Alternative model of dissipation in quantum mechanics

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The model of dissipation studied by Castro Neto and Caldeira [Phys. Rev. Lett. **67**, 1960 (1991)] is reexamined. The main results for transport are derived in a simple manner without the use of Feynman path integrals. By means of a unitary transformation, a connection is made between the model and a model previously studied in the field of quantum dissipation. Lastly, extensions of the model are discussed.

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In the past several years there has been a great deal of interest in the physics of dissipative quantum systems [1–3]. The field underwent growth during the 1980's with the development and application of path integral methods to the quantum Brownian oscillator [1,2] and the spin-boson problem [2,3]. Recently, Castro Neto and Caldeira (hereafter denoted CNC) introduced a model for dissipation in quantum mechanical systems [4]. Their work is based on an approximate form of a Hamiltonian which had previously been applied to the study of polaron dynamics [5,6]. CNC apply the path integral formalism to this model Hamiltonian in their study of the dynamics of polarons in one dimension [7], in their work on the transport properties of solitons, [8] and to the problem of the dynamics of particles coupled to a Luttinger liquid [9]. The chief result uncovered is that the quasiparticle of interest undergoes a Brownian-type motion, with a peculiar damping kernel. The model holds more than just academic interest in that the results for the temperature dependence of the mobility of the quasiparticle agree with a previous study of the one dimensional polaron problem that utilized a more complicated kinetic theory [10].

Since the path integral calculations lead to a damping of the quasiparticle motion, it would be interesting to study the dissipative model of CNC by a simple method known to lead directly to a Langevin-type equation [11–13]. The purpose of this brief report is threefold. First, we wish to provide a simple and physically clear derivation of the quasiparticle transport properties governed by the Hamiltonian of CNC without the use of the Feynman-Vernon formalism. Secondly, we wish to show a connection between the model of CNC, and a model of dissipation previously studied. Lastly, we wish to point out some features of a simple extension of the model.

We begin with the Hamiltonian [4]

$$H=\frac{\hat{\Pi}^2}{2m}+H_R, \tag{1}$$

$$\hat{\Pi}=p-\hat{h},$$

$$\hat{h}=\sum_{kk'}\hbar G_{kk'}a_k^\dagger a_{k'},$$

$$H_R=\sum_k \hbar\omega_k a_k^\dagger a_k,$$

with

$$G_{kk'}=-G_{k'k},$$

$$G_{kk'}^*=G_{k'k}. \tag{2}$$

This Hamiltonian is an approximate version of a Hamiltonian used in the theory of polaron dynamics [5,6]. Notice that, unlike previous studies on quantum Brownian motion [1,11], the Hamiltonian contains a local system-bath interaction, and the number of reservoir excitations is conserved.

We will be content to describe the dynamics of the quasiparticle to second order in the coupling constant G. This is equivalent to the Born approximation used in the functional integral study [4]. Note that

$$m\dot{x}(t)=\hat{\Pi}(t), \tag{3}$$

so that we must interpret $\hat{\Pi}(t)$ as the mechanical momentum of the quasiparticle. We now use the method employed by Lindenberg and West in their study of quantum Brownian motion [11]. The Heisenberg equation of motion is found,

$$\ddot{x}(t)=\sum_{kk'}\Gamma_{kk'}a_k^\dagger(t)a_{k'}(t), \tag{4}$$

with

$$\Gamma_{kk'}=-\frac{i\hbar}{m}G_{kk'}(\omega_k-\omega_{k'}).$$

Note that $\Gamma_{kk'}$ is real and symmetric. The equation of motion for the bath operators is found to be

$$\dot{a}_r(t)\approx -i\omega_r a_r(t)+i\sum_k G_{rk}a_k(t)\dot{x}(t), \tag{5}$$

where we have ignored the noncommutativity of the operators $\dot{x}(t)$ and $a_r(t)$ since we are concerned with the dynamics in the Born approximation limit. Equation (5) is formally integrated, and substituted into Eq. (4). The result, to second order in G is the operator equation

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$$\ddot{x}(t)+\int_0^t \hat{K}(t,\tau)\dot{x}(\tau)d\tau=\hat{F}(t), \tag{6}$$

with an operator kernel given by

$$\hat{K}(t,\tau)=i\sum_{rr'k}\Gamma_{rr'}\{G_{kr}\exp\{i[(\omega_r-\omega_{r'})t +(\omega_k-\omega_r)\tau]\}a_k^\dagger a_{r'}-G_{r'k}\exp\{i[(\omega_r-\omega_{r'})t +(\omega_{r'}-\omega_k)\tau]\}a_r^\dagger a_k\}, \tag{7}$$

and an operator "fluctuating force" of the form

$$\hat{F}(t)=\sum_{kk'}\Gamma_{kk'}\exp\{-i(\omega_k-\omega_{k'})t\}a_k^\dagger a_{k'}. \tag{8}$$

All bath operators without explicit time arguments are to be understood as the values of the operators at $t=0$. We now suppose that the bath is initially prepared in the canonical ensemble, that is

$$\rho_R(0)=\exp\{-\beta H_R\}/Z.$$

We average Eq. (6) over the initial bath state, and retain terms in the average that contribute to second order in G, giving,

$$\ddot{x}(t)+\int_0^t K(t-\tau)\dot{x}(\tau)=0, \tag{9}$$

with

$$K(t-\tau)=\frac{\hbar}{m}\sum_{kk'}G_{kk'}^2(\omega_k-\omega_{k'})[n(\omega_k)-n(\omega_{k'})] \times\cos(\omega_k-\omega_{k'})(t-\tau), \tag{10}$$

and

$$n(\omega_k)=[\exp(\beta\hbar\omega_k)-1]^{-1}.$$

Note that Eq. (9) is still an operator equation for the system operators $\ddot{x}(t)$ and $\dot{x}(t)$, and may be averaged over an arbitrary system initial state without altering the form of the equation in the Born approximation limit. Equation (9) is identical to the equation of damping obtained by CNC using the more involved path integral approach [4]. If a proper generalization of the ohmic spectral density is used [4,7,8], the quasiparticle mobility obtained from Eq. (9) agrees with that of an earlier study on the polaron dynamics in one dimension [10], which also utilized a Hamiltonian of the type (1).

From Eq. (6) we may obtain the fluctuation-dissipation relationship between the fluctuating force and the dissipative kernel [11–13]. Consider the symmetrized correlation function,

$$\tfrac{1}{2}\langle\hat{F}(t)\hat{F}(\tau)+\hat{F}(\tau)\hat{F}(t)\rangle=\sum_{kk'}\Phi_{kk'}(t-\tau), \tag{11}$$

with

$$\Phi_{kk'}(t-\tau)=\frac{\hbar^2}{m^2}|G_{kk'}|^2(\omega_k-\omega_{k'})^2\cos(\omega_k-\omega_{k'}) \times(t-\tau)n(\omega_k)[(n(\omega_{k'})+1)],$$

which is related to the diffusion function $D(t)$ of CNC [1,4,7,8]. The fluctuation-dissipation relation is now manifest, taking the form,

$$K(t-\tau)=\frac{m}{\hbar}\sum_{kk'}\Phi_{kk'}(t-\tau) \times\frac{[n(\omega_{k'})-n(\omega_k)]}{(\omega_k-\omega_{k'})\{n(\omega_k)[n(\omega_{k'})+1]\}}. \tag{12}$$

In the classical limit, the dissipative kernel is directly proportional to the symmetrized fluctuating force correlation function as expected,

$$\tfrac{1}{2}\langle\{\hat{F}(t),\hat{F}(\tau)\}\rangle=\frac{k_bT}{m}K(t-\tau).$$

We may note that the fluctuation-dissipation relation (12) is essentially identical to a fluctuation-dissipation relation obtained by Cortés, West, and Lindenberg [12], for the Hamiltonian,

$$\frac{p^2}{2m}+H_R+x\sum_{kk'}W_{kk'}a_k^\dagger a_{k'}. \tag{13}$$

In their study, the dynamics were also accounted for through second order in W. To see the relationship between the Hamiltonian (13) and (1), consider the unitary transformation

$$\tilde{H}=U^{-1}HU,$$

with

$$U=\exp(ix\hat{h}/\hbar). \tag{14}$$

If we are again concerned with dynamics to second order in G, we may write,

$$\tilde{H}=\frac{p^2}{2m}+H_b+x\sum_{kk'}iG_{kk'}(\omega_k-\omega_{k'})a_k^\dagger a_k+\mathcal{O}(G^2), \tag{15}$$

which has the form (13) to first order in G. Note that in this picture $m\dot{x}(t)=p(t)$, so that p is in fact the quasiparticle momentum. The unitary transformation (14) is, in spirit, similar to the Göppert-Mayer transformation in nonrelativistic quantum electrodynamics, where the interaction Hamiltonian $\mathbf{p}\cdot\mathbf{A}$ is transformed into $\mathbf{r}\cdot\mathbf{E}$ in the electric dipole approximation [14]. In the case of the Hamiltonian (1), the interaction Hamiltonian is given by $p\hat{h}$. One can immediately infer, from the analogy to the Göppert-Mayer transformation, that the transformed interaction Hamiltonian would be $x\hat{h}$, which is, to first order in G, identical to the third term on the right-hand side of Eq. (15). This shows that the two pictures represented by the Hamiltonians (1) and (15) are in fact identical in the weak coupling limit. Indeed, this is a manifestation of the gauge invariance.

For completeness, we start with Eq. (15) and use the same procedure as before. We find the operator equation

$$\ddot{x}(t)+\int_0^t \hat{K}(t,\tau)\dot{x}(\tau)d\tau+\hat{\Omega}(t)x(t)=\hat{R}(t), \tag{16}$$

with

$$\hat{R}(t)=-\frac{i\hbar}{m}\sum_{kk'} G_{kk'}\exp[i(\omega_k-\omega_{k'})t]\Big\{a_k^\dagger a_{k'}-i\hbar x(0)\times\sum_r (G_{kr}a_r^\dagger a_{k'}+G_{k'r}a_k^\dagger a_r)\Big\}, \tag{17}$$

and

$$\hat{\Omega}(t)=-\frac{i\hbar}{m}\sum_{kk'} G_{kk'}\{G_{kr}a_r^\dagger a_{k'}\exp[-i(\omega_{k'}-\omega_r)t]+G_{k'r}a_k^\dagger a_r\exp[-i(\omega_r-\omega_k)t]\}. \tag{18}$$

Note that the form of Eq. (16) is slightly different than that of Eq. (6). Equation (16) could be put in a more standard, Langevin-type form by modifying the system Hamiltonian as discussed by Lindenberg and West [11]. However, if we are concerned only with the reduced (bath averaged) properties of Eq. (16), then such a modification is not necessary. Our original initial conditions for the density matrix were of the factorized form $\rho(0)=\sigma(0)\rho_R(0)$. In the gauge transformed picture, the initial conditions take the form $U^{-1}\rho(0)U$. If we are concerned with dynamics in the weak coupling limit, we may again average over the cannonical ensemble of the bath ρ_R reducing Eq. (16) to Eq. (9). Furthermore, the fluctuation-dissipation relation for Eq. (16) is identical to Eq. (12). This establishes the relationship between the Hamiltonian (1) of CNC and the Hamiltonian (13) studied by Cortés, West, and Lindenberg [12] in the Born approximation limit.

Lastly, we would like to briefly comment on the extensions of the Hamiltonian (1). If terms are included in (1) that do not conserve the number of bath excitations, then the modified Hamiltonian takes the form [7,8]

$$H=\frac{1}{2m}[p-\hat{j}]^2+H_R, \tag{19}$$

with

$$\hat{j}=\hbar\sum_{kk'}\left\{G_{kk'}a_k^\dagger a_{k'}+\frac{Q_{kk'}}{2}(a_k a_{k'}-a_k^\dagger a_{k'}^\dagger)\right\}, \tag{20}$$

with $Q_{kk'}^*=-Q_{k'k}, Q_{kk'}=Q_{k'k}$. The energy nonconserving terms could correspond to the absorption or emission of phonons by the polaron (Cerenkov process) or high-frequency oscillations in the soliton problem. Such terms may be easily handled with the methods employed here. Effectively, the damping kernel will contain the sum of two terms, one term from the energy conserving portion of the Hamiltonian that takes the form (10), and a term from the counterrotating portion of (20) with the form [12],

$$\xi(t-\tau)=\frac{2\hbar}{m}\sum_{kk'}|Q_{kk'}|^2[n(\omega_k)+n(\omega_{k'})+1]\times(\omega_k+\omega_{k'})\cos(\omega_k+\omega_{k'})(t-\tau). \tag{21}$$

Note that the Hamiltonian (19) gives a damping that does not vanish as the temperature approaches zero.

To summarize our results, we have presented a derivation of the transport properties of the Hamiltonian (1) in a simple and physical manner without the use of the path integral method. The approach utilizes the method of Lindenberg and West [11], which leads naturally to a generalized Langevin equation in the weak coupling limit. The relationship between the Hamiltonian (1) and the one studied by Cortés, West, and Lindenberg [12] is demonstrated. Lastly, we have sketched how the transport properties are modified when counterrotating terms are included in the Hamiltonian.

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