Generalized Mobility Theory

MELVIN LAX
Bell Telephone Laboratories, Murray Hill, New Jersey
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A formal theory of mobility is presented that does not depend on the existence of a transport equation. In particular the Hamiltonian describing the electron plus scattering system is not decomposed into an unperturbed part plus a perturbation. Only the applied field is treated as small. Our result is shown to reduce to the usual transport result when the scattering perturbation is weak, without assuming the existence of a relaxation time. Further verification of the validity of our result is obtained by using it to demonstrate a *complex* Nyquist theorem. Mathematical convergence factors introduced in previous theories are shown to arise naturally here by allowing a weak interaction between the electron plus scattering systems and the universe. The relation between a many-electron treatment and the one-electron treatment is demonstrated for the case of Fermi as well as Boltzmann statistics.

1. INTRODUCTION

MANY authors[1] have recognized that the usual transport theory for the mobility of electrons may not be valid if the coupling between the electrons and the lattice vibrations[2] is too strong. In the first place, it will no longer be possible, precisely, to consider the electrons and lattice as *separately* in equilibrium when no fields are present. In the second place, the Boltzmann transport equation may no longer be valid: The usual transport equations deal with probabilities of occupancy of certain states, and not with probability amplitudes, or phases. In other words, after each collision, the electron must lose all phase information before having the next collision.[3] This condition can be obeyed only if the average time between collisions is long compared to the "duration" (i.e., forgetting time) of a single collision.

When the coupling is too strong for the above conditions to be met (e.g., if the time between collisions becomes comparable to the reciprocal of the Debye frequency) one has a complicated many-body problem to solve. The purposes of the present remarks are the following:

1. To call attention to the fact that even though a transport theory for the strong-coupling case does not exist, one can derive a formally correct expression for the mobility by treating only the external field as small as discussed by the authors of reference 1.

2. To indicate enough of the proof of the generalized mobility expression to understand how irreversibility results from a treatment that starts from the reversible Liouville equation.

3. To give a proof, not (I believe) heretofore presented, that the generalized mobility reduces to the usual mobility in the weak-coupling limit—even in case when a relaxation time does not exist.

4. To verify that our result is in agreement with the Nyquist theorem.

2. PERTURBED DENSITY MATRIX

In this section, and the two following, we shall, for simplicity, adopt a one-electron viewpoint. The generalization to a many-electron viewpoint is easy to carry out formally, and is presented in Sec. 5. The density matrix obeys an equation of the form

$$i\partial\rho/\partial t+[\rho, H+V(t)]+i(\rho-\rho_0)/\tau=0 \qquad (2.1)$$

where H is the Hamiltonian of the electron plus the scattering system plus the interaction between the two and V is the interaction with the external applied field. (We have used units in which $\hbar=1$.) The last term represents the fact that the crystal is not isolated but may interact weakly with the surroundings in such a way that in the absence of a field the system approaches the equilibrium density matrix:

$$\rho_0=Z^{-1}\exp(-\beta H)$$
$$\text{or } \rho_0=[1+\exp\beta(H-E_F)]^{-1}=\rho^F, \qquad (2.2)$$

where $\beta=1/(kT)$ and $Z=\text{trace}[\exp(-\beta H)]$. The second form applies when Fermi statistics is necessary and E_F, the Fermi level, is chosen so that trace $\rho^F=N$ = the total number of electrons.

The use of a one-electron viewpoint is equivalent to the assumption of an assembly of electrons that do not interact directly, or indirectly, except through the requirements of the Pauli principle. The fact that correlations introduced by antisymmetry requirements

[1] R. Kubo, Can. J. Phys. **34**, 1274 (1956); M. Lax, Phys. Rev. **100**, 1808 (1955); H. Mori, J. Phys. Soc. Japan **11**, 1029 (1956); H. Nakano, Progr. Theoret. Phys. Japan **15**, 77 (1956); R. P. Feynman (private communication).

[2] The approach to be used in the remainder of this paper is applicable to any scattering mechanism, e.g., impurity scattering (or even the motion of electrons in impurity bands), but we speak of lattice vibrations as the scattering mechanism in order to have a definite physical picture of the problem under discussion.

[3] L. Van Hove has demonstrated in detail, for the case of sufficiently weak coupling, how this phase information is lost, and has in the limit of weak coupling established the validity of the usual (Pauli) transport equation; see Physica **21**, 517 (1955). W. Kohn and J. Luttinger [Phys. Rev. **108**, 590 (1957)] have made the same assumptions as Van Hove and have also demonstrated that validity of the Pauli transport equation in a simple straightforward manner by making legitimate approximations in the density matrix equation. The loss of phase is therefore also demonstrated by Kohn and Luttinger, although in a less direct way than Van Hove's explicit examination of the solution to the density matrix equation.

can be taken into account simply by using ρ^F as the equilibrium density matrix in a one-electron description is established in Sec. 6.

The interaction with the universe is needed to prevent the crystal from heating up indefinitely, if an electric field is applied over an infinite time. It also serves the purpose of damping out oscillatory transients which would otherwise appear in ρ. For calculating conductivity, one needs a solution accurate only to first order in the electric field. To this order, no heating effects occur. Also transients can be circumvented by building up the field from $t=-\infty$ very slowly—by assuming a time dependence of the form $\exp(\alpha t)$ and taking the limit as $\alpha\to 0$. Thus a derivation can be based on the equation with no interactions with the surroundings if handled with care (i.e., first let the electric field $\mathbf{E}$ approach zero, and then let the process become completely adiabatic).

We shall prefer, however, to retain the interaction with the surroundings, as a more physically meaningful viewpoint. The same solution is then obtained as in the case of no interaction with the surroundings, with the mathematical convergence factor $\exp(\alpha t)$ replaced by the physical convergence factor $\exp(t/\tau)$.

If the term in $[\rho,V(t)]$ in (2.1) is regarded as known, Eq. (2.1) can be solved exactly subject to the initial condition $\rho(-\infty)=\rho_0$:

$$\rho(t)=\rho_0+ie^{-t/\tau}\int_{-\infty}^{t}e^{t'/\tau}e^{iH(t'-t)}\times[\rho(t'),V(t')]e^{-iH(t'-t)}dt'. \quad (2.3)$$

If the external potential V is regarded as small, one may solve (2.3) by interaction $\rho=\rho_0+\rho_1+\rho_2+\cdots$, where the term ρ_1 is linear in the applied field, ρ_2 is quadratic, etc. For the purposes of calculating the ohmic conductivity, only ρ_1 is needed and this is given precisely by

$$\rho_1(t)=i\int_0^\infty e^{-t''/\tau}e^{-iHt''}[\rho_0,\ V(t-t'')]e^{iHt''}dt'', \quad (2.4)$$

where we have introduced $t''=t-t'$. If we assume that $V(t)$ has a single frequency dependence,

$$V(t)=e^{i\omega t}V,$$

then (2.4) can be rewritten in the form

$$\rho_1(t)e^{-i\omega t}=i\int_0^\infty e^{-i\omega t}e^{-t/\tau}e^{-iHt}[\rho_0,V]e^{iHt}dt, \quad (2.5)$$

where the double prime has been dropped on the right-hand side. We see therefore that $\rho_1\exp(-i\omega t)$ is independent of time, i.e., a steady state has been reached at any finite time.

The factor $\exp(-t/\tau)$ is just a convergence factor which arises because the crystal is not isolated but interacts with the universe. The result for ρ_1 is not sensitive to τ (unless the latter is unusually short) and we may write more simply

$$\rho_1e^{-i\omega t}=i\int_0^\infty e^{-i\omega t}e^{-iHt}[\rho_0,V]e^{iHt}dt, \quad (2.6)$$

with the understanding that ω has a small negative imaginary part which may be allowed to approach zero after it has served its function of causing otherwise oscillatory expressions to vanish at the upper limit.

3. THE CURRENT

When the Hamiltonian H is invariant against an arbitrary displacement, we can show easily that the current density $\mathbf{j}(\mathbf{r})$ becomes independent of $\mathbf{r}$, i.e., uniform. It is therefore sufficient for us to calculate the volume average current density $\mathbf{j}$. If there are n noninteracting particles per cm^3 of charge e, the current density $\mathbf{j}$ is given by

$$\mathbf{j}=ne\langle\mathbf{v}\rangle_{\mathrm{Av}}=ne\ \mathrm{trace}[\mathbf{v}\rho], \quad (3.1)$$

where

$$\mathbf{v}=[\mathbf{r},H]/i. \quad (3.2)$$

Note that the use of the unperturbed density matrix ρ_0 in (3.1) yields vanishing current.

If no magnetic fields are present, and if the interaction between the electron and the scattering system does not depend on the electron momentum, then $p^2/2m$ will be the only part of H that does not commute with $\mathbf{r}$ and we can replace (3.2) by $\mathbf{v}=\mathbf{p}/m$.

For the case of a uniform applied electric field, we can write

$$V(t)=-e\mathbf{E}(t)\cdot\mathbf{r}, \quad (3.3)$$

where $\mathbf{E}(t)=\mathbf{E}_0\exp(i\omega t)$.

Substitution of the perturbed density matrix ρ_1 into (3.1) leads to an expression for the current of the usual ohmic form:

$$\mathbf{j}=\boldsymbol{\sigma}\cdot\mathbf{E}, \quad (3.4)$$

where the dyadic $\boldsymbol{\sigma}$ is given by

$$\boldsymbol{\sigma}=\frac{ne^2}{m}\frac{1}{i}\int_0^\infty e^{-i\omega t}\ \mathrm{trace}\{\mathbf{p}[\rho_0,\ e^{-iHt}\mathbf{r}e^{iHt}]\}dt, \quad (3.5)$$

or

$$\boldsymbol{\sigma}=(ne^2/m)\boldsymbol{\tau},$$

where

$$\boldsymbol{\tau}=-i\int_0^\infty dt\exp(-i\omega t)\ \mathrm{trace}\{\mathbf{p}(t)[\rho_0,\mathbf{r}]\} \quad (3.6)$$

represents a dyadic relaxation time and

$$\mathbf{p}(t)=\exp(iHt)\mathbf{p}\exp(-iHt) \quad (3.7)$$

is the Heisenberg operator for the momentum.

It is sometimes convenient for purposes of interpretation to rewrite (3.6) in the form

$$\boldsymbol{\tau}=-i\int_0^\infty\exp(-i\omega t)\ \mathrm{trace}\{[\mathbf{r},\mathbf{p}(t)]\rho_0\}dt. \quad (3.8)$$

If, for example, no scattering occurs, then $\mathbf{p}(t)=\mathbf{p}$, $[\mathbf{r},\mathbf{p}]=i\mathbf{1}$, and

$$\boldsymbol{\tau}=\mathbf{1}\int_0^\infty \exp(-i\omega t)dt=\mathbf{1}/i\omega, \tag{3.9}$$

where the small imaginary part in ω assures convergence of the integral and $\mathbf{1}$ is the unit dyadic. Thus we obtain the conductivity of a free-electron gas:

$$\sigma=ne^2/(im\omega). \tag{3.10}$$

Since the conductivity σ always appears in conjunction with a dielectric constant ϵ in the combination $\sigma+i(\omega\epsilon/4\pi)$, (3.10) is equivalent to the usual result,

$$\Delta\epsilon=-4\pi ne^2/m\omega^2, \tag{3.11}$$

for the contribution to the dielectric constant of the free-electron gas.

If scattering occurs that is describable in some approximation by a viscous energy-independent damping:

$$\mathbf{p}(t)\simeq\mathbf{p}\exp(-t/\tau),$$

then

$$\boldsymbol{\tau}\simeq\mathbf{1}\tau/(1+i\omega\tau).$$

4. PROOF OF EQUIVALENCE OF THE USUAL TRANSPORT THEORY RESULT IN THE CASE OF WEAK COUPLING

The reduction from a density matrix equation to a transport equation requires the destruction of the phase information contained in the off-diagonal elements of the density matrix.[3,4] Our reduction of ρ [Eq. (3.6)] to the usual transport results requires two steps: (1) weak coupling; (2) the elimination of phase coherence in Eq. (3.6). In order not to duplicate previous work, we shall make the approximation of weak coupling and try to express our results in such a form that the conclusions of Van Hove concerning phase destruction can be applied directly.

Equation (2.6) with the insertion $V=-e\mathbf{E}(t)\cdot\mathbf{r}$ can be rewritten in the form

$$\rho_1=-\frac{e}{m}\mathbf{E}(t)\cdot\int_0^\infty e^{-i\omega t}e^{-iHt}\frac{\partial\rho_0}{\partial\mathbf{v}}e^{iHt}dt, \tag{4.1}$$

where $\partial\rho_0/\partial\mathbf{v}$ is defined by the equation

$$\partial\rho_0/\partial\mathbf{v}\equiv-im[\mathbf{r},\rho_0]. \tag{4.2}$$

If we work in a representation in which $\mathbf{v}=\mathbf{p}/m$ is diagonal, the current (3.1) is given by

$$j=ne\int\mathbf{v}d^3v\langle\mathbf{v}|\rho_1|\mathbf{v}\rangle, \tag{4.3}$$

so that only the diagonal matrix element of ρ_1 is needed.

[4] W. Pauli's original derivation in *Festschrift Zum 60 Geburtstage A. Sommerfeld* (S. Hirzel, Leipzig, 1928) simply made the random-phase assumption before the start of each collision.

Equation (4.1) yields for this matrix element

$$\langle\mathbf{v}|\rho_1|\mathbf{v}\rangle=-\frac{e}{m}\mathbf{E}(t)\cdot\int_0^\infty e^{-i\omega t}dt\int\int\langle\mathbf{v}|e^{-iHt}|\mathbf{v}'\rangle d\mathbf{v}'\times\left\langle\mathbf{v}'\left|\frac{\partial\rho_0}{\partial\mathbf{v}}\right|\mathbf{v}''\right\rangle d\mathbf{v}''\langle\mathbf{v}''|e^{iHt}|\mathbf{v}\rangle. \tag{4.4}$$

So far, the equations are rigorous. We now wish to obtain the limiting behavior of the above expression as the coupling strength λ goes to zero, where

$$H=H_0+\lambda H_1;\quad H_0=p^2/2m. \tag{4.5}$$

This limit must be taken with care since the expression $\exp[(H_0+\lambda H_1)t]$ contains λt and t is integrated over an infinite domain. However, t does not occur in ρ_0 so that it is permissible to let $\lambda\to0$ in $\rho_0(H)=\rho_0(H_0+\lambda H_1)$; therefore $\rho_0\simeq\rho_0(H_0)$ and $\partial\rho_0/\partial\mathbf{v}$ are diagonal in the $\mathbf{v}$ representation. Thus Eq. (4.4) can be rewritten in the form

$$\langle\mathbf{v}|\rho_1|\mathbf{v}\rangle=-\frac{e}{m}\mathbf{E}(t)\cdot\int_0^\infty\exp(-i\omega t)dt\times\int W(\mathbf{v},\mathbf{v}',t)d\mathbf{v}'\partial\rho_0(\mathbf{v}')/\partial\mathbf{v}', \tag{4.6}$$

where

$$W(\mathbf{v},\mathbf{v}',t)=|\langle\mathbf{v}|\exp(-iHt)|\mathbf{v}'\rangle|^2 \tag{4.7}$$

has the significance of the probability of finding the electron at $\mathbf{v}$ at time t if it was with certainty at $\mathbf{v}'$ at time zero.

Instead of trying to reduce (4.6) completely to the classical form, we shall bring the usual transport theory into a form directly comparable to (4.6). For this purpose, the classical transport equation can be written in the form

$$\partial f/\partial t+[e\mathbf{E}(t)/m]\cdot\partial f/\partial\mathbf{v}+Kf=0, \tag{4.8}$$

where K is a linear operator and Kf is an abbreviated way of writing the collision terms.

To bring (4.8) into a form analogous to (4.6), we must regard the electric field as a perturbation and solve to first order in the electric field. Thus we may write $f=f_0+f_1+\cdots$, where f_0 is independent of the field and f_1 is linear in the field. Equation (4.8) can be rewritten in the form

$$\partial f_1/\partial t+Kf_1=\phi=-[e\mathbf{E}(t)/m]\cdot\partial f_0/\partial\mathbf{v}. \tag{4.9}$$

To solve Eq. (4.9), we introduce Green's function $W(\mathbf{v},\mathbf{v}',t-t')$ that has the following properties:

$$\begin{aligned}&(1)\ W\text{ vanishes for }t<t',\\ &(2)\ W=\delta(\mathbf{v}-\mathbf{v}')\quad\text{for }t=t'+0,\\ &(3)\ \partial W/\partial t+KW=0\quad\text{for }t\neq t',\end{aligned} \tag{4.10}$$

i.e., W is the probability at a later time t of an electron

having the velocity $\mathbf{v}$ if it started with velocity $\mathbf{v}'$ at the earlier time t'. The necessary jump in W from $t=t'-0$ to $t'+0$ can be incorporated automatically by stating that W obeys

$$\partial W/\partial t+KW=\delta(\mathbf{v}-\mathbf{v}')\delta(t-t'). \tag{4.11}$$

The solution to (4.9) can then be written in the form

$$f_1(\mathbf{v},t)=\int d\mathbf{v}'\int_{-\infty}^{t} dt'\, W(\mathbf{v},\mathbf{v}',t-t')\phi(\mathbf{v}',t'), \tag{4.12}$$

where the upper limit t arises because W vanishes for $t'>t$. If we insert $t''=t-t'$, make use of $\mathbf{E}(t)=\exp(i\omega t)\times\mathbf{E}(0)$, and later drop the double prime (4.12) becomes

$$f_1(\mathbf{v},t)=-\frac{e}{m}\mathbf{E}(t)\cdot\int\frac{\partial f_0(\mathbf{v}')}{\partial\mathbf{v}'}d\mathbf{v}'\int_0^{\infty} W(\mathbf{v},\mathbf{v}',t)\times\exp(-i\omega t)dt. \tag{4.13}$$

Equation (4.13) is identical with (4.6) if we identify ρ_0 with f_0 [which has already been done in replacing $\rho_0(H)$ by $\rho_0(H_0)$] and if we identify the W's appearing in the two equations.

It is clear from their definitions that the two W's have the same physical meaning. The work of Van Hove demonstrates that the W defined by (4.7) obeys the classical transport equation (4.10) in the weak coupling limit so that the two quantities are indeed identical. (In fact an elementary proof based on Weisskopf-Wigner perturbation theory will be presented in a future publication.)

5. NYQUIST NOISE

The classical expression[5] for the noise power $G(\nu)d\nu$ in the frequency interval $d\nu$ associated with a fluctuating function $I(t)$ is given by

$$G(\nu)=\lim_{T\to\infty}\left(\frac{2}{T}\right)\left|\int_{-\frac{1}{2}T}^{\frac{1}{2}T} I(t)e^{-2\pi i\nu t}dt\right|^2, \tag{5.1}$$

where the factor 2 arises because of the convention that the total dissipated "power" is given by

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T I^2(t)dt=\int_0^{\infty} G(\nu)d\nu, \tag{5.2}$$

so that $G(\nu)$ includes the contribution from frequencies ν and $-\nu$. For a bibliography of early work, including derivations of (5.1), the reader is referred to Rice[5] and Wiener.[6] A recent illuminating derivation of (5.1) based on an analysis of the measurement process has been given by Ekstein and Rostoker.[7]

[5] S. O. Rice, Bell System Tech. J. **23**, 282 (1944); **24**, 46 (1945).
[6] N. Wiener, Acta Math. **55**, 117 (1930); J. Math. Phys. **5**, 99 (1926).
[7] H. Ekstein and N. Rostoker, Phys. Rev. **100**, 1023 (1955).

For quantum mechanical systems, $I(t)$ is to be regarded as an operator and the expression (5.1) must be made Hermitian, i.e.,

$$G_{\mathrm{op}}(\nu)=\lim_{T\to\infty}\frac{1}{T}\int_{\frac{1}{2}T}^{\frac{1}{2}T}\int_{-\frac{1}{2}T}^{\frac{1}{2}T}[I(t)I(t')+I(t')I(t)]\times\exp[-i\omega(t-t')]dtdt', \tag{5.3}$$

where $\omega=2\pi\nu$. The mean value of the operator $G_{\mathrm{op}}(\nu)$ must be taken with respect to a quantum-mechanical state ψ, or more properly an average should be taken over an ensemble of states:

$$G(\nu)=\mathrm{trace}[G_{\mathrm{op}}(\nu)\rho_0], \tag{5.4}$$

when ρ_0 is the equilibrium density matrix $Z^{-1}\exp(-\beta H)$.

The operator $I(t)$ is the Heisenberg operator

$$I(t)=\exp(iHt)I\exp(-iHt). \tag{5.5}$$

Equation (5.3) may be generalized to include correlation spectra between components of the current by replacing $I(t)$ by $I_r(t)$ and $I(t')$ by $I_s(t')$, where r and s take any of the values x, y, z. The off-diagonal elements of $G_{rs}(\nu)$ can be complex since an "out-of-phase" contribution to the correlation is possible. The invariance of traces against unitary transformation, and in particular a negative time displacement of amount t', permits $G_{rs}(\nu)$ to be rewritten in the form

$$G_{rs}(\nu)=\int_{-\infty}^{\infty}\exp(-i\omega t)dt\times\mathrm{trace}\{[I_r(t)I_s(0)+I_s(0)I_r(t)]\rho_0\}. \tag{5.6}$$

If the trace (5.6) is written in the energy representation, and the summation indices n,n' are interchanged in the second term, Eq. (5.6) becomes

$$G_{rs}(\nu)=2\pi\textstyle\sum_{n,n'}(\rho_n+\rho_{n'})\delta(\omega-(E_n-E_{n'}))\times\langle n|I_r|n'\rangle\langle n'|I_s|n\rangle, \tag{5.7}$$

where $\rho_n=Z^{-1}\exp(-\beta E_n)$. (Degeneracy is permitted among the states n. For simplicity of notation we do not introduce other quantum numbers.)

The x component of the current, I_x, is given by

$$I_x=L_x^{-1}\textstyle\sum_i e_i v_{ix}=j_x L_y L_z, \tag{5.8}$$

where L_x is the length of the specimen between electrodes, j_x is the x component of the volume average current density [see Eq. (5.11)], and L_yL_z is the cross-sectional area of the electrodes. Equation (5.7) for $G_{xx}(\nu)$ is then identical to Ekstein and Rostoker's Eq. (15).

The *complex* Nyquist theorem can be written in the form

$$G_{rs}(\nu)=2kT[Y_{rs}(\omega)+Y_{sr}(-\omega)][\tfrac{1}{2}\beta\omega\coth(\tfrac{1}{2}\beta\omega)], \tag{5.9}$$
$$r=x,y,z;\quad s=x,y,z,$$

where the last factor is the quantum mechanical correction, and the admittance $\mathbf{Y}(\omega)$ at the frequency ω

is related to the conductivity $\boldsymbol{\sigma}(\omega)$ by

$$Y_{rs}(\omega)=(V/L_rL_s)\sigma_{rs}(\omega), \tag{5.10}$$

where V is the volume of the specimen.

Callen and Welton[8] and Ekstein and Rostoker have given derivations of the real part of (5.9) in which the admittance is obtained by a calculation of the power dissipation. (Such a calculation yields Reσ but not Imσ) As a check on our work, we shall take our expression (3.5) for the conductivity and verify the Nyquist relation.

Our expression (3.5) for σ is based on a one electron treatment. However our entire treatment applies formally also to the many-body case if we simply regard H as a many-electron Hamiltonian and use the Boltzmann form $\rho_0=(1/Z)\exp(-\beta H)$ for the equilibrium many-electron density matrix. Two minor changes in detail takes place: the interaction with the field—$e\mathbf{r}\cdot\mathbf{E}$ is replaced by—$\sum e_j\mathbf{r}_j\cdot\mathbf{E}$ and the volume average current density is calculated from

$$\mathbf{j}=(\textstyle\sum_i e_i\mathbf{v}_i)/V, \tag{5.11}$$

instead of $ne\mathbf{v}$. Thus Eq. (3.5) is replaced by

$$\boldsymbol{\sigma}=(Vi)^{-1}\int_0^\infty dt\exp(-i\omega t)\times\operatorname{trace}\{\textstyle\sum_i e_i\mathbf{v}_i(t)[\rho_0,\sum_j e_j\mathbf{r}_j]\}. \tag{5.12}$$

If we introduce the variables Q_s $(s=x,y,z)$, with Q_x defined by

$$Q_x=(L_x)^{-1}\textstyle\sum e_jx_j,$$

such that $\dot{Q}_s=I_s$, the conductivity, can be written more compactly as

$$\sigma_{rs}=L_rL_s(Vi)^{-1}\int_0^\infty dt\exp(-i\omega t)\times\operatorname{trace}\{I_r(t)[\rho_0,Q_s]\}. \tag{5.13}$$

In the energy representation, $\dot{Q}_s=I_s$ implies that

$$\langle n'|Q_s|n\rangle=i\langle n'|I_s|n\rangle/(E_n-E_{n'}), \tag{5.14}$$

so that Eq. (5.13) becomes

$$\sigma_{rs}=\frac{L_rL_s}{V}\int_0^\infty dte^{-t/\tau}e^{-i\omega t}\sum_{nn'}e^{i(E_n-E_{n'})t}\times\langle n|I_r|n'\rangle\langle n'|I_s|n\rangle(\rho_{n'}-\rho_n)/(E_n-E_n'), \tag{5.15}$$

where we have reinserted the convergence factor $\exp(-t/\tau)$ associated with the interaction with the "universe" as discussed in Sec. 2. Taking the limit as $1/\tau\to 0$, we find that

$$\tfrac{1}{2}[Y_{rs}(\omega)+Y_{sr}(-\omega)]=\pi\sum_{n,n'}\delta(\omega-E_n+E_{n'})\times\langle n|I_r|n'\rangle\langle n'|I_s|n\rangle(\rho_{n'}-\rho_n)/(E_n-E_{n'}). \tag{5.16}$$

[8] H. B. Callen and T. R. Welton, Phys. Rev. **83**, 34 (1951).

If we note that

$$\frac{\rho_n+\rho_{n'}}{\rho_{n'}-\rho_n}(E_n-E_{n'})=\frac{\exp(\beta\omega)+1}{\exp(\beta\omega)-1}(\omega) \tag{5.17}$$

is independent of the summation indices n,n' when one replaces $E_n-E_{n'}$ by ω because of the delta function, the Nyquist theorem (5.9) follows immediately.

It is to be noted that in the above derivation the Hamiltonian H may contain interactions between the electrons. Also Fermi statistics may be obeyed. Correlations introduced by statistics and by interactions undoubtedly affect the noise, but they affect the conductivity in precisely the same way, preserving the validity of the Nyquist theorem.*

6. MANY-BODY TO ONE-BODY REDUCTION

If the Hamiltonian H can be split into a set of terms

$$H=\textstyle\sum H_j, \tag{6.1}$$

such that H_j depends only on electron j, the motions of the electrons are uncorrelated except through statistics.

For the case of classical Boltzmann statistics, $\mathbf{r}_i$ and $\mathbf{r}_j$ are truly uncorrelated. In Eq. (5.12) only the terms $i=j$ contribute, and they all contribute equally resulting in a factor N. When N/V is replaced by the density n, Eq. (5.12) reduces to the one-body formula (3.6).

For the case of Fermi-Dirac statistics the motions of the electrons are correlated even when the Hamiltonian as in (6.1) contains no interactions. It is not clear, then, that the conductivity can be calculated as in Secs. 2 and 3 by one-body methods making only the modification of replacing the initial density matrix by

$$\rho_0=\rho^F\equiv\{1+\exp[\beta(H_1-E_F)]\}^{-1}, \tag{6.2}$$

where H_1 is the one-body Hamiltonian.

We shall therefore verify that our one-body result is a consequence of the many-body conductivity formula (5.12). For the purposes of the proof it is most con-

* *Note added in proof.*—The equations of this section remain valid in the presence of a magnetic field. However time-reversal symmetry implies that the Hamiltonian is invariant under the operation K of taking the complex conjugate *and* reversing the vector potential $\mathbf{A}$:

$$KH(\mathbf{A})K=H^*(-\mathbf{A})=H(\mathbf{A}). \tag{5.18}$$

Thus the states $|n\rangle=|n(\mathbf{A})\rangle$ can be chosen to be invariant under K. But $I_s(\mathbf{A})$, which is proportional to $-i\nabla-e\mathbf{A}$, reverses sign under K (i.e., velocity is odd under time reversal). It follows then that

$$\langle n(-\mathbf{A})|I_s(-\mathbf{A})|n'(-\mathbf{A})\rangle=-\langle n'(\mathbf{A})|I_s(\mathbf{A})|n(\mathbf{A})\rangle, \tag{5.19}$$

and from Eq. (5.16) we obtain the Onsager relations,

$$Y_{sr}(\omega,\mathbf{A})=Y_{rs}(\omega,-\mathbf{A}). \tag{5.20}$$

The combination

$$Y_{rs}(\omega,\mathbf{A})+Y_{sr}(-\omega,\mathbf{A})=Y_{rs}(\omega,\mathbf{A})+Y_{rs}(-\omega,-\mathbf{A})$$

is real when $\mathbf{A}=0$ so that there is no out-of-phase noise except in the presence of a magnetic field.

venient to work in a second-quantized notation. The Hamiltonian (6.1) is then replaced by

$$H=\sum\epsilon_k N_k=\sum\epsilon_k a_k^\dagger a_k, \tag{6.3}$$

where the ϵ_k are the eigenvalues associated with the one-body Hamiltonian H_1 and a_k, $a_\kappa^\dagger$ and the usual Fermi destruction and creation operators. In this respresentation we may write

$$\begin{aligned}\sum\mathbf{r}_j&=\sum_{l,k}\langle l|\,\mathbf{r}\,|k\rangle a_l^\dagger a_k,\\ \sum_i\mathbf{p}_i(t)&=\sum_{n,m}\langle n|\,\mathbf{p}\,|m\rangle a_n^\dagger(t)a_m(t),\end{aligned} \tag{6.4}$$

where

$$a_m(t)=a_m\exp(-i\epsilon_m t),\quad a_n^\dagger(t)=a_n^\dagger\exp(i\epsilon_n t). \tag{6.5}$$

In the second-quantized notation the total number of particles is not fixed and one must use a grand canonical ensemble:

$$\rho_0=\exp[-\beta H+\mu N], \tag{6.6}$$

where

$$N=\sum_k a_k^\dagger a_k, \tag{6.7}$$

or, for the noninteracting case:

$$\rho_0=\exp[-\beta\textstyle\sum_k(\epsilon_k-E_F)a_k^\dagger a_k], \tag{6.8}$$

when $E_F=\mu/\beta=$the Fermi energy is chosen so as to yield the desired density for $\langle N\rangle/V$.

The conductivity (5.12), with the help of (6.4) and (6.5), can now be written:

$$\begin{aligned}\boldsymbol{\sigma}=\frac{e^2}{m}\frac{1}{Vi}\sum_{lknm}&\langle n|\,\mathbf{p}\,|m\rangle\langle e|\,\mathbf{r}\,|k\rangle\\ &\times\operatorname{trace}\{a_n^\dagger a_m[\rho_0,a_l^\dagger a_k]\}\\ &\times\int_0^\infty\exp(-i\omega t)dt\exp[i(\epsilon_n-\epsilon_m)t].\end{aligned} \tag{6.9}$$

The trace can readily be evaluated in the representation in which the $N_k=a_k^\dagger a_k$ are all diagonal:

$$\operatorname{trace}\{a_n^\dagger a_m[\rho_0,a_l^\dagger a_\kappa]\}=\delta_{nk}\delta_{ml}[f(\epsilon_m)-f(\epsilon_k)], \tag{6.10}$$

where

$$f(\epsilon)=\frac{1}{\exp[\beta(\epsilon-E_F)]+1}. \tag{6.11}$$

The creation and destruction operators have now all disappeared and we must perform sums over states $|k\rangle$ that are eigenstates of the one-body Hamiltonian H_1 into which H is decomposed by (6.1). The notation can now be simplified by writing

$$\begin{aligned}\langle n|\,\mathbf{p}\,|m\rangle\exp[i(\epsilon_n-\epsilon_m)t]&\\ =\langle n|\exp(iH_1t)\mathbf{p}\exp(-iH_1t)\,|m\rangle&\\ =\langle n|\,\mathbf{p}(t)\,|m\rangle,&\end{aligned} \tag{6.12}$$

and

$$\langle m|\,\mathbf{r}\,|k\rangle[f(\epsilon_m)-f(\epsilon_k)]=\langle m|\,[\rho^F,\mathbf{r}]\,|k\rangle, \tag{6.13}$$

where ρ^F is defined by (6.2). Thus

$$\begin{aligned}\sigma=\frac{e^2}{mVi}\int_0^\infty&\exp(-i\omega t)dt\\ &\times\sum_{m,k}\langle k|\,\mathbf{p}(t)\,|m\rangle\langle m|\,[\rho^F,\mathbf{r}]\,|k\rangle,\\ \sigma=\frac{e^2}{mVi}\int_0^\infty&\exp(-i\omega t)\operatorname{trace}\{\mathbf{p}(t)[\rho^F,\mathbf{r}]\},\end{aligned} \tag{6.14}$$

where the trace is now over one-body states, and the Fermi energy is chosen so that

$$V^{-1}\operatorname{trace}\rho^F=n. \tag{6.15}$$

Equation (6.14) is identical to our one-body result (3.5).

7. SUMMARY

We have demonstrated that an assembly of N noninteracting electrons in a volume V will have the conductivity

$$\boldsymbol{\sigma}(\omega)=\frac{e^2}{mi\hbar V}\int_0^\infty dt\exp(-i\omega t)\operatorname{trace}\{\mathbf{p}(t)[\rho_0,\mathbf{r}]\}, \tag{7.1}$$

where

$$\mathbf{p}(t)=\exp(iHt/\hbar)\mathbf{p}\exp(-iHt/\hbar),$$

and H is the Hamiltonian describing *one* electron plus the scattering system plus the interaction between the two. For Boltzmann statistics,

$$\rho_0=\rho^B=N\exp(-\beta H)/\operatorname{trace}[\exp(-\beta H)]; \tag{7.2}$$

and for Fermi statistics,

$$\rho_0=\rho^F=\{\exp[\beta(H-E_F)]+1\}^{-1}, \tag{7.3}$$

where our formulas are *now* both written with the convention trace $\rho_0=N$ for comparison.

For the many-body case [see (5.12)] one simply takes (7.1) and replaces $\mathbf{p}(t)$ by $\sum_i\mathbf{p}_i(t)$ and $\mathbf{r}$ by $\sum\mathbf{r}_j$. H is now interperted to be the many-body Hamiltonian (possibly including interactions between electrons). The *complex* Nyquist theorem is verified for this general many-body case including interactions and a magnetic field.

The conductivity (7.1) is shown in Sec. 4 to reduce to the usual transport result for the case of weak coupling without assuming the existence of a relaxation time.