Adiabatic and isothermal resistivities

R. S. Fishman

Solid State Division, Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, Tennessee 37831-6032 and Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996-1200 (Received 24 June 1988)

The force-balance method is used to calculate the isothermal resistivity to first order in the electric field. To lowest order in the impurity potential, the isothermal resistivity disagrees with the adiabatic results of the Kubo formula and the Boltzmann equation. However, an expansion of the isothermal resistivity in powers of the impurity potential is divergent, with two sets of divergent terms. The first set arises from the density matrix of the relative electron-phonon system. The second set arises from the explicit dependence of the density matrix on the electric field, which was ignored by force-balance calculations. These divergent contributions are calculated inductively, by applying a recursion relation for the Green's functions. Using the $\lambda^2 t \rightarrow \infty$ limit of van Hove, I show that the resummation of these divergent terms yields the same result for the resistivity as the adiabatic calculations, in direct analogy with the work of Argyres and Sigel, and Huberman and Chester.

I. INTRODUCTION

Recent work¹ has suggested that there are two inequivalent methods for calculating the electrical resistivity. Calculations of the conductivity based on the Kubo formula or the Boltzmann equation^{2,3} are supposedly valid only under adiabatic conditions, when the closed system of electrons is driven out of equilibrium by the electric field. In the presence of a heat bath, which keeps the electrons at a fixed temperature, an isothermal calculation of the resistivity is required. Isothermal conditions are ensured by the force-balance (FB) method, 1,4-15 which couples the electrons to a heat bath of phonons. Under steady-state conditions, the energy generated by Joule heating of the electrons is transferred to this heat bath. Calculations of the isothermal resistivity based on the FB theory produce a different result than the adiabatic calculations based on the Kubo formula or the Boltzmann equation, even to linear order in the electric field.^{2,5} In this paper, I show that the expansion of the isothermal resistivity in powers of the impurity potential is divergent. When the divergent terms in this expansion are resummed with the limiting prescription of van Hove,¹⁶ the isothermal resistivity is brought into agreement with the adiabatic result.

The disagreement between the isothermal and adiabatic resistivities is reminiscent of an earlier disagreement between the Kubo formula and the resistivity formulas of Rousseau¹⁷ and of Kenkre and Dresden.¹⁸ The impurity resistivity calculated by those authors agrees with the result of the FB method. In terms of the electron mass m, the electron charge e, the scattering relaxation time τ , and the number of electrons N, these calculations find that

$$\rho_i = \frac{m}{Ne^2} \left\langle \frac{1}{\tau} \right\rangle \tag{1}$$

is the linearized resistivity to lowest order in the impurity potential. This expression should be contrasted with the result of the Kubo formula or the Boltzmann equation for the conductivity

$$\sigma_i = \frac{1}{\rho_i} = \frac{Ne^2}{m} \langle \tau \rangle . \tag{2}$$

The expectation value is defined by Eq. (38) as an average over the electron energies.

For a degenerate distribution of electron energies at zero temperature, $1/\langle \tau \rangle = \langle 1/\tau \rangle$ and the two methods produce the same result. For a nondegenerate distribution, however, $1/\langle \tau \rangle$ and $\langle 1/\tau \rangle$ are different.^{2,5} In a classical system, it is simple to show¹⁹ that $\langle 1/\tau \rangle$ is about three times larger than $1/\langle \tau \rangle$. This difference between the isothermal and adiabatic resistivities can have important physical consequences. For example, calculations of the electron temperature⁵ and the infrared absorption²⁰ of metals depend on which model is assumed.

The appeal of the FB method, and of the formalisms developed earlier by Rousseau¹⁷ and others, ^{18,21,22} is that an exact result for the resistivity can be expanded in powers of the impurity potential. In order to evaluate the Kubo formula for the conductivity to lowest order in the impurity potential, an infinite number of Feynman diagrams must be summed.³ The original motivation²¹ behind the development of resistivity formulas was that weak interactions might be treated perturbatively. These efforts were encouraged when it was realized that the lowest-order term in an expansion of the resistivity agrees with the Kubo formula at T = 0.

It was originally shown by Argyres and Sigel²³ and by Huberman and Chester¹⁹ that the early theories of resistivity do not permit a straightforward expansion in powers of the scattering interaction. These authors demonstrated that such an expansion is actually diver-

gent. A formal prescription for resumming this divergent series is therefore required. As first discussed by van Hove,¹⁶ the evaluation of the steady-state resistivity to lowest order in the impurity potential $\lambda \phi$ requires that the long time limit $(t \rightarrow \infty)$ precede the limit of weak scattering $(\lambda \rightarrow 0)$. Using this limiting procedure to resum the divergent series for the impurity resistivity, Argyres and Sigel demonstrated that the theory of Kenkre and Dresden¹⁸ produces the same result as the Kubo formula. Because the evaluation of the resistivity to lowest order in λ also requires the summation of an infinite number of terms, the resistivity formulas of Rousseau and of Kenkre and Dresden offer no advantages over the Kubo formula. Indeed, the presence of divergences in these theories makes them unsuitable for most applications.

The FB method was likewise motivated⁴ by the desire for an exact result for the resistivity. This formalism separates the electron positions and momenta into center-of-mass variables **R** and **P**, which are treated classically, and relative variables, which are second quantized in the usual way. When the expectation value of **P** is zero, the electric force acting on the center of mass of the electrons is balanced by the frictional forces provided by the phonons and impurities. The phonon and impurity resistivities can then be obtained from a force-balance relation. To lowest order in λ , the impurity resistivity is given by $\rho_i = m \langle 1/\tau \rangle / Ne^2$, in disagreement with linear response theory.

In an attempt to explain this discrepancy, Horing *et al.*¹ claim that the FB result for ρ_i is correct under isothermal conditions, such as in the presence of a phonon heat bath. Indeed, these authors suggest that the work of Kenkre and Dresden can be rehabilitated under such conditions, when the objections of Argyres and Sigel are no longer supposed to apply. Horing *et al.* argue that linear response theory is correct only under adiabatic conditions, when the electric field drives the electron system out of equilibrium.

In this paper, I use the limiting prescription of van Hove to resum the divergent contributions to the FB resistivity, in analogy with the work of Argyres and Sigel and of Huberman and Chester. There are two classes of divergent contributions to the FB resistivity. The first class of divergent terms arises from the density matrix of the relative electron-phonon system. The second class arises from the explicit dependence of the density matrix on the electric field. Because the center-of-mass variables **R** and **P** were treated classically by the FB method, this explicit dependence was ignored.

To obtain the full density matrix, all variables must be treated quantum mechanically. Expanded in powers of the impurity interaction, the density matrix then involves commutators of the operator $R_i(t)$ at different times. Only after these commutators are evaluated can the thermodynamic limit $N \rightarrow \infty$ be used to set terms of order \hbar/N to zero. Both sets of divergent contributions are unaffected by this limit.

The divergent terms in the FB resistivity are identical to the divergent terms found by Huberman and Chester in the theory of Rousseau. In the $\lambda^2 t \rightarrow \infty$ limit, the FB

resistivity reduces to the adiabatic result. If the dependence of the density matrix on the electric field is neglected, the resummed resistivity vanishes in this limit.

Of course, the equivalence of the isothermal and adiabatic resistivities could have been anticipated. To first order in the electric field, the electron energy is not affected by Joule heating and the presence of a phonon heat bath is irrelevant. This work demonstrates that isothermal and adiabatic calculations must produce the same result for the linearized resistivity.

This paper is divided into three main sections. In Sec. I the FB formalism is reviewed and the density matrix is derived. In Sec. II the impurity resistivity is expanded in powers of λ , to lowest order in the electric field and in the electron-phonon interaction. In Sec. III, I evaluate the divergent contributions to ρ_i , using a recursion relation for the Green's functions. These divergent terms are then resummed using the limiting prescription of van Hove. Appendixes A, B, and C provide details of the inductive method used to calculate the divergent contributions to ρ_i . A summary of the arguments presented here is given in the preceding paper.²⁴

The existence of divergences in the isothermal resistivity means that, like its predecessors, the FB formalism offers no advantages over the Kubo formula. In both cases an infinite number of terms must be considered to obtain the limit of weak interactions. Because of these divergences, the FB theory is not useful for studying nonlinear effects in strong electric fields.

II. FORCE-BALANCE THEORY

The starting point⁶ of the FB theory is the separation of the electron positions and momenta into center-ofmass and relative variables. The Hamiltonian for a system of electrons, phonons, and impurities can be written

$$H = H_c + H_e + H_{\rm ph} + H_{ei} + H_{e-\rm ph} , \qquad (3)$$

where

$$H_c = \frac{P^2}{2M} - Ne \mathbf{E} \cdot \mathbf{R} , \qquad (4)$$

$$H_e = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} , \qquad (5)$$

$$H_{\rm ph} = \sum_{\mathbf{q},\gamma} \Omega_{\mathbf{q}\gamma} b_{\mathbf{q}\gamma}^{\dagger} b_{\mathbf{q}\gamma} , \qquad (6)$$

$$H_{ei} = \lambda \sum_{\mathbf{q},\alpha} \phi(q) e^{i\mathbf{q} \cdot (\mathbf{R} - \mathbf{R}_{\alpha})} \rho_{\mathbf{q}} , \qquad (7)$$

$$H_{e\text{-ph}} = \sum_{\mathbf{q},\gamma} M(\mathbf{q},\gamma) (b_{\mathbf{q}\gamma} + b_{-\mathbf{q}\gamma}^{\dagger}) e^{i\mathbf{q}\cdot\mathbf{R}} \rho_{\mathbf{q}} .$$
(8)

Here $b_{q\gamma}^{\dagger}(c_{k\sigma}^{\dagger})$ and $b_{q\gamma}(c_{k\sigma})$ are creation and destruction operators for phonons (electrons), $\Omega_{q\gamma}(\varepsilon_k = k^2/2m)$ is the phonon (electron) energy, $M(q,\gamma)$ is the phonon interaction matrix element, and

$$\rho_{\mathbf{q}} = \sum_{\mathbf{k},\sigma} c^{\dagger}_{\mathbf{k}+\mathbf{q},\sigma} c_{\mathbf{k}\sigma} \tag{9}$$

is the electron density operator. The subscripts σ and γ

in the creation and destruction operators are electronspin and phonon-branch indices, respectively. Of course, M = Nm is the total mass of the electrons and \mathbf{R}_{α} are the positions of the N_i impurities. In analogy with Huberman and Chester,¹⁹ the dimensionless parameter λ is used to keep count of powers in the impurity potential $\phi(q)$. The center-of-mass momentum **P** and position **R** obey the commutation relation

$$[R_i, P_i] = i\delta_{ii} , \qquad (10)$$

with $\hbar = 1$. For convenience, the Coulomb interactions between the electrons have been ignored. Notice that the electric field acts on the relative electron-phonon system through the exponential factors $e^{i\mathbf{q}\cdot\mathbf{R}}$ in H_{ei} and $H_{e\text{-ph}}$.

Before time t=0, it is assumed that the electronimpurity and electron-phonon interactions are absent, so that the electrons and phonons are decoupled from the center of mass and from each other. The electric field is also assumed to be turned off for t < 0, so that the center of mass is moving with some constant momentum $\mathbf{P}_0 = M v_d \hat{x}$. The electrons and phonons are separately considered⁶ to be in states of thermal equilibrium, with electron temperature T_e and phonon temperature T not necessarily equal.

At time t = 0, the interactions of the electrons with the impurities and phonons are switched on to their full values $\phi(q)$ and $M(\mathbf{q}, \gamma)$. The frictional forces associated with these interactions will then begin to act on the center of mass of the electrons. Of course, these frictional forces will reach their steady-state values only after some characteristic times, determined by the strength of the electron-phonon and electron-impurity interactions. The electric field $\mathbf{E}(t) = \mathbf{E}(t)\hat{\mathbf{x}}$ is chosen to exactly balance these forces, so that the center-of-mass momentum \mathbf{P}_0 remains constant.

An expression for the resistivity can be obtained from the force-balance equation

$$\frac{d}{dt} \operatorname{Tr}\{\rho(t)\mathbf{P}\} = i \operatorname{Tr}\{\rho(t)[H, \mathbf{P}]\} = \mathbf{0} , \qquad (11)$$

which states that the total force acting on the center of mass is zero. The commutator

$$i[H, \mathbf{P}] = Ne\mathbf{E} - i\sum_{\mathbf{q}, \gamma} M(\mathbf{q}, \gamma) \mathbf{q} e^{i\mathbf{q}\cdot\mathbf{R}} (b_{\mathbf{q}\gamma} + b_{-\mathbf{q}\gamma}^{\dagger}) \rho_{\mathbf{q}}$$
$$-i\lambda \sum_{\mathbf{q}, \alpha} \phi(q) \mathbf{q} e^{i\mathbf{q}\cdot(\mathbf{R}-\mathbf{R}_{\alpha})} \rho_{\mathbf{q}}$$
(12)

is evaluated in the Schrödinger representation. Since the current of the electrons is $J = Nev_d$, the total resistivity is

$$\rho_T(t) = \rho_{\rm ph}(t) + \rho_i(t) = \frac{E(t)}{Nev_d} , \qquad (13)$$

where

$$\rho_{\rm ph}(t) = \frac{i}{N^2 e^2 v_d} \sum_{\mathbf{q},\gamma} M(\mathbf{q},\gamma) q_x \\ \times \operatorname{Tr}\{\rho(t) e^{i\mathbf{q}\cdot\mathbf{R}} (b_{\mathbf{q}\gamma} + b_{-\mathbf{q}\gamma}^{\dagger}) \rho_{\mathbf{q}}\}, \quad (14)$$

$$\rho_i(t) = \frac{i\lambda}{N^2 e^2 v_d} \sum_{\mathbf{q},\alpha} \phi(q) q_x e^{-i\mathbf{q}\cdot\mathbf{R}_\alpha} \mathrm{Tr}\{\rho(t) e^{i\mathbf{q}\cdot\mathbf{R}}\rho_{\mathbf{q}}\}$$
(15)

are the phonon and impurity resistivities. The density matrix $\rho(t)$ is discussed below. An average over impurity positions \mathbf{R}_{α} is implied in Eqs. (14) and (15) for the resistivities.

The other central relation of the FB theory, the energy-balance equation, is obtained in the steady-state limit $(t \rightarrow \infty)$ from the condition that the electron energy is constant:

$$\lim_{t \to \infty} \frac{d}{dt} \operatorname{Tr}\{\rho(t)H_e\} = 0 .$$
 (16)

This implies that the energy supplied per unit time by the electric field JE(t) is absorbed by the phonon heat bath. Therefore, Eq. (16) is equivalent to the relation

$$Nev_d \lim_{t \to \infty} E(t) = \lim_{t \to \infty} \frac{d}{dt} \operatorname{Tr}\{\rho(t)H_{\mathrm{ph}}\} .$$
(17)

These equations indicate that the electron-phonon interaction is responsible for keeping the electron energy constant. Because the electron-impurity scattering is elastic, the impurities cannot absorb the Joule heat generated by the electric field.

In the steady-state limit, Eq. (11) can be used with Eq. (16) to solve for the drift velocity v_d and the electron temperature T_e in terms of the electric field, the electron interactions, and the phonon temperature T. It can be shown⁶ that the difference between T_e and T is due to the nonlinear effects of Joule heating. To linear order in the electric field, then, the electron and phonon temperatures are equal. Also to this order, the drift velocity v_d is proportional to the steady-state limit of E(t).

To calculate the density matrix $\rho(t)$, all variables must be treated as quantum mechanical. Then $\rho(t)$ obeys the Liouville equation

$$\frac{d\rho}{dt} = -i[H_e + H_{\rm ph} + H_P, \rho] - i[H_I + H_E, \rho] , \quad (18)$$

where

$$H_P = \frac{P^2}{2M} , \qquad (19)$$

$$H_E \equiv E(t)H_X = -NeE(t)X , \qquad (20)$$

$$H_I = H_{ei} + H_{e-\mathrm{ph}} \ . \tag{21}$$

If the interaction representation for any operator A(t) is defined by

$$\widehat{A}(t) = e^{i(H_e + H_{\rm ph} + H_p)t} A(t) e^{-i(H_e + H_{\rm ph} + H_p)t}, \qquad (22)$$

then Eq. (18) has the formal solution

$$\hat{\rho}(t) = \rho_0 - i \int_0^t dt' [\hat{H}_I(t') + \hat{H}_E(t'), \hat{\rho}(t')] , \qquad (23)$$

which can be expanded in powers of the electron interactions and the electric field.

At time t = 0 the center-of-mass system is prepared in an eigenstate of momentum with eigenvalue P_0 and the relative electron-phonon system is prepared in a state of thermal equilibrium with temperatures T_e and T. Therefore, the density matrix at t = 0 is

$$\hat{\rho}(t=0) = \rho_0 = \frac{1}{Z} e^{-H_e/T_e} e^{-H_{\rm ph}/T} |\mathbf{P}_0\rangle \langle \mathbf{P}_0| , \qquad (24)$$

where the partition function Z is defined so that $Tr(\rho_0)=1$. All traces are evaluated by summing both over eigenstates $|\mathbf{P}\rangle$ of the center-of-mass system and over eigenstates of H_e and $H_{\rm ph}$.

To calculate the linearized resistivities, the density matrix must be expanded to first order in the electric field. The zero-order term $\hat{\rho}_r(t)$, which obeys Eq. (23) with $H_E(t)=0$, can be written

$$\widehat{\rho}_{r}(t) = S \exp\left[-i \int_{0}^{t} dt' \mathcal{H}_{I}(t')\right] \rho_{0} , \qquad (25)$$

where

$$\mathcal{H}_{I}(t_{1})\hat{A}(t_{2}) = [\hat{H}_{I}(t_{1}), \hat{A}(t_{2})]$$
(26)

and S is the time-ordering operator. To first order in the electric field, the electron temperature T_e can be set equal to T in Eq. (24) for ρ_0 . Using Eq. (23), the full density matrix $\hat{\rho}(t)$ is then expanded in powers of the electron interactions:

$$\hat{\rho}(t) = \hat{\rho}_r(t) + \sum_{n=2}^{\infty} (-i)^{n-1} \int_0^t dt_2 \int_0^{t_2} dt_3 \cdots \int_0^{t_{n-1}} dt_n [\hat{H}_I(t_2), [\hat{H}_I(t_3), \cdots [\hat{H}_E(t_n), \hat{\rho}_r(t_n)] \cdots]], \qquad (27)$$

so that $\hat{\rho}(t=0)=\hat{\rho}_r(t=0)=\rho_0$.

If the center-of-mass variables were treated classically, the commutator of $\hat{H}_E(t)$ with $\hat{\rho}_r(t)$ would vanish. By mixing classical and quantum-mechanical treatments of the electron variables, the FB method has previously neglected the explicit dependence of the density matrix on the electric field. Because the center-of-mass coordinates do not commute at different times,

$$[\hat{R}_{i}(t_{1}), \hat{R}_{j}(t_{2})] = i\delta_{ij}\frac{1}{M}(t_{2}-t_{1}), \qquad (28)$$

the additional terms in the density matrix affect the evaluation of the resistivities in Eqs. (14) and (15). To fourth and higher order in the electron-impurity interactions, these new terms in $\hat{\rho}(t)$ are responsible for a second class of divergent contributions to the impurity resistivity, as shown below.

III. IMPURITY RESISTIVITY

To calculate the impurity resistivity, it is convenient to ignore the contribution of the electron-phonon interactions to $\rho_i(t)$. The result is the lowest-order term in an expansion of $\rho_i(t)$ in powers of $M(\mathbf{q}, \gamma)$. This lowestorder result becomes exact when the electron-phonon interaction becomes negligible compared to the electronimpurity interaction. Of course, to second order in the electric field, the electron-phonon interaction plays the crucial role of maintaining isothermal conditions in the electron system.

To lowest order in $M(\mathbf{q}, \gamma)$, the impurity resistivity can be expanded in powers of the electron-impurity interaction. Using Eq. (13), I find that $\rho_i(t)$ is given by

$$\rho_{i}(t) = \frac{i\lambda}{N^{2}e^{2}v_{d}} \sum_{\mathbf{q},\alpha} \phi(q)q_{x}e^{-i\mathbf{q}\cdot\mathbf{R}_{\alpha}} \left[\operatorname{Tr}\{\widehat{\rho}_{r}(t)e^{i\mathbf{q}\cdot\widehat{\mathbf{R}}(t)}\widehat{\rho}_{\mathbf{q}}(t)\} + Nev_{d} \sum_{n=2}^{\infty} i^{n-1} \int_{0}^{t} dt_{2} \int_{0}^{t_{2}} dt_{3} \cdots \int_{0}^{t_{n-1}} dt_{n} \rho_{i}(t_{n}) \right] \times \operatorname{Tr}\{\widehat{\rho}_{r}(t_{n}) [\widehat{H}_{X}(t_{n}), [\widehat{H}_{ei}(t_{n-1}), \cdots [\widehat{H}_{ei}(t_{2}), e^{i\mathbf{q}\cdot\widehat{\mathbf{R}}(t)}\widehat{\rho}_{\mathbf{q}}(t)] \cdots]]\} , \qquad (29)$$

where the contribution of H_{e-ph} to $\hat{\rho}_r(t)$ should be ignored. Notice that the second set of terms, which arises from the noncommutivity of the center-of-mass coordinates, itself involves the resistivity $\rho_i(t)$ at previous times. These additional terms in Eq. (29) begin to affect the result for $\rho_i(t)$ at fourth order in λ .

The commutator of $\hat{H}_{X}(t)$ with the exponential factors in Eq. (29) can be evaluated with the relation

$$[\hat{X}(t_{n+1}), e^{i\mathbf{q}_{n}\cdot\hat{\mathbf{R}}(t_{n})}\cdots e^{i\mathbf{q}_{1}\cdot\hat{\mathbf{R}}(t_{1})}] = \frac{1}{M} \{t_{n+1}(q_{1x}+\cdots+q_{nx}) - (q_{1x}t_{1}+\cdots+q_{nx}t_{n})\}e^{i\mathbf{q}_{n}\cdot\hat{\mathbf{R}}(t_{n})}\cdots e^{i\mathbf{q}_{1}\cdot\hat{\mathbf{R}}(t_{1})}.$$
 (30)

Notice that Eq. (29) also involves commutators of the form

$$[e^{i\mathbf{q}_{1}\cdot\hat{\mathbf{R}}(t_{1})}, e^{i\mathbf{q}_{2}\cdot\hat{\mathbf{R}}(t_{2})}] = -2ie^{i[\mathbf{q}_{1}\cdot\hat{\mathbf{R}}(t_{1})+\mathbf{q}_{2}\cdot\hat{\mathbf{R}}(t_{2})]}\sin\left[\frac{1}{2M}\mathbf{q}_{1}\cdot\mathbf{q}_{2}(t_{1}-t_{2})\right],$$
(31)

which introduce phase factors into the time integrals of $\rho_i(t)$. Because the thermodynamic limit $M = Nm \to \infty$ is taken before²⁵ the steady-state limit $t \to \infty$, these phase factors can be neglected. So, after the evaluation of the commutators involving $\hat{X}(t)$, the coordinates $\hat{\mathbf{R}}(t)$ can be treated classically.

To second order in the electron-impurity interaction, then, the impurity resistivity is given by

$$\rho_{i}(t) = -\frac{\lambda^{2}}{N^{2}e^{2}v_{d}} \sum_{\mathbf{q}_{1},\mathbf{q}_{2}} \sum_{\alpha_{1},\alpha_{2}} \phi(q_{1})\phi(q_{2})q_{1x} \int_{0}^{t} dt_{2} e^{i\mathbf{q}_{1}\cdot[\mathbf{R}(t)-\mathbf{R}_{\alpha_{1}}]} e^{i\mathbf{q}_{2}\cdot[\mathbf{R}(t_{2})-\mathbf{R}_{\alpha_{2}}]} \frac{1}{Z_{e}} \mathrm{Tr}_{e} \{ e^{-H_{e}/T} [\hat{\rho}_{\mathbf{q}_{2}}(t_{2}), \hat{\rho}_{\mathbf{q}_{1}}(t)] \} , \qquad (32)$$

2997

where $\mathbf{R}(t_2) - \mathbf{R}(t_1) = v_d(t_2 - t_1) \hat{\mathbf{x}}$ and

$$Z_{e} = \operatorname{Tr}_{e} \exp(-H_{e}/T) \tag{33}$$

is the partition function for the noninteracting electron system, defined as a trace over the eigenstates of H_e . The average over impurities in Eq. (32) is easily²⁶ evaluated:

$$\sum_{\alpha_{1},\alpha_{2}} e^{-i\mathbf{q}_{1}\cdot\mathbf{R}_{\alpha_{1}}} e^{-i\mathbf{q}_{2}\cdot\mathbf{R}_{\alpha_{2}}} = N_{i}^{2}\delta_{\mathbf{q}_{1},0}\delta_{\mathbf{q}_{2},0} + N_{i}\delta_{\mathbf{q}_{2},-\mathbf{q}_{1}}.$$
(34)

Thus, in the limit $t \rightarrow \infty$, $\rho_i(t)$ can be rewritten

$$\lim_{t \to \infty} \rho_i(t) = \frac{iN_i \lambda^2}{N^2 e^2 v_d} \sum_{\mathbf{q}} |\phi(q)|^2 q_x \int_0^\infty dt \ e^{iq_x v_d t} \Pi^{(1)}(\mathbf{q};t) ,$$
(35)

where

$$\Pi^{(1)}(\mathbf{q};t_{1}-t_{2}) = i\Theta(t_{1}-t_{2})\frac{1}{Z_{e}}$$

$$\times \mathrm{Tr}_{e}\{e^{-H_{e}/T}[\hat{\rho}_{-\mathbf{q}}(t_{2}),\hat{\rho}_{\mathbf{q}}(t_{1})]\}.$$
(36)

Using the result of Appendix A for the density-density correlation function $\Pi^{(1)}(\mathbf{q};t)$, Eq. (35) can be evaluated to lowest order in v_d :

$$\rho_i^{(0)} = \lambda^{-2} \lim_{t \to \infty} \rho_i(t) = \frac{m}{Ne^2} \left(\frac{1}{\tau}\right) , \qquad (37)$$

where, for any quantity $A(\mathbf{p})$,

$$\langle A \rangle = -\frac{2}{3} \frac{1}{N} \sum_{\mathbf{p}} \frac{df}{d\varepsilon_{\mathbf{p}}} \frac{p^2}{m} A(\mathbf{p})$$
 (38)

is defined in terms of the Fermi function

$$f(\varepsilon_{\rm p}) = \frac{1}{1 + e^{\varepsilon_{\rm p}/T}} .$$
(39)

Finally, the inverse relaxation time for an electron of momentum **p** is given by

$$\frac{1}{\tau(\mathbf{p})} = \frac{mN_i p}{(2\pi)^2} \int d\Omega |\phi[2p\sin(\phi/2)]|^2 (1-\cos\phi) .$$
(40)

Equation (37) is the result of the FB method when the steady-state $t \rightarrow \infty$ limit is taken *after* the limit of small λ . Notice that this result disagrees with linear response theory.

IV. RESUMMATION OF DIVERGENT TERMS

To obtain the correct steady-state limit of the resistivity, it is convenient to introduce the Laplace transform²⁷

$$\rho_i(\delta) = \delta \int_0^\infty dt \, \rho_i(t) e^{-\delta t} , \qquad (41)$$

so that

$$\lim_{t \to \infty} \rho_i(t) = \lim_{\delta \to 0^+} \rho_i(\delta) .$$
(42)

As shown below, an expansion of $\rho_i(\delta)$ in powers of λ contains contributions that diverge as $\delta \rightarrow 0^+$. The first such divergent contribution occurs to fourth order in λ .

These divergent contributions can be treated by using the limiting procedure of van Hove.¹⁶ This procedure is motivated by the observation that the relaxation time $\tau(\mathbf{p})$ is of order λ^{-2} . Hence, the steady-state limit of the resistivity is reached only after a time t that is long compared to λ^{-2} , so that $\lambda^2 t \to \infty$. In terms of the Laplace transform $\rho_i(\delta)$, the weak scattering limit is attained by first taking the limit of $\lambda \to 0$ and $\delta \to 0^+$ but $\lambda^2/\delta \neq 0$ and then the limit $\lambda^2/\delta \to \infty$:

$$\rho_i^{(0)} = \lim_{\lambda^2/\delta \to \infty} \lim_{\lambda \to 0, \delta \to 0^+} \left[\lambda^{-2} \rho_i(\delta) \right].$$
(43)

This limiting prescription can also be written

$$\rho_i^{(0)} = \lim_{\lambda \to 0} \lim_{\delta \to 0^+} \left[\lambda^{-2} \rho_i(\delta) \right], \qquad (44)$$

with the long time limit $(\delta \rightarrow 0^+)$ taken *before* the limit of weak interaction. The naive result of the FB theory, given by Eq. (37), was evaluated with these limits reversed.

In the first limit $(\lambda \rightarrow 0, \delta \rightarrow 0^+; \lambda^2/\delta \neq 0)$, only the divergent contributions proportional to $(\lambda^2/\delta)^n$ survive. Terms of order $\lambda^m (\lambda^2/\delta)^n (m > 0)$ are neglected. The dominant divergent contributions are obtained by pairing the internal momentum \mathbf{q}_i in Eq. (29) for the resistivity.

To demonstrate this, rewrite Eq. (29) as the sum over components

$$\rho_i(t) = \sum_{n=1}^{\infty} g_n(t) , \qquad (45)$$

where

$$g_{1}(t) = \frac{i\lambda}{N^{2}e^{2}v_{d}} \sum_{\mathbf{q},\alpha} \phi(q)q_{x}e^{i\mathbf{q}\cdot[\mathbf{R}(t)-\mathbf{R}_{\alpha}]} \mathrm{Tr}\{\hat{\rho}_{r}(t)\hat{\rho}_{q}(t)\}$$
(46)

and, for $n \ge 2$,

$$g_{n}(t) = -i^{n}\lambda \sum_{\mathbf{q},\alpha} \phi(q)q_{x}e^{-i\mathbf{q}\cdot\mathbf{R}_{\alpha}} \int_{0}^{t} dt_{2} \int_{0}^{t_{2}} dt_{3} \cdots \int_{0}^{t_{n-1}} dt_{n} \rho_{i}(t_{n}) \times \operatorname{Tr}\{\widehat{\rho}_{r}(t_{n}) [\widehat{X}(t_{n}), [\widehat{H}_{ei}(t_{n-1}), \cdots [\widehat{H}_{ei}(t_{2}), e^{i\mathbf{q}\cdot\widehat{\mathbf{R}}(t)}\widehat{\rho}_{\mathbf{q}}(t)] \cdots]]\}.$$
(47)

The Laplace transform of these components contains integrals of the form

$$\lambda^{2n} \int_{0}^{\infty} d(t-t_{2}) \int_{0}^{\infty} d(t_{2}-t_{3}) \cdots \int_{0}^{\infty} d(t_{2n-1}-t_{2n}) e^{-\delta(t-t_{2})} e^{-\delta(t_{2}-t_{3})} \cdots e^{-\delta(t_{2n-1}-t_{2n})} \\ \times [\hat{\rho}_{q_{2n}}(t_{2n}), [\hat{\rho}_{q_{2n-1}}(t_{2n-1}), \cdots [\hat{\rho}_{q_{2}}(t_{2}), \hat{\rho}_{q_{1}}(t)] \cdots]].$$
(48)

2998

The divergent contributions that survive in the first limit contain momenta that are paired with $q_{2m} = -q_{2m-1}$ for m = 1, 2, ..., n. A recursion relation for the commutator in Eq. (48) with paired momenta is derived in Appendix A, where it is shown that this commutator does not depend on the variables $t_{2m} - t_{2m+1}$ for m = 1, 2, ..., n - 1. Integration over these variables generates the factor $1/\delta^n$, so Eq. (48) would then be proportional to $(\lambda^2/\delta)^n$. It is straightforward to show that commutators with any unpaired momenta will reduce this divergent contribution by at least one factor of δ .

Note that if the phase factors generated by commutators of the form of Eq. (31) had been kept up to this point, they would contribute additively to the Laplace parameters δ . Since the thermodynamic limit $N \rightarrow \infty$ is taken before²⁵ the long time limit $\delta \rightarrow 0^+$, these factors do not affect the evaluation of the divergent terms.

Now consider the divergent contributions of the first component $g_1(\delta)$. After expanding the density matrix $\hat{\rho}_r(t)$, the divergent term of order $\lambda^2 (\lambda^2 / \delta)^m$ can be written

$$g_{1}^{(2m+2)}(\delta) = \frac{iN_{i}^{m+1}}{N^{2}e^{2}v_{d}}\lambda^{2m+2} \\ \times \sum_{\mathbf{q}_{1},\dots,\mathbf{q}_{m+1}} |\phi(q_{1})|^{2} \cdots |\phi(q_{m+1})|^{2}q_{1x} \\ \times \int_{0}^{\infty} dT_{2} \int_{0}^{\infty} dT_{3} \cdots \int_{0}^{\infty} dT_{2m+2} e^{iq_{1x}v_{d}T_{2}} e^{iq_{2x}v_{d}T_{4}} \cdots e^{iq_{m+1,x}v_{d}T_{2m+2}} \\ \times e^{-\delta T_{2}}e^{-\delta T_{3}} \cdots e^{-\delta T_{2m+2}} \\ \times \Pi^{(m+1)}(\mathbf{q}_{1},\mathbf{q}_{2},\dots,\mathbf{q}_{m+1};T_{2},T_{3},\dots,T_{2m+2}),$$
(49)

where $\Pi^{(n)}(\mathbf{q}_i; T_i)$ is a generalization of the density-density correlation function defined in Eq. (36):

$$\Pi^{(n)}(\mathbf{q}_{i};T_{i}) = i^{2n-1}\Theta(T_{2})\Theta(T_{3})\cdots\Theta(T_{2n}) \times \frac{1}{Z_{e}}\operatorname{Tr}_{e}\left\{e^{-H_{e}/T}[\hat{\rho}_{-\mathbf{q}_{n}}(t_{2n}),[\hat{\rho}_{\mathbf{q}_{n}}(t_{2n-1}),\cdots[\hat{\rho}_{-\mathbf{q}_{1}}(t_{2}),\hat{\rho}_{\mathbf{q}_{1}}(t_{1})]\cdots]\right\},$$
(50)

where $T_i = t_{i-1} - t_i$ for i = 2, 3, ..., 2n. In Appendix B, I show that to lowest order in v_d ,

$$g_1^{(2m+2)}(\delta) = (-1)^m \frac{\lambda^{2m+2}}{\delta^m} \frac{m}{Ne^2} \left\langle \left[\frac{1}{\tau} \right]^{m+1} \right\rangle$$
(51)

for $m \ge 0$. Notice that the lowest-order m = 0 term agrees with the result of Eq. (37).

The divergent contributions to $g_{n>1}(\delta)$ that survive the first limit can be found in a similar way. For each component $g_n(\delta)$, $\hat{\rho}_r(t)$ can be expanded in powers of λ . In Appendix C it is shown that only the lowest-order term in this expansion remains nonzero after the first limit. In order to pair all the internal momenta, only odd terms $g_{2n+1}(\delta)$ are considered:

$$g_{2n+1}(\delta) = -\lambda^{2n} \frac{N_i^n}{M} \delta \sum_{\mathbf{q}_1, \dots, \mathbf{q}_n} |\phi(q_1)|^2 \cdots |\phi(q_n)|^2 q_{1x} \\ \times \int_0^{\infty} dT_2 \int_0^{\infty} dT_3 \cdots \int_0^{\infty} dT_{2n+1} \\ \times \int_0^{\infty} dt_{2n+1} e^{-\delta T_2} e^{-\delta T_3} \cdots e^{-\delta T_{2n+1}} e^{-\delta t_{2n+1}} \\ \times \rho_i(t_{2n+1})(q_{1x}T_2 + q_{2x}T_4 + \cdots + q_{nx}T_{2n}) \\ \times \Pi^{(n)}(\mathbf{q}_1, \mathbf{q}_2, \dots, \mathbf{q}_n; T_2, T_3, \dots, T_{2n})$$
(52)

for
$$n \ge 1$$
. This term is evaluated in Appendix B, with the result

$$g_{2n+1}(\delta) = (-1)^{n+1} \frac{\lambda^{2n}}{\delta^n} \rho_i(\delta) \left\langle \left[\frac{1}{\tau} \right]^n \right\rangle, \qquad (53)$$

which involves the Laplace transform of the resistivity.

Summing Eqs. (51) and (53) over the divergent contributions yields the result

$$\lim_{\lambda \to 0, \delta \to 0^{+}} \left[\lambda^{-2} \rho_{i}(\delta) \right] = \frac{m}{Ne^{2}} \frac{\sum_{n=0}^{\infty} \left[-\frac{\lambda^{2}}{\delta} \right]^{n} \left\langle \left[\frac{1}{\tau} \right]^{n+1} \right\rangle}{1 + \sum_{n=1}^{\infty} \left[-\frac{\lambda^{2}}{\delta} \right]^{n} \left\langle \left[\frac{1}{\tau} \right]^{n} \right\rangle},$$
(54)

which is exactly the same relation obtained by Huberman

and Chester¹⁹ in their analysis of the theory of Rousseau.¹⁷ The numerator arises from $g_1(\delta)$ and the divergent terms in the denominator from $g_{n>1}(\delta)$. If the center-of-mass position were treated classically, these divergent terms in the denominator would be absent. Equation (54) can now be formally resummed:

$$\lim_{\lambda \to 0, \delta \to 0^+} \left[\lambda^{-2} \rho_i(\delta) \right] = \frac{m}{Ne^2} \frac{\left\langle \frac{1}{\tau} \frac{1}{1 + \lambda^2 / (\delta \tau)} \right\rangle}{\left\langle \frac{1}{1 + \lambda^2 / (\delta \tau)} \right\rangle} .$$
(55)

Finally, upon performing the limit $\lambda^2/\delta \rightarrow \infty$, I find that

$$\rho_i^{(0)} = \frac{m}{Ne^2 \langle \tau \rangle} , \qquad (56)$$

in agreement with the Kubo formula for the conductivity. Notice that if the additional contributions to the density matrix had been left out, the resistivity would have vanished in this limit.

V. CONCLUSION

This work has shown that the FB resistivity contains two sets of divergent terms, which are the same as those found by Huberman and Chester.¹⁹ The first set of divergent terms arises from the density matrix of the relative electron-phonon system. The second set arises from the explicit dependence of the density matrix on the electric field, which was previously ignored by FB calculations. Upon resumming these divergent terms with the prescription of van Hove,¹⁶ the FB result is brought into agreement with the Kubo formula. When the second set of divergent terms is ignored, the FB resistivity is formally equivalent to the result of Rousseau,¹⁷ who also neglected the explicit dependence of the density matrix on the electric field.

It is worth emphasizing that, without the extra terms in the density matrix, the resummed result for the FB resistivity would vanish. When this new set of terms is included, by treating all variables as quantum mechanical, the resummed expression agrees with the Kubo formula. Thus, the FB theory is formally equivalent to linear response theory only when the full density matrix is used.

The discrepancy between the lowest-order FB resistivity and the Kubo formula cannot be explained by the presence of a heat bath. To first order in the electric field, the effects of Joule heating can be neglected and the existence of a heat bath is irrelevant. To this order, the electron-phonon interaction merely provides an additional frictional force that acts on the center of mass of the electrons. Isothermal and adiabatic calculations of the resistivity must then produce the same result.

Like its predecessors, the theories of Rousseau¹⁷ and of Kenkre and Dresden,¹⁸ the FB theory is formally exact. This work has shown that, when the full density matrix is used, the FB method is consistent with linear response theory for the conductivity, as are the formalisms of Rousseau and of Kenkre and Dresden. Unfortunately, like its predecessors, the FB method contains an infinite number of divergent terms that must be resummed to obtain the limit of weak scattering. The presence of divergences in all these formalisms severely limits their applications and eliminates their advantages over the Kubo formula.

This paper has been concerned with the evaluation of the zero-frequency resistivity in the presence of a constant electric field. When an oscillating electric field with frequency ω is applied, the drift velocity and the steadystate resistivity become time dependent. In their study of the work of Kenkre and Dresden, Argyres and Sigel concluded that the expansion of the frequency-dependent resistivity in powers of λ is convergent if $\omega \langle \tau \rangle \gg 1$. In this high-frequency regime, the lowest-order term in an expansion of the resistivity does agree with the Kubo formula. For frequencies that satisfy the condition $\omega \langle \tau \rangle \gg 1$, the FB method can also be used to obtain a convergent expansion of the resistivity. Provided that the full density matrix is used, this expansion should also agree with the Kubo formula. However, to evaluate the resistivity for arbitrary $\omega \langle \tau \rangle$ requires the summation over an infinite number of terms of the form $\lambda^{2n}/(\omega+i\delta)^n$. For $\omega\langle \tau \rangle \leq 1$, this expansion diverges.

The calculations of this paper have been performed to lowest order in the electric field and in the electronphonon coupling $M(\mathbf{q}, \gamma)$. To higher order in the electric field, the effects of Joule heating must be considered and the cross terms between the electron-impurity and electron-phonon interactions may become important. Other authors²⁸ have shown that the effects of Joule heating can be consistently incorporated into a calculation of the conductivity based on the Kubo formula. Calculations of such nonlinear effects with the FB theory will be frustrated by the presence of divergences even to lowest order in $M(\mathbf{q}, \gamma)$. It would be surprising if higher-order terms in an expansion of $\rho_i(\delta)$ in powers of $M(\mathbf{q}, \gamma)$ were not also divergent.

The FB method has recently²⁹ been recast into the form of a quantum Langevin equation for the center-ofmass position $R_i(t)$. Though this reformulation does not use a density matrix, the same flaws of the original method are retained: the noncommutivity of the centerof-mass operators is ignored and the divergence of the resistivity is not addressed. The result for the zerofrequency resistivity is again in disagreement with linear response theory.

Some FB calculations^{10,29} have reported that fluctuations in the center-of-mass position affect the impurity resistivity. Since this effect occurs to second order in λ , it is unrelated to the divergences in the higher-order contributions to the FB resistivity, which first occur at fourth order in λ . The predicted change in the resistivity is proportional to 1/N. The present work did not find such a lowest-order change because the thermodynamic limit $N \rightarrow \infty$ preceeded²⁵ the steady-state limit $\delta \rightarrow 0^+$.

It is unlikely that the present work will end the search for a nondivergent theory of the resistivity, nor is it so intended. However, the future designers of resistivity formulas would be well advised to heed the lessons of Argyres and Sigel and of Huberman and Chester: the first test for any theory of the resistivity is that it agrees with the Kubo formula to lowest order in the electric field. Note added in proof. After this work was submitted for publication, I received results from Argyres,³⁰ who uses projection techniques to show that the FB resistivity is divergent. With the uncorrected density matrix $\hat{\rho}_r(t)$, Argyres proves that the FB resistivity resums to zero, in agreement with this work. I have also recently become aware of papers by Peeters and Devreese³¹ and by Cox et al.,³² who treat related problems.

ACKNOWLEDGMENTS

I would like to acknowledge support under U.S. Department of Energy (DOE) Contract No. DE-AC05-84OR21400 with Martin Marietta Energy Systems, Inc., and under National Science Foundation (NSF) Grant No. DMR-87-04210. I would like to thank Dr. G. Y. Hu for his comments on this paper. It is also a pleasure to thank Dr. T. Kaplan and Professor G. D. Mahan for many useful and stimulating conversations.

APPENDIX A

In this Appendix, I develop a recursion relation for the correlation function $\Pi^{(m)}(\mathbf{q}_i;T_i)$ defined by Eq. (50). From the definition of the electron density operator ρ_q , it can be readily shown that

$$[\hat{\rho}_{-\mathbf{q}_{1}}(t_{2}), \hat{\rho}_{\mathbf{q}_{1}}(t_{1})] = -\sum_{\mathbf{k},\sigma} A_{\mathbf{k},\mathbf{q}_{1},\sigma} e^{i\omega_{\mathbf{k},\mathbf{q}_{1}}T_{2}}, \qquad (A1)$$

where $T_i = t_{i-1} - t_i$,

$$\omega_{\mathbf{k},\mathbf{q}} = \varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}} , \qquad (A2)$$

and

$$A_{\mathbf{k},\mathbf{q},\sigma} = c_{\mathbf{k}+\mathbf{q},\sigma}^{\dagger} c_{\mathbf{k}+\mathbf{q},\sigma} - c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} .$$
 (A3)

It is also easily shown that for any function F_k ,

$$\left[\hat{\rho}_{-\mathbf{q}_{2}}(t_{2}),\left[\hat{\rho}_{\mathbf{q}_{2}}(t_{1}),\sum_{\mathbf{k},\sigma}A_{\mathbf{k},\mathbf{q}_{1},\sigma}F_{\mathbf{k}}\right]\right] = \sum_{\mathbf{k},\sigma}A_{\mathbf{k},\mathbf{q}_{2},\sigma}e^{i\omega_{\mathbf{k},\mathbf{q}_{2}}T_{2}}(F_{\mathbf{k}}-F_{\mathbf{k}-\mathbf{q}_{1}}+F_{\mathbf{k}-\mathbf{q}_{1}+\mathbf{q}_{2}}-F_{\mathbf{k}+\mathbf{q}_{2}}).$$
(A4)

Therefore, if the correlation function is written

$$\Pi^{(m)}(\mathbf{q}_{1},\mathbf{q}_{2},\ldots,\mathbf{q}_{m};T_{2},T_{3},\ldots,T_{2m}) = 2i(-1)^{m}\Theta(T_{2})\Theta(T_{3})\cdots\Theta(T_{2m})\sum_{\mathbf{k}}\left[f(\varepsilon_{\mathbf{k}+\mathbf{q}_{m}})-f(\varepsilon_{\mathbf{k}})\right]e^{i\omega_{\mathbf{k},\mathbf{q}_{m}}T_{2m}}G_{\mathbf{k}}^{(m)},$$
(A5)

then for $m \ge 1$,

$$G_{\mathbf{k}}^{(m+1)} = G_{\mathbf{k}}^{(m)} e^{i\omega_{\mathbf{k},\mathbf{q}_{m}}T_{2m}} - G_{\mathbf{k}-\mathbf{q}_{m}}^{(m)} e^{-i\omega_{\mathbf{k},-\mathbf{q}_{m}}T_{2m}} + G_{\mathbf{k}-\mathbf{q}_{m}+\mathbf{q}_{m+1}}^{(m)} e^{-i\omega_{\mathbf{k}+\mathbf{q}_{m+1},-\mathbf{q}_{m}}T_{2m}} - G_{\mathbf{k}+\mathbf{q}_{m+1}}^{(m)} e^{i\omega_{\mathbf{k}+\mathbf{q}_{m+1},\mathbf{q}_{m}}T_{2m}}$$
(A6)

and $G_k^{(1)} = 1$. Note that $G_k^{(m)}$ is a function of $\{q_1, q_2, \ldots, q_m\}$ and $\{T_2, T_4, \ldots, T_{2m-2}\}$. Equations (A5) and (A6) permit an inductive calculation of the divergent contributions to the resistivity. Two symmetry relations that facilitate this calculation are

$$G_{\mathbf{k}-\mathbf{q}_{n}}^{(n)} = -G_{\mathbf{k}}^{(n)}(\mathbf{q}_{1},\mathbf{q}_{2},\ldots,\mathbf{q}_{n-1},-\mathbf{q}_{n}), \quad n \ge 2$$
(A7)

$$G_{-k}^{(n)} = G_{k}^{(n)}(-\mathbf{q}_{1}, -\mathbf{q}_{2}, \dots, -\mathbf{q}_{n}), \quad n \ge 1$$
(A8)

which follow from Eq. (A6).

APPENDIX B

In this Appendix the dominant divergent contributions to $g_1(\delta)$ and $g_{2n+1}(\delta)$ $(n \ge 1)$ are evaluated inductively. Consider first the contributions to $g_1^{(2m+2)}(\delta)$. Using the recursion relation of Eqs. (A5) and (A6), Eq. (49) can be written, for m > 1,

$$g_{1}^{(2m+2)}(\delta) = (-1)^{m+1} \frac{2\pi N_{i}^{m+1}}{N^{2}e^{2}} \frac{\lambda^{2m+2}}{\delta^{m}} \sum_{q_{1}, \dots, q_{m+1}} |\phi(q_{1})|^{2} \cdots |\phi(q_{m+1})|^{2} q_{1x} q_{m+1,x}$$

$$\times \sum_{\mathbf{k}} \frac{df}{d\varepsilon_{\mathbf{k}}} \delta(\varepsilon_{\mathbf{k}+\mathbf{q}_{m+1}} - \varepsilon_{\mathbf{k}}) \int_{0}^{\infty} dT_{2} \int_{0}^{\infty} dT_{4} \cdots \int_{0}^{\infty} dT_{2m} e^{-\delta T_{2}} e^{-\delta T_{4}} \cdots e^{-\delta T_{2m}} G_{\mathbf{k}}^{(m+1)}$$

$$= (-1)^{m+1} \frac{8\pi^{2} N_{i}^{m+1}}{N^{2}e^{2}} \frac{\lambda^{2m+2}}{\delta^{m}}$$

$$\times \sum_{q_{1}, \dots, q_{m+1}} |\phi(q_{1})|^{2} \cdots |\phi(q_{m+1})|^{2} q_{1x} q_{m+1,x}$$

$$\times \sum_{\mathbf{k}} \frac{df}{d\varepsilon_{\mathbf{k}}} \delta(\varepsilon_{\mathbf{k}+\mathbf{q}_{m+1}} - \varepsilon_{\mathbf{k}}) \delta(\varepsilon_{\mathbf{k}+\mathbf{q}_{m}} - \varepsilon_{\mathbf{k}}) \int_{0}^{\infty} dT_{2} \int_{0}^{\infty} dT_{4} \cdots \int_{0}^{\infty} dT_{2m-2} e^{-\delta T_{2}} e^{-\delta T_{4}} \cdots e^{-\delta T_{2m-2}} G_{\mathbf{k}}^{(m)} .$$

(B1)

Now note that

$$N_{i} \sum_{\mathbf{q}_{m+1}} |\phi(q_{m+1})|^{2} \mathbf{q}_{1} \cdot \mathbf{q}_{m+1} \delta(\varepsilon_{\mathbf{k}+\mathbf{q}_{m+1}} - \varepsilon_{\mathbf{k}}) = -\frac{1}{2\pi} \mathbf{k} \cdot \mathbf{q}_{1} \frac{1}{\tau(\mathbf{k})} , \qquad (B2)$$

where $\tau(\mathbf{k})$ is defined by Eq. (40). So, for m > 2,

$$g_{1}^{(2m+2)}(\delta) = (-1)^{m} \frac{4\pi N_{l}^{m}}{N^{2} e^{2}} \frac{\lambda^{2m+2}}{\delta^{m}}$$

$$\times \sum_{q_{1},\dots,q_{m}} |\phi(q_{1})|^{2} \cdots |\phi(q_{m})|^{2}$$

$$\times \sum_{\mathbf{k}} \frac{df}{d\varepsilon_{\mathbf{k}}} \delta(\varepsilon_{\mathbf{k}+q_{m}} - \varepsilon_{\mathbf{k}}) \frac{1}{\tau(\mathbf{k})}$$

$$\times \int_{0}^{\infty} dT_{2} \int_{0}^{\infty} dT_{4} \cdots \int_{0}^{\infty} dT_{2m-2} e^{-\delta T_{2}} e^{-\delta T_{4}} \cdots e^{-\delta T_{2m-2}} G_{\mathbf{k}}^{(m-1)}(e^{i\omega_{\mathbf{k},\mathbf{q}_{m-1}}T_{2m-2}} + e^{-i\omega_{\mathbf{k},\mathbf{q}_{m-1}}T_{2m-2}})$$

$$\times [\mathbf{k} \cdot \mathbf{q}_{1} - (\mathbf{k} + \mathbf{q}_{m}) \cdot \mathbf{q}_{1}]$$

$$= (-1)^{m} \frac{4\pi N_{l}^{m-1}}{N^{2} e^{2}} \frac{\lambda^{2m+2}}{\delta^{m}}$$

$$\times \sum_{q_{1},\dots,q_{m-1}} |\phi(q_{1})|^{2} \cdots |\phi(q_{m-1})|^{2}$$

$$\times \sum_{\mathbf{k}} \frac{df}{d\varepsilon_{\mathbf{k}}} \delta(\varepsilon_{\mathbf{k}+\mathbf{q}_{m-1}} - \varepsilon_{\mathbf{k}}) \left[\frac{1}{\tau(\mathbf{k})} \right]^{2}$$

$$\times \int_{0}^{\infty} dT_{2} \int_{0}^{\infty} dT_{4} \cdots \int_{0}^{\infty} dT_{2m-4} e^{-\delta T_{2}} e^{-\delta T_{4}} \cdots e^{-\delta T_{2m-4}} G_{\mathbf{k}}^{(m-1)} \mathbf{k} \cdot \mathbf{q}_{1}.$$
(B3)

By iterating this procedure, it is apparent that

$$g_{1}^{(2m+2)}(\delta) = (-1)^{m} \frac{4\pi N_{i}^{2}}{N^{2} e^{2}} \frac{\lambda^{2m+2}}{\delta^{m}}$$

$$\times \sum_{\mathbf{q}_{1}, \mathbf{q}_{2}} |\phi(q_{1})|^{2} |\phi(q_{2})|^{2}$$

$$\times \sum_{\mathbf{k}} \frac{df}{d\varepsilon_{\mathbf{k}}} \delta(\varepsilon_{\mathbf{k}+\mathbf{q}_{2}} - \varepsilon_{\mathbf{k}}) \left[\frac{1}{\tau(\mathbf{k})}\right]^{m-1} \int_{0}^{\infty} dT_{2} e^{-\delta T_{2}} (e^{i\omega_{\mathbf{k},\mathbf{q}_{1}}T_{2}} + e^{-i\omega_{\mathbf{k},\mathbf{q}_{1}}T_{2}}) [\mathbf{k} \cdot \mathbf{q}_{1} - (\mathbf{k}+\mathbf{q}_{2}) \cdot \mathbf{q}_{1}]$$

$$= (-1)^{m} \frac{\lambda^{2m+2}}{\delta^{m}} \frac{m}{N e^{2}} \left\langle \left[\frac{1}{\tau}\right]^{m+1} \right\rangle.$$
(B4)

as stated in Eq. (51). This result is also valid for m = 1 and 2, as can be shown explicitly. The calculation of the divergent contributions to $g_{2n+1}(\delta)$ $(n \ge 1)$ proceeds in a similar fashion. It is simple to show that only the term involving $q_{nx}T_{2n}$ survives in Eq. (52). Using the relation

$$\int_{0}^{\infty} dT_{2n} T_{2n} e^{-\delta T_{2n}} \sum_{\mathbf{k}} \left[f(\varepsilon_{\mathbf{k}+\mathbf{q}_{n}}) - f(\varepsilon_{\mathbf{k}}) \right] e^{i\omega_{\mathbf{k},\mathbf{q}_{n}} T_{2n}} G_{\mathbf{k}}^{(n)} = \pi i \sum_{\mathbf{k}} \frac{df}{d\varepsilon_{\mathbf{k}}} \delta(\varepsilon_{\mathbf{k}+\mathbf{q}_{n}} - \varepsilon_{\mathbf{k}}) G_{\mathbf{k}}^{(n)} , \qquad (B5)$$

Eq. (52) can be rewritten

$$g_{2n+1}(\delta) = 2\pi (-1)^n \frac{N_i^n}{M} \rho_i(\delta) \frac{\lambda^{2n}}{\delta^n} \\ \times \sum_{\mathbf{q}_1, \dots, \mathbf{q}_n} |\phi(q_1)|^2 \cdots |\phi(q_n)|^2 q_{1x} q_{nx} \\ \times \sum_{\mathbf{k}} \frac{df}{d\varepsilon_{\mathbf{k}}} \delta(\varepsilon_{\mathbf{k}+\mathbf{q}_n} - \varepsilon_{\mathbf{k}}) \int_0^\infty dT_2 \int_0^\infty dT_4 \cdots \int_0^\infty dT_{2n-2} e^{-\delta T_2} e^{-\delta T_4} \cdots e^{-\delta T_{2n-2}} G_{\mathbf{k}}^{(n)} .$$
(B6)

Comparison of this result with Eq. (B1) for $g_1^{(2m+2)}(\delta)$ reveals that

3002

$$g_{2n+1}(\delta) = (-1)^{n+1} \frac{\lambda^{2n}}{\delta^n} \rho_i(\delta) \left\langle \left[\frac{1}{\tau} \right]^n \right\rangle,$$

as stated in Eq. (53).

APPENDIX C

In this Appendix, I show that higher-order terms in an expansion of $\hat{\rho}_r(t)$ in Eq. (47) for $g_{n\geq 2}(t)$ are suppressed by powers of δ compared with the dominant contributions. Consider, for example, the 2*m*th-order term in the expansion of $\hat{\rho}_r(t)$. Only even powers are used so that the internal momenta of the correlation function can be paired. The contribution of this term is

$$g_{2n+1,2m}(\delta) \propto \delta N_{i}^{n+m} \sum_{\mathbf{q}_{1},\dots,\mathbf{q}_{n+m}} |\phi(q_{1})|^{2} \cdots |\phi(q_{n+m})|^{2} q_{1x}$$

$$\times \int_{0}^{\infty} dt_{1} \int_{0}^{\infty} dt_{2} \cdots \int_{0}^{\infty} dt_{2(n+m)+1} e^{-\delta T_{2}} e^{-\delta T_{3}} \cdots e^{-\delta T_{2(n+m)+1}} e^{-\delta t_{2(n+m)+1}}$$

$$\times \rho_{i}(t_{2n+1})(q_{1x}T_{2}+q_{2x}T_{4}+\cdots+q_{nx}T_{2n})\Theta(T_{2n+1})\Theta(T_{2n+2})$$

$$\times \Pi^{(n+m)}(\mathbf{q}_{1},\mathbf{q}_{2},\dots,\mathbf{q}_{n+m};T_{2},T_{3},\dots,T_{2n},t_{2n}-t_{2n+2},T_{2n+3},T_{2n+4},\dots,T_{2(n+m)+1}). \quad (C1)$$

To lowest order in δ ,

$$\delta \int_0^\infty dt_{2n+1} \rho_i(t_{2n+1}) e^{-\delta(t_{2n+1}-t_{2n+2})} \Theta(t_{2n+1}-t_{2n+2}) = \rho_i(\delta) .$$
(C2)

It can be shown that higher-order terms in δ , proportional to $(\delta t_{2n+2})^r \rho_i(\delta)$, will also suppress the divergent contributions from $g_{n\geq 2}(\delta)$. Shifting indices and considering only the lowest-order term in δ , I find that

$$g_{2n+1,2m}(\delta) \propto \rho_{i}(\delta) N_{i}^{n+m} \frac{\lambda^{2(n+m)}}{\delta^{n+m}} \\ \times \sum_{\mathbf{q}_{1}, \dots, \mathbf{q}_{n+m}} |\phi(q_{1})|^{2} \cdots |\phi(q_{n+m})|^{2} q_{1x} \\ \times \int_{0}^{\infty} dT_{2} \int_{0}^{\infty} dT_{4} \cdots \int_{0}^{\infty} dT_{2(n+m)} e^{-\delta T_{2}} e^{-\delta T_{4}} \cdots e^{-\delta T_{2(n+m)}} \\ \times (q_{1x} T_{2} + q_{2x} T_{4} + \cdots + q_{nx} T_{2n}) \\ \times \sum_{\mathbf{k}} [f(\varepsilon_{\mathbf{k}+\mathbf{q}_{n+m}}) - f(\varepsilon_{\mathbf{k}})] G_{\mathbf{k}}^{(n+m)} e^{i\omega_{\mathbf{k},\mathbf{q}_{n+m}} T_{2(n+m)}} .$$
(C3)

But, after performing the time integral, it can be shown that

$$\sum_{\mathbf{q}_{n+m}} |\phi(q_{n+m})|^2 \sum_{\mathbf{k}} \int_0^\infty dT_{2(n+m)} e^{-\delta T_{2(n+m)}} e^{i\omega_{\mathbf{k},\mathbf{q}_{n+m}} T_{2(n+m)}} [f(\varepsilon_{\mathbf{k}+\mathbf{q}_{n+m}}) - f(\varepsilon_{\mathbf{k}})] G_{\mathbf{k}}^{(n+m)} \propto \delta .$$
(C4)

Therefore, $g_{2n+1,2m}(\delta)$ (m > 0) is suppressed by at least one factor of δ compared to $(\lambda^2/\delta)^{n+m}$. In the first limit $(\lambda \rightarrow 0, \delta \rightarrow 0^+; \lambda^2/\delta \neq 0)$, this term will vanish. Therefore, only the lowest-order term in the expansion of $\hat{\rho}_r(t)$ needs to be considered.

- ¹N. J. M. Horing, X. L. Lei, and H. L. Cui, Phys. Rev. B **33**, 6929 (1986).
- ²R. Kubo, M. Toda, and N. Hashitsume, *Statistical Physics II* (Springer, New York, 1985).
- ³G. D. Mahan, *Many Particle Physics* (Plenum, New York, 1981).
- ⁴C. S. Ting, S. Ying, and J. J. Quinn, Phys. Rev. Lett. **37**, 215 (1976).
- ⁵W. Y. Lai and C. S. Ting, Phys. Rev. B 24, 7206 (1981).
- ⁶X. L. Lei and C. S. Ting, Phys. Rev. B **30**, 4809 (1984); J. Phys. C **18**, 77 (1985); Phys. Rev. B **32**, 1112 (1985).
- ⁷W. Cai, X. L. Lei, and C. S. Ting, Phys. Rev. B **31**, 4070 (1985).
- ⁸X. L. Lei, J. Birman, and C. S. Ting, J. Appl. Phys. 58, 2270

(1985).

- ⁹C. S. Ting and T. Nee, Phys. Rev. B 33, 7056 (1986).
- ¹⁰D. Y. Xing and C. S. Ting, Phys. Rev. B **35**, 3971 (1987).
- ¹¹Z. B. Su, L. Y. Chen, and J. L. Birman, Phys. Rev. B **35**, 9744 (1987).
- ¹²X. L. Lei, D. Y. Xing, M. Liu, C. S. Ting, and J. L. Birman, Phys. Rev. B 36, 9134 (1987).
- ¹³H. L. Cui, X. L. Lei, and N. J. M. Horing, Phys. Rev. B 37, 8223 (1988).
- ¹⁴D. Y. Xing, M. Liu, and C. S. Ting, Phys. Rev. B 37, 10283 (1988).
- ¹⁵X. L. Lei, J. Cai, and L. M. Xie, Phys. Rev. B 38, 1529 (1988).
- ¹⁶L. van Hove, Physica (Utrecht) **21**, 517 (1955).

<u>39</u>

(**B7**)

- ¹⁸V. Kenkre and M. Dresden, Phys. Rev. A 6, 769 (1972); V. Kenkre, *ibid.* 7, 772 (1973).
- ¹⁹M. Huberman and G. V. Chester, Adv. Phys. 24, 489 (1975).
- ²⁰J. W. Wu and G. D. Madan, Phys. Rev. B 29, 1769 (1984).
- ²¹S. F. Edwards, Proc. Phys. Soc. 86, 977 (1965).
- ²²W. G. Chambers, J. Phys. C 6, 2586 (1973).
- ²³P. N. Argyres and J. L. Sigel, Phys. Rev. Lett. **31**, 1397 (1973); Phys. Rev. B **9**, 3197 (1974).
- ²⁴R. S. Fishman and G. D. Mahan, preceding paper, Phys. Rev. B 39, 2990 (1989).
- ²⁵D. N. Zubarev, Nonequilibrium Statistical Thermodynamics (Plenum, New York, 1974).

- ²⁶See, for example, S. Doniach and E. H. Sondheimer, in Green's Functions for Solid State Physicists (Benjamin, Reading, 1974), Chap. 5.
- ²⁷W. Kohn and J. M. Luttinger, Phys. Rev. 108, 590 (1957).
- ²⁸A. M. Tremblay, B. Patton, P. C. Martin, and P. F. Maldague, Phys. Rev. A **19**, 1721 (1979).
- ²⁹G. Y. Hu and R. F. O'Connell, Phys. Rev. B 36, 5798 (1987); Physica A 149A, 1 (1988); Phys. Rev. B 38, 1721 (1988).
- ³⁰P. N. Argyres, this issue, Phys. Rev. B **39**, 2982 (1989).
- ³¹F. M. Peeters and J. T. Devreese, Phys. Status Solidi B 115, 539 (1983).
- ³²D. L. Cox, C. Tannous, and J. W. Wilkins, Phys. Rev. B 33, 2132 (1986).