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Gauge-independent statistical mechanics of free electrons in a magnetic field

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The equilibrium distribution function which satisfies the gauge-independent Boltzmann equation is derived using a nonunitary transformation of the exact equilibrium density matrix for free electrons in a magnetic field. An integral representation of this distribution is obtained which approaches continuously the zero-field Fermi-Dirac distribution in the limit of vanishing magnetic field. Moreover, the integral can be evaluated analytically in the limit of nondegenerate statistics and in the extreme quantum limit when quantum oscillations are no longer present. As a check, expressions for the low-field diamagnetic susceptibility and high-field Hall effect are calculated using this distribution. The results are in exact agreement with those obtained by the more-usual density-matrix approach.

I. INTRODUCTION

The galvanomagnetic transport properties of solids for moderate magnetic fields can be explained quite successfully in terms of the Boltzmann transport equation. That this approach is justified for noninteracting electrons in small magnetic fields was first shown rigorously by Stinchcombe[1] and later using an apparently different method by Thomas.[2] The equivalence of the two methods was subsequently demonstrated by Mertsching and Streitwolf[3] who pointed out that the Boltzmann equation could be obtained from a simple nonunitary transformation of the Liouville equation. An interesting aspect of this transformation is that the transformed equilibrium density matrix is diagonal in the momentum representation. Thomas[4] studied the form of this new distribution function in the limit of small magnetic fields and classical Boltzmann statistics and showed that it approaches continuously the zero-field Boltzmann distribution. This result was significant since it also provided some justification for using the zero-field equilibrium distribution in the semiclassical analysis of transport for a nondegenerate system in a magnetic field. Since, in the semiclassical theory of transport in metals, the zero-field Fermi-Dirac distribution is always used, it is important to know whether a result similar to that obtained by Thomas also holds for the degenerate case. The main purpose of this paper is to show that the Thomas[4] work, which assumed classical Boltzmann statistics, can in fact be generalized to include Fermi-Dirac statistics by applying the nonunitary transformation (in the form given by Mertsching and Streitwolf[3]) to the equilibrium density matrix for free electrons in a magnetic field.

We begin with a brief discussion of the derivation of the Boltzmann equation in order to properly define the transformation of the equilibrium density matrix. An exact integral representation of the transformed equilibrium distribution is then obtained for arbitrary magnetic fields and Fermi-Dirac statistics. The low-field behavior of this distribution is considered and is shown to reduce to the zero-field Fermi-Dirac distribution. To show that the expression for the transformed distribution is correct, the low field diamagnetic susceptibility and the Hall effect in the absence of scattering are calculated. The well-known results obtained by the more standard density matrix are reproduced.

II. BOLTZMANN EQUATION

Consider a system of noninteracting free electrons in a uniform magnetic field $\vec{H}$ and uniform electric field $\vec{E}$. The statistical mechanics of the system can be described in terms of the single-particle density matrix ρ, which satisfies the Liouville equation

$$i\hbar\frac{\partial\rho}{\partial t}=[\mathcal{H},\rho] \ , \tag{1}$$

where $\mathcal{H}$ is the Hamiltonian for the system,

$$\mathcal{H}=(1/2m)[\vec{p}-(e/c)\vec{A}]^2-e\vec{E}\cdot\vec{r} \ ,$$

$\vec{A}$ is the vector potential defined by $\vec{H}=\vec{\nabla}\times\vec{A}$, e is the electronic charge, c is the speed of light, and $\hbar$ is Planck's constant divided by 2π. As shown in Refs. 1–3 there exists an operator f, which satisfies the Boltzmann equation

$$i\hbar\frac{\partial f}{\partial t}=\frac{1}{2m}[p^2,f]-e\vec{E}\cdot[\vec{r},f] -\frac{e}{2mc}\{\vec{p}\times\vec{H}\cdot[\vec{r},f]+[\vec{r},f]\cdot\vec{p}\times\vec{H}\} \ , \tag{2}$$

and f is related to ρ by a nonunitary transformation which is expressed most simply in the coordinate representation as

$$f_{rr'}=\rho_{rr'}\exp(-i\lambda_{rr'}/\hbar) \ , \tag{3}$$

with

$$\lambda_{rr'}=(e/2c)\vec{r}\cdot\vec{H}\times\vec{r}'+(e/c)(\Phi_r-\Phi_{r'}) \ ,$$

and where

$$\vec{A}_r=\tfrac{1}{2}\vec{H}\times\vec{r}+\nabla_r\Phi_r$$

defines Φ_r.

The following results are also obtained and will be used later: For the number of particles N (this defines the normalization),

$$N=\mathrm{Tr}(\rho)=\mathrm{Tr}(f) \ , \tag{4a}$$

and for the current density $\vec{J}$,

$$\vec{J}=(e/m)\,\mathrm{Tr}\{[\vec{p}-(e/c)\vec{A}]\rho\}=(e/m)\,\mathrm{Tr}(\vec{p}f) \ . \tag{4b}$$

III. EQUILIBRIUM DISTRIBUTION

Using Cartesian coordinates with the direction of $\vec{H}$ defining the z axis, $\vec{H}=(0,0,H)$, and choosing the Landau gauge, $\vec{A}=(0,Hx,0)$, the expression for $\lambda_{rr'}$ can be written

$$\lambda_{rr'}=(eH/2c)(x+x')(y-y') \ . \tag{5}$$

In this gauge and in zero electric field, the eigenfunctions and eigenvalues of $\mathcal{H}$ are, respectively,

$$\psi_\alpha(\vec{r})=(1/2\pi)\exp(iK_y y+iK_z z)\phi_n(x-x_0) \tag{6a}$$

and

$$\epsilon_\alpha=(n+\tfrac{1}{2})\hbar\omega+\epsilon_z \ , \tag{6b}$$

where α denotes the set of quantum numbers, $\alpha=\{n,K_y,K_z\}$, $n=0,1,2,\ldots$, $\phi_n(x-x_0)$ is the normalized nth harmonic-oscillator wave function centered about

$$x_0=\frac{\hbar c}{eH}K_y, \quad \epsilon_z=\frac{\hbar^2K_z^2}{2m} \ , \quad \omega=\frac{|e|H}{mc} \ .$$

In the energy representation, the single-particle equilibrium density matrix is diagonal and is given simply by the Fermi-Dirac distribution function

$$\rho_\alpha=\{\exp[\beta(\epsilon_\alpha-\mu)+1]\}^{-1} \ , \tag{7}$$

where $\beta=(k_BT)^{-1}$, k_B is Boltzmann's constant, T is the temperature, and μ is the chemical potential. Applying the transformation defined by Eq. (3) one obtains the transformed operator f which is diagonal in the momentum representation ($\vec{K}$ representation). For this new distribution function, one has

$$f(\vec{K})=2\int_{-\infty}^{\infty}dx\sum_{n=0}^{\infty}(-1)^n\rho_n(K_z)\times\exp(-2iK_xx)\phi_n(x-x_0)\phi_n(x+x_0) \ . \tag{8}$$

The integral in Eq. (8) can be done and the result expressed in terms of the Laguerre polynomials L_n as

$$f(\vec{K})=2\exp(-u)\sum_n(-1)^nL_n(2u)\rho_n(K_z) \ , \tag{9}$$

where $u=(\hbar/m\omega)(K_x^2+K_y^2)$. The details of the above integration are given in the Appendix.

At this point one should calculate $\mathrm{Tr}(f)$ to check the normalization and show that $\mathrm{Tr}(f)=\mathrm{Tr}(\rho)$. Using either Eq. (8) or Eq. (9), one obtains

$$\begin{aligned}\mathrm{Tr}(f)&=\frac{2}{(2\pi)^3}\int d^3K\,f(\vec{K})\\&=\frac{2}{(2\pi)^2}\frac{m\omega}{\hbar}\sum\int dK_z\,\rho_n(K_z)\\&=\mathrm{Tr}(\rho) \ .\end{aligned} \tag{10}$$

As shown in the Appendix, $f(\vec{K})$ is also given by the following exact integral representation:

$$f(\vec{K})=\frac{1}{4}\int_{-\infty}^{\infty}dv\,\frac{\exp\{-\beta(\epsilon_z-\mu)[\frac{1}{2}(1+iv)]\}\exp(-u\tanh\{\frac{1}{2}\beta\hbar\omega[\frac{1}{2}(1+iv)]\})}{\cosh(\frac{1}{2}\pi v)\cosh\{\frac{1}{2}\beta\hbar\omega[\frac{1}{2}(1+iv)]\}} \ , \tag{11}$$

where u is the same as defined in Eq. (9). The integral in Eq. (11) can be done by closing the contour in the appropriate half-planes. However, when $\epsilon_z<\mu-\frac{1}{2}\hbar\omega$, the contour must be closed in the upper half-plane where there are essential singularities coming from the poles of $\tanh\{\frac{1}{2}\beta\hbar\omega[\frac{1}{2}(1+iv)]\}$. The results are in that case very complicated and not easily interpreted as to their physical significance. It is better in fact to leave the integral as it is; that is, when f is used to calculate some physical quantity, the integration over K_x and K_y can often be done first which will eliminate the term containing the essential singularities. On the other hand, when $\epsilon_z>\mu-\frac{1}{2}\hbar\omega$, the contour can be closed in the lower half-plane where there are only the simple poles of $[\cosh(\frac{1}{2}\pi v)]^{-1}$. That case corresponds to either the high-temperature limit when μ becomes negative or the extreme quantum limit when $\frac{1}{2}\hbar\omega>\mu$. Closing the contour then in the lower half-plane, one obtains, for $f(\vec{K})$,

$$f(\vec{K}) = \sum_{m=0}^{\infty} (-1)^m \frac{\exp[-(m+1)\beta(\epsilon_z - \mu)] \exp\{-u \tanh[\frac{1}{2}(m+1)\beta\hbar\omega]\}}{\cosh[\frac{1}{2}(m+1)\beta\hbar\omega]} \tag{12}$$

IV. SMALL-FIELD APPROXIMATION

When $\beta\hbar\omega << 1$, the field-dependent terms in Eq. (11) can be expanded in powers of $\beta\hbar\omega$. Keeping terms to order $(\beta\hbar\omega)^2$ one obtains, for the distribution,

$$f(\vec{K}) = g(\epsilon) - \left(\frac{\hbar\omega}{2}\right)^2 \left(\frac{1}{2}\frac{d^2g}{d\epsilon^2} + \frac{1}{3}\epsilon_\perp \frac{d^3g}{d\epsilon^3}\right) . \tag{13}$$

In Eq. (13), $\epsilon = \hbar^2K^2/2m$, $\epsilon_\perp = \epsilon - \epsilon_z$, and $g(\epsilon) = \{\exp[\beta(\epsilon-\mu)]+1\}^{-1}$ which, apart from the quadratic dependence of μ on H is simply the zero-field Fermi-Dirac distribution function. In the two limiting cases of degenerate ($k_BT << \mu$) and nondegenerate ($k_BT >> \mu$) statistics, one can do the integral in Eq. (4a) using the small field expression for $f(\vec{K})$ in Eq. (13). The results of these integrations give the following expressions for μ as a function of magnetic field:

$$\mu = \mu_0\left[1 + \frac{1}{12}\left(\frac{\hbar\omega}{2\mu_0}\right)^2\right], \quad k_BT << \mu \tag{14a}$$

and

$$\mu = \mu_0\left[1 + \frac{1}{12}(\beta\hbar\omega)\left(\frac{\hbar\omega}{2\mu_0}\right)\right], \quad k_BT >> \mu , \tag{14b}$$

where μ_0 is the chemical potential in zero field, $\mu_0 = \mu(T,H=0)$. The expansions of $f(\vec{K})$ about the respective zero-field distribution functions are

$$f(\vec{K}) = g^0(\epsilon) - \left(\frac{\hbar\omega}{2}\right)^2 \left(\frac{1}{12\mu_0}\frac{dg^0}{d\epsilon} + \frac{1}{2}\frac{d^2g^0}{d\epsilon^2} + \frac{1}{3}\epsilon_\perp \frac{d^3g^0}{d\epsilon^3}\right), \quad k_BT << \mu \tag{15a}$$

and

$$f(\vec{K}) = g^0(\epsilon)[1 + \tfrac{1}{12}(\beta\hbar\omega)^2(\beta\epsilon_\perp - 1)] , \quad k_BT >> \mu , \tag{15b}$$

where $g^0(\epsilon)$ is precisely the zero-field Fermi-Dirac distribution

$$g^0(\epsilon) = \{\exp[\beta(\epsilon-\mu_0)]+1\}^{-1} ,$$

which of course reduces to the classical Boltzmann distribution in the high-temperature limit; i.e., in Eq. (15b),

$$g^0(\epsilon) = \exp[-\beta(\epsilon-\mu_0)] .$$

One should note that while Eq. (15a) is a new result, Eq. (15b) is exactly the expression obtained by Thomas[4] for the classical Boltzmann electron gas.

V. LANDAU DIAMAGNETISM

As a check on the validity of this transformed distribution, we consider the susceptibility for the two cases, $k_BT << \mu$ and $k_BT >> \mu$. In either case one needs the thermodynamic potential Ω, which can be obtained from the expression for the number of particles $N = -(\partial\Omega/\partial\mu)_{T,H}$. Using Eqs. (4a) and (13) yields the following expression for Ω:

$$\Omega = \frac{2}{(2\pi)^3}\int d^3K \left[k_BT \ln(1-g) - \left(\frac{\hbar\omega}{2}\right)^2\left(\frac{1}{2}\frac{dg}{d\epsilon} + \frac{1}{3}\epsilon_\perp\frac{d^2g}{d\epsilon^2}\right)\right] , \tag{16}$$

which is valid for all temperatures. For the two limiting cases then,

$$\Omega = -\tfrac{2}{3}\,\mathrm{Tr}(\epsilon g) + \tfrac{1}{6}\nu(\mu_0)(\tfrac{1}{2}\hbar\omega)^2 , \quad k_BT << \mu \tag{17a}$$

and

$$\Omega = -\tfrac{2}{3}\,\mathrm{Tr}(\epsilon g) + \tfrac{1}{6}N\beta(\tfrac{1}{2}\hbar\omega)^2 , \quad k_BT >> \mu , \tag{17b}$$

where $\nu(\mu_0)$ is the zero-field density of states evaluated at $\epsilon = \mu_0$. The susceptibility is calculated according to

$$\chi = \frac{d}{dH}\left[-\left(\frac{\partial\Omega}{\partial H}\right)_{T,\mu}\right] .$$

From Eqs. (17a) and (17b), one then obtains the results of Landau[5]

$$\chi = -\tfrac{1}{3}\nu(\mu_0)(e\hbar/2mc)^2 , \quad k_BT << \mu \tag{18a}$$

and

$$\chi = -\tfrac{1}{3}N\beta(e\hbar/2mc)^2 , \quad k_BT >> \mu . \tag{18b}$$

VI. HALL EFFECT

When the effects of scattering can be neglected ($\omega \mathcal{T} \gg 1$, where $\mathcal{T}$ is an average lifetime), Eq. (2) is appropriate to describe the transport. Expressing Eq. (2) in the momentum representation and considering only the steady state, the following equation remains to be solved:

$$[\vec{E} + (\hbar/mc)\vec{K}\times\vec{H}]\cdot\vec{\nabla}_K f_T = 0 \ , \tag{19}$$

where f_T represents the total distribution. In the linear-response approximation, the solution of Eq. (19) is

$$f_T = f - \frac{\hbar c}{H}\frac{\partial f}{\partial \epsilon_\perp}(K_x E_y - K_y E_x) \ . \tag{20}$$

The current is calculated using Eq. (4b) and yields for the x component

$$J_x = (Nec/H)E_y \ . \tag{21}$$

Therefore, the well-known result for the Hall coefficient[6] R_H is obtained

$$R_H = 1/Nec \ . \tag{22}$$

VII. CONCLUSIONS

An equilibrium distribution which is diagonal in the momentum representation and which satisfies the ordinary Boltzmann transport equation has been considered for free electrons in a uniform magnetic field. When transforming to the momentum representation, an exact summation over the Landau levels is possible and an integral representation of the distribution is obtained. The form of the distribution makes it possible to show by a simple calculation that the Hall coefficient is given by its semiclassical value for arbitrarily large values of the field when scattering effects can be neglected. The distribution can also be expanded about the zero-field Fermi-Dirac distribution function and the leading term is quadratic in the magnetic field. Using this small-field expansion of the distribution, the well-known Landau diamagnetism for spinless electrons is correctly predicted.

In the usual semiclassical treatment of transport in a magnetic field, the zero-field equilibrium distribution is always used. A problem presently under consideration is determing to what extent neglect of field-dependent terms in the equilibrium distribution is justified. This problem is complicated when scattering effects are included but is (nonetheless) one which needs clarification.

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APPENDIX

The details leading to Eqs. (9) and (11) are presented here. Consider first the derivation of Eq. (9) from Eq. (8). The nth harmonic-oscillator wave function ϕ_n is expressed in terms of the nth Hermite polynomial H_n as[7]

$$\phi_n(x) = (1/2^n n!)^{1/2}(m\omega/\pi\hbar)^{1/4}\exp[(-m\omega/2\hbar)x^2]H_n[(m\omega/\hbar)^{1/2}x] \ . \tag{A1}$$

Using the Rodrigues formula[8] for the H_n, the product $\phi_n(x+x_0)\phi_n(x-x_0)$ can be written in the form

$$\phi_n(x-x_0)\phi_n(x+x_0) = \frac{(-1)^n}{2^{2n}n!}\left(\frac{m\omega}{\hbar}\right)^{1/2}\exp\left(\frac{-m\omega}{\hbar}(x^2+x_0^2)\right)\sum_{s=0}^{n}\binom{n}{s}(-1)^s H_{2s}\left[\left(\frac{2m\omega}{\hbar}\right)^{1/2}x\right]H_{2n-2s}\left[\left(\frac{2m\omega}{\hbar}\right)^{1/2}x_0\right] \ , \tag{A2}$$

and for the Fourier transform, one then obtains

$$\int dx\,\exp(-2iK_x x)\phi_n(x-x_0)\phi_n(x+x_0) = \frac{(-1)^n}{2^{2n}n!}\exp\left(\frac{-\hbar}{m\omega}(K_x^2+K_y^2)\right)\sum_{s=0}^{n}\binom{n}{s}H_{2s}\left[\left(\frac{2\hbar}{m\omega}\right)^{1/2}K_x\right]H_{2n-2s}\left[\left(\frac{2\hbar}{m\omega}\right)^{1/2}K_y\right] \ . \tag{A3}$$

The sum on the right-hand side of Eq. (A3) is simply $(-1)^n 2^{2n} n! L_n$, where L_n is the nth Laguerre polynomial,[8] and Eq. (A3) becomes

$$\int dx\,\exp(-2iK_x x)\phi_n(x-x_0)\phi_n(x+x_0) = \exp(-u)L_n(2u) \ , \tag{A4}$$

where $u = (\hbar/m\omega)(K_x^2+K_y^2)$ is defined in Eq. (9).

To obtain Eq. (11) from Eq. (9), first write the distribution in the form

$$\rho_n(K_z) = \exp(an+b)/\cosh(an+b) \ , \tag{A5}$$

where $a \equiv -\frac{1}{2}\beta\hbar\omega$ and $b \equiv -\frac{1}{2}\beta(\epsilon_z + \frac{1}{2}\hbar\omega - \mu)$. Next, Fourier transform $[\cosh(an+b)]^{-1}$ to obtain

$$f(\vec{K}) = \frac{1}{2}\exp(-u)\int_{\infty}^{\infty} d\nu \frac{\exp[b(1+i\nu)]}{\cosh(\frac{1}{2}\pi\nu)} \sum_{n=0}^{\infty} L_n(2u)\{-\exp[a(1+i\nu)]\}^n \ . \tag{A6}$$

Then using the generating function for the Laguerre polynomials[8]

$$\sum_{n=0}^{\infty} L_n(t) z^n = \left(\frac{1}{1-z}\right)\exp\left(\frac{tz}{z-1}\right) \ , \quad |z|<1 \ , \tag{A7}$$

one obtains the integral representation of $f(\vec{K})$ given by Eq. (11).

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