Thermodynamics of dissipative quantum systems by effective potential

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Classical-like formulas are given in order to evaluate thermal averages of observables belonging to a quantum nonlinear system with dissipation described by the Caldeira-Leggett model [Phys. Rev. Lett. **46**, 211 (1981); Ann. Phys. (N.Y.) **149**, 374 (1983)]. The underlying scheme is the *pure-quantum self-consistent harmonic approximation*, which leads to expressions with a Boltzmann factor involving an *effective potential* and with a Gaussian average. The latter describes the effect of the fluctuations of purely quantum origin. As an illustration we calculate the coordinate probability distribution for a double-well potential in the presence of various degrees of Ohmic dissipation. [S1063-651X(97)50405-3]

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The concept of effective potential, meant to reduce quantum statistical mechanics calculations to classical ones, was first introduced by Feynman [1,2]. He introduced a variational principle for the path-integral expression of the partition function—the *Feynman-Jensen* (FJ) *inequality*—and used it with a ''free particle'' trial action.

A significant improvement has been achieved by Giachetti and Tognetti [3,4] and independently by Feynman and Kleinert [5] using a quadratic trial action with the same variational principle. For nonstandard systems, where the FJ inequality is generally not valid, the *pure-quantum self-consistent harmonic approximation* (PQSCHA) gives a way to construct an effective Hamiltonian, thus recovering the phase-space concept and the classical-like formulas for thermal averages [6,7].

Several successful applications in different branches of condensed matter physics pointed out the power of the approach [7]. In the case of open systems, little work has been done for taking into account the quantum dissipation in the effective potential formalism; indeed, in a *system-plus-reservoir* model, only the effective potential for expressing the partition function as a configuration integral has been given, both for linear [8,9] and nonlinear coupling [10] with environmental oscillators.

By using the PQSCHA approach, that is equivalent to the variational method, we present here an accurate derivation of the density matrix of a nonlinear system interacting with a heat bath through the *Caldeira-Leggett* (CL) *model* [11]. This model considers the system of interest as linearly interacting with a bath of harmonic oscillators, whose coordinates can be integrated out from the path integral, leaving the CL Euclidean action

$$S[q(u)]=\int_0^{\beta\hbar}\frac{du}{\hbar}\left[\frac{m}{2}\,\dot{q}^2(u)+V(q(u))\right]-\int_0^{\beta\hbar}\frac{du}{4\hbar}\int_0^{\beta\hbar}du'\,k(u-u')(q(u)-q(u'))^2. \tag{1}$$

The kernel $k(u)=k(\beta\hbar-u)$ is a function that depends on temperature $T=1/\beta$ and on the spectral density of the environmental bath [9]. The density matrix elements in the coordinate representation are expressed by Feynman's path integral as

$$\rho(q'',q')\equiv\langle q''|\hat{\rho}|q'\rangle=\int_q^{q''}\mathcal{D}[q(u)]e^{-S[q(u)]}, \tag{2}$$

where the path integration is defined as a sum over all paths $q(u)$, with $u\in[0,\beta\hbar]$, $q(0)=q'$, and $q(\beta\hbar)=q''$.

As suggested by Feynman [2], we can rearrange the path integral (1) summing over classes of paths that share the same average point

$$\rho(q'',q')=\int d\overline{q}\;\overline{\rho(q}''\overline{,q';q)}, \tag{3}$$

$$\overline{\rho(q}''\overline{,q';q)}=\int_{q'}^{q''}\mathcal{D}[q(u)]\,\delta(\overline{q}-\overline{q}[q(u)])\;e^{-S[q(u)]}, \tag{4}$$

where $\overline{q}[q(u)]=(\beta\hbar)^{-1}\int_0^{\beta\hbar}du\;q(u)$ is the average point functional. Furthermore, as only paths with a fixed average point $\overline{q}$ appear in the path integral (4), from action (1) we define a trial action $S_0[q(u)]$ by replacing $V(q(u))$ with a trial quadratic ''potential''

$$V_0(q;\overline{q})=w(\overline{q})+\tfrac{1}{2}m\omega^2(\overline{q})(q-\overline{q})^2, \tag{5}$$

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where the parameters $w(\overline{q})$ and $\omega^2(\overline{q})$ are now to be optimized, so that the trial reduced density $\overline{\rho_0}(q,q;\overline{q})$ at best approximates $\overline{\rho}(q,q;\overline{q})$, *for each value of* q. Note that $V_0(q,\overline{q})$ is not related to a quantum observable, since it depends on $\overline{q}$: so, the first part of the trial action is also nonlocal.

The evaluation of the trial reduced density $\overline{\rho_0}(q'',q';\overline{q})$, in spite of the fact that the action is quadratic, is rather tricky: on the one hand, the known general method of calculating the minimal action fails since its minimization gives rise to infinite order equations of motion, and, on the other hand, the method of Fourier expansion of the paths in terms of discrete Matsubara components conflicts with the openness of the paths, since we are indeed looking also for the off-diagonal part of the density matrix ($q''\neq q'$). However, the second way may still be followed by transforming as

$$\overline{\rho}(q'',q';\overline{q})=\lim_{\varepsilon\to 0}\left\{\frac{1}{\mathcal{F}_\varepsilon}\oint \mathcal{D}[q(u)]\,\delta(\overline{q}-\overline{q[q(u)]})\times e^{-S[q(u)]}\right\}; \tag{6}$$

the integral is over all *closed* paths $\{q(u)|u\in[0,\beta\hbar]\}$ that satisfy the constraints $q(\varepsilon)=q'$ and $q(\beta\hbar-\varepsilon)=q''$. $\mathcal{F}_\varepsilon$ is the integral over the open paths $\{q(u)|u\in[-\varepsilon,\varepsilon]\}$ (the range $[\beta\hbar-\varepsilon,\beta\hbar]$ is periodically mapped onto $[-\varepsilon,0]$) with end points $q(-\varepsilon)=q''$ and $q(\varepsilon)=q'$; for small ε it is dominated by the kinetic contribution

$$\mathcal{F}_\varepsilon=\left(\frac{m}{4\pi\hbar^2\varepsilon}\right)^{1/2}\exp\left[-\frac{m}{4\hbar\varepsilon}(q''-q')^2+O(\varepsilon)\right]. \tag{7}$$

Now the paths in Eq. (6) can be Fourier expanded,

$$q(u)=\overline{q}+2\sum_{n=1}^{\infty}(x_n\cos\nu_n u+y_n\sin\nu_n u); \tag{8}$$

$\nu_n=2\pi n/(\beta\hbar)$ are the Matsubara frequencies and the ν_0 component is just $\overline{q}$, as it appears from the inverse transformation. The measure of the path integral then becomes [2]

$$\left(\frac{m}{2\pi\hbar^2\beta}\right)^{1/2}\int d\overline{q}\prod_{n=1}^{\infty}\frac{m\beta\nu_n^2}{\pi}\int dx_n dy_n, \tag{9}$$

and the trial action takes then the form

$$S_0[q(u)]=\beta w(\overline{q})+\beta m\sum_{n=1}^{\infty}[\nu_n^2+\omega^2(\overline{q})+\nu_n\gamma(\nu_n)](x_n^2+y_n^2). \tag{10}$$

Here we have made use of the relation that connects the kernel $k(u)$ with the Laplace transform $\gamma(z)$ of the real-time memory damping function $\gamma(t)$ [9]

$$k(u)=\frac{m}{\beta\hbar}\sum_{n=-\infty}^{\infty}e^{i\nu_n u}|\nu_n|\,\gamma(z=|\nu_n|). \tag{11}$$

While it is trivial to manage the δ function that fixes $\overline{q}$, the end-point constraints are implemented by inserting the δ functions $\delta(q(\beta\hbar-\varepsilon)-q'')$ and $\delta(q(\varepsilon)-q')$, and then using their Fourier representation. The calculation of $\overline{\rho_0}$ can then be carried forward by Gaussian quadratures giving

$$\overline{\rho_0}(q'',q';q)=\left(\frac{m}{2\pi\hbar^2\beta}\right)^{1/2}\frac{e^{-\beta w(\overline{q})}}{\mu(\overline{q})}\times\lim_{\varepsilon\to 0}\left[\frac{1}{\mathcal{F}_\varepsilon}\frac{e^{-\xi^2/c_\varepsilon}}{\sqrt{\pi c_\varepsilon}}\frac{e^{-\zeta^2/s_\varepsilon}}{\sqrt{\pi s_\varepsilon}}\right], \tag{12}$$

where $\xi\equiv\frac{1}{2}(q'+q'')-\overline{q}$ and $\zeta\equiv q''-q'$,

$$\mu(\overline{q})=\prod_{n=1}^{\infty}\frac{\nu_n^2+\omega^2(\overline{q})+\nu_n\gamma(\nu_n)}{\nu_n^2}, \tag{13}$$

$$c_\varepsilon=\frac{4}{\beta m}\sum_{n=1}^{\infty}\frac{\cos^2\nu_n\varepsilon}{\nu_n^2+\omega^2(\overline{q})+\nu_n\gamma(\nu_n)}, \tag{14}$$

$$s_\varepsilon=\frac{16}{\beta m}\sum_{n=1}^{\infty}\frac{\sin^2\nu_n\varepsilon}{\nu_n^2+\omega^2(\overline{q})+\nu_n\gamma(\nu_n)}. \tag{15}$$

In the last expressions, the leading terms for small ε are $c_\varepsilon=2\alpha(\overline{q})+O(\varepsilon)$, and, in a less straightforward way [11,12], $s_\varepsilon=4\hbar\varepsilon/m[1-(2\varepsilon/\hbar m)\lambda(\overline{q})+o(\varepsilon)]$, with

$$\alpha(\overline{q})=\frac{2}{\beta m}\sum_{n=1}^{\infty}\frac{1}{\nu_n^2+\omega^2(\overline{q})+\nu_n\gamma(\nu_n)}, \tag{16}$$

$$\lambda(\overline{q})=\frac{m}{\beta}\sum_{n=-\infty}^{\infty}\frac{\omega^2(\overline{q})+|\nu_n|\gamma(|\nu_n|)}{\nu_n^2+\omega^2(\overline{q})+|\nu_n|\gamma(|\nu_n|)}. \tag{17}$$

Eventually, the limit in ε can be easily taken, and the result reads

$$\overline{\rho_0}(q'',q';\overline{q})=\left(\frac{m}{2\pi\hbar^2\beta}\right)^{1/2}\frac{e^{-\beta w(\overline{q})}}{\mu(\overline{q})}\frac{e^{-\xi^2/2\alpha(\overline{q})-\lambda(\overline{q})\zeta^2/2\hbar^2}}{\sqrt{2\pi\alpha(\overline{q})}}. \tag{18}$$

Now, if $\rho_0(q'',q')$—obtained using the last result in Eq. (3)—is taken as an approximation for the exact density matrix $\rho(q'',q')$, we have a way to explicitly calculate any quantum thermal average by two Gaussian quadratures plus a single integral in $\overline{q}$. A more convenient formalism deals with phase space: let us briefly show it.

The Weyl symbol for an observable $\hat{\mathcal{O}}=\hat{\mathcal{O}}(\hat{p},\hat{q})$ is the phase-space function $\mathcal{O}(p,q)$ that is defined in terms of the matrix elements in coordinate space as [13]

$$\mathcal{O}(p,q)=\int d\zeta\, e^{-ip\zeta/\hbar}\left\langle q+\tfrac{1}{2}\,\zeta|\hat{\mathcal{O}}|q-\tfrac{1}{2}\zeta\right\rangle. \tag{19}$$

By means of a simple property of Weyl symbols the average of $\hat{\mathcal{O}}$ takes the form of a phase-space integral,

$$\langle\hat{\mathcal{O}}\rangle=\frac{1}{\mathcal{Z}}\int\frac{dpdq}{2\pi\hbar}\rho(p,q)\mathcal{O}(p,q). \tag{20}$$

From Eqs. (3) and (18) the Weyl symbol for the trial density operator turns out to be

$$\rho_0(p,q)=2\pi\hbar\left(\frac{m}{2\pi\hbar^2\beta}\right)^{1/2}\int d\overline{q}\,\frac{e^{-\beta w(\overline{q})}}{\mu(\overline{q})}\times\frac{e^{-\xi^2/2\alpha(\overline{q})}}{\sqrt{2\pi\alpha(\overline{q})}}\,\frac{e^{-p^2/2\lambda(\overline{q})}}{\sqrt{2\pi\lambda(\overline{q})}}, \tag{21}$$

where $\xi\equiv q-\overline{q}$. Therefore, the average of any observable $\hat{\mathcal{O}}(\hat{p},\hat{q})$ can be expressed as a classical formula

$$\langle\hat{\mathcal{O}}\rangle=\frac{1}{\mathcal{Z}}\left(\frac{m}{2\pi\hbar^2\beta}\right)^{1/2}\int d\overline{q}\langle\!\langle\mathcal{O}(p,\overline{q}+\xi)\rangle\!\rangle e^{-\beta V_{\rm eff}(\overline{q})}, \tag{22}$$

where the double bracket is the Gaussian average operating over p and ξ, with moments $\langle\!\langle\xi^2\rangle\!\rangle=\alpha(q)$ and $\langle\!\langle p^2\rangle\!\rangle=\lambda(\overline{q})$; the effective potential is defined as

$$V_{\rm eff}(\overline{q})\equiv w(\overline{q})+\beta^{-1}\ln\mu(\overline{q}). \tag{23}$$

In order to determine the functions $w(\overline{q})$ and $\omega^2(\overline{q})$ we impose the PQSCHA condition, i.e., we require that the potential $V(q)$ and the trial potential $V_0(q;\overline{q},)$ together with their derivatives up to second order, have equal averages with respect to the reduced (diagonal) density $\overline{\rho_0(q,q;\overline{q})}$. The condition for the first derivatives is overcome by the definition of the average point, so that we are left with

$$\langle\!\langle V(\overline{q}+\xi)\rangle\!\rangle=\langle\!\langle V_0(\overline{q}+\xi)\rangle\!\rangle\equiv w(\overline{q})+\frac{m}{2}\omega^2(\overline{q})\alpha(\overline{q}),$$

$$\langle\!\langle V''(\overline{q}+\xi)\rangle\!\rangle=\langle\!\langle V_0''(\overline{q}+\xi)\rangle\!\rangle\equiv m\omega^2(\overline{q}). \tag{24}$$

The latter condition must be solved self-consistently with the definition of $\alpha(\overline{q})$ in terms of $\omega^2(\overline{q})$, Eq. (16). Now we have all the necessary ingredients to explicitly evaluate the effective potential and all the thermal averages through the classical-like expression (22). As in the case of no dissipation, it can be seen that for the most usual potentials the self-consistent solution for $\alpha(\overline{q})$ turns out to be always positive, even though $\omega^2(\overline{q})$ can be negative [4,5]. Indeed, what matters is that α, Eq. (16), is a decreasing function of ω^2, with a divergence to $+\infty$ [which in the dissipative case happens at $\omega^2\to-\nu_1^2-\nu_1\gamma(\nu_1)$].

In the case of *Ohmic dissipation*, corresponding to $\gamma(z)=\gamma=$const [i.e., the memory is Markovian, $\gamma(t)=\gamma\delta(t-0)$], one can see that the ($\overline{q}$-dependent) mean-square momentum $\lambda(\overline{q})$, Eq. (17), is divergent in the Ohmic case. Correspondingly, also $\mu(\overline{q})$, Eq. (13) diverges. The physical reason for this, basically related to the uncertainty principle, is well discussed in Refs. [9,11]. Here we note that the coordinate mean-square fluctuation $\alpha(\overline{q})$ is still well defined, and that the effective potential can be made finite by subtraction of the infinite but $\overline{q}$-independent quantity $\beta^{-1}\ln\mu_1$, with $\mu_1=\Pi_{n=1}^{\infty}[1+\gamma(\nu_n)/\nu_n]$. Therefore, Eq. (22) is still meaningful in the case of observables that do not depend on momentum.

For a given potential $V(\hat{q})$, it is convenient to devise a characteristic energy scale ϵ (e.g., the barrier height for a double-well potential, the well depth for physical potentials that vanish at infinity, etc.) and a length scale σ (such that variations of V comparable to ϵ occur on this length scale) and write $V(\hat{q})=\epsilon v(\hat{q}/\sigma)$. In this way one better deals with the dimensionless coordinate $\hat{x}=\hat{q}/\sigma$. If x_m is the absolute minimum of $v(x)$, the harmonic approximation (HA) of the system is characterized by the frequency $\omega_0=\sqrt{\epsilon v''(x_m)/m\sigma^2}$; a dimensionless coupling parameter g for the system can be defined as the ratio between the HA quantum energy level splitting $\hbar\omega_0$ and the overall energy scale ϵ,

$$g=\frac{\hbar\omega_0}{\epsilon}=\left(\frac{\hbar^2 v''(x_m)}{m\epsilon\sigma^2}\right)^{1/2}. \tag{25}$$

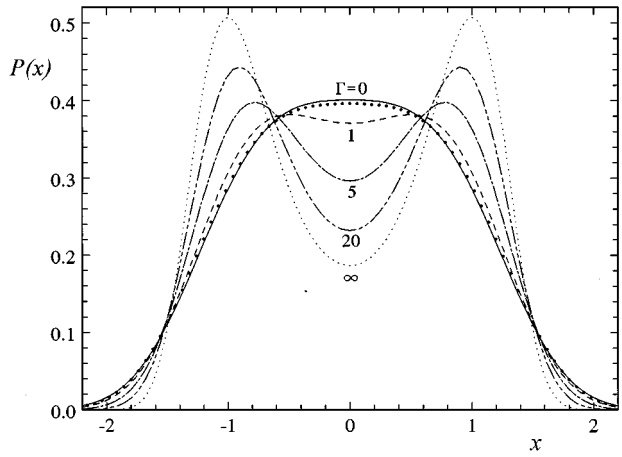

FIG. 1. Configuration density $\mathcal{P}(x)=\langle\delta(\hat{x}-x)\rangle$ of the double-well quartic potential for $g=5$, $t=1$, and different values of the Ohmic damping parameter $\Gamma=\gamma/\omega_0$. The filled circles are the exact result for $\Gamma=0$; the dotted curve at $\Gamma=\infty$ corresponds to the classical limit.

The case of weak (strong) quantum effects occurs when g is small (large) compared to 1. In the following application we shall make use of the dimensionless variables only, i.e., energies are given in units of ϵ, lengths in units of σ, frequencies in units of ω_0, and so on; the reduced temperature is $t=1/(\epsilon\beta)$.

Let us then consider the double-well quartic potential

$$v(x)=(1-x^2)^2. \tag{26}$$

It has two degenerate symmetric minima in $x_m=\pm1$, with $v''(x_m)=8$. From the PQSCHA equations (24) and the definitions (23) and (16) we obtain

$$v_{\rm eff}(x)=(1-x^2)^2-3\alpha^2(x)+t\,\ln\mu(x), \tag{27}$$

$$\mu(x)=\prod_{n=1}^{\infty}\frac{(\pi n)^2+f^2(x)+\pi n\tilde{\gamma}(n)}{(\pi n)^2}, \tag{28}$$

$$f^2(x)=\frac{g^2}{8t^2}[3x^2+3\alpha(x)-1], \tag{29}$$

$$\alpha(x)=\frac{g^2}{16t}\sum_{n=1}^{\infty}\frac{1}{(\pi n)^2+f^2(x)+\pi n\tilde{\gamma}(n)}, \tag{30}$$

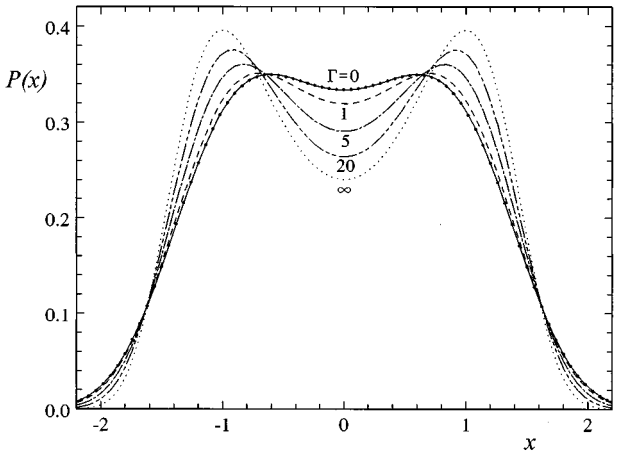

FIG. 2. Same as Fig. 1, for $g=5$, $t=2$.

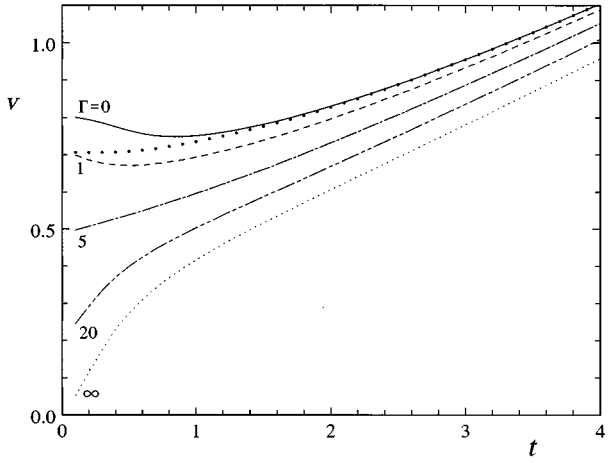

FIG. 3. Average potential energy $v=\langle v(x)\rangle$ of the double-well quartic potential vs temperature, for $g=5$ and different values of $\Gamma=\gamma/\omega_0$. The filled circles are the exact result for $\Gamma=0$; the dotted curve at $\Gamma=\infty$ corresponds to the classical limit.

where

$$f(x)=\frac{\beta\hbar\omega(x)}{2}=\frac{g}{2t}\,\frac{\omega(x)}{\omega_0}\,, \tag{31}$$

$$\tilde{\gamma}(n)=\frac{\beta\hbar\gamma(\nu_n)}{2}=\frac{g}{2t}\,\frac{\gamma(\nu_n)}{\omega_0}\,, \tag{32}$$

and $\nu_n=(2\pi t/g)\omega_0 n$. Equations (29) and (30) have to be solved self-consistently. This task is done numerically; exact reference data can be obtained only for $\gamma=0$ by numerical solution of the Schrödinger equation.

In Figs. 1 and 2 we report the shapes of the coordinate probability distribution $\mathcal{P}(x)=\langle\delta(\hat{x}-x)\rangle$ in the case of Ohmic damping, $\gamma(\nu_n)=\Gamma\omega_0=\text{const}$, at a very strong value of the coupling, $g=5$; this gives a (nondissipative) ground state energy $e_0=1.394$, and the first excited level is $e_1=e_0+2.355$. When dissipation is switched on $\mathcal{P}(x)$ tends towards the classical distribution $\mathcal{P}_c\sim e^{-v(x)/t}$.

Figure 3 shows typical results found for the average potential energy $v(t)=\langle v(x)\rangle$. By comparing with the exact data at $\Gamma=0$ it appears that the PQSCHA gives very accurate results, in spite of the strong coupling. At lowest temperatures the PQSCHA tends to the ordinary self-consistent harmonic (or one-loop) approximation, since the effective Boltzmann factor tends to a δ function.

However, a more physical model should involve a non-Markovian memory damping function; in such a model there would be at least one more characteristic frequency scale (e.g., the frequency ω_D in the Drude model [9]) above which $\gamma(z)$ rapidly vanishes. In this case all averages make sense, and whereas the averages of coordinate-dependent observables tend again to the classical behavior (in other words, the environment quenches the pure-quantum coordinate fluctuations), those of momentum-dependent ones go in the opposite direction due to the momentum exchanges with the environment. Of course, the PQSCHA expressions are even more useful in these physical situations. Further details and applications, as well as the extension to the case of many degrees of freedom, will be given in a forthcoming paper.

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