Force-balance theory of resistivity

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The recently proposed force-balance theory of resistivity is examined critically in the context of a simple model. It is shown that this theory's basic formula, when evaluated correctly, yields in general a vanishing resistivity. This renders this theory untenable.

I. INTRODUCTION

There has recently been renewed interest in the theory of transport properties of solids, especially in the regime of nonlinear response to an electric field. [1,2] For the case of linear response the theory of Kubo and others [3–6] has given the generally accepted standard formula for the conductivity σ. The evaluation[7–17] of this formula, however, presents considerable difficulty even in the case of weak scattering due to the imperfections. This is due to the fact that σ is of order λ^{-2}, where λ denotes the strength of the scattering interaction. Specifically, the evaluation of σ requires the summation of an infinite number of appropriate terms (or diagrams) and it results in an integral equation for the steady-state distribution function, similar to the semiclassical Boltzmann transport equation[18,19] in the simplest cases. A different method of evaluation, the method of kinetic equations,[20–26] leads more simply to identical integral equations.

Because of this difficulty, a number of different formulations[27–31] have been proposed which give explicit expression for the resistivity $\rho=\sigma^{-1}$, rather than the conductivity σ. These were expected to be easier to evaluate for small λ, because ρ is of order λ^2 and thus, it was thought, it was necessary to evaluate only the first nonvanishing term in the expansion of ρ in powers of λ. If correct, these formulations would have been of extreme practical usefulness. However, all of them have been shown[32–34] to be in error. If correctly evaluated, they too require the summation of an infinite number of appropriate terms even for small λ. The physical results are identical to those of the standard theory[3–26] for σ, as they should be, since both formulations evaluate the same physical quantity, i.e., the adiabatic conductivity σ or its inverse ρ.

Recently a new formulation has been proposed, the force-balance theory,[35–41] for the linear and nonlinear resistivity ρ. It is claimed to have a simple mathematical structure for small λ, and many applications have been reported to complicated systems that involve electron-electron, electron-impurity, and electron-phonon scattering. This theory is *not* mathematically equivalent to the standard theory[3–6] in the case of linear response. It has been stated[38] that it represents the *isothermal* resistivity (linear and nonlinear).

In order to examine critically this new theory, we consider here for simplicity the case of independent electrons and scattering only by fixed impurities. This case (including electron-electron interaction) has been considered in detail by the authors[36,38] of this theory. We are going to accept, for the sake of argument, all explicit and implicit assumptions in the formulation of this theory, and we shall concentrate only on the *evaluation* of the formula for the resistivity that this theory produces. We shall show that the correct evaluation of ρ according to this theory requires the summation of an infinite number of appropriate terms even for small λ. Furthermore, it will be shown that such a calculation gives a resistivity (linear and nonlinear) equal in general to zero for small λ. Finally, it is shown that $\rho=0$ even for arbitrary λ, in general. On the basis of this result it is clear that any discussion of the physical basis of this formulation, *as it has been presented so far,* is unnecessary.

In the following section we present a succinct formulation of this new theory for the simple system of independent electrons with electron-impurity scattering, which forms the basis of our considerations. The resulting formula for ρ is evaluated "simply" up to order λ^2 and it constitutes the main result of this theory.[36–38] In Sec. III we examine the formula for ρ critically after rewriting it in a more convenient form, and we evaluate it correctly for small λ. We find it to give $\rho=0$, in general. We point out that the same argument gives $\rho=0$ for all λ, in general. We conclude with a brief discussion.

II. THE FORCE-BALANCE EQUATION FOR RESISTIVITY

We present here briefly the new theory[35–38] of resistivity (linear and nonlinear) in the simplest case of a system of N independent electrons in N_i random impurities driven by a homogeneous electric field $\mathbf{E}$.

The Hamiltonian of the system is

$$H_T=\sum_{i=1}^{N}[H(\mathbf{p}_i,\mathbf{r}_i)-e\mathbf{E}\cdot\mathbf{r}_i]\,, \tag{2.1}$$

where

$$H(\mathbf{p},\mathbf{r})=H_0+V=\frac{\mathbf{p}^2}{2m}+V(\mathbf{r})=\frac{\mathbf{p}^2}{2m}+\sum_{a}^{N_i}u(\mathbf{r}-\mathbf{r}_a) \tag{2.2}$$

and $u(\mathbf{r}-\mathbf{r}_a)$ is the electron-impurity potential centered at $\mathbf{r}_a$. The central point for this formalism is the intro-

duction of the variables for the center of mass (c.m.), $\mathbf{R},\mathbf{P}$, and for the relative electrons, $\mathbf{r}_i',\mathbf{p}_i'$, namely

$$\mathbf{R}=(1/N)\sum_i \mathbf{r}_i,\quad \mathbf{P}=\sum_i \mathbf{p}_i \tag{2.3}$$

$$\mathbf{r}_i'=\mathbf{r}_i-\mathbf{R},\quad \mathbf{p}_i'=\mathbf{p}_i-(1/N)\mathbf{P}\ , \tag{2.4}$$

which satisfy canonical commutation relations (we take $\hbar=1$)

$$[R_\alpha, P_\beta]=i\delta_{\alpha\beta} \tag{2.5}$$

$$[r_{i\alpha}', p_{j\beta}']=i\delta_{\alpha\beta}(\delta_{ij}-1/N)\cong i\delta_{\alpha\beta}\delta_{ij}\ , \tag{2.6}$$

while $(\mathbf{P},\mathbf{R})$ commute with $(\mathbf{p}_i',\mathbf{r}_i')$. Thus

$$H_T=H_c+H_e+H_{ei}\ , \tag{2.7}$$

where

$$H_c=\frac{\mathbf{P}^2}{2M}-Ne\mathbf{E}\cdot\mathbf{R}\ , \tag{2.8}$$

$$H_e=\sum_i \frac{(\mathbf{p}_i')^2}{2m}=\sum_{\mu\nu}(H_o)_{\mu\nu}c_\mu^\dagger c_\nu\ , \tag{2.9}$$

$$H_{ei}=\sum_i V(\mathbf{r}_i'+\mathbf{R})=\sum_{\mu,\nu}[V(\mathbf{R})]_{\mu\nu}c_\mu^\dagger c_\nu\ . \tag{2.10}$$

Here H_c represents the motion of the c.m. as an effective particle of mass $M=Nm$ driven by the field and H_e describes the system of relative electrons taken as unconstrained fermions, with $c_\mu^\dagger$ and c_ν being the creation and annihilation operators for the arbitrary one-electron states $|\mu\rangle$ and $|\nu\rangle$, respectively. H_{ei} gives the coupling between these two subsystems due to the electron-impurity interaction. The operator for the total force on the electrons is, according to (2.7)–(2.10),

$$\dot{\mathbf{P}}=-i[\mathbf{P},H_T]=Ne\mathbf{E}+\mathbf{F}_T(\mathbf{R})\ , \tag{2.11}$$

where

$$\mathbf{F}_T(\mathbf{R})=-\frac{\partial}{\partial\mathbf{R}}\sum_i V(\mathbf{r}_i'+\mathbf{R})=\sum_i \mathbf{F}(\mathbf{r}_i'+\mathbf{R})$$
$$=\sum_{\mu,\nu}[\mathbf{F}(\mathbf{R})]_{\mu\nu}c_\mu^\dagger c_\nu \tag{2.12}$$

and

$$\mathbf{F}(\mathbf{r}')=-\frac{\partial V(\mathbf{r}')}{\partial\mathbf{r}'} \tag{2.13a}$$

is the operator for the force on a relative electron due to the impurities, while

$$\mathbf{F}(\mathbf{R})=\mathbf{F}(\mathbf{r}'+\mathbf{R})\ . \tag{2.13b}$$

For the time development of the system it is assumed that the c.m., due to its enormous mass $M=Nm$, behaves like a classical system and thus $\mathbf{R}(t)$ becomes a time-dependent c number. It is then taken that the subsystem of relative electrons evolves in time under the influence of a t-dependent Hamiltonian

$$H_e+H_{ei}(t)=\sum_{\mu,\nu}[H_0+V(\mathbf{R}(t))]_{\mu\nu}c_\nu^\dagger c_\nu\ , \tag{2.14}$$

where

$$V(\mathbf{R})=V(\mathbf{r}'+\mathbf{R})\ . \tag{2.14a}$$

Thus its density matrix $\rho(t)$ satisfies the Liouville equation

$$i\frac{d}{dt}\rho(t)=[H_e+H_{ei}(t),\rho(t)]\ . \tag{2.15}$$

Now it is assumed that the steady state is described by the solution of (2.15) in the limit $t\to\infty$ with the initial condition[42]

$$\rho(0)=e^{-\beta(H_e-\mu N)}/\mathrm{Tr}e^{-\beta(H_e-\mu N)} \tag{2.16}$$

while

$$\mathbf{R}(t)=\mathbf{v}t+\mathbf{R}_0 \tag{2.17}$$

and H_{ei} is turned on adiabatically. Here $\mathbf{v}$ is the constant velocity of the c.m. in the steady state. It is determined by the condition that the average of the total force (2.11) in the steady state vanishes, i.e., by the force-balance equation

$$Ne\mathbf{E}+\mathbf{D}=0\ , \tag{2.18}$$

where

$$\mathbf{D}=\lim_{t\to\infty}\mathrm{Tr}\{\mathbf{F}_T(\mathbf{R}(t))\rho(t)\}=\mathbf{D}(\mathbf{v})\ , \tag{2.19}$$

with $\mathbf{R}(t)$ given by (2.17) in (2.12), (2.14), and (2.15). Tr denotes the trace in the space of the many relative electrons and it includes the ensemble average over the random impurity centers $\{\mathbf{r}_a\}$. From (2.18), $\mathbf{v}$ is determined in terms of $\mathbf{E}$ and thus the electric resistivity (nonlinear) in the simple case of an isotropic system is

$$\rho=\frac{E}{Nev}=-\frac{D(v)}{(Ne)^2v}\ , \tag{2.20}$$

where all vector quantities are in the direction of $\mathbf{E}$.

Thus, the quantity $\mathbf{D}$, defined by (2.19) and (2.14)–(2.17), is the basic formula of this theory, as it determines through (2.20) the resistivity (linear and nonlinear).

Now, the simplicity in mathematical structure which is the most important aspect of the present method, according to the authors,[37] arises from the expectation that the evaluation of $\mathbf{D}$, Eq. (2.19), for weak electron-impurity interaction is simple. Specifically, if λ denotes the strength of the impurity interaction V and

$$\mathbf{D}=\sum_{n=2}^{\infty}\lambda^n\mathbf{D}_n\ , \tag{2.21}$$

$$\rho(t)=\sum_{n=0}^{\infty}\lambda^n\rho_n(t)\ , \tag{2.22}$$

it is taken[36–38] that

$$\mathbf{D}_2=\lim_{t\to\infty}\mathrm{Tr}\{\mathbf{F}_T(\mathbf{R}(t))\rho_1(t)\}\ , \tag{2.23}$$

where

$$\rho_1(t)=\frac{1}{i}\int_0^t dt'\, e^{iH_e(t'-t)}[H_{ei}(t'),\rho(0)]e^{-iH_e(t'-t)}, \tag{2.24}$$

since $\mathbf{F}_T$ is of order λ. It is clear that $\rho_0(t)=\rho(0)$ and $\mathbf{D}_0=\mathbf{D}_1=0$.

From (2.23) and (2.24), $\mathbf{D}_2(\mathbf{v})$ is found to be, when $|\mu\rangle$ is taken as the plane-wave representation $|\mathbf{k}\sigma\rangle$,

$$\mathbf{D}_2(\mathbf{v})=\lim_{\varepsilon\to 0^+}(-i)N_i\sum_{\mathbf{q}}\mathbf{q}|u(\mathbf{q})|^2 2\sum_{k}\frac{f_o(\varepsilon_{k+q})-f_0(\varepsilon_k)}{i\varepsilon+\varepsilon'_{k+q}-\varepsilon'_k}$$
$$=2\sum_k f_0(\varepsilon_k)\sum_{k'}W_{kk'}(\mathbf{k}'-\mathbf{k}), \tag{2.25}$$

where

$$W_{kk'}=2\pi\langle|V_{kk'}|^2\rangle\delta(\varepsilon'_k-\varepsilon'_{k'}) \tag{2.26}$$

with $\langle\ \rangle$ denoting the impurity average,

$$\varepsilon'_k=\varepsilon_k+\mathbf{v}\cdot\mathbf{k}=k^2/2m+\mathbf{v}\cdot\mathbf{k}, \tag{2.27}$$

$f_0(\varepsilon)$ is the Fermi-Dirac distribution function and $u(\mathbf{q})$ is the Fourier transform of the single impurity potential $u(\mathbf{r})$ of (2.2). This is the result of Refs. 36 and 38 where the impurity scattering was considered in detail.

III. EVALUATION OF D

We show here that the proposed expression (2.23) for $\mathbf{D}_2$, and thus the resistivity up to order λ^2, is in error. We prove that a correct evaluation of (2.19) yields $\mathbf{D}=0$, and thus zero resistivity, in general.

We first simplify the mathematical structure of this theory, taking advantage of the fact that we are not considering electron-electron or electron-phonon interactions. Thus from (2.12) we see that $\mathbf{D}$ of (2.19) can be written in terms of the one-electron density operator

$$f(t)_{\mu\nu}=\mathrm{Tr}\{c_\mu\rho(t)c_\nu^\dagger\} \tag{3.1}$$

(without the impurity average), namely

$$\mathbf{D}=\lim_{t\to\infty}\mathrm{tr}\{\mathbf{F}(\mathbf{r}+\mathbf{R}(t))f(t)\}. \tag{3.2}$$

Here tr is the trace over the one-electron free-particle states $|\mathbf{k}\sigma\rangle$ with periodic boundary conditions and it includes the impurity average, while $\mathbf{F}(\mathbf{r})$, given by (2.13), is the operator for the force on an electron due to the impurities and $\mathbf{R}(t)$ is given by (2.17). From (3.1), (2.15) and (2.16) we have the Liouville equation for $f(t)$:

$$i\frac{d}{dt}f(t)=[H_0+V(\mathbf{r}+\mathbf{R}(t)),f(t)], \tag{3.3}$$

$$f(0)=f_0(H_0)=[e^{\beta(H_0-\mu)}+1]^{-1}, \tag{3.4}$$

where, as in (2.9), $H_0=\mathbf{p}^2/2m$, and $\mathbf{p},\mathbf{r}$ now refer to the relative electron. Since now

$$\mathbf{F}(\mathbf{r}+\mathbf{R})=e^{i\mathbf{p}\cdot\mathbf{R}}\mathbf{F}(\mathbf{r})e^{-i\mathbf{p}\cdot\mathbf{R}} \tag{3.5}$$

and similarly for $V(\mathbf{r}+\mathbf{R})$, we have from (3.2)

$$\mathbf{D}=\lim_{t\to\infty}\mathrm{tr}\{\mathbf{F}g(t)\} \tag{3.6}$$

where

$$g(t)=e^{-i\mathbf{p}\cdot\mathbf{R}(t)}f(t)e^{i\mathbf{p}\cdot\mathbf{R}(t)} \tag{3.7}$$

and $\mathbf{F}=\mathbf{F}(\mathbf{r})=-\partial V(\mathbf{r})/\partial\mathbf{r}$. From (3.3), (3.4), and (3.7) we get for $g(t)$

$$i\frac{d}{dt}g(t)=[H',g(t)]=L'g(t) \tag{3.8}$$

$$g(0)=f_0(H_0), \tag{3.9}$$

where, since $d\mathbf{R}/dt=\mathbf{v}$,

$$H'=H_0+\mathbf{v}\cdot\mathbf{p}+V(\mathbf{r})=H'_0+V(\mathbf{r}) \tag{3.10}$$

and correspondingly

$$L'=L'_0+L_1,\quad L'_0X=[H'_0,X],\quad L_1X=[V,X]. \tag{3.11}$$

In order to find the limit of $g(t)$ for $t\to\infty$, it proves convenient[21,33,34] to introduce the Laplace average

$$\hat{g}(\varepsilon)=\varepsilon\int_0^\infty e^{-\varepsilon t}g(t)dt \tag{3.12}$$

with ε a positive number. Now if $\lim_{t\to\infty}g(t)$ exists we have[21,33,34] for the steady state

$$\lim_{t\to\infty}g(t)=\lim_{\varepsilon\to 0^+}\hat{g}(\varepsilon). \tag{3.13}$$

From (3.12), (3.8), and (3.9) we find that $\hat{g}(\varepsilon)$ is given by the compact but convenient expression

$$\hat{g}(\varepsilon)=i\varepsilon(i\varepsilon-L')^{-1}f_0(H_0). \tag{3.14}$$

From (3.6), (3.13), and (3.14) we have

$$\mathbf{D}=\lim_{\varepsilon\to 0^+}\mathbf{D}(\varepsilon), \tag{3.15}$$

where

$$\mathbf{D}(\varepsilon)=\mathrm{tr}\{\mathbf{F}i\varepsilon(i\varepsilon-L')^{-1}f_0(H_0)\}. \tag{3.16}$$

Or, since

$$i\varepsilon(i\varepsilon-L')^{-1}=1+(i\varepsilon-L')^{-1}L', \tag{3.17}$$

we have equivalently

$$\mathbf{D}(\varepsilon)=\mathrm{tr}\{\mathbf{F}(i\varepsilon-L')^{-1}L_1f_0\}, \tag{3.18}$$

since $\mathrm{tr}\{\mathbf{F}f_0\}=0$ and $L'_0f_0=0$. Furthermore, since

$$\mathbf{F}=-\frac{\partial V(\mathbf{r})}{\partial\mathbf{r}}=iL_1\mathbf{p}, \tag{3.19}$$

we get

$$\mathbf{D}(\varepsilon)=i\,\mathrm{tr}\{(L_1\mathbf{p})(i\varepsilon-L')^{-1}L_1f_0\}. \tag{3.20}$$

Finally, since $\mathrm{tr}\{AB\}=\mathrm{tr}\{BA\}$ and

$$\mathrm{tr}\{A(i\varepsilon-L')^{-1}B\}=\mathrm{tr}\{B(i\varepsilon+L')^{-1}A\}, \tag{3.21}$$

we have the convenient expression

$$\mathbf{D}(\varepsilon)=-i\,\mathrm{tr}\{f_0L_1G(i\varepsilon)L_1\mathbf{p}\}, \tag{3.22}$$

where

$$G(i\varepsilon)=(i\varepsilon+L')^{-1}. \tag{3.22a}$$

From this we can generate easily an expansion of $\mathbf{D}(\varepsilon)$ in powers of λ, i.e.,

$$\mathbf{D}(\varepsilon)=\sum_{n=2}^{\infty}\lambda^n\mathbf{D}_n(\varepsilon)\ , \tag{3.23}$$

since

$$G(i\varepsilon)=(i\varepsilon+L_0'+L_1)^{-1}$$
$$=\sum_{n=0}^{\infty}(-1)^n[G_0(i\varepsilon)L_1]^nG_0(i\varepsilon)\ , \tag{3.24}$$

where

$$G_0(i\varepsilon)=(i\varepsilon+L_0')^{-1}\ . \tag{3.25}$$

Thus we have

$$\mathbf{D}_2(\varepsilon)=-i\ \mathrm{tr}\{f_0L_1G_0(i\varepsilon)L_1\mathbf{p}\}\ . \tag{3.26}$$

If we now take, with the authors of the force-balance theory,[36-38] as in (2.23),

$$\mathbf{D}_2=\lim_{\varepsilon\to0^+}\mathbf{D}_2(\varepsilon)\ , \tag{3.27}$$

we obtain from (3.26) simply

$$\mathbf{D}_2=2\sum_k f_0(\varepsilon_k)\sum_{k'}W_{kk'}(\mathbf{k}'-\mathbf{k}) \tag{3.28}$$

which is identical, of course, to (2.25).

But we now prove that such a procedure is erroneous. The error lies in the fact that expansion (3.23) of $\mathbf{D}(\varepsilon)$ in powers of λ is invalid in the limit $\varepsilon\to0^+$, since there are terms of order λ^n $(n\geq3)$ that diverge as $\varepsilon\to0^+$. These divergent terms appear whenever, in expansion (3.24), $G_0(i\varepsilon)$ operates on the part X_d of any operator X that is diagonal in the plane-wave representation $|k\rangle$, which diagonalizes $H_0'=H_0+\mathbf{v}\cdot\mathbf{p}$. For then

$$[G_0(i\varepsilon)X_d]_{kk'}=\frac{1}{i\varepsilon}X_{kk}\delta_{kk'}\ , \tag{3.29}$$

and thus such terms diverge as $\varepsilon\to0^+$. By contrast we note that for the nondiagonal part X_{nd} of X,

$$[G_0(i\varepsilon)X_{nd}]_{kk'}=(i\varepsilon-\varepsilon_k'+\varepsilon_{k'}')^{-1}X_{kk'}\quad(k'\neq k) \tag{3.30}$$

presents no divergence as $\varepsilon\to0^+$, since when the thermodynamic limit is taken first (in order to avoid the Poincaré cycle) this becomes

$$[G_0(i\varepsilon)X_{nd}]_{kk'}\longrightarrow-[(\varepsilon_k'-\varepsilon_k')_p^{-1}+i\pi\delta(\varepsilon_k'-\varepsilon_{k'}')]X_{kk'}$$
$$\text{as }\varepsilon\to0^+\quad(k'\neq k)\ . \tag{3.31}$$

Thus the procedure of keeping only the term of the lowest order in λ in the expansion of $\mathbf{D}(\varepsilon)$ in order to obtain the corresponding term of $\mathbf{D}$ in the limit $\varepsilon\to0^+$ is invalid. Instead, we must sum the infinite subset of terms in the expansion of $\mathbf{D}(\varepsilon)$ that are of the form $(\lambda^2/i\varepsilon)^n(n\geq1)$. These are the dominant terms for sufficiently small λ. In other words, evaluating $\mathbf{D}_2$ as

$$\mathbf{D}_2=\lim_{\varepsilon\to0^+}\lim_{\lambda\to0}[\lambda^{-2}\mathbf{D}(\varepsilon)]\ , \tag{3.32}$$

as it was done in (3.26) and (3.27), is *incorrect.* The correct way is

$$\mathbf{D}_{2c}=\lim_{\lambda\to0}\lim_{\varepsilon\to0^+}[\lambda^{-2}\mathbf{D}(\varepsilon)]\ . \tag{3.33}$$

This is equivalent to the "λ^2t limit" technique of van Hove[34] which gives

$$\mathbf{D}_{2c}=\lim_{\lambda^2/\varepsilon\to\infty}\lim_{\substack{\lambda\to0,\varepsilon\to0\\(\lambda^2/\varepsilon\neq0)}}[\lambda^{-2}\mathbf{D}(\varepsilon)]\ . \tag{3.34}$$

The physical basis of this limiting procedure has been discussed by van Hove,[43] Argyres and Sigel[32,33], and Huberman and Chester,[34] and it amounts to the technique of Argyres and Sigel[32-34] we mentioned above. It is important to point out that it is this procedure that has been used[7-17] in the evaluation of the Kubo formula for the linear conductivity for this system. We now extend the technique of Argyres and Sigel[32,33] to obtain the correct evaluation of $\mathbf{D}$. In the Appendix we show that the same technique yields the standard result for the evaluation of the Kubo formula for σ. In fact, it does so much more simply than the earlier derivations,[7-17] which are quite lengthy.

The isolation of the divergent terms of $\mathbf{D}(\varepsilon)$ is greatly facilitated with the introduction of the operator Δ that projects the diagonal part X_d of X, i.e.,

$$(\Delta X)_{kk'}=X_{kk}\delta_{kk'}\ . \tag{3.35}$$

The projection operator for the nondiagonal part of X is then $\Delta'=1-\Delta$, with the obvious properties $\Delta^2=\Delta$, $\Delta'^2=\Delta'$, $\Delta\Delta'=\Delta'\Delta=0$. The divergent terms now arise whenever $G_0(i\varepsilon)$ operates on a diagonal operator, since, as we saw in (3.29),

$$G_0(i\varepsilon)\Delta=\frac{1}{i\varepsilon}\Delta\ , \tag{3.36}$$

whereas $G_0(i\varepsilon)\Delta'$ yields regular terms according to (3.30). Thus it is convenient *not* to use expansion (3.24) of $G(i\varepsilon)$ in powers of L_1, but rather to expand $G(i\varepsilon)$ in powers of ΔL_1. We have

$$G(i\varepsilon)=(i\varepsilon+L_0'+\Delta'L_1+\Delta L_1)^{-1}$$
$$=\sum_{n=0}^{\infty}(-1)^n[G'(i\varepsilon)\Delta L_1\Delta']^nG'(i\varepsilon)\ , \tag{3.37}$$

where

$$G'(i\varepsilon)=(i\varepsilon+L_0'+\Delta'L_1)^{-1}$$
$$=G_0(i\varepsilon)-G_0(i\varepsilon)\Delta'L_1G_0(i\varepsilon)+\cdots \tag{3.38}$$

and we made use of the fact $\Delta L_1\Delta=0$. We note that $G'(i\varepsilon)\Delta'$ has no divergent terms, whereas $G'(i\varepsilon)\Delta$ does have divergent terms with a *single* $(1/i\varepsilon)$ factor. By a simple rearrangement we can exhibit them by writing

$$G'(i\varepsilon)\Delta=\frac{1}{i\varepsilon}[\Delta+G'(i\varepsilon)\Delta'L_1\Delta] \tag{3.39}$$

from which it follows that

$$\Delta'G'(i\varepsilon)\Delta=\frac{1}{i\varepsilon}\Delta'G'(i\varepsilon)\Delta'L_1\Delta\ . \tag{3.40}$$

Finally, from (3.37) and (3.40) we have

$$\Delta' G(i\varepsilon)\Delta' = \sum_{n=0}^{\infty} \left[\frac{-1}{i\varepsilon}\right]^n [\Delta' G'(i\varepsilon)\Delta' L_1 \Delta L_1 \Delta']^n \times \Delta' G'(i\varepsilon)\Delta' , \tag{3.41}$$

where *all* divergences are exhibited since $G'(i\varepsilon)\Delta'$ has no divergent terms. We now note that the quantity of interest, $\mathbf{D}(\varepsilon)$ of (3.22), when the trace is evaluated in the $|k\rangle$ representation, is

$$\mathbf{D}(\varepsilon) = -i \operatorname{tr}\{f_0 \Delta L_1 \Delta' G(i\varepsilon)\Delta' L_1 \mathbf{p}\} , \tag{3.42}$$

since $\operatorname{tr}\{f_0 X\} = \operatorname{tr}\{f_0 \Delta X\}$ and $\Delta L_1 \mathbf{p} = \mathbf{0}$. Using (3.41) in (3.42) and rearranging the series, we have

$$\mathbf{D}(\varepsilon) = -i \operatorname{tr}\left[f_0 \sum_{n=0}^{\infty} \left[\frac{-1}{i\varepsilon}\right]^n [S(\varepsilon)]^{n+1}\mathbf{p}\right] , \tag{3.43}$$

where

$$S(\varepsilon) = \Delta L_1 \Delta' G'(i\varepsilon)\Delta' L_1 \Delta = \Delta L_1 G'(i\varepsilon) L_1 \Delta , \tag{3.44}$$

since $\Delta L_1 \Delta = 0$. In (3.43) all divergent terms are shown explicitly, since $S(\varepsilon)$ produces no divergencies as $\varepsilon \to 0^+$.

For the evaluation of $\mathbf{D}$ to the lowest order of λ we need all divergent terms of $\mathbf{D}(\varepsilon)$ of the form $(\lambda^2/i\varepsilon)^n$, as we explained earlier. These are obtained from (3.43) and (3.44) by introducing λ and putting $G'(i\varepsilon) \cong G_0(i\varepsilon)$ [from (3.38)] in $S(\varepsilon)$, the neglected terms of (3.38) generating contributions of the form $(\lambda^3/i\varepsilon)^n$, $(\lambda^4/i\varepsilon)^n$, etc. We thus obtain

$$\mathbf{D}(\varepsilon) \cong -i\lambda^2 \operatorname{tr}\left[f_0 \sum_{n=0}^{\infty} \left[\frac{-\lambda^2}{i\varepsilon}\right]^n [S_2(\varepsilon)]^{n+1}\mathbf{p}\right] , \tag{3.45}$$

where

$$S_2(\varepsilon) = \Delta L_1 \Delta' G_0(i\varepsilon)\Delta' L_1 \Delta = \Delta L_1 G_0(i\varepsilon) L_1 \Delta . \tag{3.46}$$

All other terms vanish in the limiting procedure of (3.34). We recall now that the trace in (3.45) includes the ensemble average over the impurity centers, which we now denote explicitly by $\langle\ \rangle$. Because of the randomness of their distribution we find[20] that in the thermodynamic limit $\langle S_2^n \rangle = \langle S_2 \rangle^n$, and thus upon summation of the series

$$\mathbf{D}(\varepsilon) \cong -i\lambda^2 \operatorname{tr}\left[f_0 \left[1 + \frac{\lambda^2}{i\varepsilon}\langle S_2(\varepsilon)\rangle\right]^{-1} \langle S_2(\varepsilon)\rangle \mathbf{p}\right] . \tag{3.47}$$

According to the correct limiting procedure (3.33) or (3.34) for $\mathbf{D}_{2c}$, we thus find from (3.47) that, since $\langle S_2(0^+)\rangle$ exists,

$$\mathbf{D}_{2c} = 0 . \tag{3.48}$$

More explicitly, we have from (3.47)

$$\mathbf{D}_{2c} = \lim_{\varepsilon \to 0^+} \operatorname{tr}[f_0 \mathbf{Q}(\varepsilon)] = 2 \sum_k f_0(\varepsilon_k) \mathbf{Q}_k , \tag{3.49}$$

where $\mathbf{Q}_k = \lim_{\varepsilon \to 0^+} \langle k | \mathbf{Q}(\varepsilon) | k \rangle$ and the diagonal operator $\mathbf{Q}(\varepsilon)$ is determined by

$$[i\varepsilon + \langle S_2(\varepsilon)\rangle]\mathbf{Q}(\varepsilon) = \varepsilon \langle S_2(\varepsilon)\rangle \mathbf{p} , \tag{3.50}$$

or, equivalently, $\mathbf{Q}_k$ is given by the integral equation

$$\sum_{k'} W_{kk'}(\mathbf{Q}_{k'} - \mathbf{Q}_k) = \lim_{\varepsilon \to 0^+} \left[\varepsilon \sum_{k'} W_{kk'}(\mathbf{k}' - \mathbf{k})\right] = 0 , \tag{3.50a}$$

with $W_{kk'}$ given by (2.26). Equation (3.50a) yields, in general,[44] $\mathbf{Q}_k = 0$ and thus (3.48). By contrast, the incorrect procedure (3.32) yields from (3.47)

$$\mathbf{D}_2 = -i \lim_{\varepsilon \to 0^+} \operatorname{tr}\{f_0 \langle S_2(\varepsilon)\rangle \mathbf{p}\} = 2 \sum_k f_0(\varepsilon_k) \sum_{k'} W_{kk'}(\mathbf{k}' - \mathbf{k}) \tag{3.51}$$

which is, of course, identical to the earlier expressions (3.28) and (2.25).

A similar argument shows, in fact, that $\mathbf{D} = \mathbf{0}$ to all order in λ. In the expression (3.43) for $\mathbf{D}(\varepsilon)$, which shows explicitly *all* divergent terms for $\varepsilon \to 0^+$, we note that we have, in the thermodynamic limit for the impurity average, $\langle S^n \rangle = \langle S \rangle^n$. Therefore, from (3.15)

$$\mathbf{D} = \lim_{\varepsilon \to 0^+} (-i) \operatorname{tr}\left[f_0 \left[1 + \frac{1}{i\varepsilon}\langle S(\varepsilon)\rangle\right]^{-1} \langle S(\varepsilon)\rangle \mathbf{p}\right] . \tag{3.52}$$

Since now $\langle S(0^+)\rangle$, given by (3.44), exists, we have as in the previous paragraph that

$$\mathbf{D} = \mathbf{0} . \tag{3.53}$$

Thus, the force-balance theory[35-38] predicts, in general, zero direct-current resistivity (linear and nonlinear), at least for the system of independent electrons in random impurities of arbitrary strength.

IV. DISCUSSION

It has been argued[38] that this force-balance theory gives the *isothermal* resistivity (linear and nonlinear), in contrast to the other expressions[27-31] for the *adiabatic* resistivity (linear), which have been shown[32-34] to be erroneous. As a result, it has been stated[38] that a critical analysis like the one presented above *cannot* in fact be applicable to the force-balance theory. We have not discussed the question whether this theory[36-38] gives the isothermal rather than the adiabatic resistivity. Our point of view has been that whatever the physical meaning of the expression for $\mathbf{D}$ [Eq. (2.19)] is according to this theory, the method of *evaluation* of this quantity is in error. A correct evaluation of $\mathbf{D}$—at least for the case of independent electrons in random impurities—yields in general a vanishing result for the resistivity. Thus a discussion of the physical meaning of ρ as given by Eq. (2.20) becomes superfluous. We conclude that the force-balance theory, as it has been presented so far, is untenable.

Finally, we present an argument which without detailed calculations indicates that $\mathbf{D} = 0$. From (3.6) we see that $\mathbf{D} = \operatorname{tr}\{\mathbf{F} g(t \to \infty)\}$ is the average value of the

force $\mathbf{F}$ of the impurities on an electron for a steady state produced by the Hamiltonian H', Eq. (3.10), starting from the initial condition (3.9). Now we note that equation (3.8) for $g(t)$ can be written equivalently as

$$i\frac{d}{dt}g(t)=\left[\frac{(\mathbf{p}+m\mathbf{v})^2}{2m}+V(\mathbf{r}),\, g(t)\right] . \tag{4.1}$$

If we now carry a gauge transformation

$$g'(t)=e^{im\mathbf{v}\cdot\mathbf{r}}g(t)e^{-im\mathbf{v}\cdot\mathbf{r}} \tag{4.2}$$

we find that

$$i\frac{d}{dt}g'(t)=\left[\frac{\mathbf{p}^2}{2m}+V(\mathbf{r}),\, g'(t)\right]=[H,\, g'(t)] \tag{4.3}$$

and

$$g'(0)=f_0[(\mathbf{p}-m\mathbf{v})^2/2m] \tag{4.4}$$

while

$$\mathbf{D}=\mathrm{tr}\{\mathbf{F}g'(t\to\infty)\} , \tag{4.5}$$

since $\mathbf{F}=\mathbf{F}(\mathbf{r})$. But, according to (4.3) and (4.4), $g'(t\to\infty)$ is the equilibrium value of the one-electron density operator for the independent electrons with total one-electron Hamiltonian $H=H_0+V$ starting from the displaced unperturbed equilibrium distribution (4.4). Since we expect such a system to reach an equilibrium state as $t\to\infty$,[43,45-48] $g'(t\to\infty)$ must be a function of $H=H_0+V$. But, in view of the fact that

$$\mathbf{F}=i[V,\, \mathbf{p}]=i[H,\, \mathbf{p}] , \tag{4.6}$$

we immediately get $\mathbf{D}=-\mathrm{tr}\{[H,\, g'(t\to\infty)]\mathbf{p}\}=\mathbf{0}$. Although clearly this is not a rigorous argument as presented here, it provides an understanding of the result $\mathbf{D}=\mathbf{0}$ on more physical grounds.

Note added in proof. This argument can be genezalized to apply to the more complicated system of electrons and phonons with electron-electron, electron-impurity and electron-phonon interactions.

APPENDIX

We derive here the standard results of the linear response theory for the conductivity of the system under study, Eqs. (2.1) and (2.2), using the technique we developed in Sec. III. This should be compared with the other existing methods[7-17] for the same problem.

For the system of electrons described by Eqs. (2.1) and (2.2) we can write

$$H_T=\sum_{\mu,\nu}(H-e\mathbf{E}\cdot\mathbf{r})_{\mu\nu}c_\mu^\dagger c_\nu , \tag{A1}$$

where $H=H_0+V$ is given by (2.2). The current density is

$$\mathbf{J}_T=\lim_{t\to\infty}\left[\frac{e}{m}\right]\mathrm{Tr}\{\mathbf{P}\rho_T(t)\} , \tag{A2}$$

where

$$\mathbf{P}=\sum_{\mu,\nu}(\mathbf{p})_{\mu\nu}c_\mu^\dagger c_\nu \tag{A3}$$

is the total momentum and $\rho_T(t)$ is the statistical density operator determined by

$$i\frac{d}{dt}\rho_T(t)=[H_T,\, \rho_T(t)] , \tag{A4}$$

$$\rho_T(0)=e^{-\beta(\tilde{H}-\mu\tilde{N})}/\mathrm{Tr}e^{-\beta(\tilde{H}-\mu\tilde{N})} . \tag{A5}$$

Here $\tilde{H}=\sum_{\mu,\nu}H_{\mu\nu}c_\mu^\dagger c_\nu$, $\tilde{N}=\sum_\mu c_\mu^\dagger c_\mu$, and Tr includes the impurity average.

This reduces immediately to a one-electron system, since from (A2) and (A3) we get

$$\mathbf{J}_T=\lim_{t\to\infty}\left[\left[\frac{e}{m}\right]\mathrm{tr}\{\mathbf{p}f_T(t)\}\right] , \tag{A6}$$

where $f_T(t)$ is the one-electron density matrix,

$$[f_T(t)]_{\mu\nu}=\mathrm{Tr}\{c_\mu\rho_T(t)c_\nu^\dagger\} , \tag{A7}$$

and tr is the trace in the space of one-electron operator and includes the impurity average. From (A1), (A4), and (A5) it is easily seen that

$$i\frac{d}{dt}f_T(t)=[H-e\mathbf{E}\cdot\mathbf{r},\, f_T(t)] , \tag{A8}$$

$$f_T(0)=f_0(H)=(e^{\beta(H-\mu)}+1)^{-1} . \tag{A9}$$

For the linear response we get from (A8),

$$f_T(t)=f_0(H)+f(t) , \tag{A10}$$

where

$$i\frac{d}{dt}f(t)=Lf(t)+C=(L_0+L_1)f(t)+C , \tag{A11}$$

$$f(0)=0 , \tag{A12}$$

$$C=-e\mathbf{E}\cdot[\mathbf{r},\, f_0(H)] . \tag{A13}$$

In (A11) we have introduced $LX=[H,X]$, $L_0X=[H_0,X]$, and $L_1X=[V,X]$. The ohmic current density for the steady state is then

$$\mathbf{J}=\lim_{t\to\infty}\left[\left[\frac{e}{m}\right]\mathrm{tr}\{\mathbf{p}f(t)\}\right] . \tag{A14}$$

In order to consider more easily the steady state, we introduce the Laplace average

$$\hat{f}(\varepsilon)=\varepsilon\int_0^\infty dt\, e^{-\varepsilon t}f(t) . \tag{A15}$$

From (A11), (A12), and (A15) we get

$$\hat{f}(\varepsilon)=K(i\varepsilon)C , \tag{A16}$$

where

$$K(i\varepsilon)=(i\varepsilon-L)^{-1} . \tag{A17}$$

Since now $f(t\to\infty)=\hat{f}(\varepsilon\to0^+)$, we have from (A14)

$$\mathbf{J}=\lim_{\varepsilon\to0^+}\left[\frac{e}{m}\right]\mathrm{tr}\{\mathbf{p}\hat{f}(\varepsilon)\}=\lim_{\varepsilon\to0^+}\left[\frac{e}{m}\right]\mathrm{tr}\{\mathbf{p}\Delta K(i\varepsilon)C\} . \tag{A18}$$

In order to evaluate (A18) we expand $K(i\varepsilon)$ and C in powers of V. We note that while

$$C=\sum_{n=0}^{\infty} C_n \ , \tag{A19}$$

$$C_0=-e\mathbf{E}\cdot[\mathbf{r},f_0(H_0)]=(-ie/m)\mathbf{E}\cdot\mathbf{p}f_0'(H_0) \tag{A19a}$$

presents no difficulty,

$$K(i\varepsilon)=\sum_{n=0}^{\infty}[K_0(i\varepsilon)L_1]^nK_0(i\varepsilon) \tag{A20}$$

with

$$K_0(i\varepsilon)=(i\varepsilon-L_0)^{-1} \tag{A21}$$

generates divergent terms such as $\varepsilon\to 0^+$. Specifically, since

$$K_0(i\varepsilon)\Delta=\frac{1}{i\varepsilon}\Delta \ , \tag{A22}$$

such an expansion diverges term by term as $\varepsilon\to 0^+$ and we must sum the divergent terms. In order to carry this out, it is convenient to expand $K(i\varepsilon)$ in powers of ΔL_1, rather than L_1 as in (A20), i.e.,

$$\begin{aligned}K(i\varepsilon)&=(i\varepsilon-L_0-\Delta' L_1-\Delta L_1)^{-1}\\&=\sum_{n=0}^{\infty}[K'(i\varepsilon)\Delta L_1\Delta']^nK'(i\varepsilon) \ ,\end{aligned} \tag{A23}$$

where

$$\begin{aligned}K'(i\varepsilon)&=(i\varepsilon-L_0-\Delta' L_1)^{-1}\\&=K_0(i\varepsilon)+K_0(i\varepsilon)\Delta' L_1K_0(i\varepsilon)+\cdots \ .\end{aligned} \tag{A24}$$

We note that $K'(i\varepsilon)\Delta'$ has no divergent terms, whereas $K'(i\varepsilon)\Delta$ does have divergent terms with a single $(1/i\varepsilon)$ factor, namely

$$K'(i\varepsilon)\Delta=\frac{1}{i\varepsilon}[\Delta+K'(i\varepsilon)\Delta' L_1\Delta] \ . \tag{A25}$$

We thus have

$$\Delta K'(i\varepsilon)\Delta=\frac{1}{i\varepsilon}\Delta \ , \tag{A26}$$

$$\Delta K'(i\varepsilon)\Delta'=0 \ , \tag{A27}$$

$$\Delta' K'(i\varepsilon)\Delta=\frac{1}{i\varepsilon}\Delta' K'(i\varepsilon)\Delta' L_1\Delta \ , \tag{A28}$$

while $\Delta' K'(i\varepsilon)\Delta'$ has no singular terms. Finally, from (A23) and (A26)–(A28) we get, after reorganizing the series,

$$\Delta K(i\varepsilon)\Delta=\frac{1}{i\varepsilon}\sum_{n=0}^{\infty}\left[\frac{1}{i\varepsilon}\right]^n[S(\varepsilon)]^n\Delta \ , \tag{A29}$$

$$\Delta K(i\varepsilon)\Delta'=\frac{1}{i\varepsilon}\sum_{n=0}^{\infty}\left[\frac{1}{i\varepsilon}\right]^n[S(\varepsilon)]^n\Delta L_1\Delta' K'(i\varepsilon)\Delta' \ , \tag{A30}$$

where

$$S(\varepsilon)=\Delta L_1\Delta' K'(i\varepsilon)\Delta' L_1\Delta=\Delta L_1K'(i\varepsilon)L_1\Delta \ . \tag{A31}$$

Taking now the impurity average and noting that $\langle[S(\varepsilon)]^n\rangle=\langle S(\varepsilon)\rangle^n$ and $\langle S(\varepsilon)A\rangle=\langle S(\varepsilon)\rangle\langle A\rangle$ for any operator A in the thermodynamic limit, we have, upon summing the series,

$$\begin{aligned}\langle\Delta K(i\varepsilon)C\rangle&=\Delta\langle K(i\varepsilon)\rangle\Delta\langle C\rangle+\Delta\langle K(i\varepsilon)\Delta' C\rangle\\&=[i\varepsilon-\langle S(\varepsilon)\rangle]^{-1}[\langle\Delta C\rangle+D(\varepsilon)] \ ,\end{aligned} \tag{A32}$$

where

$$D(\varepsilon)=\langle\Delta L_1K'(i\varepsilon)\Delta' C\rangle \ . \tag{A33}$$

Since now $S(\varepsilon),D(\varepsilon)$ have no singular terms as $\varepsilon\to 0^+$, we have from (A18)

$$\mathbf{J}=2\left[\frac{e}{m}\right]\sum_{\mathbf{k}}\mathbf{k}f_k \ , \tag{A34}$$

where $f_k=\langle k|f|k\rangle$ and f is the diagonal operator:

$$f=-\langle S(0^+)\rangle^{-1}[\langle\Delta C\rangle+D(0^+)] \ , \tag{A35}$$

or equivalently

$$\langle S(0^+)\rangle f=-[\langle\Delta C\rangle+D(0^+)] \ . \tag{A36}$$

This is an integral equation for the distribution function f_k. In the lowest order in $\lambda(V\to\lambda V)$, we have clearly that f_k is of order λ^{-2}, and it is given by the standard Boltzmann equation

$$\sum_{k'}w_{kk'}(f_{k'}-f_k)=(e/m)\mathbf{E}\cdot\mathbf{k}f_0'(\varepsilon_k) \ , \tag{A37}$$

where

$$w_{kk'}=2\pi\langle|V_{kk'}|^2\rangle\delta(\varepsilon_k-\varepsilon_{k'}) \ . \tag{A38}$$

All these results can be obtained more simply by the method of kinetic equations.[20–26]

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