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On Diamagnetism and Non-Dissipative Transport

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Abstract. The states of free electrons in a magnetic field confined to a box of finite volume are determined and used to calculate the average magnetic moment and the non-dissipative electric and heat current in an unambiguous way. It is shown that for infinite volume the average magnetic moment coincides with the magnetization calculated by Landau. Similarly, for infinite volume, the non-dissipative transport coefficients coincide with those calculated by Zyryanov and Silin who use Landau's method and subtract the purely diamagnetic parts from the total currents. We think that our considerations give an answer to the often discussed question, why the Landau calculation of the magnetization and similar calculations of the non-dissipative transport coefficients are correct for a large system.

1. Introduction

In the eyes of many physicists, the Landau diamagnetism of free electrons in a box [1] is simple text book knowledge. Others, however, are of the opinion that Landau's calculation of magnetization is either incomprehensible or not convincing—even in those cases when they do not doubt the correctness of Landau's formula for susceptibility. This is undoubtedly one of the reasons why there are numerous alternative theories, of which those by Teller [2], Kubo [3], and Ohtaka and Moriya [4] should be particularly mentioned. Perhaps the most important objection to Landau's theory is that the role of the "surface electrons" which are reflected on the surface of the box is not clarified. This omission is particularly regrettable because it is precisely the consideration of the surface electrons which leads to the well known theorem of classical statistics, according to which the total magnetic moment of free point charges in the box disappears. As this objection is often formulated, it is not clear just how far the surface electrons are correctly taken into account when, in the counting of states, one neglects those states which correspond to circular orbits, the center of which lies outside of the box. In any case, Landau calculates the free energy using an incomplete set of states (Landau states) without any further justification. It is clear that in such a calculation the identity of the thermodynamic magnetization and the thermal average of the total magnetic moment is violated. To the best of our knowledge, however, this fact has not yet been fully appreciated in the literature.

The aim of the paper by Teller quoted above is the calculation of the magnetization via the surface current. Although Teller "essentially" confirms the result of Landau, his work doesn't give any real insight into the implications of Landau's theory; the theories of Landau and Teller are actually much too different to be compared.

In Section 2 of the present paper we calculate the thermal average of the magnetic moment of free electrons in a box. The finite extension of the box will be taken account of by homogeneous boundary conditions in the eigenvalue problem which replaces Landau's normalization condition. Although the eigenvalue problem can then not be solved exactly in a closed form, general symmetry relations and approximate formulae [5] can be obtained, which are sufficient for our present purposes. In the calculation of the magnetic moment we employ a device used by Teller in which the integrals are divided into surface parts and volume parts. We can then show that, in the limit of an infinite system, the average of the magnetic moment and the magnetization calculation by Landau become identical. At finite volumes, corrections occur which can be calculated explicitely.

The diamagnetism is closely related to the non-dissipative currents which occur in thermally inhomogeneous systems of free electrons [6–21]. The controversy (cf. [18, 19]) among those authors who have made essential contributions to this topic is mainly caused by the fact that some follow Landau's and others follow Teller's procedure. Particularly controversial is the question of how the purely diamagnetic surface currents has to be taken account of.

In Section 3 the currents which flow on the surface of the box are calculated directly. Special treatment for the diamagnetic currents is not necessary. The expressions of the transport coefficients coincide which those obtained by the procedure similar to Landau's after the diamagnetic contributions have been subtracted. Thus, our method of calculation gives justification for such a treatment.

2. Diamagnetism

1. To begin we briefly review Landau's calculation of the magnetization. Landau considers free electrons in a magnetic field $\mathbf{B}=(0,0,B)$ confined to a box of volume $V=L_x L_y L_z$. Choosing the vector potential $\mathbf{A}=(0, Bx, 0)$ he requires, for the energy eigenfunctions, periodic boundary conditions in y and z and normalization condition over the infinite interval $-\infty<x<+\infty$ which corresponds to an infinite length $L_x\to\infty$. In this case the quantum numbers are $\alpha=(n, k_y, k_z)$, $k_y=-x_0/R^2$, $R^2=\hbar c/|e|B$. In the classical description x_0 is the x-coordinate of the center of the cyclotron motion of the electrons in the plane perpendicular to the magnetic field. The eigenfunctions are in y and z plane waves and in x Hermite functions which depend on $x-x_0$. The energy eigenvalues $\varepsilon_\alpha^L=\hbar\omega(n+1/2)+\hbar^2 k_z^2/2m$, $\omega=|e|B/mc$ are in x_0 degenerate. The crucial point is now that, in the counting of states, Landau restricts himself to states with $0\leqq x_0\leqq L_X$, i.e. he neglects those states the center of which lies outside of the box. In the calculation of the thermodynamic potential

$$\Omega=-kT2\sum_\alpha \ln\{1+\exp[(\zeta-\varepsilon_\alpha)/kT]\} \tag{1}$$

the summation over k_y leads to the degeneracy factor

$$L_y\int\frac{dk_y}{2\pi}=\frac{L_y}{2\pi R^2}\int_0^{L_x} dx_0=\frac{L_x L_y}{2\pi R^2}=\frac{L_x L_y}{2\pi\hbar}\frac{|e|B}{c}$$

$$\Omega_L=-kT2\frac{V}{(2\pi\hbar)^2}\frac{|e|B}{c}$$

$$\cdot\sum_n\int_{-\infty}^{\infty} dp_z \ln\{1+\exp[(\zeta-\varepsilon_\alpha^L)/kT]\}.$$

The index L here and in the following denotes that the labeled quantity is calculated by using Landau eigenfunctions, eigenstates, and Landau counting of states. Due to the incomplete counting of states, the identity of the magnetization $\mathfrak{M}=-(\partial\Omega/\partial B)$ and the average of the magnetic moment $\langle M\rangle=2\sum_\alpha f_\alpha^0\left(-\frac{\partial\varepsilon_\alpha}{\partial B}\right)$, where f_α^0 is the Fermi distribution function, is violated. One obtains instead

$$\mathfrak{M}_L=\langle M\rangle_L-\Omega_L/B. \tag{3}$$

It seems therefore desirable to omit the Landau normalization condition and counting of states by taking account of the finite extension of the system in the formulation of the eigenvalue problem.

2. In order to describe an electron in a finite box we require, in place of the Landau normalization condition, that the energy eigenfunctions

$$\psi_\alpha(\mathbf{r})=\frac{1}{\sqrt{L_y L_z}}\exp[i(p_y y+p_z z)/\hbar]\,\mathscr{W}_\alpha(x) \tag{4}$$

vanish outside the interval boundaries $x=0$ and $x=L_x$. The solution to the eigenvalue problem

$$\left\{\frac{\hbar^2}{2m}\frac{d^2}{dx^2}-\frac{m\omega^2}{2}(x-x_0)^2+\left(\varepsilon_\alpha-\frac{\hbar^2 k_z^2}{2m}\right)\right\}\mathscr{W}_\alpha(x)=0 \tag{5}$$

with boundary conditions $\mathscr{W}_\alpha(0)=\mathscr{W}_\alpha(L_x)=0$ leads, for $R\ll L_x$, to the eigenvalues

$$\varepsilon_\alpha=\hbar\omega(n+\tfrac{1}{2})+\frac{\hbar\omega}{\sqrt{2\pi}}\left(\frac{x_0}{R}\right)^{2n+1}\exp\{-x_0^2/2R^2\}+\frac{\hbar^2 k_z^2}{2m} \tag{6}$$

for internal electrons ($x_0>R$) and

$$\varepsilon_\alpha=\hbar\omega[(2n+1)+\tfrac{1}{2}]-\frac{\sqrt{2}}{\pi}\frac{\Gamma(n+\frac{1}{2})}{n!}(2n+1)\hbar\omega\frac{x_0}{R} \tag{7}$$

for surface electrons ($x_0<R$). Here x_0 is measured from the surface at $x=0$.

The energy spectrum is symmetrical in respect to $x_0=L_x/2$,

$$\varepsilon(n, x_0, k_z)=\varepsilon(n, L_x-x_0, k_z) \tag{8a}$$

and correspondingly

$$\mathscr{W}_{n,x_0}(x)=\mathscr{W}_{n,L_x-x_0}(L_x-x). \tag{8b}$$

3. Using "Feynman's Theorem" $\langle\alpha|\frac{\partial H}{\partial\lambda}|\alpha\rangle=\frac{\partial\varepsilon_\alpha}{\partial\lambda}$

$$\frac{\partial\varepsilon_\alpha}{\partial B}=\frac{e^2 B}{m c^2}\int_0^{L_x} x(x-x_0)\,\mathscr{W}_\alpha^2(x)\,dx \tag{9}$$

and with

$$\sum_\alpha\cdots\rightarrow\frac{L_y L_z}{(2\pi\hbar)^2}\frac{|e|B}{c}\sum_n\int_{-\infty}^{\infty}dx_0\int_{-\infty}^{\infty}dp_z\ldots \tag{10}$$

$$\langle M\rangle=-\frac{2L_y L_z}{(2\pi\hbar)^2}\frac{|e|^3 B^2}{m c^3}\sum_n\int dp_z\int dx_0\, f_\alpha^0 \cdot\int_0^{L_x} x(x-x_0)\,\mathscr{W}_\alpha^2(x)\,dx. \tag{11}$$

According to point 2 above we can always find for $R\ll L_x$ an internal state characterized by $\bar{x}_0$, such that up to the exponential correction $\exp\{-x_0^2/2R^2\}$, $\left.\frac{\partial\varepsilon_\alpha}{\partial x_0}\right|_{x_0=\bar{x}_0}=\left.\frac{\partial\varepsilon_\alpha}{\partial x_0}\right|_{x_0=L_x-\bar{x}_0}=0$ holds true.

Corresponding to the division

$$\int_{-\infty}^{\infty}dx_0=\int_{-\infty}^{\bar{x}_0}dx_0+\int_{\bar{x}_0}^{L_x-\bar{x}_0}dx_0+\int_{L_x-\bar{x}_0}^{\infty}dx_0 \tag{12}$$

we obtain three contributions to the average magnetic moment

$$\langle M\rangle=\langle M\rangle_1+\langle M\rangle_2+\langle M\rangle_3 \tag{13}$$

which we now consider successively. Performing the transformation of variables $x_0\rightarrow L_x-x_0$ and $x\rightarrow L_x-x$, and using the symmetry relations (8) and the relation

$$\frac{\partial\varepsilon_\alpha}{\partial x_0}=-\frac{e^2 B^2}{m c^2}\int_0^{L_x}(x-x_0)\,\mathscr{W}_\alpha^2(x)\,dx \tag{14}$$

we obtain

$$\langle M\rangle_3=\langle M\rangle_1-\frac{2V}{(2\pi\hbar)^2}\frac{|e|B}{c}\sum_n\int_{-\infty}^{\infty}dp_z \cdot\int_{-\infty}^{\bar{x}_0}dx_0\, f_\alpha^0\frac{\partial\varepsilon_\alpha}{\partial x_0}. \tag{15}$$

Since, for the quantum number $x_0=\bar{x}_0$, $\varepsilon_\alpha=\varepsilon_\alpha^L$ and therefore

$$\langle M\rangle_3=\langle M\rangle_1+\frac{2V}{(2\pi\hbar)^2}\frac{|e|}{c} \cdot kT\sum_n\int_{-\infty}^{\infty}dp_z\ln\{1+\exp[(\zeta-\varepsilon_\alpha^L)/kT]\}$$

$$=\langle M\rangle_1-\Omega_L/\mathrm{B} \tag{16}$$

holds.

In the expression for $\langle M\rangle_2$, we can replace $\mathscr{W}_\alpha(x)$ by the corresponding Hermite function and extend the integration in respect to x from $-\infty$ to ∞. We obtain then

$$\langle M\rangle_2=\langle M\rangle_L-\frac{2\bar{x}_0}{L_x}\langle M\rangle_L \tag{17}$$

and finally

$$\langle M\rangle=\langle M\rangle_L-\Omega_L/B+K(L_x) \tag{18}$$

where the correction

$$K(L_x)=2\langle M\rangle_1-\frac{2\bar{x}_0}{L_x}\langle M\rangle_L \tag{19}$$

depends explicitely on the extension of the system. Since the choice of $\bar{x}_0$ is independent of L_x, and $\langle M\rangle_1/V$ is of the order $\bar{x}_0/L_x$ we obtain, with Eq. (3) in the limit $L_x\rightarrow\infty$

$$\langle M\rangle=\mathfrak{M}_L. \tag{20}$$

Thus, for an infinite system, the average of the magnetic moment agrees with Landau's expression for the magnetization $\mathfrak{M}_L=-(\partial\Omega_L/\partial B)_{\zeta,T}$. As the preceeding calculations show (c.f. Eq. (15)), the surface electrons (with $\partial\varepsilon_\alpha/\partial x_0\neq 0$) give an essential contribution to the magnetic moment. Although the relative number of surface electrons decreases, their magnetic moment $\left(\frac{e}{2c}\mathbf{r}\times\mathbf{v}\right)$ increases with increasing volume [2].

3. Non-Dissipative Transport

1. From the grand canonical density operator of local equilibrium

$$\rho^l=\frac{\exp\{-\int\beta(\mathbf{r})[\mathscr{H}(\mathbf{r})-\zeta(\mathbf{r})\mathscr{N}(\mathbf{r})]\,d^3r\}}{\operatorname{Tr}\exp\{-\int\beta(\mathbf{r})[\mathscr{H}(\mathbf{r})-\zeta(\mathbf{r})\mathscr{N}(\mathbf{r})]\,d^3r\}} \tag{21}$$

one obtains for independent electrons the single particle density operator

$$f^l=\{\exp\int\beta(\mathbf{r})[H(\mathbf{r})-\zeta(\mathbf{r})\,n(\mathbf{r})]\,d^3r+1\}^{-1} \tag{22}$$

$$=\{\exp[\{\beta(\hat{\mathbf{r}}),H\}-\beta(\hat{\mathbf{r}})\,\zeta(\hat{\mathbf{r}})]+1\}^{-1} \tag{23}$$

where

$$H(\mathbf{r})=\{H,n(\mathbf{r})\}=\tfrac{1}{2}(H\,n(\mathbf{r})+n(\mathbf{r})\,H),\quad n(\mathbf{r})=\delta(\mathbf{r}-\hat{\mathbf{r}}).$$

We assume that the temperature and the chemical potential are smoothly varying functions of x,

$$T(\mathbf{r})=T(x)=T+\frac{\partial T}{\partial x}x,\qquad \zeta(\mathbf{r})=\zeta(x)=\zeta+\frac{\partial\zeta}{\partial x}x. \tag{24}$$

Then, in linear approximation

$$f^l_{\alpha\beta}=f^0_\alpha\,\delta_{\alpha\beta}-\frac{f^0_\alpha-f^0_\beta}{\varepsilon_\alpha-\varepsilon_\beta}\left\{\frac{\partial\zeta}{\partial x}+\left(\frac{\varepsilon_\alpha+\varepsilon_\beta}{2T}-\frac{\zeta}{T}\right)\frac{\partial T}{\partial x}\right\}\hat{x}_{\alpha\beta} \quad (25)$$

holds where f^0_α is again the Fermi distribution function. The stationary single electron density dperator f which describes the non-dissipative transport is defined by the conditions

$$[H,f]=0,\quad \mathrm{Tr}\,f=1,\quad \mathrm{Tr}\,Hf=\mathrm{Tr}\,Hf^0. \quad (26)$$

Putting

$$f=f^l+f^1 \quad (27)$$

with a linearized expression (25) for f^l and $\hat{x}=\hat{x}_0+\hat{\xi}$ with $\langle\alpha|\hat{x}_0|\beta\rangle=x_0\,\delta_{\alpha\beta}$ and $\langle\alpha|\hat{\xi}|\alpha\rangle=0$ the conditions (26) give $f^1_{\alpha\beta}=-f^l_{\alpha\beta}$ for $\alpha\neq\beta$ and $f^1_{\alpha\alpha}=0$. Thus, the stationary density operator is

$$f_{\alpha\beta}=f_\alpha(x_0)\,\delta_{\alpha\beta} \quad (28)$$

$$f_\alpha(x_0)=f^0_\alpha-\frac{\partial f^0}{\partial\varepsilon_\alpha}\left\{\frac{\partial\zeta}{\partial x}+\frac{\varepsilon_\alpha-\zeta}{T}\frac{\partial T}{\partial x}\right\}x_0 \quad (29)$$

i.e.

$$f_\alpha(x_0)=\{\exp[(\varepsilon_\alpha-\zeta(x_0))/kT(x_0)]+1\}^{-1} \quad (30)$$

in linear approximation. Thereby it has been shown that the intuitive distribution function (30) is – at least in linear approximation – the exact stationary distribution.

2. Now we want to calculate the average of the electric current and the heat current in the stationary state characterized by the distribution function (28). The averages of the corresponding current densities can be written as

$$j_y(x)=2\sum_\alpha f_\alpha(x_0)\,j_{y\alpha}(x), \quad (31)$$

$$q_y(x)=2\sum_\alpha f_\alpha(x_0)\,q_{y\alpha}(x) \quad (32)$$

with

$$j_{y\alpha}(x)=-\frac{\hbar|e|}{2mi}\left\{\psi^*_\alpha\left(\frac{\partial}{\partial y}+\frac{i|e|}{\hbar c}Bx\right)\psi_\alpha+h.c.\right\}$$
$$=-\frac{|e|\,\omega}{L_y L_z}(x-x_0)\,\mathscr{W}^2_\alpha(x) \quad (33)$$

and

$$q_{y\alpha}(x)=\frac{\omega}{L_y L_z}(x-x_0)(\varepsilon_\alpha-\zeta)\,\mathscr{W}^2_\alpha(x). \quad (34)$$

It should be pointed out that these expressions differ essentially from the formally similar expressions in [6, 7] since, in our expressions, the contribution of the surface electrons is fully taken account of. We can, therefore, in the following calculation of the total charge and heat transport

$$J_y=\int j_y(x)\,d^3r,\qquad Q_y=\int q_y(x)\,d^3r \quad (35)$$

perform the integration with respect to x and the summation in respect to x_0 in arbitrary order. With (14) and the linearized distribution function (29) we obtain

$$J_y=-\frac{2c}{B}\sum_\alpha\frac{\partial f^0}{\partial x_0}x_0\left\{\frac{\partial\zeta}{\partial x}+\frac{\varepsilon_\alpha-\zeta}{T}\frac{\partial T}{\partial x}\right\} \quad (36)$$

$$Q_y=\frac{2c}{|e|B}\sum_\alpha\frac{\partial f^0_\alpha}{\partial x_0}x_0(\varepsilon_\alpha-\zeta)\left\{\frac{\partial\zeta}{\partial x}+\frac{\varepsilon_\alpha-\zeta}{T}\frac{\partial T}{\partial x}\right\} \quad (37)$$

and herewith, after using (10) and partial integration

$$J_y=\sigma_{yx}\left\{-\frac{1}{e}\frac{\partial\zeta}{\partial x}\right\}+\beta_{yx}\left\{-\frac{1}{T}\frac{\partial T}{\partial x}\right\} \quad (38)$$

$$Q_y=\gamma_{yx}\left\{-\frac{1}{e}\frac{\partial\zeta}{\partial x}\right\}+\kappa_{yx}\left\{-\frac{1}{T}\frac{\partial T}{\partial x}\right\} \quad (39)$$

with transport coefficients

$$\sigma_{yx}=2\frac{L_y L_z}{(2\pi\hbar)^2}e^2\sum_n\int_{-\infty}^{\infty}dp_z\int_{-\infty}^{\infty}dx_0\,f^0_\alpha=-\frac{ce}{B}N \quad (40)$$

$$\beta_{yx}=\gamma_{yx}=2\frac{L_y L_z}{(2\pi\hbar)^2}|e|\sum_n\int_{-\infty}^{\infty}dp_z\int_{-\infty}^{\infty}dx_0$$
$$\cdot\frac{\partial f^0_\alpha}{\partial x_0}x_0(\varepsilon_\alpha-\zeta) \quad (41)$$

$$\kappa_{yx}=-2\frac{L_y L_z}{(2\pi\hbar)^2}\sum_n\int_{-\infty}^{\infty}dp_z\int_{-\infty}^{\infty}dx_0\frac{\partial f^0_\alpha}{\partial x_0}x_0(\varepsilon_\alpha-\zeta)^2 \quad (42)$$

N is the number of electrons in the volume V.

Up to corrections of the order $\bar{x}_0/L_x$, the coefficient β_{yx} can be written as

$$\beta_{yx}=\frac{2V}{(2\pi\hbar)^2}|e|\sum_n\int_{-\infty}^{\infty}dp_z\int_{L_x-\bar{x}_0}^{\infty}dx_0(\varepsilon_\alpha-\zeta)\frac{\partial f^0_\alpha}{\partial x_0}$$
$$=\frac{cT}{B}\left(\frac{\partial\Omega_L}{\partial T}\right)_{\zeta,B} \quad (43)$$

and furthermore, since for a large system $\Omega_L\simeq\Omega$ holds, and $S=-(\partial\Omega/\partial T)_{\zeta,B}$ the total entropy is,

$$\beta_{yx}=-\frac{cST}{B}. \quad (44)$$

Analogous calculations lead to

$$\kappa_{yx}=-\frac{c}{eB}\int_{-\infty}^{\zeta}T^2\left(\frac{\partial S}{\partial T}\right)_{\zeta',B}d\zeta'. \quad (45)$$

The expressions (40) (44) and (45) for the transport coefficients have been derived with different methods in the papers [6–19] (c.f. also [20, 21]). The direct calculation of the currents and transport coefficients given in the present paper doesn't require a separate treatment of the diamagnetic contributions (as in the papers [6–8, 11–15, 21]). Our treatment can be understood as a refinement and a justification of Obratzov's theory [9, 10, 19].

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