Ground State Energy Fluctuations of a System Coupled to a Bath

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It is often argued that a small non-degenerate quantum system coupled to a bath has a fixed energy in its ground state since a fluctuation in energy would require an energy supply from the bath. We consider a simple model of a harmonic oscillator (the system) coupled to a linear string and determine the mean squared energy fluctuations. We also analyze the two time correlator of the energy and discuss its behavior for a finite string.

The coupling of two subsystems is a central problem in many areas of physics. The interaction of atoms with the radiation field has been central in the development of quantum mechanics. The division into subsystems often depends on the questions asked: For instance dephasing in mesoscopic systems investigates the quantum motion of a single electron in a conductor viewing all other conduction electrons as the bath. In this work we are interested in the energy fluctuations in a test system coupled to another system. Of particular interest is the zero-temperature limit. It is often argued that in the zero-temperature limit two subsystems can not exchange energy. The argument is based on the assumption that both subsystems are in their separate ground state (which they would assume in the absence of any coupling). Since both the test system and the bath are in their ground state neither of the two can supply an energy to the other. Below we consider a simple system of an oscillator (the test system) coupled to a linear string (the bath) and investigate the energy fluctuations of the test system. This is an exactly solvable model which demonstrates the existence of energy fluctuations in the zero-temperature limit. These fluctuations are a consequence of the finite coupling energy between the test system and the bath.

Often the interaction of two subsystems is treated in terms of the Einstein coefficients for the absorption and the spontaneous and stimulated emission of the test system. In such an approach rates of transitions of the test system. This is an exactly solvable model which demonstrates the existence of energy fluctuations in the zero-temperature limit. These fluctuations are a consequence of the finite coupling energy between the test system and the bath.

The role of zero-point fluctuations in mesoscopic conductors is a hotly debated issue and we cite here only Ref. 7 as an entry to the literature. The point of view taken here has been applied to investigate the persistent current of a small mesoscopic loop with a quantum dot capacitively coupled to a transmission line. The persistent current is a measure of the quantum coherence of the ground state. It was found that the ground state undergoes a crossover from a state with a well defined persistent current much larger than its mean square fluctuations to a state in which the magnitude of the persistent current is much smaller than its mean square fluctuations as the coupling to the bath increases.

Vacuum fluctuations can have important effects on the system considered. The Lamb shift is a widely appreciated example. Another example is the Casimir effect. In both of these examples the effect of the vacuum can be thought of in terms of a renormalization of the original parameters characterizing the system. In contrast, the energy fluctuations which we discuss here can not be obtained from the uncoupled system simply by renormalizing its parameters: After all, a harmonic oscillator in its ground state does not fluctuate.

The system we consider is a harmonic oscillator with mass $m_0$ and frequency $\omega_0$ described by the energy operator

$$\hat{H}_0 = \frac{1}{2m_0} \hat{q}^2 + \frac{m_0 \omega_0^2}{2} \hat{q}^2. \quad (1)$$

The oscillator is coupled to a harmonic bath, which leads to a dissipation linear in its velocity with a friction constant $\eta$. The expectation value of the mean energy of the test oscillator in the ground state of the system is to the linear order in the friction constant $\eta$

$$\langle \hat{H}_0 \rangle = \frac{\hbar \omega_0}{2} + \frac{\hbar \eta}{2\pi} \left[ \ln \left( \frac{\omega_c}{\omega_0} \right) - 1 \right] \quad (2)$$

and the mean squared energy $\langle \delta \hat{H}_0^2 \rangle = \langle (\hat{H}_0 - \langle \hat{H}_0 \rangle)^2 \rangle$ is

$$\langle \delta \hat{H}_0^2 \rangle = \frac{\hbar^2 \omega_0 \eta}{2\pi} \left[ \ln \left( \frac{\omega_c}{\omega_0} \right) - 1 \right]. \quad (3)$$

where $\omega_c$ is a (high-frequency) Debye cut-off of the spectrum of the bath. Thus both the mean energy and the mean squared fluctuations in energy increase (for weak coupling) linearly with the coupling constant $\eta$. Note that the mean squared fluctuations are proportional to $\hbar^2$. The result for the mean energy is well known. \hfill $\square$
In contrast, the result for the energy fluctuations seems novel. Below we extend Eq. (3) to all orders in η and investigate also the two time correlator of the energy (a fourth order correlation). Eqs. (2) and (3) are valid for the infinitely long string. To emphasize that the overall energy (system plus coupling energy plus bath) is conserved despite the energy fluctuations in the test system alone, we will later also consider a string with a finite number of particles only.

The mean squared energy fluctuations can be determined from the coordinate correlation function of the oscillator which is conveniently obtained using the classical response of the oscillator and the fluctuation-dissipation relation at a finite temperature $T$

$$\langle \hat{q}(t)\hat{q}(0) \rangle = \frac{\hbar}{2\pi m_0} \int_{-\infty}^{\infty} d\omega \frac{\omega \exp(i\omega t)}{(\omega^2 - \omega_0^2)^2 + \eta^2 \omega^2} \times \left[ \coth \left( \frac{\omega}{2T} \right) + 1 \right],$$

and then passing to the limit $T \to 0$. Introducing $\Omega_+ = (\omega_0^2 - \eta^2/4)^{1/2}$, for $\omega_0 > \eta/2$ and $\Omega_- = (\eta/4 - \omega_0^2)^{1/2}$ for $\omega_0 < \eta/2$.

$$\langle q^2 \rangle = \frac{\hbar}{2m_0 \Omega_+} \left[ 1 - \frac{2}{\pi} \arctan \left( \frac{\eta}{2\Omega_+} \right) \right],$$

where $\langle q^2 \rangle$ is given by Eq. (3). Expanding Eq. (5) up to terms linear in $\eta$ gives Eq. (4). The full result Eq. (3) is shown in Fig. 1 together with the mean energy $\langle \hat{H}_0 \rangle = \langle \hbar \eta/2\pi \rangle \ln(\omega_c/\omega_0) + m_0 \Omega_+^2 \langle q^2 \rangle > q^2 >$

of the test oscillator.

So far we considered the system consisting of the oscillator and the bath in a thermodynamic equilibrium at a given temperature $T$, which was then set equal to zero. It is also instructive to trace the origin of the energy fluctuations by using a microscopic model of the bath and purely quantum-mechanical considerations without involving any thermodynamic relations.

It is well known that a harmonic bath can be modeled by a semi-infinite string of identical particles with mass $m_0$ and frequency $\omega_0$. The electrical analog of this system consists of an LC-oscillator coupled to a transmission line. In the continuous limit where $m_0 \to 0$ and $\omega_0 \to \infty$, the string leads to dissipation that is linear in the velocity of the oscillator with friction constant $\eta = (m h/m_0)\omega_0$. In this limit, the interaction with the string does not shift the resonance frequency of the test oscillator and results only in a finite damping. The role of the high-frequency cutoff $\omega_c$ is played now by $\omega_h$.

For $\omega_0 > \eta/2$ and

$$\langle q^2 \rangle = \frac{\hbar}{\pi m_0 \Omega_-} \ln \left( \frac{\eta + 2\Omega_-}{2\omega_0} \right),$$

for $\omega_0 < \eta/2$. The energy fluctuations are determined by the fourth order correlations of the momentum and coordinate. The momentum is related to the coordinate via $p = m_0 \dot{q}$ and thus the momentum correlations can be reduced to time-derivatives of coordinate correlations. We next make use of the fact that the fluctuations are Gaussian and thus fourth order correlations can be expressed as sums of products of second order correlations. Thus we obtain the energy correlator in the form

$$\langle \delta \hat{H}_0(t)\delta \hat{H}_0(0) \rangle = \langle \hat{H}_0(t)\hat{H}_0(0) \rangle - \langle \hat{H}_0 \rangle^2$$

where

$$\langle \delta \hat{H}_0(t)\delta \hat{H}_0(0) \rangle = \frac{1}{2} m_0^2 \left[ \frac{\partial^2}{\partial t^2} \langle \hat{q}(t)\hat{q}(0) \rangle \right]^2 + m_0^2 \omega_0^2 \left[ \frac{\partial}{\partial t} \langle \hat{q}(t)\hat{q}(0) \rangle \right]^2 + \frac{1}{2} m_0^2 \omega_0^4 \langle \hat{q}(t)\hat{q}(0) \rangle^2.$$

For the mean squared fluctuations we need the time derivatives of the correlator at $t = 0$. Evaluating the resulting integrals yields,

$$\langle \delta \hat{H}_0(t)\delta \hat{H}_0(0) \rangle = \langle \hat{H}_0(t)\hat{H}_0(0) \rangle - \langle \hat{H}_0 \rangle^2$$

where

$$\langle \delta \hat{H}_0(t)\delta \hat{H}_0(0) \rangle = \frac{\hbar^2}{2\pi} \eta^2 \ln \left( \frac{\omega_0}{\omega_c} \right) + \frac{\hbar}{\pi} m_0 \eta (\omega_0^2 - \eta^2/2) \ln \left( \frac{\omega_c}{\omega_0} \right) \langle q^2 \rangle + \frac{1}{8} m_0^2 (8\omega_0^4 - 4\omega_0^2 \eta^2 + \eta^4) \langle q^2 \rangle^2 - \frac{\hbar^2}{4} \omega_0^2,$$

of the test oscillator.

To address a system with a well defined ground-state energy, we consider a test system attached to a chain of a finite length consisting of $N$ oscillators. The Hamiltonian of a system coupled to a linear harmonic string is conveniently split into the following three parts

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_i + \hat{\mathcal{H}}_b,$$

where

$$\hat{\mathcal{H}}_0 = \frac{1}{2m_0} \dot{q}_0^2 + \frac{1}{2} (m_0 \omega_0^2 + m_h \omega_h^2) q_0^2,$$

$$\hat{\mathcal{H}}_i = -m_h \omega_h^2 \dot{q}_0 \vec{x}_1,$$

$$\hat{\mathcal{H}}_b = \frac{1}{2m_h} \sum_{\alpha=1}^N \dot{p}_\alpha^2 + \frac{1}{2} m_h \omega_h^2 \vec{x}_\alpha^2.$$
matrix forms large even for one oscillator. Instead, we perform a linear mechanical diagonalization of \( \langle \eta \rangle \) in the ground state as a function of the coupling constant \( \eta \) in units with \( \hbar = 1 \).

\[
+ \frac{1}{2} m_k \omega_k^2 \sum_{\alpha=1}^{N-1} (\dot{x}_{\alpha+1} - \dot{x}_\alpha)^2. \tag{12}
\]

A transition from a finite to the infinite system is most conveniently traced by watching the behavior of a two-time correlator of energy. We introduce the exact classical normal modes of the total Hamiltonian \( \hat{H} \) and calculate the correlator \( \langle \eta \rangle \). Note that this is not the quantum-mechanical diagonalization of \( \hat{H} \) in the basis of its eigenstates because the number of these states is infinitely large even for one oscillator. Instead, we perform a linear transformation of coordinates \( x_\alpha \) with an \( N + 1 \times N + 1 \) matrix \( \hat{U} \) that will simultaneously bring the quadratic forms

\[
K = \frac{1}{2m_0} p^2 + \frac{1}{2m_k} \sum_{\alpha} p_\alpha^2 - \frac{1}{2} \sum_{\alpha, \beta} K_{\alpha, \beta} p_\alpha p_\beta,
\]

\[
\Pi = \frac{1}{2} \sum_{\alpha, \beta} \Pi_{\alpha, \beta} x_\alpha x_\beta
\]

describing the kinetic and potential energy of the system to a diagonal form. To this end, we introduce the classical normal modes of the system \( \psi_k \), which obey the set of equations

\[
- \omega_k^2 \psi_k(0) = - (\omega_0^2 + \mu \omega_k^2) \psi_k(0) + \mu \omega_k^2 \psi_k(1), \tag{13}
\]

\[
- \omega_k^2 \psi_k(1) = \omega_k^2 [\mu \psi_k(0) + \psi_k(2) - 2 \psi_k(1)], \tag{14}
\]

\[
- \omega_k^2 \psi_k(\alpha) = \omega_k^2 [\psi_k(\alpha + 1) + \psi_k(\alpha - 1) - 2 \psi_k(\alpha)], \tag{15}
\]

\[
2 \leq \alpha < N,
\]

\[
- \omega_k^2 \psi_k(N) = \omega_k^2 [\psi_k(N - 1) - \psi_k(N)]. \tag{16}
\]

Here \( \mu = (m_k/m_0)^{1/2} \) is the ratio of the mass of the bath oscillators and the mass of the test oscillator. We search the eigenvectors in the form

\[
\psi_k(0) = A_k/\mu,
\]

\[
\psi_k(\alpha \geq 1) = A_k \cos(\lambda_k \alpha) + B_k \sin(\lambda_k \alpha). \tag{17}
\]

On applying the transformation \([17]\) to the Hamiltonian \( \hat{H}_L \), it assumes the form

\[
\hat{H}_L = \frac{1}{2} \sum_{k=1}^{N+1} \left( \frac{1}{m_h} \hat{\pi}_k^2 + m_h \omega_k^2 \hat{x}_k^2 \right). \tag{18}
\]

The quantum-mechanical coordinate of the test oscillator \( \hat{q} \) can be written in terms of the normal coordinates \( \hat{\xi}_k \) of the transformed Hamiltonian \( \hat{H}_L \) \([18]\)

\[
\hat{q}(t) = \sum_{k=1}^{N+1} A_k \hat{\xi}_k(t), \tag{19}
\]

and the latter can be presented in the form

\[
\hat{\xi}_k(t) = \frac{\hbar^{1/2}}{\sqrt{2m_h \omega_k}} (\hat{a}_k e^{-i \omega_k t} + \hat{a}_k^+ e^{i \omega_k t}), \tag{20}
\]

where \( \hat{a}_k \) and \( \hat{a}_k^+ \) are time-independent annihilation and creation operators with the standard commutation rules.

Now one easily obtains from Eq. \([18]\) an expression for the correlation function of energy fluctuations

\[
C(t) \equiv \frac{1}{2} \langle \delta \hat{H}_0(t) \delta \hat{H}_0(0) + \delta \hat{H}_0(0) \delta \hat{H}_0(t) \rangle = \frac{\hbar^2}{8 m_h} \left[ \left( \sum_k \omega_k A_k^4 \cos \omega_k t \right)^2 - \left( \sum_k \omega_k A_k^2 \sin \omega_k t \right)^2 \right] + \frac{\hbar^2}{4 m_h} \left[ \left( \sum_k A_k^2 \cos \omega_k t \right)^2 - \left( \sum_k A_k^2 \omega_k \cos \omega_k t \right)^2 \right] + \frac{\hbar^2}{4 m_h} \left[ \left( \sum_k A_k^2 \omega_k \cos \omega_k t \right)^2 - \left( \sum_k A_k^2 \omega_k \sin \omega_k t \right)^2 \right]. \tag{21}
\]
The amplitudes $A_k$ and eigenfrequencies $\omega_k$ were numerically calculated and equation (21) was evaluated for $\omega_0/\omega_h = 1$, $m_h/m_0 = 0.1$, and different values of $N$. The results are shown in Fig. 3.

Since the string is finite, we now have a recurrence phenomenon. As shown in Fig. 2, the correlation function initially oscillates and its envelope decreases rapidly (as it would for the infinite chain), but it rebuilds after a time it takes a signal to travel along the string and to return to the oscillator after reflection at the opposite end. The built-up time is different from the decay time of the correlation and in detail the reconstituted correlation is clearly not the same as the initial correlation. This behavior is a consequence of the fact that the eigenfrequencies $\omega_k$ of our problem are only nearly exact multiples of the lowest eigenfrequency. Even in the limit of a continuous yet finite string ($m_h \to 0$, $\omega_h \to \infty$), the equidistant levels of the system are disturbed near the test-oscillator frequency $\omega_0$. The fact that the eigenfrequencies are not exact multiples leads to the more complex phenomenon depicted in Fig. 3. The above results suggest that a transition to the thermodynamic limit is possible if the travel time of a perturbation through the system is longer than the duration of an experiment.

The exact diagonalization demonstrates that the energy of a small system coupled to a bath fluctuates as a function of time despite the fact that the overall energy of the system is fixed. This is a consequence of the finite coupling energy between the system and the bath. As a result the test oscillator is not in a normal mode of the total system but as shown by Eq. (19) in a superposition of the true normal modes of the total system. It is for this reason that the simple argument mentioned in the introduction fails.

The results presented in this work demonstrate that even at zero temperatures vacuum fluctuations of the bath give rise to a ground state that exhibits a non-trivial dynamics. Textbook statistical mechanics assumes that the coupling energy between the test system and the bath can be neglected. In contrast, here the coupling energy is essential. The effect discussed here can not simply be absorbed into renormalized parameters of the test system. We believe that these observations are crucial in understanding the zero-temperature properties of systems and that they are applicable not only to the particular system investigated here but are of a very general nature.

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