A New Method for Quantum Processes in Fermionic Heat Baths

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The general path-integral formalism for real-time dynamics for a quantum system in a fermionic environment proposed previously is investigated by using a new method called local adiabatic transformation. This method is based on the observation that in the long-time limit (the time scale of the system is much larger than that of the environment, typically characterized by the inverse of the cutoff frequency of the environment), most degrees of freedom of the environment will follow the dynamics adiabatically. This feature is utilized by transforming the original problem of coordinate coupling into a problem of velocity coupling. This is achieved by making some simple unitary transformation on the fermion field (before path-integrating out of that field). By doing perturbations on the new problem, all the previous important results are recovered. Furthermore, generalizations to more realistic situations [for example, a particle traveling over a large distance and coupled to a Fermi gas through the phase factor $\exp(i\mathbf{k} \cdot \mathbf{R})$ (the coupling may involve many channels of angular momentum)] are considered and significant results obtained.

KEY WORDS: Adiabatic transformation; fermion bath; Grassmann algebra; influence functional; path integral; real-time density matrix.

1. INTRODUCTION

Quantum dynamics of a general particle coupled to a dissipative environment involves, in general, a large number of degrees of freedom, which substantially complicates the problem even if the original system might be very simple, for example, a two-state system. Recently, this topic has attracted a great deal of interest in the context of macroscopic quantum coherence

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(MQC) and macroscopic quantum tunneling (MQT),[2] since a macroscopic quantity cannot be isolated from its environment. There also has been interest in the behavior of a heavy particle (or defect) inside or on the surface of a solid, which involves coupling(s) to either the metallic electrons or the phonon modes in the solid.[3] Many introductory comments on these two fields can be found in the literature (especially those in our previous work[5]).

Due to the profound differences between Bose and Fermi statistics, it is in general necessary to study the two major kinds of "heat baths," either boson or fermion baths. A boson bath is usually represented by a set of harmonic oscillators, whereas a fermion bath consists of fermion excitations obeying anticommutation rules. Nevertheless, it is generally believed that if the coupling between a system and its environment is sufficiently weak, any environment can be cast into a bath of harmonic oscillators.[1,6] Moreover, it has been shown that for a certain kind of coupling, a fermion bath can be cast into one or several boson baths (no matter how strong the couplings), provided one makes suitable mappings between the corresponding couplings.[5,7,8] Once such mappings are achieved, the fermion-bath problem can be greatly simplified by utilizing all the corresponding properties of the boson bath.

Most of the previous work[5,7,8] along this line is based on the solution of a special type of singular integral equation. However, there are severe limitations on their generalizations. For instance, it is very difficult to explore the transport behavior of a particle with coupling to a fermionic environment. In addition, the rigorousness of the solution procedure has been subject to some suspicion (despite the considerable amount of algorithm associated with these works).

In this work, a new method is introduced to the fermion bath problem. Our goal is to give a rather simple and physical picture for the previous results. This is achieved by employing the previously obtained path-integral formalism for the fermion-bath problem.[5] In this method (which shall be called local adiabatic transformation), the fermion field in the presence of coupling is diagonalized at an arbitrary given time.[4] Based on this, a new interaction (between the system and the environment) in the form of velocity coupling appears. One then can integrate out of the transformed fermion field and evaluate the corresponding Feynman influence

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[2] There is a rich literature in the field of MQT and MQC. For general interest, see Refs. 1–3; special topics related to this work will be mentioned subsequently.

[3] A nice discussion of this is given by Sols and Guinea.[4]

[4] Note that the transformation is performed in the framework of the path-integral formalism; thus, no operators are involved. Direct unitary transformation on an operator basis has not succeeded in reducing the complexity of the problem.

functional[6,9,10] via a simple second-order perturbation. Quite remarkably, it recovers all the previous important results, and yet serves as a promising approach to further developments. As an example, the transport of a particle in a Fermi liquid is investigated,[5] where the previous method falls into difficulties.

This paper is arranged as follows. In Section 2, the basic path-integral formalism for the real-time density matrix is reviewed. The local adiabatic transformation is introduced in Section 3. The simplest situation, where all the coupling matrix elements are identical, is considered first in Section 4. Section 5 involves the more general case where many angular momentum channels enter. In Section 6, we study a more realistic example, where the coupling is realized through the phase factor $\exp(i\mathbf{k} \cdot \mathbf{R})$. Finally, a discussion is given in Section 7. In the Appendix, a simple exercise related to the problem of phase shift is presented.

2. FORMULATION OF THE DYNAMICS

In this section, we review briefly previous work[5] on the path-integral formalism for the real-time density matrix. We use the same general Hamiltonian as before (the chemical potential term $-\mu \hat{N}_e$ has been included by setting the Fermi surface at ε_f equal to zero):

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}) + \sum_{i,j=1}^{\Omega} C_{ij}(\hat{x}) \, \hat{b}_i^\dagger \hat{b}_j + \sum_{i=1}^{\Omega} \hat{b}_i \varepsilon_i \hat{b}_i + \hat{H}_{\text{int}}(\{\hat{b}_i^\dagger, \hat{b}_i\}) \quad (2.1)$$

where the notations are standard and transparent. To study the real-time properties of this kind of complete quantum system, the most relevant quantity to look into is always the real-time density matrix, given via the definition (taking $\hbar \equiv 1$)

$$\hat{\rho}(x, y, t) \equiv \langle x | \exp(-i\hat{H}t) \, \hat{\rho}(0) \exp(+i\hat{H}t) \, | y \rangle \quad (2.2)$$

Note that Eq. (2.2) is still an operator equation with respect to the environment. Concerning the initial density matrix $\hat{\rho}(0)$, we choose most conventionally the factorized one

$$\langle x' | \, \hat{\rho}(0) \, | y' \rangle = \tilde{\rho}(x', y', 0) \exp(-\beta \hat{H}_e) \quad (2.3a)$$

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[5] Only the bulk problem is studied here. The surface problem, e.g., a particle traveling on the surface of a metal, is mentioned in the last section.

where $\hat{H}_e$ is the Hamiltonian for the environment only [as can be found in Eq. (2.1)]. This gives

$$\hat{\rho}(x, y, t) = \int dx' \, dy' \, \langle x| \exp(-i\hat{H}t) |x'\rangle [\exp(-\beta\hat{H}_e)]$$

$$\times \langle y'| \exp(i\hat{H}t) |y\rangle \, \tilde{\rho}(x', y', 0) \qquad (2.3b)$$

Notice that nothing is particular about this choice. One can of course replace the factor $\exp(-\beta\hat{H}_e)$ by $\exp\{-\beta[\hat{H}_{e\text{-}p}(x') + \hat{H}_e]\}$ to emphasize that initially the environment is under equilibrium with the particle at the position x' (which may be the better choice when the coupling between the particle and the environment is strong).

Because the behavior of the environment is beyond the scope of interest, the environmental degrees of freedom should be traced out,

$$\rho(x, y, t) = \text{Tr}_e[\hat{\rho}(x, y, t)]$$

$$= \int dx' \, dy' \, \tilde{\rho}(x', y', 0) \, J(x, y, t; x', y', 0) \qquad (2.4)$$

where $\rho(x, y, t)$ is known as the reduced density matrix for the system alone and the function $J(x, y, t; x', y', 0)$ is given by

$$J(x, y, t; x', y', 0)$$
$$= \text{Tr}_e[\exp(-\beta\hat{H}_e) \, \langle y'| \exp(+i\hat{H}t) |y\rangle\langle x| \exp(-i\hat{H}t) |x'\rangle] \qquad (2.5a)$$

It is now a matter of expressing the right-hand side of Eq. (2.5a) in terms of path integrals. This procedure is quite lengthy, but somewhat straightward (see Appendix A of Ref. 5). We then arrive at the formula

$$J(x, y, t; x', y', 0)$$

$$\equiv \oint Dz(\tau) \int_{\gamma} \prod_{i=1}^{\Omega} Db_i^{\dagger}(\tau) \, Db_i(\tau) \exp\left(i \oint d\tau \left[\frac{1}{2} m\dot{z}^2 - V(z) \right] \right.$$

$$\left. + i \int_{\gamma} \left[\sum_{i=1}^{\Omega} b_i^{\dagger}(i\partial_{\tau} - \varepsilon_i) \, b_i - \sum_{i,j=1}^{\Omega} C_{ij}(z) \, b_i^{\dagger}b_j - H_{\text{int}}(\{b_i^{\dagger}, b_i\}) \right] \right)$$

$$(2.5b)$$

where the integral contour γ is the so-called Baym–Kadanoff contour, as shown in Fig. 1, and $\oint$ neglects the segment $(0 - i\varepsilon, -i\beta)$; the path integral over the fermion variables $\{b_i^{\dagger}, b_i\}$ is defined in Grassmann algebra. Note
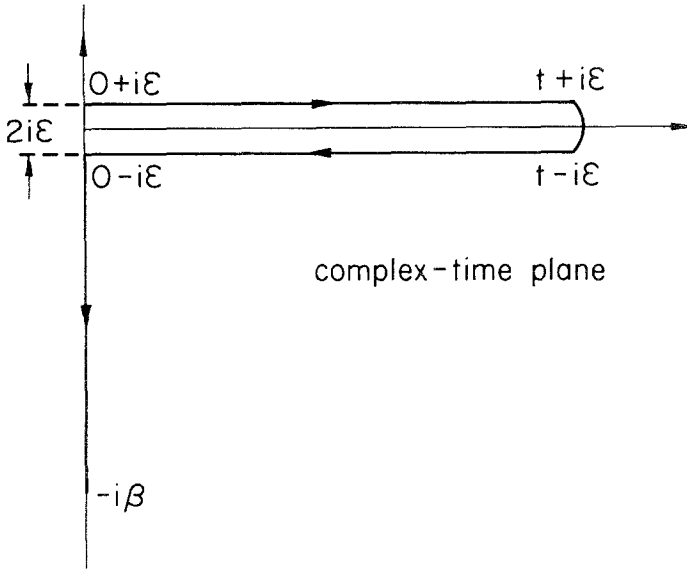
Fig. 1.   A schematic representation of the contour γ (Baym–Kadanoff contour). Note that the quantity ε is infinitesimal. Also, the integral $\oint$ does not include the infinitesimal segments between the ends at 0, t.

that for $\oint$ we also exclude the infinitesimal segments between those ends at 0, t. A few boundary conditions are imposed on this path integral:

$$z(0 + i\varepsilon) = x', \qquad z(0 - i\varepsilon) = y', \qquad b_i(0 + i\varepsilon) = -b_i(-i\beta)$$

$$z(t + i\varepsilon) = x, \qquad z(t - i\varepsilon) = y, \qquad b_i^\dagger(0 + i\varepsilon) = -b_i^\dagger(-i\beta)$$

$$C_{ij}(z(\tau)) \equiv 0 \qquad \text{for} \quad \tau \in (0 - i\varepsilon, -i\beta)$$

This path-integral formalism, as one can see, involves no specific assumptions on either the environment or the system itself. In particular, the usual tight-binding treatment[7,8] is not necessary. Nevertheless, in this work, most of the time we shall set $\hat{H}_{\text{int}} = 0$ and concentrate on the long-time limit, where the time scale of the system is slow compared to that of the environment, the latter typically characterized by the inverse of the cutoff frequency of the environment. Several important examples will be given.

3. LOCAL ADIABATIC TRANSFORMATION

In the case where the fermion field is noninteracting, the exponent in Eq. (2.5b) is bilinear for the fermion variables, and thus, is subject to

possible diagonalization. Suppose that one indeed can find a unitary transformation $\mathbf{T}(z)$ such that

$$\mathbf{T}^\dagger(z)[\mathbf{E} + \mathbf{C}(z)]\,\mathbf{T}(z) = \tilde{\mathbf{E}} \tag{3.1}$$

where matrix notations are implied, with

$$(\mathbf{E})_{ij} = \varepsilon_i \delta_{ij}, \qquad (\tilde{\mathbf{E}})_{ij} = E_i \delta_{ij}, \qquad (\mathbf{C})_{ij} = C_{ij}$$

The fields can be written in the corresponding vector notations, e.g.,

$$\mathbf{B}^\dagger = (b_1^\dagger, b_2^\dagger, \ldots, b_\Omega^\dagger), \qquad \tilde{\mathbf{B}}^\dagger = \mathbf{B}^\dagger \mathbf{T}$$

The transformed action becomes (writing down only the fermion part of the action)

$$S_{\text{en}} = \int_\gamma d\tau \,\{\tilde{\mathbf{B}}^\dagger[i\partial_\tau - \tilde{\mathbf{E}} - \mathbf{T}^\dagger(-i\partial_\tau \mathbf{T})]\,\tilde{\mathbf{B}}\} \tag{3.2}$$

One thus obtains the new coupling

$$\tilde{\mathbf{C}} = -i\dot{z}\mathbf{T}^\dagger(z)[\partial_z \mathbf{T}(z)] \tag{3.3}$$

which is proportional to the "velocity" of the particle, indicating the nature of the adiabatic transformation. Before proceeding further, one has to determine the Jacobian of transformation for the path integral (2.5b). Note that, for a given time,

$$\prod_{i=1}^{\Omega} db_i^\dagger\, db_i \equiv \prod_{i=1}^{\Omega} \left\{\left[\sum_{k=1}^{\Omega} (\mathbf{T}^\dagger)_{ik}\, d\tilde{b}_k^\dagger\right]\left[\sum_{l=1}^{\Omega} (\mathbf{T})_{il}\, d\tilde{b}_l\right]\right\} \tag{3.4}$$

Since the fields $\mathbf{B}$, $\tilde{\mathbf{B}}$ are in Grassmann algebra, one has $-d\tilde{b}_k^\dagger\, d\tilde{b}_{k'}^\dagger = d\tilde{b}_{k'}^\dagger\, d\tilde{b}_k^\dagger$, namely,

$$\prod_{i=1}^{\Omega} db_i^\dagger = \left[\sum_{k_1, k_2, \ldots, k_\Omega = 1}^{\Omega} \varepsilon_{k_1, k_2, \ldots, k_\Omega}^{1, 2, \ldots, \Omega} (\mathbf{T}^\dagger)_{1k_1} (\mathbf{T}^\dagger)_{2k_2} \cdots (\mathbf{T}^\dagger)_{\Omega k_\Omega}\right] \prod_{i=1}^{\Omega} d\tilde{b}_i^\dagger$$

$$= (\text{Det } \mathbf{T}^\dagger) \prod_{i=1}^{\Omega} d\tilde{b}_i^\dagger \tag{3.5}$$

and likewise for the other part. Therefore, the Jacobian is simply the *inverse* of $(\text{Det } \mathbf{T}^\dagger)(\text{Det } \mathbf{T}) = 1$. Eventually, one arrives at the new path-integral expression for the function J,

$$J(x, y, t; x', y', 0) = \oint Dz(\tau) \exp\left\{i\oint d\tau\left[\frac{1}{2}m\dot{z}^2 - V(z)\right] - \text{tr}\log\tilde{\mathbf{G}}\right\} \tag{3.6}$$

where the Green's function satisfies [the matrix products in Eq. (3.7a) involve summations over time indices]

$$\tilde{\mathbf{G}} = \mathbf{G}^0 + \mathbf{G}^0(\tilde{\mathbf{C}} + \tilde{\mathbf{E}} - \mathbf{E})\,\tilde{\mathbf{G}} \tag{3.7a}$$

$$(i\partial_\tau - \varepsilon_i)(\mathbf{G}^0)_{ij}\,(\tau, \tau') = \delta_{ij}\delta_\gamma(\tau, \tau') \tag{3.7b}$$

We need to worry a little about the boundary conditions and the poorness of the new coupling[6] when τ crosses over those ends at times 0, t. For the original field $\mathbf{B}$, its Green's function satisfies the antiperiodic boundary condition because the field does the same. But now

$$\tilde{\mathbf{B}}(0 + i\varepsilon) = \mathbf{T}^\dagger(z(0 + i\varepsilon))\,\mathbf{B}(0 + i\varepsilon) = -\mathbf{T}^\dagger(z(0 + i\varepsilon))\,\mathbf{T}(z(-i\beta))\,\tilde{\mathbf{B}}(-i\beta)$$

Thus, one sees a rather sophisticated boundary condition. However, an easy way out of the difficulty is to add an extra infinitesimal time piece $-i\delta\beta$ (at $\tau = -i\beta$) to the contour γ to ensure the antiperiodicity of $\tilde{\mathbf{B}}$, namely $z(-i\beta - i\delta\beta) \equiv z(0 + i\varepsilon) = x'$, or equivalently $z(\tau)$ obeying a periodic boundary condition. As regards the poorness of $\tilde{\mathbf{C}}$, the same trick can be used by making $z(\tau)$ join continuously across those ends. The fact that these manipulations affect neither the original field $\mathbf{B}$ nor its Green's function legitimizes the procedure. In this way, we have the zeroth-order Green's function for Eqs. (3.7),

$$(\mathbf{G}^0)_{ij}\,(\tau, \tau') = -i\delta_{ij}e^{-\varepsilon_i(\tau - \tau')}[\theta_\gamma(\tau, \tau') - f(\varepsilon_i)] \tag{3.8}$$

where $f(\varepsilon_i)$ is the Fermi distribution function and $\theta_\gamma(\tau, \tau')$ is the step function on the contour γ.

4. COUPLING WITH IDENTICAL MATRIX ELEMENTS

Of particular interest is the simplest case where $C_{ij}(\hat{x}) = CF(\hat{x})$ [for simplicity, we take $F(\hat{x}) = \hat{x}$], which forms the basis of all the further developments. One needs to diagonalize the following $\Omega \times \Omega$ matrix: $M_{ij} = \varepsilon_i\delta_{ij} + Cz$. Assume for the moment that $\{\varepsilon_i\}$ is nondegenerate (the case of degeneracy will be discussed later); it is then a simple exercise to find that the new eigenvalues are the solutions of the equation

$$\sum_{i=1}^{\Omega} \frac{1}{\varepsilon_i - E} + \frac{1}{Cz} = 0 \tag{4.1}$$

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[6] Note that there are no such problems for the corresponding Euclidean action in imaginary time. Thus, some way out of this difficulty is desired.

and the eigenstates are

$$a_i(E) = \frac{1}{\varepsilon_i - E} \left\{ \sum_{i=1}^{\Omega} \frac{1}{(\varepsilon_i - E)^2} \right\}^{-1/2} \tag{4.2}$$

For a uniform equal-spacing energy spectrum, $\varepsilon_i - \varepsilon_j = \varepsilon_0(i-j) = (i-j)/\rho_0$ (where ρ_0 is the density of states), Eq. (4.1) says (in the limit of infinite number of states)

$$E_i = \varepsilon_i + \frac{\arctan(\pi\rho_0 Cz)}{\pi\rho_0} \tag{4.3a}$$

$$\sum_{i=1}^{\Omega} \left(\frac{1}{\varepsilon_i - E_j} \right)^2 = \left(\frac{1}{Cz} \right)^2 + (\pi\rho_0)^2 \tag{4.3b}$$

The unitary transformation[7] is then

$$(\mathbf{T})_{ij} = a_i(E_j) \tag{4.4a}$$

and the new coupling is

$$(\tilde{\mathbf{C}})_{ij} = -i\dot{z} \sum_{k=1}^{\Omega} a_k(E_i) \, \partial_z a_k(E_j) \tag{4.4b}$$

Note that $(\tilde{\mathbf{C}})_{ii} \equiv 0$ and by virtue of the orthogonality one need not differentiate on the normalization factor. For $i \neq j$, one has

$$(\tilde{\mathbf{C}})_{ij} = i \frac{(d/d\tau)\{\arctan[\pi\rho_0 Cz(\tau)]\}}{\pi\rho_0(E_i - E_j)} \tag{4.5}$$

where Eqs. (4.3) have been used.

Going back to Eqs. (3.6) and (3.7), one can expand

$$-\operatorname{tr} \log \tilde{\mathbf{G}} = -\operatorname{tr} \log \mathbf{G}^0 - \operatorname{tr} \mathbf{G}^0(\tilde{\mathbf{E}} - \mathbf{E} + \tilde{\mathbf{C}})$$

$$-\frac{1}{2} \operatorname{tr} \mathbf{G}^0(\tilde{\mathbf{E}} - \mathbf{E} + \tilde{\mathbf{C}}) \, \mathbf{G}^0(\tilde{\mathbf{E}} - \mathbf{E} + \tilde{\mathbf{C}}) + O(\tilde{\mathbf{C}}^3) \tag{4.6}$$

In the right-hand side of Eq. (4.6), the first term will cancel with the normalization of the path integral in Eq. (3.6); the second term is purely adiabatic and will renormalize the particle potential $V(z)$; only the third term contains information on dissipation. After some algebra, one has

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[7] In the case where $\{\varepsilon_i\}$ has degeneracies, $\{E_i\}$ does not exhaust all the states. Thus, Eq. (4.4a) gives only the relevant part of the transformation. It is easy to show that the rest of the whole transformation is confined within each of the degeneracies; cf. Section 5.

$$-\operatorname{tr} \log \tilde{\mathbf{G}} = -\operatorname{tr} \log \mathbf{G}^0 - \operatorname{tr} \mathbf{G}^0(\tilde{\mathbf{E}} - \mathbf{E})$$

$$+\frac{1}{2\pi^2} \oint d\tau \, d\tau' \, \delta_0(z(\tau)) \, \delta_0(z(\tau'))$$

$$\times \frac{1}{\rho_0^2} \sum_{i,j=1}^{\Omega} e^{-i(\varepsilon_i - \varepsilon_j)(\tau - \tau')} [\theta_\gamma(\tau, \tau') - f(\varepsilon_i)][\theta_\gamma(\tau', \tau) - f(\varepsilon_j)]$$

$$+\frac{i}{2\pi^2} \oint d\tau \, \delta_0^2(z(\tau)) \frac{1}{\rho_0^2} \sum_{i,j=1}^{\Omega} \left[\frac{f(\varepsilon_i) - f(\varepsilon_j)}{\varepsilon_i - \varepsilon_j} \right] + O(\tilde{\mathbf{C}}^3) \qquad (4.7a)$$

where some intermediate processes of integrating by parts[8] have been performed to utilize the boundary conditions discussed above. $\delta_0(z(\tau))$ is called the phase shift on the Fermi surface (to be discussed in the Appendix),

$$\delta_0(z(\tau)) = -\arctan[\pi\rho_0 z(\tau)] \qquad (4.7b)$$

Equations (4.7) are identical to the previous result[5] (apart from some possible adiabatic potential renormalization, which is beyond the scope of this work, since it depends on the details of the high-energy cutoff of the spectrum of the environment). The remaining algebra goes nearly the same as before. For convenience, we simply quote the expression for the Feynman influence functional[5]:

$$F[z_1, z_2] = \exp\left\{ \frac{i}{2\pi} \int_0^t d\tau \left\{ \left[\frac{d}{d\tau} \delta_0(z_1(\tau)) \right] \delta_0(z_2(\tau)) \right. \right.$$

$$\left. - \delta_0(z_1(\tau)) \left[\frac{d}{d\tau} \delta_0(z_2(\tau)) \right] \right\}$$

$$- \int_0^t d\tau \int_0^\tau d\tau' \left\{ [\delta_0(z_1(\tau)) - \delta_0(z_2(\tau))] \right.$$

$$\left. \left. \times K(\tau - \tau')[\delta_0(z_1(\tau')) - \delta_0(z_2(\tau'))] \right\} \right\} \qquad (4.8a)$$

where the contour has been separated into two branches and the Fourier transform of $K(t)$ is

$$K(\omega) = \frac{\omega}{\pi} \coth \frac{\beta\omega}{2} \qquad (4.8b)$$

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[8] An adiabatic potential term appears in Eq. (4.7a) (the last term in the right-hand side). It, however, will be canceled by the adiabatic part imbeded in the double-time integral.

In the case where $\{\varepsilon_i\}$ is uniformly degenerate (e.g., spin degeneracy), the result (4.8) remains the same provided one defines properly the total density of states, although the situation is somewhat subtle (cf. Section 5). There is a short discussion in the last section concerning possible spin complications.

5. MANY ANGULAR MOMENTUM CHANNELS

In practice, the environment for certain systems is often known as some sort of Fermi liquid, and the coupling between them then induces scattering of fermions near the Fermi surface. Again we do not consider the interactions between fermions. Consider the following Hamiltonian:

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}) + \sum_{\mathbf{k},\mathbf{k}'} \hat{b}_{\mathbf{k}}^{\dagger} (V_{\mathbf{k},\mathbf{k}'}(\hat{x}) + \delta_{\mathbf{k},\mathbf{k}'}\varepsilon_{\mathbf{k}}) \, \hat{b}_{\mathbf{k}'} \qquad (5.1)$$

where we have labeled the fermion states by their wave vectors $\mathbf{k}$ and $\mathbf{k}'$ as usual. Since all relevant physical processes take place only near the Fermi surface, the following expansion would be quite general:

$$V_{\mathbf{k},\mathbf{k}'}(\hat{x}) = \sum_{l=0}^{\infty} (2l+1) \, V_l(\hat{x}) \, P_l\!\left(\frac{\mathbf{k}\cdot\mathbf{k}'}{|\mathbf{k}|\,|\mathbf{k}'|}\right)$$

$$= 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} V_l(\hat{x}) \, Y_{lm}\!\left(\frac{\mathbf{k}}{|\mathbf{k}|}\right) Y_{lm}^*\!\left(\frac{\mathbf{k}'}{|\mathbf{k}'|}\right) \qquad (5.2)$$

The main task left is to find a unitary transformation to diagonalize (5.1); for this we assert the following form:

$$(\mathbf{T})_{\mathbf{k},nlm}(\tau) = N_l (4\pi)^{1/2} \frac{Y_{lm}(\mathbf{k}/|\mathbf{k}|)}{\varepsilon_{\mathbf{k}} - E_{nlm}} \qquad (5.3)$$

where E_{nlm} are the new eigenvalues given via

$$4\pi \sum_{\mathbf{k}} \frac{Y_{lm}(\mathbf{k}/|\mathbf{k}|) \, Y_{l'm'}^*(\mathbf{k}/|\mathbf{k}|)}{\varepsilon_{\mathbf{k}} - E_{nlm}} + \frac{\delta_{ll'}\delta_{mm'}}{V_l(z(\tau))} = 0 \qquad (5.4)$$

With regard to the summation over $\mathbf{k}$, one can imagine that states are divided into various energy shells with equal spacing between two neighbors, and the degeneracy of each of the shells is large. Thus, one can first sum over these degenerate states to obtain the factor $\delta_{ll'}\delta_{mm'}$, then perform the usual procedure of summing over different energy shells as in the last section. In fact, $\{E_{nlm}\}$ gives an alternative way of labeling the fermion

states. In the limit of zero coupling, i.e., $V_l(\hat{x}) \to 0$, we have $E_{nlm} \to E^0_{nlm}$, which is nothing but an eigenenergy if we label the fermion states in terms of angular momentum. It is not difficult to show

$$(\mathbf{T}^\dagger \mathbf{T})_{nlm,n'l'm'} = N_l^2 4\pi \sum_{\mathbf{k}} \frac{Y_{lm}(\mathbf{k}/|\mathbf{k}|)\, Y^*_{l'm'}(\mathbf{k}/|\mathbf{k}|)}{(\varepsilon_\mathbf{k} - E_{nlm})^2} \delta_{nlm,n'l'm'} \qquad (5.5)$$

Moreover, one gets, from Eqs. (5.4) and (5.5),

$$E_{nlm} = E^0_{nlm} + \frac{g}{\pi \rho_0} \arctan[\pi \rho_0 V_l(z)] \qquad (5.6a)$$

$$N_l^2 = g\, \frac{V_l^2}{1 + (\pi \rho_0 V_l)^2} \qquad (5.6b)$$

where g is the number of states in one energy shell and ρ_0 is the total density of states (We do not include the spin of fermions, but it will be discussed in the last section.) The new coupling is, for $nlm \neq n'l'm'$,

$$(\tilde{\mathbf{C}})_{nlm,n'l'm'} = \frac{-ig\delta_{ll'}\delta_{mm'}}{\pi \rho_0 (E_{nlm} - E_{n'lm})} \left[\frac{d}{d\tau} \delta_l(z(\tau)) \right] \qquad (5.7)$$

where δ_l is the lth-channel phase shift (to be justified in the Appendix)

$$\delta_l = -\arctan \pi \rho_0 V_l(z) \qquad (5.8)$$

The generalization of Eqs. (4.7) and (4.8) to this section is obvious (the same generalization is also obtained in previous work[5]). Note that $(g/\rho_0)\sum_n \to \int dE_{nlm}$ (l, m fixed) in the continuous limit.

6. A PARTICLE IN A FERMI LIQUID

To discuss, for example, the transport behavior of a particle in a Fermi liquid (say, an electron gas), one needs to deal with the following rather different situation:

$$\hat{H} = \frac{\hat{\mathbf{P}}}{2m} + U(\mathbf{R}) + \sum_{\mathbf{k},\mathbf{k}'} \{ \exp[-i(\mathbf{k} - \mathbf{k}') \cdot \mathbf{R}] \} \hat{b}_\mathbf{k}^\dagger V_{\mathbf{k},\mathbf{k}'} \hat{b}_{\mathbf{k}'} + \sum_\mathbf{k} \varepsilon_\mathbf{k} \hat{b}_\mathbf{k}^\dagger \hat{b}_\mathbf{k} \qquad (6.1)$$

The phase $\exp(i\mathbf{k} \cdot \mathbf{R})$ contains essentially the coupling information. However, it can be absorbed into $\hat{b}_\mathbf{k}$, resulting in a new "Lagrangian" for the fermion field (keeping only the environmental part)

$$L_{en} = \sum_\mathbf{k} \hat{b}_\mathbf{k}^\dagger [i\partial_\tau - \varepsilon_\mathbf{k} - \mathbf{k} \cdot \dot{\mathbf{R}}(\tau)] \hat{b}_\mathbf{k} - \sum_{\mathbf{k},\mathbf{k}'} \hat{b}_\mathbf{k}^\dagger V_{\mathbf{k},\mathbf{k}'} \hat{b}_\mathbf{k} \qquad (6.2)$$

Note that the same expansion for $V_{\mathbf{k},\mathbf{k}'}$ as in Eq. (4.2) can be made, but V_l is now essentially independent of $\mathbf{R}(\tau)$. The same transformation (5.3)–(5.6) in the last section can be applied here, and transforms $\mathbf{k} \cdot \dot{\mathbf{R}}(\tau)$ into a new form (the following expression includes the limit $E_{nlm} = E_{n'l'm'}$)

$$(\varDelta)_{nlm,n'l'm'} = \frac{N_l N_{l'} [(d/d\tau) \, S_{lm,l'm'}(\tau)]}{E_{nlm} - E_{n'l'm'}} \left(\frac{1}{V_l} - \frac{1}{V_{l'}} \right) \tag{6.3a}$$

where $S_{lm,l'm'}(\tau)$ is the matrix element

$$S_{lm,l'm'}(\tau) = \int d\Omega_{\mathbf{k}} \; Y_{lm}^*(\mathbf{k}/|\mathbf{k}|) \, \mathbf{k} \cdot \mathbf{R}(\tau) \, Y_{l'm'}(\mathbf{k}/|\mathbf{k}|) \tag{6.3b}$$

Choosing $\mathbf{R}$ along the z axis for the moment, one has the selection rule $l' = l + (-)\, 1,\; m' = m$, and

$$S_{lm,(l-1)m}(\tau) = -i \left[\frac{l^2 - m^2}{(2l+1)(2l-1)} \right]^{1/2} |\mathbf{k}| R_z(\tau) \tag{6.3b'}$$

Note that

$$\sum_{m=-(l-1)}^{l-1} S_{lm,(l-1)m}(\tau) \, S_{(l-1)m,lm}(\tau')$$

$$= \frac{\mathbf{k}^2 R_z(\tau) \, R_z(\tau')}{(2l+1)(2l-1)} \sum_{m=-(l-1)}^{l-1} (l^2 - m^2) = \frac{l}{3} \, \mathbf{k}^2 R_z(\tau) \, R_z(\tau') \tag{6.4}$$

This is to be used in obtaining Eq. (6.6). In general, one should replace $R_z(\tau)\, R_z(\tau')$ by $\mathbf{R}(\tau) \cdot \mathbf{R}(\tau')$ for rotational invariance. Also, using the expression (5.8) for the phase shifts, one has

$$\sin \delta_l = -\frac{\pi \rho_0 V_l}{[1 + (\pi \rho_0 V_l)^2]^{1/2}} \tag{6.5a}$$

$$(\varDelta)_{nlm,n'l'm'} = \frac{g \dot{S}_{lm,l'm'}(\tau) \sin(\delta_l - \delta_{l'})}{\pi \rho_0 (E_{nlm} - E_{n'l'm'})} \tag{6.5b}$$

In parallel to the procedure of the last two sections, we have in Eq. (3.6) [cf. Eqs. (4.7)]

$$-\operatorname{tr} \log \tilde{\mathbf{G}} = -\operatorname{tr} \log \mathbf{G}^0$$

$$+ \frac{1}{2\pi} \oint d\tau \, d\tau' \left\{ \eta \mathbf{R}(\tau) \cdot \mathbf{R}(\tau') \int dE \, dE' \right.$$

$$\times e^{-i(E-E')(\tau - \tau')} [\theta_\gamma(\tau, \tau') - f(E)][\theta_\gamma(\tau', \tau) - f(E')] \Big\}$$

$$+ \frac{i}{2\pi} \oint d\tau \left\{ \eta \mathbf{R}^2(\tau) \int dE \, dE' \, \frac{f(E) - f(E')}{E - E'} \right\} + O(\varDelta^3) \tag{6.6a}$$

where

$$\eta = \sum_{l=1}^{\infty} \frac{2l}{3\pi} \mathbf{k}_f^2 \sin^2(\delta_l - \delta_{l-1}) \qquad (6.6b)$$

The same influence functional can be trivially written down in analogy to Eqs. (4.8). Here one sees that the original problem has been reduced to a simple boson-bath problem with three-dimensional linear coupling. This result differs from that claimed in Ref. 8, where one needs a large number of baths of harmonic oscillators in order to complete the mapping. It is also interesting to compare it with the result of Ref. 4, where a similar conclusion is found in the limit of small distance, i.e., $|\mathbf{R}(\tau) - \mathbf{R}(\tau')| < |\mathbf{k}_f|^{-1}$. No such limitation is required for Eq. (6.6a). In the quasiclassical limit[10,11] a quantum Langevin equation can be found, which then gives the viscosity η as stated in Eq. (6.6b). This is in agreement with the formula used by Echenique et al.[12]

7. DISCUSSION

In this section, we discuss several interesting points concerning this new method and comment on its relation to other work. The first point concerns the spin complications, since fermions always have nonzero spins, such as $s = 1/2$ for an electron. If the coupling interaction in Eq. (2.1) does not flip fermions into different spin states, then one can simply double (say, for an electron gas) the number of the coupling channels in Section 5. The other simple case is that the coupling is insensitive to the spin, namely, it scatters the fermions regardless of their spin states. Again one can simply double the total density of states. The real complications come from the case in which the coupling is spin-dependent (similar to the Kondo problem). This case is not intended here, but we suspect it can be incorporated into this work.

Another point concerns the convergence of the higher order contributions. Throughout this work, only the second-order perturbations on the new couplings are used. Remarkably, such a simple approach recovers all the previous significant results[5,7,8]; the latter are claimed to be exact in the long-time limit, i.e., the time scale of the system considered is much longer than that of environment, typically characterized by the inverse of the cutoff frequency ω_c of the spectrum of the environment. Thus, it is quite possible that the second-order results here have the same status. Unfortunately, we have not been able to show that all the higher order contributions can be ignored in that limit; for example, they are $O(|\dot{\mathbf{R}}|/\omega_c)$.

Adiabatic potential renormalizations are not well treated in this paper. They are cutoff-dependent, and so are beyond the scope of this approach. In previous work,[5] very careful arguments are given on the separation of adiabatic and dissipative contributions. A nice analytic expression is presented there for a certain choice of the high-energy cutoff. Note that for the problem considered in Section 6, there are no adiabatic potential shifts due to the coupling, in agreement with the result of similar boson-bath problems and Ref. 8.

For a surface problem such as quantum diffusion of heavy particles in a metallic surface, the spherical symmetry breaks down, so that one cannot directly make use of the spherical harmonics $Y_{lm}(\mathbf{k}/|\mathbf{k}|)$. In this situation perhaps both the fermion field and the coupling should be rewritten in proper form. The version of Section 6 needs to be revised because the transformation used there no longer holds. One needs to find a new set of orthogonal functions to complete the diagonalization. Nevertheless, this is merely a matter of algebra. I suspect that the changes will only be quantitative.[9]

Finally, we mention some other work relevant to the current problem. Aslangul *et al.*[14] explore successfully the real-time dynamics for some boson-bath problems by using a "displaced Hamiltonian." This Hamiltonian results from a direct unitary transformation in an operator basis. However, for the fermion-bath problem, a similar technique does not seem to reduce the complexity of the problem. On the other hand, our results show the equivalence between the two kinds of baths. This allows one to utilize those results on boson-bath problems.

For the transport properties, work[8,15] has been done based on a combination of path-integral (tight-binding limit) and scaling techniques. The results all indicate similarities to the behavior of boson-bath coupling. A rather different approach[16,17] associated with the Anderson orthogonality theorem can also deal with several angular momentum channels. It will be very interesting to explore the relations between these approaches.

APPENDIX. PHASE SHIFTS ON THE FERMI SURFACE

In the text, it is claimed that the quantity $-\arctan(\pi\rho_0 V_l)$ is identical to the phase phift of the lth (angular momentum) scattering channel between the particle and a fermion on the Fermi surface. In this Appendix we give a formal derivation of this claim, which allows one to check clearly its validity, since, in principle, the determination of phase shifts is a complicated matter.

From Eqs. (123.15), (130.9), and (130.12) of Ref. 13, the scattering amplitude can be expanded into

$$f(\mathbf{n}, \mathbf{n}') = \sum_{l=0}^{\infty} f_l (2l+1) P_l(\mathbf{n} \cdot \mathbf{n}') \tag{A1}$$

$$f_l = \frac{1}{2ik} (e^{2i\delta_l} - 1) \tag{A2}$$

where δ_l is the lth-channel phase shift. The question here is whether it is identical to the phase shift defined in the text in certain limit(s). In fact, in the momentum representation, the scattering amplitude satisfies

$$f(\mathbf{n}, \mathbf{n}') = \left(\frac{m}{2\pi\hbar^2} \right) F(k\mathbf{n}, k\mathbf{n}') \tag{A3}$$

where

$$F(\mathbf{k}, \mathbf{q}) = -V_{\mathbf{k},\mathbf{q}} - \frac{2m}{\hbar^2} \int \frac{d^3 q'}{(2\pi)^3} \frac{F(\mathbf{k}, \mathbf{q}') V_{\mathbf{q},\mathbf{q}'}}{(2\pi)^3 \, q'^2 - k^2 - i0} \tag{A4}$$

If now the matrix element $V_{\mathbf{k},\mathbf{q}}$ is nonzero only within a thin layer of Fermi surface, it is then fair to assume that $F(\mathbf{k}, \mathbf{q})$ only depends on the direction of $\mathbf{k}, \mathbf{q}$ within the layer and is zero outside it. However, even though the layer is thin with respect to the Fermi sphere, it may well be large with respect to the typical energy scale considered in a specific problem, for example, the long-time limit of our problem. In such a case

$$\frac{2m}{\hbar^2} \int \frac{d^3 q'}{(2\pi)^3} \frac{F(\mathbf{k}, \mathbf{q}') V_{\mathbf{q},\mathbf{q}'}}{q'^2 - k^2 - i0} \simeq \frac{imk_f \pi}{\hbar^2 (2\pi)^3} \int d\Omega_{\mathbf{q}'} \, F(\mathbf{k}, \mathbf{q}') V_{\mathbf{q}',\mathbf{q}} \tag{A5}$$

where we have kept only the imaginary part coming from the vicinity of the Fermi surface. After these arguments, one has (a unit volume of normalization for plane waves is always assumed)

$$f(\mathbf{n}, \mathbf{n}') = -\pi\rho_0 V_{\mathbf{n},\mathbf{n}'} - \tfrac{1}{4} i\pi\rho_0 \int d\Omega_{n''} f(\mathbf{n}, \mathbf{n}'') V_{\mathbf{n}'',\mathbf{n}'} \tag{A6}$$

Using expansions (A1) and (5.2), it is not difficult to find

$$f_l = \frac{-\pi\rho_0 V_l}{1 + i\pi\rho_0 V_l} \tag{A7}$$

where we have used

$$\rho_0 = \frac{mk_f}{2\pi^2 \hbar^2} \qquad \text{(without spin)} \tag{A8a}$$

$$\int d\Omega_{n''} P_l(\mathbf{n}, \mathbf{n}'') P_{l'}(\mathbf{n}'', \mathbf{n}') = \frac{4\pi}{2l+1} \delta_{l,l'} P_l(\mathbf{n}, \mathbf{n}') \qquad \text{(addition theorem)} \tag{A8b}$$

Comparing Eq. (A7) to Eq. (A2), one finds

$$\delta_l = -\arctan(\pi\rho_0 V_l) \tag{A9}$$

[9] In fact, important progress has already been achieved, and will be presented elsewhere.

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