}x$, where $P_1(x)$ is synonymous with $P(x)$. Since $P_2(-\Delta E) = \int_{-\infty}^{\infty} P_1(-\Delta E - x)P_1(x)\mathrm{d}x = \int_{-\infty}^{\infty} P(-\Delta E + x)P(-x)\mathrm{d}x = \int_{-\infty}^{\infty} P(\Delta E - x)\exp(\beta(-\Delta E + x))P(x)\exp(-\beta x)\mathrm{d}x = \exp(-\beta\Delta E)P_2(\Delta E)$, the symmetry of the pdf for a single oscillator is retained for a system of two oscillators. By iteration, it can be shown that

$$P_M(\Delta E) = P_M(-\Delta E)\exp(\beta\Delta E). \tag{31}$$

For a cyclic process with $C_1 = 2$ we show numerically generated pdfs in Figure 5 for one, two, three and ten oscillators. All of them satisfy (31) in spite of their varying shape as M increases.

These symmetries of the work distribution, however, are not immediately equivalent to the Crooks relation, which refers to forward and backward processes. But it has been remarked that the harmonic oscillator is rather special [15, 22] and that fluctuation relations of a specific kind emerge. Since the Crooks relation states that $P_{\mathrm{F}}(\Delta E) = P_{\mathrm{B}}(-\Delta E)\exp(\beta\Delta E)$ for an isolated cyclic process it must be the case that $P_{\mathrm{F}}(\Delta E) = P_{\mathrm{B}}(\Delta E)$: the distribution of energy change for the oscillator is the same whether we process the system according to a forward cyclic sequence $\omega(t)$ or the reverse sequence $\bar{\omega}(t) = \omega(\tau - t)$. The special nature of the oscillator allows us to understand this in the following way.

The process matrices for the forward and backward cycles, S_{F} and S_{B} respectively, are related by $S_{\mathrm{F}}\hat{S}S_{\mathrm{B}}\hat{S} = I$ where

$$\hat{S} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{32}$$

is a velocity inversion matrix since it transforms phasor A into A^*, and these represent oscillator configurations with the same position but opposite velocities. The relation is simply the statement that a deterministic forward process, followed by velocity inversion, the backward process and another velocity inversion, should restore the initial state of the system in phase space. Hence, if

$$S_{\rm F} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \quad \text{then} \quad S_{\rm B} = \begin{pmatrix} d & b \\ c & a \end{pmatrix}, \tag{33}$$

and clearly, both matrices have the same value of C_1 according to (9), in spite of corresponding to quite different transformations of the initial phasor A. We showed in (28) that the distribution of energy change is the same for two cyclic processes with equal values of C_1 and $\langle \Delta E \rangle$, and hence $P_{\rm F}(\Delta E) = P_{\rm B}(\Delta E)$.

We noted with reference to Figure 2 that if $C_2^2 + C_3^2 < C_1^2$ then a distribution with only positive or negative values of ΔE emerges. For $C_1 > 0$, we find $\Delta E_- > 0$ and the distribution would then take the form

$$P(\triangle E) \propto \int_{\Delta E L_+}^{\Delta E L_-} \Phi(\triangle E, E) \exp(-\beta E)\,{\rm d}E, \tag{34}$$

for positive ΔE and $P(\Delta E) = 0$ otherwise, which again can best be understood with reference to Figure 3. However, this does not appear to reduce to a simple form in general and a symmetry about the point $\Delta E = 0$ is obviously absent. However, a special case for $C_2^2 + C_3^2 = C_1^2$ does simplify since it corresponds to $L_- \to \infty$ and $L_+ = 1/(2C_1)$. We find that

$$\begin{aligned} P(\Delta E) &\propto \int_{\Delta E L_+}^{\infty} \frac{{\rm e}^{-\beta E} {\rm d}E}{(\triangle E\,(E - \Delta E L_+))^{1/2}} \\ &\propto \frac{{\rm e}^{-\beta \Delta E L_+}}{\Delta E^{1/2}} = \left(\frac{\beta}{2C_1 \pi \Delta E} \right)^{1/2} {\rm e}^{-\beta \Delta E/(2C_1)}. \end{aligned} \tag{35}$$

An example process where this applies is a step up from ω_0 to $\omega_1 > \omega_0$: S is simply the right hand component matrix in (29) such that

$$2C_1 = \left(\frac{\omega_1}{\omega_0} \right)^2 \left(1 + \left(\frac{\omega_0}{\omega_1} \right)^2 \right) - 2 = \left(\frac{\omega_1}{\omega_0} \right)^2 - 1, \tag{36}$$

and the condition $C_2^2 + C_3^2 - C_1^2 = 2C_1 + 1 - D^2 = 0$ holds. Thus

$$P_{\rm F}(\Delta E) = \left[\frac{\beta \omega_0^2}{\pi \left(\omega_1^2 - \omega_0^2 \right) \Delta E} \right]^{1/2} \exp\left(-\frac{\beta \omega_0^2 \Delta E}{\omega_1^2 - \omega_0^2} \right), \tag{37}$$

for $\Delta E > 0$ and zero otherwise. For the reverse process consisting of a step down from ω_1 to ω_0 the pdf is

$$P_{\rm B}(\Delta E) = \left[-\frac{\beta \omega_1^2}{\pi \left(\omega_1^2 - \omega_0^2 \right) \Delta E} \right]^{1/2} \exp\left(\frac{\beta \omega_1^2 \Delta E}{\omega_1^2 - \omega_0^2} \right), \tag{38}$$

for $\Delta E < 0$ and zero otherwise. The subscripts identify these as pdfs for a forward process and its backward counterpart, and they satisfy

$$\begin{aligned} \frac{P_{\rm F}(\Delta E)}{P_{\rm B}(-\Delta E)} &= \frac{\omega_0}{\omega_1} \exp\left(-\frac{\beta \omega_0^2 \Delta E}{\omega_1^2 - \omega_0^2} \right) \exp\left(\frac{\beta \omega_1^2 \Delta E}{\omega_1^2 - \omega_0^2} \right) \\ &= \exp(\beta (\Delta E - \Delta F)), \end{aligned} \tag{39}$$

as required by the Crooks relation, where $\Delta F = \beta^{-1} \ln(\omega_1/\omega_0)$ is the free energy change in the forward process. They resemble the work distributions for a harmonic oscillator under isothermal conditions for this process [18].

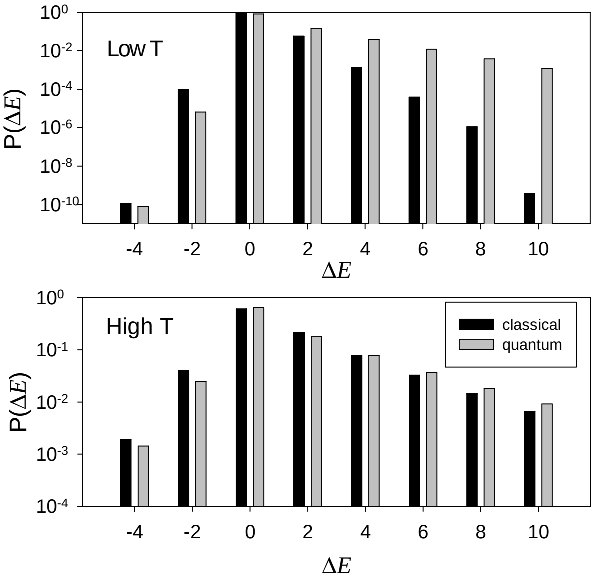

Figure 6. Probabilities of energy change ΔE (in units of $\hbar\omega_0$) for a step up-step down cyclic work process. Grey bars represent $P_{\mathrm{q}}(\Delta E)$ in (42), derived from a quantum treatment, and black bars correspond to the classical pdf (28), integrated over a range $\hbar\omega_0$ each side of the allowed quantised values of ΔE. The lower plot at $\beta\hbar\omega = 1$ illustrates the similarity of treatments at high temperature in contrast to the upper plot at $\beta\hbar\omega = 5$ (or low temperature) where the range of fluctuations is broader in the quantum treatment compared with the classical. The quantum histograms satisfy $P_{\mathrm{q}}(\Delta E) = \exp(\beta\Delta E)P_{\mathrm{q}}(-\Delta E)$: the classical counterparts do not though they are based on underlying continuous pdfs that do.

3. Quantum treatment

We expect the pdfs of energy change for a quantum treatment of forward and backward processes for an isolated oscillator to satisfy the Crooks relation, as has been demonstrated by Deffner *et al* [21, 25]. However, our interest in this section is in the symmetry in the distribution of energy change for a forward cyclic process. We employ the treatment of a 1-d quantum oscillator driven by an arbitrary $\omega(t)$ provided by Ji *et al* [26]. According to this approach, the familiar eigenfunctions $\psi_n(x)$ of a 1-d harmonic oscillator with frequency $\omega(0) = \omega_0$ evolve into

$$\hat{\psi}_n(x,t) = \frac{1}{2^n n!}\left(\frac{\omega_0}{\hbar\pi g_-(t)}\right)^{1/4} \exp\left[-\frac{(\omega_0 + \mathrm{i}g_0(t))}{2\hbar g_-(t)}x^2 \right.$$
$$\left. -\mathrm{i}\left(n+\frac{1}{2}\right)\int_0^t \frac{\omega_0}{m g_-(t')}dt'\right] H_n\left(\sqrt{\frac{\omega_0}{\hbar g_-(t)}}x\right), \qquad (40)$$

where the H_n are Hermite polynomials and the functions $g_-(t)$, $g_0(t)$ and $g_+(t)$ satisfy

$$\begin{aligned} \dot{g}_-(t) &= -2g_0(t)/m \\ \dot{g}_0(t) &= m\omega^2(t)g_-(t) - g_+(t)/m \\ \dot{g}_+(t) &= 2m\omega^2(t)g_0(t), \end{aligned} \qquad (41)$$

with initial conditions $g_-(0) = 1/m$, $g_0(0) = 0$ and $g_+(0) = m\omega_0^2$. The pdf of energy change $P_{\mathrm{q}}(\Delta E)$ for an arbitrary cyclic process is then straightforward to calculate. We write

$$P_{\mathrm{q}}(j\hbar\omega_0) = \sum_{n=0}^{\infty}\sum_{k=0}^{\infty} |T_{kn}(t)|^2 p_n \delta_{k-n,j}, \qquad (42)$$

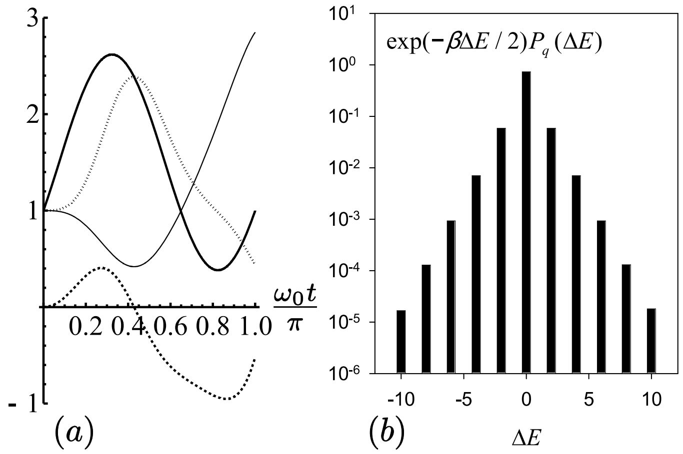

Figure 7. (*a*) The evolution of functions $mg_-(t)$ (thin solid curve), $g_0(t)$ (dashed) and $g_+(t)/m\omega_0^2$ (dotted) under time-dependent frequency driving $\omega(t)/\omega_0 = \left(1+\sin(2\omega_0 t)+\sin^2(\omega_0 t)\right)$ (thick solid curve). (*b*) The probability distribution $P_{\mathrm{q}}(\Delta E)$ of energy change ΔE (in units of $\hbar\omega_0$) for $\beta\hbar\omega_0 = 1$ is plotted in the form $f(\Delta E) = \exp(-\beta\Delta E/2)P_{\mathrm{q}}(\Delta E)$ to demonstrate the symmetry $f(\Delta E) = f(-\Delta E)$.

where $p_n \propto \exp(-(n+1/2)\hbar\omega_0\beta)$ is the initial canonical probability for state n, and $T_{kn}(t)$ is the transition amplitude, which up to an unimportant phase is given by

$$\begin{aligned} T_{kn}(t) = &\int_{-\infty}^{\infty} dx \frac{1}{2^k k!}\left(\frac{\omega_0}{\hbar\pi g_-(t)}\right)^{1/4} \\ &\times \exp\left[\frac{(\mathrm{i}g_0(t)-\omega_0)}{2\hbar g_-(t)}x^2\right] H_k\left(\sqrt{\frac{\omega_0}{\hbar g_-(t)}}x\right) \\ &\times \frac{1}{2^n n!}\left(\frac{m\omega_0}{\hbar\pi}\right)^{1/4} \exp\left[-\frac{m\omega_0}{2\hbar}x^2\right] H_n\left(\sqrt{\frac{m\omega_0}{\hbar}}x\right). \end{aligned} \tag{43}$$

Parity considerations dictate that T_{kn} is zero unless k and n differ by an even number, and hence $P_{\mathrm{q}}(j\hbar\omega_0)$ is zero unless j is even.

We study the step up and down process that was considered classically in section 2.3, namely $\omega = \omega_0$ for $t < 0$ and $t > \tau$, and $\omega = \omega_1 = 2\omega_0$ in the interval $0 \le t \le \tau$ with $\omega_1\tau = \pi/2$. The pdfs of energy change under the quantum dynamics for cases where $\beta\hbar\omega_0$ is equal to 1 and 5 are shown in Figure 6. Both pdfs satisfy the relationship $P_{\mathrm{q}}(\Delta E) = \exp(\beta\Delta E)P_{\mathrm{q}}(-\Delta E)$. The quantum pdfs may be contrasted with the classical counterparts by integrating $P(\Delta E)$ in (28) over the range $(j-1)\hbar\omega_0 \le \Delta E \le (j+1)\hbar\omega_0$ and comparing the result with $P_{\mathrm{q}}(j\hbar\omega_0)$. We see that the classical and quantum treatments coincide rather well for $\beta\hbar\omega_0 = 1$, but that differences emerge for $\beta\hbar\omega_0 = 5$. The latter is evidently a low temperature regime and the energy change brought about by the process is distributed more broadly due to the relatively more substantial quantum fluctuations.

The step up-step down process has a very simple time-dependence of $\omega(t)$. We investigate driving the system with the more complicated frequency history $\omega(t) = \omega_0\left(1+\sin(2\omega_0 t)+\sin^2(\omega_0 t)\right)$ over the interval $0 \le \omega_0 t \le \pi$ such that the g-functions evolve with time as in Figure 7(*a*). The resulting distribution $P_{\mathrm{q}}(\Delta E)$ for $\beta\hbar\omega_0 = 1$ is shown in Figure 7(*b*) in a form that demonstrates the symmetry $P_{\mathrm{q}}(\Delta E) = \exp(\beta\Delta E)P_{\mathrm{q}}(-\Delta E)$.

4. Conclusions

We have calculated the probability distribution function $P(\Delta E)$ of energy change brought about by taking a 1-d harmonic oscillator, initially in thermal equilibrium, through a process of external work while isolated from the environment. If the process is cyclic, then the pdf extends over positive and negative ΔE and exhibits a symmetry $P(\Delta E) = \exp(\beta \Delta E) P(-\Delta E)$ with respect to the reversal of the sign of the energy change. This is reminiscent of the Crooks relation, which is also satisfied by the system, but is distinct, since it involves a forward process only and not its reverse. But the symmetry is also a special case of the result $P(\Delta E) = \exp(\beta L \Delta E) P(-\Delta E)$ that is valid for a class of non-cyclic processes for this system. These symmetries are a consequence of the simple dynamics of an oscillator. We have demonstrated that the symmetry is retained if the system consists of M independent oscillators subjected to the same process, even though the $P_M(\Delta E)$ take a variety of forms. The symmetry is also retained when an oscillator undergoing a cyclic process is treated quantum mechanically. At high temperatures the results of the classical and quantum treatments are similar, while at low temperatures there is a relative broadening of the pdf in the quantum treatment, as would be expected from the inclusion of quantum uncertainty in the dynamics.

The understanding of nonequilibrium thermodynamic processes has advanced tremendously in the last decade or so as a result of the development of fluctuation relations and particular identities such as the Crooks relation and the Jarzynski equality [15, 3]. The explicit calculation of probability distribution functions satisfying these relations is a challenging task, but has considerable pedagogical value. The harmonic oscillator has been a popular system for such activity, but it is a rather special case in that further symmetries emerge that are not present in general. Using an approach based on phasors and a geometrical consideration of phase space trajectories and their weighting in canonical averages, we have demonstrated some of this richness. It offers a contrast to approaches offered elsewhere [21, 22, 23, 24, 25] with the intention that it might make an additional contribution to this understanding.

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