Thermal Reservoir coupled to External Field and Quantum Dissipation

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Abstract

In the framework of the Caldeira -Leggett model of dissipative quantum mechanics, we investigate the effects of the interaction of the thermal reservoir with an external field. In particular, we discuss how the interaction modifies the conservative dynamics of the central particle, and the mechanism of dissipation. We briefly comment on possible observable consequencies.

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1. Introduction.

By quantum dissipation we conventionally denote the problem of the quantum mechanics of a particle in contact with a dissipative environment. After pioneering work by Feynman and Vernon [1], an exactly solvable lagrangian was put forward by Ullersma [2] in the slightly different context of quantum brownian motion. Ullersma introduced a mechanical model for the thermal reservoir as a set of independent harmonic oscillators; he then showed that in the limit of an infinite number of oscillators and of continuously distributed frequencies the dynamics of the particle is governed by the damped Langevin equation. Caldeira and Leggett [3] addressed the problem of the effect of dissipation on quantum tunnelling by applying the formalism of the effective action in the framework of the Feynman path integral quantization. In their analysis they considered systems subject to both dissipative and “true” external forces, thereby ruled in the quasiclassical region by the damped equation of motion

$$M\ddot{q} + \eta\dot{q} + \frac{dV}{dq} = F_{\text{ext}}(t). \quad (1)$$

They studied in detail the problem of the modification of tunnelling rates in the presence of dissipation and pioneered a new broad field of research, mesoscopic physics, where one is considering situations when both thermal and quantum fluctuations are important. For recent comprehensive reviews on quantum brownian motion, dissipative quantum tunnelling, and mesoscopic physics see references [4]-[7]. The problem of quantum brownian motion and the Ullersma -Caldeira -Leggett model of quantum dissipation have also been recently reformulated [8] in the framework of stochastic mechanics at finite temperature [9]. In this letter we address the question of how the coupling of an external field with the thermal reservoir affects the dynamics of a dissipative quantum system.

2. The model without field-reservoir coupling.

We will handle the problem following the effective action approach of Caldeira and
Leggett. We start by briefly reviewing the main features of the model without an external field interacting with the thermal reservoir: for a system of $N + 1$ particles consider the lagrangian

$$L_0 = \frac{M}{2} \dot{q}^2 - V(q) + \sum_{\alpha=1}^{N} \left\{ \frac{m_{\alpha}}{2} \dot{x}_{\alpha}^2 - \frac{m_{\alpha}}{2} \omega_{\alpha}^2 x_{\alpha}^2 + \epsilon_{\alpha} x_{\alpha} q \right\},$$

(2)

which describes a particle (the so-called central particle) of mass $M$ and potential energy $V(q)$ interacting linearly with an ensemble (the thermal reservoir) of $N$ independent harmonic oscillators of masses $m_{\alpha}$ and frequencies $\omega_{\alpha}$. Irreversibility and dissipation are introduced by taking the limit of an infinite number of thermal oscillators with continuously distributed frequencies. The form of the potential $V(q)$ needs not to be specified for our purposes. By letting $V(q) = \frac{1}{2} \omega_0^2 q^2$ we recover the Ullersma lagrangian. Choosing a smooth function with a single metastable minimum we recover the Caldeira-Leggett model for dissipative quantum tunnelling. The reduction of the degrees of freedom of the thermal reservoir leads to the effective dissipative dynamics for the central particle; in the framework of the Feynman path integral quantization the effective action $S_{0\text{eff}}$ obtained from the euclidean version (with $q(t) = q(t+T)$) of the lagrangian $L_0$ reads

$$S_{0\text{eff}}[q(t)] = \int_0^T dt \left( \frac{M}{2} \dot{q}^2 + V(q) \right) + \sum_{\alpha} \frac{\epsilon_{\alpha}^2}{4m_{\alpha} \omega_{\alpha}^2} \int_0^T dt \int_{-\infty}^\infty dt' e^{-\omega_{\alpha}|t-t'|} q(t)q(t') + \sum_{\alpha} \int_0^T dt \frac{\epsilon_{\alpha}^2}{2m_{\alpha} \omega_{\alpha}^2} q^2(t),$$

(3)

where the last term is introduced to ensure that the coupling with the thermal oscillators does not lower $V(q)$ below the original uncoupled value. Recognizing the non local time-dependent term in the action as the dissipative force leads to the phenomenological equation (1) with the friction coefficient $\eta$ identified as

$$\eta(\omega) = \frac{\pi}{2} \sum_{\alpha} \frac{\epsilon_{\alpha}^2}{m_{\alpha} \omega_{\alpha}^2} \delta(\omega - \omega_{\alpha}),$$

(4)
where $\omega$ is the Fourier conjugated of $t$ for the dynamic evolution of the dissipative system. The above identification is valid as long as $\omega \ll \omega_c$, where $\omega_c$ is the frequency at which the validity of eqn.(1) begins to break down. As the number of the thermal oscillators grows indefinitely, the frequencies become continuously distributed according to a spectral density $J(\omega)$ given by

$$J(\omega) = \frac{\pi}{2} \sum_{\alpha} \frac{\epsilon_\alpha^2}{m_\alpha \omega_\alpha} \delta(\omega - \omega_\alpha). \quad (5)$$

Comparing eqn.(4) and eqn.(5) one has

$$J(\omega) = \eta \omega. \quad (6)$$

Relation (6) is a general consequence of the requirement that the particle-reservoir coupling, i.e. the dissipation, be strictly linear.

3. Field-reservoir interaction.

We now want to investigate how the picture sketched above is modified by letting an external force act on the central particle and on the thermal reservoir. We are motivated by the consideration that in many physically interesting situations the approximation of considering only the central particle affected by a deterministic external force cannot be soundly justified. Also, from a conceptual point of view it seems more satisfactory to treat the central particle and the oscillators on equal dynamical footing. It is clear that for a generic type of coupling this might become a formidable problem. As a first step in our investigation we introduce a time- and velocity-independent coupling of the system (central particle + oscillators) with an external field of strength $F_0$, and consider a dependence at most quadratic on the coordinates of the system. The new model lagrangian reads

$$L = \frac{M}{2} \ddot{q}^2 - V(q) + F_0(\delta_0 q - \frac{\delta'_0 q^2}{2}) + \sum_{\alpha=1}^{N} \left\{ \frac{m_\alpha}{2} \dot{x}_\alpha^2 - \frac{m_\alpha}{2} \omega_\alpha^2 x_\alpha^2 + \epsilon_\alpha x_\alpha q + F_0(\delta_\alpha x_\alpha - \frac{\delta'_\alpha x_\alpha^2}{2}) \right\}. \quad (7)$$
We now introduce the new variables $y_\alpha$ defined by

$$y_\alpha = x_\alpha - \frac{\delta_\alpha F_0}{m_\alpha \Omega_\alpha^2} = x_\alpha - \bar{x}_\alpha,$$

with the new frequencies $\Omega_\alpha$ defined by

$$\Omega_\alpha = \sqrt{\omega_\alpha^2 + \frac{F_0 \delta'_\alpha}{m_\alpha}},$$

and finally define the potential $V_F(q)$ as

$$V_F(q) = V(q) - F_0 (\delta_0 q - \frac{\delta'_0}{2}q^2) - \sum_\alpha \epsilon_\alpha \bar{x}_\alpha q.$$

It is then easy to show, after some straightforward transformations, that the lagrangian $L$ takes the form

$$L = \frac{M}{2} \dot{q}^2 - V_F(q) + \sum_\alpha \left\{ \frac{m_\alpha}{2} y_\alpha^2 - \frac{m_\alpha}{2} \Omega_\alpha^2 y_\alpha^2 + \epsilon_\alpha y_\alpha q \right\} + E_0.$$

We have thus recasted the lagrangian for the central particle and the oscillators interacting with the external field in the form of the Ullersma lagrangian for the central particle and the oscillators alone. The effect of the interaction amounts now to a modification of the dynamical parameters in the original non-interacting lagrangian. An obvious consequence, eqn.(9), is that the oscillators’ frequencies acquire a field-dependent renormalization. The interesting new feature is expressed by eqn.(10): in the presence of an external field interacting with the reservoir the conservative force acting on the central particle acquires not only a contribution from the field-particle coupling, but also an extra term depending on the details of the field-reservoir coupling. The last term in eqn. (11) defined by

$$E_0 = \sum_\alpha \frac{\delta^2 F_0^2}{2 m_\alpha \Omega_\alpha^2} = \frac{1}{2} \sum_\alpha m_\alpha \Omega_\alpha^2 \bar{x}_\alpha^2,$$

amounts to a constant shift of the zero-point energy of the unperturbed system of thermal oscillators, and is irrelevant to our discussion. How the interaction of the thermal reservoir with the external field affects the mechanism of dissipation is the question we want to
address next. We then consider the effective action $S_{\text{eff}}$ for the lagrangian $L$ defined by eqn. (11). Since $L$ is still of the form of an Ullersma lagrangian, we can carry over the reduction procedure of Caldeira and Leggett exactly as in the unperturbed case to obtain the following expression for $S_{\text{eff}}$

$$S_{\text{eff}}[q(t)] = \int_0^T dt \left( \frac{M}{2} \dot{q}^2 + V(q) - F_0(\delta_0 q - \frac{\delta}{2} q^2) - \sum_\alpha \epsilon_\alpha \bar{x}_\alpha q \right) +$$

$$\sum_\alpha \frac{\epsilon_\alpha^2}{4m_\alpha \Omega_\alpha^2} \int_0^T dt \int_{-\infty}^{\infty} dt' e^{-\Omega_\alpha |t-t'|} q(t)q(t') +$$

$$\sum_\alpha \int_0^T dt \frac{\epsilon_\alpha^2}{2m_\alpha \Omega_\alpha^2} q^2(t). \quad (13)$$

By comparing eqn. (13) with eqns. (3), (4), and (6) we obtain the following relations

$$\eta(\omega, F_0) = \frac{\pi}{2} \sum_\alpha \frac{\epsilon_\alpha^2}{m_\alpha \Omega_\alpha^2} \delta(\omega - \Omega_\alpha), \quad (14)$$

and

$$J(\omega, F_0) = \eta(\omega, F_0) \omega. \quad (15)$$

We then recognize that the dissipation coefficient $\eta$ and the spectral density $J$ acquire a dependence on the external field’s strength $F_0$ through the renormalized frequencies $\Omega_\alpha$ of the thermal oscillators. From the second term of eqn. (13) we see that if $\Omega_\alpha$ increases with $F_0$ the correlation $\langle q(t)q(t') \rangle$ is reduced; for large times and values of $F_0$ one gets the locally overdamped behaviour of the quasiclassical equation of motion, i.e.

$$\dot{q} = \frac{F_0}{\eta} \equiv \mu F_0, \quad (16)$$

where $\mu = 1/\eta$ can be thought as the mobility of the central particle. The above prediction could then be tested on microscopic models of concrete physical systems, for instance by studying how an external electric field applied to an electrolytic solution (where the overdamped central particles are the conducting ions) affects the mobility (the friction).
4. Discussion and conclusions.

To summarize, we have shown that the modification of the Ullersma-Caldeira-Leggett model of quantum dissipation to allow interaction of the thermal reservoir with external forces leads to some non trivial effects. In fact, besides affecting the mechanism of dissipation, the field-reservoir coupling induces a new potential in the conservative dynamics of the central particle, depending on the field strength and on the dynamical parameters of the reservoir. The question immediately arises of where to look for such effects. A possibility is that suggested in discussing the consequences of eqn. (16). However, the general strategy should be to apply the above scheme to explicit microscopic models (including models of fermionic reservoirs). In this way one could also analyse the explicit functional dependence of \( \eta \) on the external field, and investigate the existence of discontinuities and phase transitions in its behaviour for some critical value of the field. Work is also in progress to extend the analysis developed in the present paper to the case of fields with more general dependence on the system’s degrees of freedom, and to the case of time-dependent fields, i.e. to the problem of the non equilibrium.

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