Quantum Theory of Electrical Transport in a Magnetic Field. I

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The relationship between the quantum theory of electrical transport in the presence of a magnetic field and the corresponding Boltzmann transport equation is established for a simple system. The model consists of noninteracting free electrons being elastically scattered by an arbitrary potential in the presence of uniform electric and magnetic fields. Without the aid of a representation, the exact gauge-dependent Liouville equation for the density operator of this system is transformed into a completely gauge-independent equation satisfied by a new density operator. The new density operator is shown to give the correct current density, using the ordinary gauge-independent free-particle velocity operator. No approximations are made in performing the transformations, and the physical content of the new gauge-independent transport formalism is identical in all respects with that contained in the initial gauge-dependent equations. A new density matrix is defined which is essentially the Fourier sum of the matrix of the gauge-independent density operator. By considering the scattering potential resulting from a set of fixed impurity centers, it is shown that the diagonal elements of this new density matrix satisfy the ordinary time-dependent Boltzmann transport equation in which the spatial gradient term appears explicitly. The possible existence of a spatial variation in the average density of scatterers is also taken into account. The final equation for the quantum-mechanical distribution function represents the result obtained by treating the electric field and the effective scattering potential to the lowest possible order in which they contribute.

I. INTRODUCTION

THE work presented here is concerned with the problem of establishing the relationship between the correct quantum-mechanical theory of electrical transport based on the density-matrix formalism and the ordinary Boltzmann transport equation.[1–3] Because of the increasing interest in the effects of a magnetic field on the transport properties of metals and semiconductors, special attention is given to the problem of correctly establishing the form of an equivalent gauge-independent transport formalism that is directly related to the usual gauge-independent transport equation. This approach provides a way of properly treating all magnetic effects having an influence on transport properties within the familiar framework of a transport equation. In the present work, an improved derivation of the gauge-independent transport formalism is presented that avoids altogether the use of a representation.[4] The gauge-independent density operator is used to define a new spatially dependent density matrix. The diagonal elements of this new density matrix are found to satisfy a Boltzmann transport equation that includes the spatial gradient term; they, therefore, correspond exactly to the classical distribution function.

The expectation value of any observable quantity represented by the operator M is given by

$$\bar{M}(t)=\mathrm{Tr}\{\rho_T(t)M(t)\}, \tag{1.1}$$

where ρ_T is the density operator.[5] The time development of ρ_T is determined by the Liouville equation

$$ih\frac{\partial\rho_T}{\partial t}=[H_T,\rho_T], \tag{1.2}$$

where H_T is the complete Hamiltonian for the system. Once ρ_T is known, the value of any operator M representing an observable quantity can be found from (1.1). While this procedure is certainly straightforward and correct, it has not been extensively employed in the treatment of transport problems, because of the difficulty involved in solving Eq. (1.2) for the density operator. The most usual approach in dealing with transport problems has been through the use of the Boltzmann transport equation or some related transport equation. For this reason it is desirable to establish as rigorously as possible the connection between the exact density-matrix formalism, represented by Eqs. (1.1) and (1.2), and the more commonly used transport equations.

In the absence of a magnetic field, the correct relationship between the exact density-matrix formalism and the ordinary time-independent Boltzmann equation has been established by Kohn and Luttinger[6] for a simple spatially homogeneous model. For a system in the presence of a magnetic field, the vector potential appears explicitly in Eq. (1.2) for the exact density operator and in the corresponding velocity operator as well. It is then apparent that the exact magnetic-field-dependent density operator does not correspond to the ordinary classical distribution function.[7] Moreover, the matrix equations obtained from the operator relationship (1.2) contain matrix elements of the vector potential, and this leads directly to difficulty in attempting

[1] N. Ashby, Ph.D. thesis, Harvard University, 1961 (unpublished).
[2] J. H. Irving, Ph.D. thesis, Princeton University, 1965 (unpublished).
[3] S. Fujita, *Introduction to Nonequilibrium Quantum Statistical Mechanics* (W. B. Saunders Co., Philadelphia, 1966), Chap. 5.
[4] R. B. Thomas, Jr., Phys. Rev. **152**, 138 (1966).
[5] R. C. Tolman, *Principles of Statistical Mechanics* (Oxford University Press, New York, 1930), p. 327.
[6] W. Kohn and J. M. Luttinger, Phys. Rev. **108**, 590 (1957).
[7] A. H. Wilson, *The Theory of Metals* (Cambridge University Press, London, 1953), 2nd ed., Chap. 2, p. 51.

to solve them. In order to avoid this difficulty, and to ensure a description that is finally gauge-independent, a method was found of eliminating the vector potential from the operator equation at the outset. Using the methods of Kohn and Luttinger, the resulting gauge-independent operator equation was found to be directly related to a simple form of the Boltzmann equation in the presence of a magnetic field.

The original method of deriving the gauge-independent transport formalism depends on the use of a representation that tends to complicate the equations and to obscure important relationships. Actually, the use of a representation is not essential to the derivation; this is suggested by the fact that the final results can again be written in operator form. Here a simpler and somewhat more general derivation of the gauge-independent transport formalism is presented, which makes no use of a representation. The model consists in noninteracting free electrons being elastically scattered by an arbitrary spatially dependent potential in the presence of uniform electric and magnetic fields. In Sec. II, the exact gauge-dependent Liouville equation for the density operator of this system is transformed into a completely gauge-independent equation for a new density operator. In Sec. III, the corresponding gauge-independent velocity operator is found.

In Sec. IV, the relationship between the gauge-independent Liouville equation and a more general form of the Boltzmann transport equation is established. This is accomplished with the aid of a new density matrix that is essentially the Fourier sum of the matrix of the gauge-independent density operator. This quantity turns out to correspond exactly to the ordinary classical distribution function. For mathematical convenience, the scattering potential is limited to that provided by a set of fixed impurity centers, and is treated as a perturbation by means of the Born approximation. It is shown that the diagonal elements of the new density matrix satisfy the ordinary time-dependent Boltzmann equation, in which the spatial gradient term appears explicitly. The possible existence of a spatial variation in the average density of scatterers is also taken into account. This procedure can readily be extended to obtain higher-order corrections, which will include terms depending on the spatial variation of the various physical parameters used to describe the system. By an appropriate choice of basis functions, the periodic lattice potential can also be included; this would lead to interesting additional terms in the corresponding transport equation.

The transformation to the gauge-independent transport formalism (Secs. II and III) is carried out without approximation; this means that the physical content of the resulting transport equation (Sec. IV) is identical in all respects with that contained in the initial set of gauge-dependent equations (Sec. II), at least within the limitations of the model considered here. It would be interesting and instructive to make a comparison between the predictions of Eqs. (1.1) and (1.2) and those of the gauge-independent transport equation for some simple systems subjected to a uniform magnetic field. This would help to clarify the role of small but well-known magnetic effects in electrical conductivity. The results of this further investigation, where the effects of a periodic lattice potential are also included, will appear later.

II. GAUGE-INDEPENDENT LIOUVILLE EQUATION

Consider a collection of electrons so dilute that the interaction of one electron with another can be neglected. The electrons are treated as completely free, except for their interaction with an arbitrary scattering potential and the externally applied electric and magnetic fields. The exact Hamiltonian for each electron moving in such a system may be written

$$H_T=\frac{1}{2m}\left(\mathbf{p}-\frac{e}{c}\mathbf{A}(\mathbf{r})\right)^2+U(\mathbf{r})+H_E(\mathbf{r}). \tag{2.1}$$

The first term on the right-hand side is the Hamiltonian of a free electron in the presence of a magnetic field $\mathbf{B}=\nabla\times\mathbf{A}(\mathbf{r})$, where $\mathbf{A}(\mathbf{r})$ is the vector potential. $U(\mathbf{r})$ is the scattering potential, which is assumed to depend only upon the spatial coordinates; this potential can be considered to be composed of two parts: $V(\mathbf{r})$, the periodic lattice potential and $H'(\mathbf{r})$, the potential resulting from added impurity atoms and possible imperfections in the crystal lattice. The last term in (2.1) is the interaction of an electron with a uniform electric field.

The exact density operator for the system, ρ_T, satisfies Eq. (1.2), with H_T given by (2.1). Taking the magnetic field in the positive z direction and choosing for convenience the Landau gauge $\mathbf{A}(\mathbf{r})=(-yB, 0, 0)$, it is found that ρ_T satisfies the equation

$$i\hbar\frac{\partial\rho_T}{\partial t}=\left[\frac{1}{2m}\mathbf{p}^2+\omega_0 yp_x+\tfrac{1}{2}m\omega_0^2y^2+U+H_E,\ \rho_T\right], \tag{2.2}$$

where $\omega_0=eB/mc$ is the cyclotron frequency.

The exact velocity operator $\mathbf{v}$ is defined as the total time rate of change of the spatial coordinate. Then, for the Hamiltonian (2.1) the velocity operator is given by the commutator

$$\mathbf{v}=\frac{i}{\hbar}[H_T,\mathbf{r}]=(1/m)\mathbf{P}, \tag{2.3}$$

where $\mathbf{P}\equiv[\mathbf{p}-(e/c)\mathbf{A}(\mathbf{r})]$ is the momentum operator for an electron moving in a magnetic field. Placing this expression for the velocity in Eq. (1.1) and multiplying by the product of the electronic charge e and the electron density n_0 gives the exact current density

$$\mathbf{j}=en_0\,\mathrm{Tr}\{\mathbf{v}\rho_T\}. \tag{2.4}$$

It will now be shown that a pair of gauge-independent equations can be found that are physically equivalent to Eqs. (2.2) and (2.3), since they give identical current densities. First, assume that ρ_T can be written in the form of a Fourier operator integral,

$$\rho_T=\int e^{i[\mathbf{p}-(e/c)\mathbf{A}(\mathbf{r})]\cdot\xi}R(\xi,\mathbf{r},\mathbf{B},t)d\xi, \tag{2.5}$$

where $R(\xi,\mathbf{r},\mathbf{B},t)$ is taken to be independent of the field gauge. It is useful to express this integral as a series of commutators. In order to accomplish this, we consider two operators a and b which both commute with their commutator $[a,b]$. Then

$$e^{a+b}=e^ae^be^{-1/2[a,b]}. \tag{2.6}$$

Taking $a=i\omega_0 my\xi_x$ and $b=ip_y\xi_y$, we find $[a,b]=-i\omega_0 \times m\hbar\xi_x\xi_y$, which does in fact commute with both a and b as defined here. Making use of (2.6) and some well-known elementary commutation relations, it can be shown that (2.5) can be written as the double sum

$$\rho_T=\sum_{n=0}^{\infty}\sum_{n'=0}^{\infty}\frac{1}{n!}\left(\frac{m\omega_0 y}{i\hbar}\right)^n\frac{1}{n'!}\left(\frac{im\omega_0}{2\hbar}\right)^{n'} \times[x^{[n+n']},[y^{[n']},\tilde{\rho}_T]], \tag{2.7}$$

where $\tilde{\rho}_T$ is defined by

$$\tilde{\rho}_T=\int e^{i\mathbf{p}\cdot\xi}R(\xi,\mathbf{r},\mathbf{B},t)d\xi. \tag{2.8}$$

Here $[a^{[n]},b]$ is defined to be the n-fold commutator of the operator a with operator b, i.e., $[a,[a,\cdots],b]$ with n factors of a and $[a^{[0]},b]\equiv b$.

In order to find an equation satisfied by $\tilde{\rho}_T$, substitute the expression (2.7) for ρ_T into Eq. (2.2). After considerable algebra, involving the successive application of elementary commutation relations, it can be shown that

$$0=\sum_{n=0}^{\infty}\sum_{n'=0}^{\infty}\frac{1}{n!}\frac{1}{n'!}\left(\frac{m\omega_0 y}{i\hbar}\right)^n\left(\frac{im\omega_0}{2\hbar}\right)^{n'} \times\left[x^{[n+n']},\left[y^{[n']},\left\{-i\hbar\frac{\partial\tilde{\rho}_T}{\partial t}+[U(\mathbf{r})+H_E(\mathbf{r}),\tilde{\rho}_T]\right.\right.\right.$$
$$\left.\left.\left.+\frac{1}{2m}[\mathbf{p}^2,\tilde{\rho}_T]+\tfrac{1}{2}\omega_0(p_x[y,\tilde{\rho}_T]+[y,\tilde{\rho}_T]p_x -p_y[x,\tilde{\rho}_T]-[x,\tilde{\rho}_T]p_y)\right\}\right]\right]. \tag{2.9}$$

Upon examining this result it is seen that the expression contained in curly brackets depends in no way on the magnetic-field gauge, although it still depends on the magnetic field through ω_0. By setting this bracket equal to zero, (2.9) is always satisfied and $\tilde{\rho}_T$ is found to satisfy the equation

$$i\hbar\frac{\partial\tilde{\rho}_T}{\partial t}=[\tilde{H}_T,\tilde{\rho}_T]$$
$$-\frac{e}{2mc}\sum_\alpha\{(\mathbf{p}\times\mathbf{B})_\alpha[x_\alpha,\tilde{\rho}_T]+[x_\alpha,\tilde{\rho}_T](\mathbf{p}\times\mathbf{B})_\alpha\} \tag{2.10}$$

for an arbitrarily directed magnetic field, where the effective gauge-independent Hamiltonian $\tilde{H}_T=\mathbf{p}^2/2m+U+H_E$. No approximations have been made in obtaining Eq. (2.10) and the result appears to be exact within the limitations of the model.

III. GAUGE-INDEPENDENT VELOCITY OPERATOR

The velocity operator $\tilde{\mathbf{v}}$, corresponding to the density operator $\tilde{\rho}_T$ must be known before Eq. (2.10) can be used as a basis for developing a gauge-independent transport theory. In order to find such an operator, we begin with the exact expression for the current density (2.4), which must of course be the same no matter how it is calculated. Making use of (2.3) and (2.5) the current density can be written

$$\mathbf{j}=\frac{en_0}{im}\mathrm{Tr}\left\{\int(\nabla_\xi e^{i\mathbf{P}\cdot\xi})Rd\xi\right\}. \tag{3.1}$$

Assume that $R(\xi,\mathbf{r},\mathbf{B},t)$ approaches zero as ξ_α approaches infinity; this is required if ρ_T and $\tilde{\rho}_T$ are to remain finite and have bounded traces. Now perform a partial integration of (3.1) with respect to ξ; the integrated part is seen to vanish and we obtain

$$\mathbf{j}=(en_0i/m)\ \mathrm{Tr}\varrho_T', \tag{3.2}$$

where the vector ϱ_T' is defined by

$$\varrho_T'=\int e^{i\mathbf{P}\cdot\xi}\nabla_\xi Rd\xi. \tag{3.3}$$

Because $\nabla_\xi R$ is independent of the field gauge, ϱ_T' can be expanded by the same method used in Sec. II to obtain the expansion (2.7) for ρ_T from the integral expression (2.5). In this way it is found that the current density can be written

$$\mathbf{j}=\frac{ien_0}{m}\mathrm{Tr}\left\{\sum_{n=0}^{\infty}\sum_{n'=0}^{\infty}\frac{1}{n!}\frac{1}{n'!}\left(\frac{m\omega_0 y}{i\hbar}\right)^n \times\left(\frac{im\omega_0}{2\hbar}\right)^{n'}[x^{[n+n']},[y^{[n']},\tilde{\varrho}_T']]\right\}, \tag{3.4}$$

where the new vector $\tilde{\varrho}_T'$ is defined by

$$\varrho_T'=\int e^{i\mathbf{p}\cdot\xi}\nabla_\xi Rd\xi. \tag{3.5}$$

First evaluate the $n=n'=0$ term in the double sum (3.4); this turns out to be the only nonvanishing contribution to the current density. Then

$$\mathbf{j}=\frac{ien_0}{m}\,\mathrm{Tr}\left\{\int e^{i\mathbf{p}\cdot\xi}\nabla_\xi R d\xi\right\}=en_0\,\mathrm{Tr}\left\{\frac{1}{m}\mathbf{p}\tilde{\rho}_T\right\}, \quad (3.6)$$

after inegrating once by parts. If we now examine the remaining terms in the sum on the right-hand side of Eq. (3.4) for which $n+n'=0$, it can be shown that they all vanish by making use of the fact that the trace of a product of factors is invariant under a cyclic permutation of the factors. The entire contribution to the current density is then given by (3.6), the first term in the series (3.4). This expression for the current is completely equivalent to that given by (2.4), but is now expressed in terms of gauge-independent operators. If $\tilde{\rho}_T$, satisfying Eq. (2.10), is taken to be the correct density operator, then it is clear from Eq. (3.6) that the corresponding (gauge-independent) velocity operator is just $\mathbf{p}/m$, the free-particle momentum operator divided by the mass.

To complete the correspondence between ρ_T and $\tilde{\rho}_T$, it must be shown that their traces are identical in order to provide for probability normalization. This is most easily accomplished by taking the trace of Eq. (2.7), where it is found that only the first term, $\mathrm{Tr}\tilde{\rho}_T$, obtained from the sum on the left-hand side of the equation, does not vanish.

IV. BOLTZMANN TRANSPORT EQUATION

In this section, it is shown how the ordinary Boltzmann transport equation, including the spatial gradient term, is derived from the operator equation (2.10). Some care is taken to indicate clearly the approximations made, for they provide useful criteria for determining the validity of the Boltzmann equation. In order to present the essential elements of the derivation without unnecessary mathematical complication, we shall neglect the effect of the periodic potential for the present, and replace $U(\mathbf{r})$ by $H'(\mathbf{r})$ alone, which represents the scattering potential of a set of fixed impurity centers. We consider the effective Hamiltonian

$$\tilde{H}_T=H_0+H'(\mathbf{r})+H_E(\mathbf{r}), \quad (4.1)$$

where $H_0=\mathbf{p}^2/2m$. Here, $H'(\mathbf{r})$ is the interaction of an electron with the impurities; it can be written

$$H'(\mathbf{r})=\sum_{i=1}^{N}\phi(\mathbf{r}-\mathbf{r}_i)\equiv\lambda V_s. \quad (4.2)$$

In this expression, $\phi(\mathbf{r})$ is the interaction of an electron with a single scatterer located at the origin, $\mathbf{r}_i$ are the locations of the N scatterers, and λ is some dimensionless measure of the strength of the scattering interaction V_s with the electron. We now wish to consider the solution of Eq. (2.10) with $\tilde{H}_T$ given by (4.1), treating $H'(\mathbf{r})$ as a perturbation.

It is convenient to make use of a representation in which the free-particle Hamiltonian H_0 is diagonal, that is, plane waves with periodic boundary conditions. The normalized eigenfunctions of H_0 are $\psi_k(\mathbf{r})=\exp(i\mathbf{k}\cdot\mathbf{r})/V^{1/2}$, where $V=L^3$ is the volume of the container. The allowed wave vectors are $k_\alpha=(2\pi/L)n_\alpha$, where n_α are all the real positive and negative integers including zero. Then ψ_k satisfies the equation $H_0\psi_k=\epsilon_k{}^0\psi_k$, where $\epsilon_k{}^0=\hbar^2\mathbf{k}^2/2m$. It is assumed that the dimensions of the container are sufficiently large, so that k_α can be taken to be an essentially continuous variable. In cases where this condition is not satisfied, interesting effects occur which depend on the size and shape of the container.[8]

Making use of a plane-wave representation, we define a new spatially dependent distribution function[9,10] $\tilde{g}_T(\mathbf{k},\mathbf{r},t)$ in terms of a sum over the density matrix of $\tilde{\rho}_T$:

$$\tilde{g}(\mathbf{k},\mathbf{r},t)=\sum_{q}e^{i\mathbf{q}\cdot\mathbf{r}}\tilde{\rho}_{T\;k+(q/2)\;k-q/2}. \quad (4.3)$$

It will be found that $\tilde{g}_T(\mathbf{k},\mathbf{r},t)$ corresponds exactly to the ordinary classical distribution function by showing that it satisfies a Boltzmann transport equation that includes the spatial gradient term. We begin by forming the appropriate matrix of Eq. (2.10) and multiplying it by $e^{i\mathbf{q}\cdot\mathbf{r}}$. By summing the resulting equation over $\mathbf{q}$ and making use of the definition (4.3) we find, after considerable algebra, that $\tilde{g}_T(\mathbf{k},\mathbf{r},t)$ satisfies the equation

$$\begin{aligned}i\hbar\frac{\partial\tilde{g}_T}{\partial t}(\mathbf{k},\mathbf{r},t)=&-\frac{i\hbar^2}{m}\mathbf{k}\cdot\nabla_r\tilde{g}_T(\mathbf{k},\mathbf{r},t)-ie\mathbf{E}^0\cdot\nabla_k\tilde{g}_T(\mathbf{k},\mathbf{r},t)\\&-\frac{ie\hbar}{mc}(\mathbf{k}\times\mathbf{B})\cdot\nabla_k\tilde{g}_T(\mathbf{k},\mathbf{r},t)+\sum_{k'}\tilde{g}_T(\tfrac{1}{2}(\mathbf{k}+\mathbf{k}'),\mathbf{r},t)\\&\times\{e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}H'_{kk'}-e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}H'_{k'k}\}. \quad (4.4)\end{aligned}$$

In the process of obtaining this result, partial integrations have been performed with respect to $\mathbf{r}'$ and $\mathbf{k}'$ making use of the physically reasonable assumptions

$$\lim_{r_\alpha\to\infty}\tilde{g}_T(\mathbf{k},\mathbf{r},t)=0,$$

$$\lim_{k_\alpha\to\infty}\tilde{g}_T(\mathbf{k},\mathbf{r},t)=0.$$

In obtaining Eq. (4.4) no special assumptions have been made about the scattering potential other than that of its being a function only of the spatial coordinates; consequently, it can be applied equally well to a system that includes, in addition to $H'(\mathbf{r})$, a periodic lattice potential $V(\mathbf{r})$ as well.

Eq. (4.4) now has a form which closely resembles that of the Boltzmann equation; only the collision sum on the right-hand side of the equation needs further

[8] L. Friedman, Phys. Rev. **134**, A336 (1964).
[9] E. Wigner, Phys. Rev. **40**, 749 (1932).
[10] O. Von Roos, Phys. Rev. **119**, 1174 (1960).

modification. An examination of this term suggests that it would be useful to establish a relationship between $\tilde{g}_T[\frac{1}{2}(\mathbf{k}+\mathbf{k}'),\mathbf{r},t]$ and $\tilde{g}_T(\mathbf{k},\mathbf{r},t)$ in order to obtain an equation for $\tilde{g}_T(\mathbf{k},\mathbf{r},t)$ itself. In order to accomplish this we examine the matrix equation satisfied by $\tilde{\rho}_T$. Inserting (4.1) into (2.10), we find that

$$\left[\omega_{kk'}-i\hbar\frac{\partial}{\partial t}\right]\tilde{\rho}_{Tkk'}=(\tilde{\rho}_{Tk}-\tilde{\rho}_{Tk'})H'_{kk'}+\tilde{c}_{Tkk'}+\sum_{k'';\ (k''\neq k,\ k')}(\tilde{\rho}_{Tkk''}H'_{k''k'}-H'_{kk''}\tilde{\rho}_{Tk''k'})+\frac{ie\hbar}{2mc}(\mathbf{k}+\mathbf{k}')\times\mathbf{B}\cdot(\nabla_k+\nabla_{k'})\tilde{\rho}_{Tkk'},\quad(4.5)$$

where $\epsilon_k=\epsilon_k{}^0+H_{kk}'$, $\omega_{kk'}=\epsilon_k-\epsilon_{k'}$, $\tilde{\rho}_{Tk}\equiv\tilde{\rho}_{Tkk}$, and

$$\tilde{c}_{Tkk'}=-ie\mathbf{E}^0\cdot[\tilde{\rho}_T,\mathbf{r}]_{kk'}=ie\mathbf{E}^0\cdot(\nabla_k+\nabla_{k'})\tilde{\rho}_{Tkk'}.\quad(4.6)$$

Following Kohn and Luttinger, we treat the scattering potential $H'(\mathbf{r})$ as a perturbation, and assume that (4.5) can be solved by taking the diagonal and off-diagonal matrix elements of $\tilde{\rho}_T$ to begin with orders λ^{-2} and λ^{-1}, respectively [see Eq. (4.2)]. It is further assumed that the product of the cyclotron frequency ω_0 and the effective collision relaxation time τ is of order unity[4] or, equivalently, $\omega_0\tau\approx\lambda^0$. This means, effectively, that the magnetic field can be considered to contribute a factor λ^2 for the purpose of determining the order in λ of the various terms in Eq. (4.5). This follows from the fact that τ must begin with a term inversely proportional to the square of the scattering potential. Then to lowest order in λ, Eq. (4.5) becomes just

$$\left[\omega_{kk'}-i\hbar\frac{\partial}{\partial t}\right]\tilde{\rho}_{Tkk'}{}^{(-1)}=(\tilde{\rho}_{Tk}{}^{(-2)}-\tilde{\rho}_{Tk'}{}^{(-2)})H'_{kk'}+ie\mathbf{E}^0\cdot(\nabla_k+\nabla_{k'})\tilde{\rho}_{Tkk'}{}^{(-1)},\quad(4.7)$$

which is of over-all order λ^{-1}.

In general, we would like to solve Eq. (4.7) for $\tilde{\rho}_{Tkk'}$ in terms of $\tilde{\rho}_{Tk}$. However, this cannot be easily accomplished because of the differential operators. In order to simplify the equation enough to find a solution, two further assumptions are made. First, we assume that only terms linear in the electric field are important, which means that the effects of Joule heating are neglected. Then $\tilde{\rho}_T$ can be written as the sum

$$\tilde{\rho}_T(t)=\tilde{\rho}+\tilde{\rho}_E(t),\quad(4.8)$$

where $\tilde{\rho}_E(t)$ is linear in the electric field, and $\tilde{\rho}$ is the time-independent equilibrium distribution in the absence of an electric field. From (2.10), it is found that $\tilde{\rho}$ satisfies the equation

$$[H_0+H',\tilde{\rho}]-\frac{e}{2mc}\sum_\alpha\{(\mathbf{p}\times\mathbf{B})_\alpha[x_\alpha,\tilde{\rho}]+[x_\alpha,\tilde{\rho}](\mathbf{p}\times\mathbf{B})_\alpha\}=0.\quad(4.9)$$

If only terms linear in the electric field are retained, (4.7) becomes

$$\left[\omega_{kk'}-i\hbar\frac{\partial}{\partial t}\right]\tilde{\rho}_{Ekk'}{}^{(-1)}=(\tilde{\rho}_{Ek}{}^{(-2)}-\tilde{\rho}_{Ek'}{}^{(-2)})H'_{kk'},\quad(4.10)$$

because $\tilde{\rho}$ begins with order λ^0 according to Eq. (4.9). Equation (4.10) can still not be easily solved for $\tilde{\rho}_{Ekk'}{}^{(-1)}$ because of the partial time derivative. It is therefore convenient to make the second assumption, that the time derivative of $\tilde{\rho}_E$ can be written

$$\frac{\partial\tilde{\rho}_E}{\partial t}=\tfrac{1}{2}(\tilde{\rho}_E S+S\tilde{\rho}_E),\quad(4.11)$$

where S is in general an operator which may depend on $\mathbf{r}$, $\mathbf{p}$, and t. Substituting (4.11) into Eq. (4.10) gives

$$[\omega_{kk'}-\tfrac{1}{2}i\hbar(S_k+S_{k'})]\tilde{\rho}_{Ekk'}{}^{(-1)}=(\tilde{\rho}_{Ek}{}^{(-2)}-\tilde{\rho}_{Ek'}{}^{(-2)})H'_{kk'}+\tfrac{1}{2}i\hbar(\tilde{\rho}_{Ek}{}^{(-2)}-\tilde{\rho}_{Ek'}{}^{(-2)})S_{kk'}+\tfrac{1}{2}i\hbar\sum_{k'';\ (k''\neq k,\ k')}(\tilde{\rho}_{Ekk''}{}^{(-1)}S_{k''k'}+S_{kk''}\tilde{\rho}_{k''k'}{}^{(-1)}),\quad(4.12)$$

after separating out terms in the sum containing diagonal matrix elements of $\tilde{\rho}_E$ and S and letting $S_k\equiv S_{kk}$. In order to simplify Eq. (4.12) still further we admit only small time variations for which S satisfies the condition

$$\tfrac{1}{2}\hbar S_{kk'}\ll H'_{kk'}.\quad(4.13)$$

Equation (4.12) then becomes

$$\tilde{\rho}_{Ekk'}{}^{(-1)}=\frac{(\tilde{\rho}_{Ek}{}^{(-2)}-\tilde{\rho}_{Ek'}{}^{(-2)})}{\omega_{kk'}-\frac{1}{2}i\hbar(S_k+S_{k'})}H'_{kk'},\quad(4.14)$$

which is good to terms linear in the electric field.

Inverting Eq. (4.3), we find that

$$\tilde{\rho}_{Ekk'}=\frac{1}{V}\int e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}\tilde{g}_E(\tfrac{1}{2}(\mathbf{k}+\mathbf{k}'),\mathbf{r},t)d\mathbf{r},\quad(4.15)$$

where $\tilde{g}_E$ is linear in the electric field, and $\tilde{g}_T$ is now given by the sum of two terms,

$$\tilde{g}_T(t)=\tilde{g}+\tilde{g}_E(t)\quad(4.16)$$

in conformity with (4.8). Substituting (4.15) into (4.14) shows that

$$\tilde{g}_E(\tfrac{1}{2}(\mathbf{k}+\mathbf{k}'),\mathbf{r},t)=\frac{(\tilde{g}_E(\mathbf{k},\mathbf{r},t)-\tilde{g}_E(\mathbf{k}',\mathbf{r},t))}{\omega_{kk'}-\frac{1}{2}i\hbar(S_k+S_{k'})}\times e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}H'_{kk'},\quad(4.17)$$

which is understood to hold only to terms of lowest order in λ and first order in the electric field.

Using (4.17), the collision sum in Eq. (4.4) can be written

$$-\sum_{k';\,(k'\neq k)}(\tilde{g}_E(\mathbf{k},\mathbf{r},t)-\tilde{g}_E(\mathbf{k}',\mathbf{r},t))|H'_{kk'}|^2 \times\{[\omega_{kk'}-\tfrac{1}{2}i\hbar(S_k+S_{k'})]^{-1} -[\omega_{kk'}+\tfrac{1}{2}i\hbar(S_k+S_{k'})]^{-1}\}. \quad (4.18)$$

In general, (4.18) depends on S through $(S_k+S_{k'})$. However, there is a considerable range of $(S_k+S_{k'})$ for which (4.18) is practically independent of $(S_k+S_{k'})$. This range is defined by the following conditions. First,

$$\tfrac{1}{2}(S_k+S_{k'})\ll\tau_a^{-1} \quad (4.19)$$

where τ_a is an atomic time, that is, τ_a is a time associated with the dynamics of the electron, and would be of the order of $\hbar/\bar{\epsilon}$, where $\bar{\epsilon}$ is a typical energy of the electron. Further, if $\frac{1}{2}(S_k+S_{k'})\ll\Delta E/\hbar$, where ΔE is of the order of the spacing of the translational electronic levels, the sum in (4.18) can be replaced by an integral. Then the condition (4.19) enables us to use the well-known result

$$\lim_{\gamma\to+0}(x-i\gamma)^{-1}=P(1/x)+i\pi\delta(x), \quad (4.20)$$

where $\gamma\equiv\frac{1}{2}\hbar(S_k+S_{k'})$, $P(1/x)$ is the principal value of x^{-1}, and $\delta(x)$ is the Dirac delta function. With the aid of (4.20), the collision sum (4.18) becomes

$$-2\pi i\sum_{k';\,(k'\neq k)}(\tilde{g}_E(\mathbf{k},\mathbf{r},t)-\tilde{g}_E(\mathbf{k}',\mathbf{r},t)) \times|H'_{kk'}|^2\delta(\omega_{kk'}). \quad (4.21)$$

In general, the collision sum (4.21) still depends on the positions of all the scatterers. Kohn and Luttinger showed, however, that the summation over k' effectively eliminates this dependence.[11] If there is no correlation between the positions of the scatterers, (4.21) becomes a well-defined expression independent of these positions. Kohn and Luttinger define the ensemble average of a function, which depends on the positions of all the scatterers, as the average of the function over all possible arrangements of the scatterers without any correlation between them. It can then be shown, without any loss of rigor, that it is possible to replace $|H'_{kk'}|^2$ in a sum such as occurs in expression (4.21) by its ensemble average given by

$$\langle|H'_{kk'}|^2\rangle=\frac{n}{\Omega}|\phi_{kk'}|^2, \quad (4.22)$$

where n is the density of scatterers in volume Ω containing a large number of scatterers, and

$$\phi_{kk'}=\int_{-\infty}^{\infty}e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}\phi(\mathbf{r})d\mathbf{r} \quad (4.23)$$

for a potential of finite range.

[11] See Ref. 6, Appendix B.

In the present discussion, we wish to include the possibility that an average spatial gradient in the density of scatterers may exist. Then, in order to make use of the result (4.22) it must be assumed that over distances characteristic of the volume Ω, containing a sufficiently large number of scatterers to give meaning to the ensemble average, the average density of scatterers changes only by a negligible fraction of the average density. Taking $n(\mathbf{r})$ equal to the average density of scatterers at the point $\mathbf{r}$, we require the existence of a volume element Ω satisfying the conditions

$$\frac{n(\mathbf{r})}{\Omega^{1/3}}\gg|\nabla_r n(\mathbf{r})|, \quad (4.24a)$$

$$n(\mathbf{r})\Omega\gg1. \quad (4.24b)$$

For a given gradient of the average density of scatterers, $\nabla_r n(\mathbf{r})$, it is clear that the inequalities (4.24) can always be satisfied by choosing a sufficiently large value of $n(\mathbf{r})$. Once the conditions (4.24) are satisfied, the function $|H'_{kk'}|^2$ contained in a sum over $\mathbf{k}'$ can be replaced by its ensemble average (4.22) in a small region Ω near the point $\mathbf{r}$. The collision sum (4.21) then becomes

$$-\frac{2\pi i}{V}\sum_{k'}{}'(\tilde{g}_E(\mathbf{k},\mathbf{r},t)-\tilde{g}_E(\mathbf{k}',\mathbf{r},t)) \times n(\mathbf{r})|\phi_{kk'}|^2\delta(\omega_{kk'}), \quad (4.25)$$

where the prime on the summation now indicates that $k\neq k'$.

Replacing the sum in Eq. (4.4) with the expression (4.25) gives, finally,

$$0=\frac{\partial\tilde{g}_E(\mathbf{k},\mathbf{r},t)}{\partial t}+\frac{\hbar}{m}\mathbf{k}\cdot\nabla_r\tilde{g}_E(\mathbf{k},\mathbf{r},t) +\frac{1}{\hbar}e\mathbf{E}^0\cdot\nabla_k\tilde{g}(\mathbf{k},\mathbf{r})+\frac{e}{mc}(\mathbf{k}\times\mathbf{B})\cdot\nabla_k\tilde{g}_E(\mathbf{k},\mathbf{r},t) +\frac{n(\mathbf{r})}{(2\pi)^2}\int d\mathbf{k}'(\tilde{g}_E(\mathbf{k},\mathbf{r},t)-\tilde{g}_E(\mathbf{k}',\mathbf{r},t)) \times|\phi_{kk'}|^2\delta(\omega_{kk'}), \quad (4.26)$$

where the sum over k' has been replaced by an integral. In the third term of Eq. (4.25), $\tilde{g}(\mathbf{k},\mathbf{r})$ is the time-independent equilibrium distribution in the absence of an electric field. With methods similar to those used in obtaining Eq. (4.26) it can be shown, starting with (4.9), that $\tilde{g}(\mathbf{k},\mathbf{r})$ must satisfy the equation

$$0=\frac{\hbar}{m}\mathbf{k}\cdot\nabla_r\tilde{g}(\mathbf{k},\mathbf{r})+\frac{e}{mc}(\mathbf{k}\times\mathbf{B})\cdot\nabla_k\tilde{g}(\mathbf{k},\mathbf{r}) +\frac{n(\mathbf{r})}{(2\pi)^2}\int d\mathbf{k}'(\tilde{g}(\mathbf{k},\mathbf{r})-\tilde{g}(\mathbf{k}',\mathbf{r})) \times|\phi_{kk'}|^2\delta(\omega_{kk'}). \quad (4.27)$$

Equation (4.26) has the form of the customary time-dependent Boltzmann equation for a system of fixed scattering centers. It is valid to terms of first order in the electric field, and lowest nonvanishing order in the scattering potential. It is possible to extend the ordering process begun in this section and obtain corrections to Eq. (4.26) involving both the electric field and the scattering potential.

V. CONCLUSION

A system composed of noninteracting electrons scattered by an arbitrary potential in the presence of uniform electric and magnetic fields is studied. It is found that the exact equation for the gauge-independent density operator for this system can be transformed, without the aid of a representation, into a gauge-independent operator equation satisfied by a new density operator. The new density operator is shown to give the correct current density, using the ordinary gauge-independent velocity operator. This transformation to the gauge-independent transport formalism is carried out without approximation, and appears to be exact within the limitations of the present model. The results obtained here are in complete agreement with those found previously by means of a more complicated derivation.

The matrix of the gauge-independent density operator is used to define a new quantum-mechanical distribution function, which depends on the spatial as well as the momentum coordinates. Using a simplified model, it is shown that the new distribution function satisfies an ordinary time-dependent Boltzmann equation, which includes the spatial-gradient term. It can be inferred from this that the new quantum-mechanical distribution function corresponds exactly to the usual classical distribution function describing a system in the presence of a magnetic field. The results obtained here hold only up to terms linear in the electric field and lowest nonvanishing order in the scattering potential. They can, however, be extended to determine higher-order corrections.

The gauge-independent transport formalism provides a way of treating the influence of a magnetic field on a quantum-mechanical system of charged particles without the necessity of explicitly including the often troublesome vector potential. In a later publication, we hope to study some simple systems involving a magnetic field for the purpose of demonstrating the consistency of the gauge-independent equations obtained here with the more usual equations containing the vector potential. This will lead to a determination of some small additional quantum-mechanical terms in the Boltzmann equation.

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