

1-20-2006

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Recommended Citation

Ford, G., & O'Connell, R. (2006). A quantum violation of the second law?. *Physical Review Letters*, 96 (2)
<https://doi.org/10.1103/PhysRevLett.96.020402>

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A quantum violation of the second law?

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(Dated: July 24, 2018)

Abstract

An apparent violation of the second law of thermodynamics occurs when an atom coupled to a zero-temperature bath, being necessarily in an excited state, is used to extract work from the bath. Here the fallacy is that it takes work to couple the atom to the bath and this work must exceed that obtained from the atom. For the example of an oscillator coupled to a bath described by the single relaxation time model, the mean oscillator energy and the minimum work required to couple the oscillator to the bath are both calculated explicitly and in closed form. It is shown that the minimum work always exceeds the mean oscillator energy, so there is no violation of the second law.

INTRODUCTION

Widespread interest in recent years in mesoscopic systems, fundamental quantum physics and quantum computation has highlighted the critical role which dissipative environments play in such studies. This has led to a critical examination of many results that were derived for macroscopic systems. In particular, there has been considerable interest in the area of quantum and mesoscopic thermodynamics. In some instances questions have been raised about the validity of the fundamental laws of thermodynamics, especially at low temperatures where quantum effects are important [1]. Whereas many interesting new facets of old results have emerged, it is important to exercise caution before questioning the validity of fundamental laws (especially the laws of thermodynamics), since many subtle issues arise. Here we examine an apparent violation of the second law of thermodynamics that would lead to the extraction of work from the zero point fluctuations of the heat bath.

An atom in contact with a zero temperature heat bath is necessarily in an excited state. This perhaps counter-intuitive observation is a simple consequence of the fact that the Hamiltonian H_A of the isolated atom does not commute with the Hamiltonian H of the *system* of atom coupled to the bath. It follows that in the ground state of the system the energy of the atom *must* fluctuate and therefore have a mean value greater than its ground state energy E_0 [2, 3],

$$\langle H_A \rangle_{T=0} > E_0. \quad (1)$$

The existence of this energy might lead one to think that there could be a quantum violation of the second law of thermodynamics, perhaps small, but nevertheless a violation. Here the idea is to begin with the atom in its ground state. It is then dropped into a bath at zero temperature, where it comes to equilibrium with mean energy $\langle H_A \rangle_{T=0}$. The atom is then fished out and the energy of transition to the ground state is used to raise a weight. Behold, we have a cyclic process in which a weight is raised with no other effect than the extraction of energy from a reservoir. This would be a violation of the second law in its Kelvin-Planck form: "It is impossible to construct an engine which will work in a complete cycle, and produce no effect excepting the raising of a weight and the cooling of a heat reservoir" [4]. What is wrong? Because there must be something wrong. The answer is that it takes work to couple the atom to the bath and this work exceeds that obtained in the transition to the ground state. The principle of minimum work tells us that the minimum work required

to take a system from one thermodynamic state to another at the same temperature is the difference of Helmholtz free energy [5]. In the present case this would be the free energy of the system of the atom coupled to the bath minus the free energy of the bath in the absence of the atom. One should expect, therefore, that if the second law is to hold this work must be greater than the mean energy of the atom.

Our point here is that for the example of an oscillator coupled to a linear passive heat bath both the mean energy and the work required to couple the oscillator to the bath can be calculated explicitly and in closed form. With the resulting expressions we are able to show that, for all coupling strengths, the work is always greater than the mean energy and therefore second law is satisfied.

OSCILLATOR COUPLED TO THE BATH

The mean energy of an oscillator coupled to a heat bath is given by the expression

$$\langle H_O \rangle = \frac{1}{2}m \langle \dot{x}^2 \rangle + \frac{1}{2}K \langle x^2 \rangle, \quad (2)$$

where K is the oscillator force constant. To evaluate these expectations we begin with the well known formula for the correlation function [6],

$$\frac{1}{2} \langle x(t_1)x(t_2) + x(t_2)x(t_1) \rangle = \frac{\hbar}{\pi} \int_0^\infty d\omega \coth \frac{\hbar\omega}{2kT} \text{Im}\{\alpha(\omega)\} \cos \omega(t_2 - t_1). \quad (3)$$

Here $\alpha(\omega)$ is the response function, of the general form

$$\alpha(\omega) = \frac{1}{-m\omega^2 - i\omega\tilde{\mu}(\omega) + K}, \quad (4)$$

in which $\tilde{\mu}(\omega)$ is the Fourier transform of the memory function. For the single relaxation time model, this is given by

$$\tilde{\mu}(\omega) = \frac{\zeta}{1 - i\omega\tau}, \quad (5)$$

in which ζ is the Ohmic friction constant and $\tau \ll m/\zeta$ is the bath relaxation time. With this form of $\tilde{\mu}(\omega)$ the response function is a rational function, with the denominator a cubic polynomial in ω . In order to perform the integrals we need it is necessary to factor this denominator. For this purpose it is convenient to introduce in place of the parameters K , ζ and τ the parameters Ω , ω_0 and γ through the relations

$$K = m\omega_0^2 \frac{\Omega}{\Omega + \gamma}, \quad \zeta = m\gamma \frac{\Omega(\Omega + \gamma) + \omega_0^2}{(\Omega + \gamma)^2}, \quad \tau = \frac{1}{\Omega + \gamma}. \quad (6)$$

With this replacement, the response function (4) takes the form:

$$\alpha(\omega) = \frac{\omega + i(\Omega + z_1 + z_2)}{-m(\omega + i\Omega)(\omega + iz_1)(\omega + iz_2)}, \quad (7)$$

where

$$z_1 = \frac{\gamma}{2} + i\omega_1, \quad z_2 = \frac{\gamma}{2} - i\omega_1, \quad \omega_1 = \sqrt{\omega_0^2 - \frac{\gamma^2}{4}}. \quad (8)$$

The poles of the response function are therefore at $\omega = -i\Omega$, $-iz_1$, and $-iz_2$, all in the lower half plane. With this we see that the relations (6) are expressions for the physical parameters K , ζ and τ in terms of the positions of the poles. The inversion of these relations involves tedious expressions for the roots of a cubic equation. However, the region of physical interest is that of τ small, where $\Omega \sim 1/\tau$ is large, while $\omega_0^2 \cong K/m$ and $\gamma \cong \zeta/m$. Therefore, in the following expressions we use the parameters Ω , ω_0 and γ , keeping in mind that Ω is essentially the inverse of the bath relaxation time, while ω_0 and γ are the oscillator natural frequency and relaxation rate as slightly shifted by the coupling to the bath.

Setting $T = 0$ in the formula (3) and using the expression (7) for the response function, the integrals are elementary and we obtain the exact expressions,

$$\begin{aligned} \langle x^2 \rangle_{T=0} &= \hbar \frac{(\Omega^2 + \omega_0^2 - \frac{\gamma^2}{2}) \arccos \frac{\gamma}{2\omega_0} - \gamma\omega_1 \log \frac{\Omega}{\omega_0}}{\pi m \omega_1 (\Omega^2 - \gamma\Omega + \omega_0^2)}, \\ \langle \dot{x}^2 \rangle_{T=0} &= \hbar \frac{[\Omega^2(\omega_0^2 - \frac{\gamma^2}{2}) + \omega_0^4] \arccos \frac{\gamma}{2\omega_0} + \gamma\omega_1 \Omega^2 \log \frac{\Omega}{\omega_0}}{\pi m \omega_1 (\Omega^2 - \gamma\Omega + \omega_0^2)}. \end{aligned} \quad (9)$$

With this we find from (2) that the mean energy of the oscillator coupled to the heat bath at temperature zero is given by

$$\begin{aligned} \langle H_O \rangle_{T=0} &= \frac{\hbar}{2\pi} \left[\frac{(\Omega^2 + \omega_0^2)(2\Omega\omega_1^2 + \gamma\omega_0^2) - \frac{1}{2}\gamma^3\Omega^2}{\omega_1(\Omega + \gamma)(\Omega^2 - \gamma\Omega + \omega_0^2)} \arccos \frac{\gamma}{2\omega_0} \right. \\ &\quad \left. + \frac{\gamma\Omega(\Omega^2 + \gamma\Omega - \omega_0^2)}{(\Omega + \gamma)(\Omega^2 - \gamma\Omega + \omega_0^2)} \log \frac{\Omega}{\omega_0} \right]. \end{aligned} \quad (10)$$

The oscillator ground state energy is given by

$$E_0 = \frac{\hbar}{2} \sqrt{\frac{K}{m}} = \frac{\hbar\omega_0}{2} \sqrt{\frac{\Omega}{\Omega + \gamma}}. \quad (11)$$

As we have remarked, the mean energy must always be greater than the ground state energy. This is clearly seen in Fig 1 where a three-dimensional plot of $\langle H_O \rangle_{T=0}/E_0$ is shown for a wide range of γ/ω_0 and Ω/ω_0 .

Next we consider the work required to couple the oscillator to the bath. The principle of minimum work tells us that the minimum work required to take a system from one thermodynamic state to another is the difference of Helmholtz free energy [5]. In the present case this would be the free energy of the system of the oscillator coupled to the bath minus the free energy of the bath in the absence of the oscillator. For this free energy difference there is the remarkable formula which for the system at temperature T takes the form [7]:

$$F_O(T) = \frac{1}{\pi} \int_0^\infty d\omega f(\omega, T) \text{Im} \left\{ \frac{d \log \alpha(\omega + i0^+)}{d\omega} \right\}, \quad (12)$$

where $\alpha(\omega)$ is again the oscillator susceptibility. In this formula $f(\omega, T)$ is the free energy (including zero point energy) of a free oscillator of frequency ω at temperature T :

$$f(\omega, T) = kT \log \left(2 \sinh \frac{\hbar\omega}{2kT} \right). \quad (13)$$

At zero temperature $f(\omega, 0) = \hbar\omega/2$ and using again the expression (7) for the response function, the integral (12) can be evaluated exactly to give the simple result:

$$F_O(0) = \frac{\hbar}{2\pi} \left[2\omega_1 \arccos \frac{\gamma}{2\omega_0} + \gamma \log \frac{\Omega}{\omega_0} + (\Omega + \gamma) \log \frac{\Omega + \gamma}{\Omega} \right]. \quad (14)$$

In Fig. 2 we plot $F_O(0)/E_0$ and $\langle H_O \rangle_{T=0}/E_0$ vs the coupling strength as measured by γ/ω_0 . In this plot we have chosen $\Omega = 5\omega_0$ but for any $\Omega > \omega_0$ the result is the same: the minimum work required to couple the oscillator to the bath, $F_O(0)$, is always greater than the mean energy of the oscillator coupled to the bath, $\langle H_O \rangle_{T=0}$. Thus in the cyclic process described above there is a loss rather than a gain of energy and there is no violation of the second law.

REMARKS

In the limit of vanishing bath relaxation time, both $F_O(0)$ and $\langle H_O \rangle_{T=0}$ are logarithmically divergent, but it is not difficult to see that

$$F_O(0) - \langle H_O \rangle_{T=0} \rightarrow \frac{\gamma}{\pi\omega_0} E_0. \quad (15)$$

From the figure it is clear that this linear dependence on γ is a pretty good approximation even for rather long bath relaxation times. The discrepancy between the work required to couple the oscillator to the bath and that obtainable from the oscillator removed from the bath increases roughly proportional to the strength of coupling to the bath.

The free energy at zero temperature is in fact the energy. Therefore, we see that coupling the oscillator to the bath actually requires an energy greater than $\langle H_O \rangle_{T=0}$, the additional energy going to the bath. Since the bath is infinite, this finite additional energy does not raise the temperature.

The principle of minimum work becomes the principle of maximum work when the initial and final states are reversed [5]. Returning to the general case of an atom we considered in the beginning, if $F_A(T)$ is the free energy of the atom coupled to the bath at an arbitrary temperature T minus the free energy of the bath alone, then $F_A(T)$ is the minimum work required to couple the atom to the bath while it is also the maximum work that can be obtained when the atom is extracted from the bath. The net work obtained can never be positive.

Part of this work was carried out at the School of Theoretical Physics of the Dublin Institute for Advanced Studies . The authors wish to thank the School and its Director, Professor Tony Dorlas for their hospitality.

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Figure Captions

Fig. 1. Three dimensional plot of $\langle H_O \rangle_{T=0} / E_0$ as a function of γ / ω_0 and Ω / ω_0 .

Fig. 2. Plot of $F_O(0) / E_0$ and $\langle H_O \rangle_{T=0} / E_0$ as functions of the coupling strength as measured by γ / ω_0 . The relaxation time is chosen so that $\Omega = 5\omega_0$. The overdamped oscillator corresponds to $\gamma / \omega_0 > 2$.



