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Study of electrons in contact with non-Markovian baths

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Abstract. We discuss the extension of the augmented space formalism to study systems of fermions in contact with a heat bath to incorporate non-Markovian evolution of the bath variables. The formalism uses the ideas of the memory function approach. We give a simple example to show how the non-Markovian nature of the bath effects the spectral response of the electron system.

1. Introduction

The problem of fermions in contact with time fluctuating random potentials is of particular interest to condensed matter physicists. The reason for continued interest in these problems lies in the fact that a number of many-body interacting systems can be mapped onto the problem of individual fermions interacting with a time fluctuating stochastic bath. The Hubbard model is one such example [1]. Sluggish electrons in quenched disordered systems (dirty alloys) interacting with a phonon bath is another [2]. Several authors have treated the motion of excitons coupled to heat baths using ideas that originated in the Haken–Strobl model [3–5] in which the fermion degrees of freedom are treated quantum mechanically, while the evolution of the bath is treated in a stochastic manner. There are several *adiabatic* or *static* approximations that ignore the dynamics of the bath, replacing its effect by a static quenched disorder in the fermion potential. This approximation would be valid whenever the time scales associated with the bath evolution are much larger than that of the electrons that interact with it. In this category lie the *alloy analogy* CPA solutions of the Hubbard model [6] and the adiabatic approximation for the electron–phonon coupled system [7]. Difficulties with these approximations arise in many interesting situations where the bath dynamics plays an important role, such as the presence of a Fermi-liquid–non-Fermi-liquid transition in half-filled Hubbard models for the $U \rightarrow 0$ limit [8, 9] and a low-temperature anomalous temperature coefficient of resistivity in Mooij alloys [10]. The next stage of sophistication assumes the stochastic evolution of the bath to be Markovian [11]. However, memory effects, absent in the Markovian process, may also play a crucial role in many situations, for example, if we want to bridge between wave-like propagation and diffusive propagation in such systems [12]. The aim of this paper is to set up a generalized methodology to treat the fermions in contact with non-Markovian baths within the framework of the augmented space formalism (ASF) introduced by one of us [13].

The Hamiltonian of a fermion moving on a lattice in contact with a time fluctuating stochastic bath may be written as follows:

$$H = \sum_i \sum_j t_{ij} c_i^\dagger c_j + V(\{u_n(t)\}). \tag{1}$$

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The potential seen by the fermion because of the stochastic bath depends on time fluctuating *bath variables* $u_n(t)$. In the simplest model, each lattice point has a bath variable attached to it, and the Hamiltonian may be written as

$$H = \sum_i \sum_j t_{ij} c_i^\dagger c_j + \sum_i \lambda u_i(t) c_i^\dagger c_i. \tag{2}$$

The first term represents the Hamiltonian seen by the fermion in absence of the bath and may be designated as H_0. If the vector of stochastic variables $v(t) = \{u_i(t)\}$ takes on values $\xi(\tau)$ as time evolves, then the space spanned by $\xi(\tau)$ is called the *state space* of the bath. This is in exact analogy to the *state space* for quenched disorder as described in the ASF. A *history* of the bath is a set of vectors $\{\xi(\tau_j)\}$ $0 \leqslant \tau_1 \leqslant \tau_2 \leqslant \ldots \leqslant \tau_n = t$ and the set constitutes a path or curve in the state space. Note that the fermion creation and annihilation operators $c_i^\dagger$ and c_i are operators on a Hilbert space H spanning the lattice, whereas the potentials u_i operate on the state space Φ such that $\xi|\phi\rangle = \xi|\phi\rangle$ where $|\phi\rangle$ are the eigenvectors of the bath Hamiltonian H_b which span the state space Φ.

The evolution operator, averaged over different histories of the bath, may be written as

$$\langle U(t)\rangle = \int \prod \Delta u_i(\tau) P_w[u_i(\tau)]\, T_\tau \exp\left[(-i/\hbar)\int_0^t \left(H_0 + \lambda \sum_i u_i(\tau) n_i(\tau)\right) d\tau\right]. \tag{3}$$

Here τ parametrizes a point on a particular *history* of the bath from $\tau = 0$ to t, and $P_w[u_i(\tau)]$ is a weight function for i-site histories. As expressed in (3) $\langle U(t)\rangle$ is the mean evolution operator averaged over all time histories of the bath. Our aim would be to obtain an expression for this object. Notice that the Laplace transform of the averaged evolution operator is the averaged Green operator or propagator of the electron in interaction with the bath.

Any static or adiabatic approximation at this point suppresses the time dependence of the bath variables $\{u_i\}$, leading to a frozen random probability distribution of the site energies seen by the electron. Our main aim would be to keep the intrinsic dynamics of the bath variables intact. In particular we shall concentrate on the non-Markovian bath evolution. The Markovian approximation washes out all of the *reversible* behaviour of the bath, which may be of importance in the exact nature of the transport of the fermion. For example, as mentioned earlier, when the electron Hamiltonian has intrinsic static disorder, so that near the Fermi energy the electrons are *sluggish*, the non-Markovian nature of the bath evolution is essential to bridge the gap between wave-like and diffusive nature of the electron propagation in contact with the phonon bath [12].

As a first step, we shall set up the generalized Master equation for the evolution probability of the bath variables. We shall follow the procedure of Zwanzig [14] and Nakajima [15] starting from the definition of the evolution probability as the diagonal element of the density matrix for the bath in its state space Φ.

$$p(\xi, t) = \langle \xi|\rho|\xi\rangle$$

and using the equation of motion in the bath:

$$i\partial\rho/\partial t = [H_b, \rho] = \mathcal{L}\rho$$

$\mathcal{L}$ being the Liouville operator, we obtain

$$\partial p(\xi, t)/\partial t = \int_0^t ds \int d\xi' \left[W(\xi, \xi', t-s)p(\xi', s) - W(\xi', \xi, t-s)p(\xi, s)\right] + I(\xi, t) \tag{4}$$

where

$$W(\xi,\xi',t) = -\left[\mathcal{P}\mathcal{L}\exp\left(-it(1-\mathcal{P})\mathcal{L}\right)\right]_{\xi\xi,\xi'\xi'}$$
$$I(\xi,t) = i\left[\mathcal{P}\mathcal{L}\exp\left[-it(1-\mathcal{P})\mathcal{L}\right]\ (1-\mathcal{P})\rho(0)\right]_{\xi\xi}.$$

Here the projection operator $\mathcal{P}$ acts on any operator to project out the diagonal matrix element in the representation based on the states of Φ. Since $\rho(0)$ is usually itself diagonal in this basis the inhomogeneous term $I(x,t)$ usually vanishes. The function $W(\xi,\xi',t)$ is the generalized transition matrix element of the evolution Master equation. For a Markovian process the transitions have no memory, so that $W(\xi,\xi',t) = F(\xi,\xi')\delta(t)$ and our generalized Master equation reduces to the well known Pauli Master equation

$$\partial p(\xi,t)/\partial t = \int d\xi' \left[W(\xi,\xi')p(\xi',t) - W(\xi',\xi)p(\xi,t)\right]. \tag{5}$$

The Chapman–Kolmogorov equation for the Markovian bath is derived starting from the Pauli Master equation. However, in order to take into account reversible effects we shall start from the generalized version (4) and derive a generalized Chapman–Kolmogorov equation for the evolution probability

$$\frac{\partial p(\xi,t)}{\partial t} = \int \int_0^t d\xi' \hat{F}_{\xi\xi'}(t-s)p(\xi',s)\, ds. \tag{6}$$

Here $\hat{F}_{\xi\xi'}(t-s)$ is the generalized Fokker–Planck operator on the state space Φ. For a special case, we may assume that the transitions do not depend on the states in Φ. In this case the generalized Fokker–Planck operator decouples into the ordinary Fokker–Planck operator and a *memory function* $\phi(t-s)$, which is independent of the state variables. The Chapman–Kolmogorov equation then becomes

$$\frac{\partial p(\xi,t)}{\partial t} = \int_0^t ds\phi(t-s)\left[-\frac{\partial}{\partial\xi}\left(\alpha_1(\xi)p(\xi,s)\right) + \frac{1}{2}\frac{\partial^2}{\partial\xi^2}\left(\alpha_2(\xi)p(\xi,s)\right)\right]. \tag{7}$$

where $\alpha_n = \int d\xi'\xi'^n F(\xi,\xi')$. The α_1 can be thought of as the *local velocity* and α_2 the *local diffusion constant.*

If we extract the Fokker–Planck operator $\hat{F} = [-(\partial/\partial\xi)\alpha_1(\xi) + \frac{1}{2}(\partial^2/\partial\xi^2)\alpha_2(\xi)]$, then the generalized Chapman–Kolmogorov equation reduces to

$$\frac{\partial p(\xi,t)}{\partial t} = \int_0^t ds\phi(t-s)\hat{F}p(\xi,s). \tag{8}$$

Note that in several situations this partitioning of the generalized Fokker–Planck operator into state variables and time may not obtain. For example, if the bath is a phonon bath, then the state space consists of the space spanned by harmonic oscillator states $|n\rangle$ and the generalized Fokker–Planck operator becomes $(1/t)(d/dt)J^2_{m-n}(ZVt/\hbar)$ [16].

The Fokker–Planck operator has a zero eigenvalue. The corresponding eigenstate is the *stationary* solution of the generalized Chapman–Kolmogorov equation. Let $p^*(\xi)$ be a stationary solution. We note that the Fokker–Planck operator is not self-adjoint; therefore, we have to define an inner product between two functions in the state space Φ as follows:

$$(q \odot r) = \int \int d\xi\ d\xi'\ q(\xi)Q(\xi-\xi')r(\xi')$$

where $Q(\xi - \xi') = (1/p^*(\xi))\delta(\xi - \xi')$ is the kernel of the inner product.

We shall now employ the augmented space theorem of Mookerjee [2] and Paquet and Leroux-Hugon [1] to evaluate the averaged evolution operator. We shall first define a *conditionally averaged* evolution operator $U(\xi, \xi', t)$ such that the system history begins at a state ξ' at $t = 0$ and evolves to a state ξ at t. It is easy to notice that $U(\xi, \xi' t)$ is the representation of an operator $\tilde{U}$ acting on the state space Φ. The fully averaged evolution operator is summed over all histories that end up in different final states ξ'. However, each of these histories could have originated from any one of the initial states ξ, so

$$\langle U(t)\rangle = \int d\xi' \int d\xi \; U(\xi, \xi')p^*(\xi')$$

$$= \int d\xi' \int d\xi'' \int d\xi \; p^*(\xi)Q(\xi - \xi'')U(\xi'' - \xi')p^*(\xi').$$

Thus, from the definition of the inner product

$$U(t) = (p^* \odot \tilde{U} p^*) \tag{9}$$

The history average of the evolution operator has been reduced to a matrix element of an operator $\tilde{U}$ between the stationary states in the state space Φ of the bath. This is the augmented space theorem. We have augmented the Hilbert space spanned by the lattice $\mathcal{H}$ by the state space Φ. Our evolution operators are operators on the augmented space $\mathcal{H} \otimes \Phi$ and history averages reduce simply to taking specific matrix elements on this augmented space.

The next step involves noting that the electron system in contact with a bath evolves in two distinct ways: part of its evolution is governed by the Schrödinger equation and part by the generalized Chapman–Kolmogorov equation. Thus Hamiltonian H_0 is the generator of infinitesimal time translations for the quantum evolution, while the generalized Fokker–Planck operator plays the same role for the stochastic evolution. We obtain

$$i\hbar \frac{\partial \tilde{U}}{\partial t} = \tilde{H}\tilde{U}(t) + i\hbar \sum_i \int_0^t ds \; \tilde{F}_i(t - s)\tilde{U}(s). \tag{10}$$

$\tilde{F}_i(t - s)$ are operators (one for each of the bath variables u_i) on the state space Φ whose representations are our generalized Fokker–Planck operators $F_i(\xi, \xi', t - s)$.

Define $G(z) = (1/t\hbar) \int_o^\infty \exp(izt/\hbar)\, dt$, the time evolution operator. Taking the Laplace transform of both sides of (8) we obtain

$$z\tilde{G}(z) - 1 = \tilde{H}\tilde{G}(z) + \sum_i i\hbar \tilde{F}_i(z)\tilde{G}(z) \tag{11}$$

where $\tilde{F}_i(z) = \int_0^\infty \tilde{F}(s) \exp(izs/\hbar)\, ds$.

In other words, the propagator, averaged over different histories of the bath, is given by the matrix element of the resolvent of an effective Hamiltonian operator $\tilde{H}$ in the augmented space $\mathcal{H} \otimes \Phi$:

$$\langle G(z)\rangle = \left(p^* \odot \left[z\tilde{I} - \tilde{H}\right]^{-1} p^*\right) \tag{12}$$

where

$$\tilde{H} = \tilde{H}_0 + i\hbar \tilde{F}(z). \tag{13}$$

2. Illustrative examples

We shall illustrate the formalism introduced in the previous section by specific examples. We shall first take the case of an electron interacting with an Ehrenfest bath. In this model the local velocities and diffusion constants are written in terms of a single lifetime τ_0: $\alpha_1 = -(x/\tau_0)$ and $\alpha_2 = (2/\tau_0)$. The Markovian approximation of this problem has already been illustrated in an earlier article [11]. The Markovian memory function is a delta function in time. In this model we have shown that the state space is spanned by the set of oscillator eigenfunctions

$$\gamma_n^i(x) = \left(2^n n! \pi\right)^{-1/2} H_n(x/2) \exp\left(-x^2/2\right).$$

In the representation in which the Fokker–Planck operator is diagonal, the interaction potential part of the electron Hamiltonian is tridiagonal with diagonal matrix elements $a_n = 0$, and off-diagonal matrix elements $b_n = n$. This was appropriate for a static Gaussian distribution of the potentials. In the static or adiabatic approximation this is the result of Sumi [7].

Let us now go beyond the Markovian approximation by introducing generalizations to the memory function. Kenkre and Knox [12] and our earlier work [11] have shown that the Markovian memory is appropriate to a diffusive evolution of the bath. However, if we take the telegrapher's equation [17] as the basis of our bath evolution:

$$\left(c/\alpha_2\right)\frac{\partial p(x,t)}{\partial t} = c\alpha_1 \frac{\partial p(x,t)}{\partial t} + c\frac{\partial^2 p(x,t)}{\partial x^2} - \frac{\partial^2 p(x,t)}{\partial t^2} \tag{14}$$

then in the limit of c much larger than α_2 we recover the Markovian diffusive behaviour with a delta function memory, whereas, in the opposite limit, the evolution equation of the bath is wave like with long memory, and the memory function is a theta function in time with the evolution at a time t depending upon all the earlier times. Kenkre and Knox have shown that the generalized memory functions of the telegraphers equation has the form $\phi(t) = c\exp(-ct/\alpha_2)$. It is easy to check that this function smoothly interpolates between the theta and delta function forms.

Incorporating this in our formalism in equation (11), the effective augmented space Hamiltonian becomes

$$\tilde{H} = \sum_i \sum_j t_{ij} c_i^\dagger c_j + \sum_i \tilde{M}^{(i)} c_i^\dagger c_i + i\hbar\left[c/\left(\frac{c}{\alpha_2} - iz\right)\right] \sum_i c_i^\dagger c_i. \tag{15}$$

In order to calculate the propagator of the electron, we may carry out the dynamical CPA approximation proposed by one of us [11]. The idea behind this approximation can be expressed either in terms of *walks* on the augmented space or em scattering diagrams. The former is a graphical representation of the renormalized perturbation expansion for the propagator. The path counting method has been described in detail by Mookerjee [18] and Haydock [19]. The CPA involves neglecting the contributions of all paths that connect more than one site and their configurations. Paquet and Leroux-Hugon [1] have shown that this is identical to neglecting crossed or correlated scattering diagrams involving more than one site. This is exactly what the single-site CPA should mean. Within this approximation Mookerjee [11] has shown that the *cardinality*-dependent self-energy is given by

$$\Sigma_q = -iq\hbar w(z) + S_q$$

$$S_{q+r} = \frac{(r+1)\lambda^2}{1/G_{q+r+1} + \Sigma_{q+1} + i(q+1)\hbar w(z) - S_{q+r+1}} \tag{16}$$

$$w(z) = \left[c/\left(\frac{c}{\alpha x_2} - iz\right)\right]$$

with $G_q(z) = g_{ii}(z - \Sigma_q)$ and $G_{ii}(z) = g_{ii}(z - \Sigma_0)$.

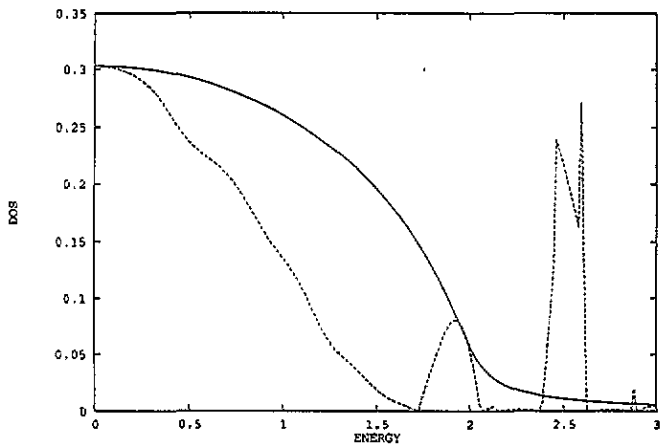

Figure 1. The density of states (shown only for positive energies) for an electron interacting with a Markovian bath (solid curve) and a non-Markovian bath with long memory (dashed curve).

Since it is simple to show that $\lim_{q\to\infty} \Sigma_q = 0$, we can start our iterative calculation with a $q = Q$ so chosen that we remain within a prescribed accuracy when we increase Q. We choose an unperturbed density as a semicircular density in the range $-2 \leqslant E \leqslant 2$. We choose such a featureless density for the specific reason that we want to identify *only* structures introduced by the non-Markovian nature of the bath.

Figure 1 (solid curve) shows half the density of states (the density is symmetric around the y-axis at $E = 0$) for a c/α_2 ratio of 10. This approximates the Markovian bath very well, and our results agree closely with the earlier calculations by Paquet and Leroux-Hugon [1] and Mookerjee [2]. The dashed curve is for the opposite limit c/α_2 ratio of 0.1. This should extrapolate to the limit of a very long memory bath, whose dynamics is governed by a wave equation. Note that the self-energy introduced by the dynamics in the Markovian regime is totally imaginary, leading to a lifetime effect. However, in the opposite regime, the dynamics-induced self-energy has a real part, which leads to a shift in the energy spectrum. Moreover, the real part has a strong energy dependence. This leads to considerable structure in the density of states, as shown in figure 1. If we slowly decrease the c/α_2 ratio from 10 down to 0.1, we can see the growth of the structures from the simple tailing in the lifetime effect in the Markovian regime.

Next we have introduced an oscillatory part to the memory function. This is motivated by the fact that the memory function of a phonon bath has an oscillatory character specific to the Bessel function mentioned earlier. However, a full accurate study of the phonon bath would require the memory to depend on the bath states as well. We have modelled the situation by a cosine modulation of the telegrapher equation memory. Note that it is the large-c/α_2 regime that models the phonon bath. Figure 2 shows the modification of

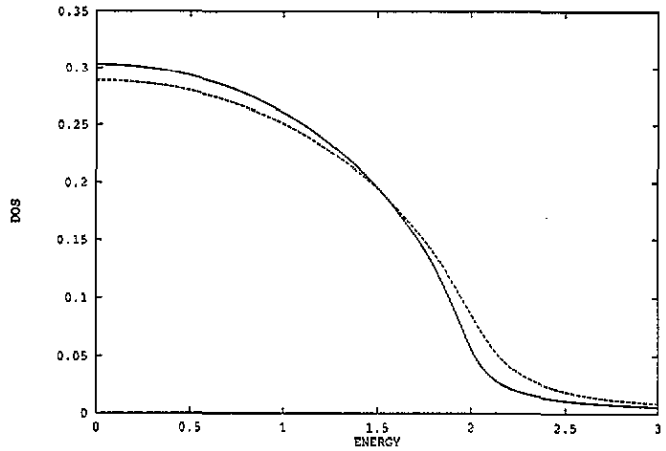

Figure 2. The density of states for an electron interacting with a Markovian bath (solid curve) and a bath with oscillatory decaying memory function (dashed curve).

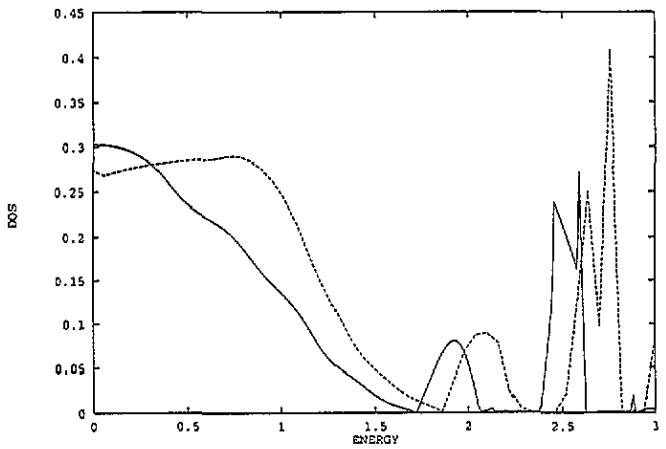

Figure 3. The density of states of an electron interacting with a non-Markovian bath with long-time memory (solid curve) and long-time memory modulated with an oscillatory function (dashed curve).

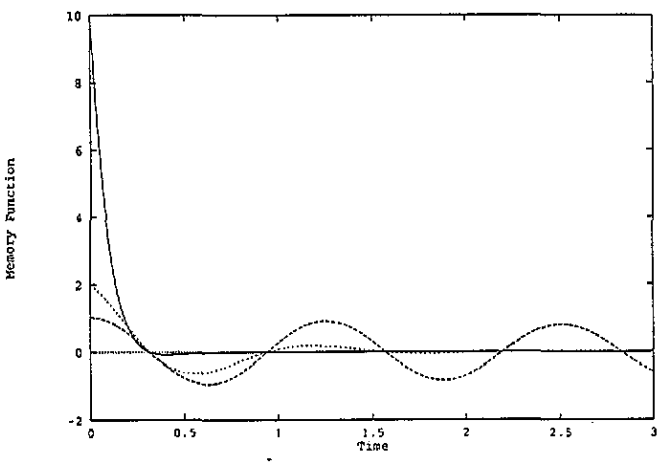

Figure 4. The memory functions considered in the earlier figures: a fast decaying almost Markovian bath (solid curve), a long-time oscillatory memory (dashed curve) and a memory intermediate between the two (dotted curve) (for a ratio $c/\alpha_2 \sim 1$).

the purely Markovian memory result (bold curve) by the cosine modulation (dashed curve). In this regime the effect is not large. The conjecture was earlier made by Mookerjee [11] when he argued that the approximation of the phonon bath by a Markovian memory was qualitatively not bad. However, the effect of cosine modulation on the structures in the long-time memory regime is considerable. The structures move outwards, while the low-energy regime is also modified. Figure 4 shows the different cosine modulated memory functions used: Markovian, diffusion like (full curve), long-time wave like (dashed curve) and an intermediate regime (dotted curve).

The aim of this illustration is not only to demonstrate how to work with non-Markovian baths within the augmented space methodology, but also to illustrate in a few simple examples that long-time memory may have considerable effect on the density of states, which may reflect for example line shapes in resonance experiments. It is our claim that the methodology proposed, coupled with methods for obtaining the memory functions in specific cases, will form a significant improvement over the Markovian treatments tried earlier.

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