Rigorous Formalism for Landau Diamagnetism

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Abstract

The magnetic moment at a finite temperature $M(H, \mu, T)$ is expressed as a superposition of $M(H, \nu, O)$. The rigorous calculation about $M(H, \mu, O)$ for a potential of general shape is given. The rigorous relations among the total current I, $\Sigma^{x}\langle jx\rangle$, $\Sigma^{a}\langle jx\rangle$, and the size effect ΔM are derived, which will be powerful for the derivation of some integral theorems in some specified potential in the succeeding paper.

Introduction

There have been a number of papers concerning to the size effect in Landau diamagnetism and to the current distribution near the boundary. However, a clear answer has not, the author believes, been given as yet in the sixty years elapse since the first paper of Landau[1~4].

Two different methods for this answer are found. The first is the direct calculation of wave functions using some approximation such as W.K.B., leading to much different conclusions by different authors[5~8]. It has an intrinsic difficulty. Enormous magnitudes of the magnetic moments e.g. $\propto H^{-1}$ are derived in the process of calculation, and the answer is their minute difference e.g. $\propto H^{0}$. In order to obtain an approximate answer e.g. $\propto H^{0}$, the calculation of the term e.g. $\propto H^{-1}$ must be exact and no approximation is allowable.

The second is the calculation of linear response by Green's function, leading to a conclusion of very small size effect[9,10]. Although it is elegant and powerful, the theoretical basis for its validity is not clear. The moment at $T=0°$K is known to have an intrinsic singularity at $H=0$ as a function of the magnetic field H[4]. It happens to be linear at a finite temperature or in an inhomogeneous field, as a result of smoothing effect. However, it doesn't imply that other quantity such as the size effect ΔM or the current density $J(x)$ is linear at a finite temperature.

In this paper discussions are given of some rigorous formulas valid in a potential of general form, which will be used in the succeeding paper in order to derive some integral formulas in the potential of an infinite step function. And also of some features often regarded to be somewhat paradoxical.

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Fundamental Processes

Let us consider free electrons confined in a box LL_yL_z in a homogeneous magnetic field H in the z-direction, expressed by the vector potential $[0, (L+x)H, 0]$. The appearance of Landau diamagnetism with infinitely slowly increasing field is viewed to be a quasi-static process consisting of three fundamental processes;

1) Drift of orbits in the x-direction and compression of density. The Lorentz force by this drift and the electric field in the y-direction just cancel.

2) Energy increase by the inhomogeneous electric field and dilation of density in the E-space (E; energy). The compression in x-space and the dilation in E-space conserve the density in E-x-space constant.

3) Non-dissipasive relaxation near Fermi level.

These three processes complete the circulation of the center of orbit in E-x-space. For infinitely large L, the drift velocity at $x=0$ is infinitely large. Here exists the reason of the paradoxical arguments at the ealier period. Landau's approach is first to calculate the grand potential Ω neglecting the contribution from the surface and next to calculate its derivative[1].

$$\Omega = -kT\Sigma \log[1+\exp\{(\mu-E_i)/kT\}]$$
$$-M = \partial\Omega/\partial H$$

Teller's approach is first to calculate the derivative concerning to an individual electron and next to calculate the sum[2]. The contribution from the surface is by no means negligible. Both the contribution from the bulk and that from the surface are enormous, and the sum is their minute difference.

$$-M = \Sigma(\partial E_i/\partial H)/[1+\exp\{(\mu-E_i)/kT\}]$$

Once it is noticed that both approaches are just similar to the Euler's or Lagrange's in fluid mechanics, the apparent paradox completely vanishes. An individual electron near the surface drifts infinitely quickly for infinitely large L. So that the derivative $\partial E_i/\partial H$ near the surface doesn't give the contribution to $\partial\Omega/\partial H$ in the surface but to that in the bulk. So that both approaches naturally give same result.

It should be stated in addition, that such an explanation often found in the text is erroneous that the state density is scarce near the surface so that the paramagnetic current near the surface is smaller than the diamagnetic current inside the bulk. As shown later and more explicitly in the succeeding paper, the state density is surely lower, but the normalized wave function is localized near the surface so that it has larger charge density compared to that of a complete orbit inside the bulk. The average charge density in E-space are quite the same in surface and in bulk. The reason of the appearance of the diamagnetic moment is that it is similar to an alterating series as a function of E. The initial term at the lowest level is always diamagnetic so that the statistical average is diamagnetic.

Calculation

Let us start from the formula for the magnetic moment M derived from the grand potential Ω,

$$M(H, \mu, T) = -\partial\Omega(H, \mu, T)/\partial H \tag{1}$$

$$\Omega = -kT\sum \log[1+\exp\{(\mu - E_i)/kT\}] \tag{2}$$

This is rewritten as,

$$\begin{aligned} M(H, \mu, T) &= \int_0^\infty \left[-\int_0^\nu \rho \frac{\partial E_i}{\partial H} dE\right] \Big/ [(2kT)\{1+\cosh((\nu-\mu)/kT)\}]\, d\nu \\ &= \int_0^\infty M(H, \nu, 0) \Big/ [(2kT)\{1+\cosh((\nu-\mu)/kT)\}]\, d\nu \end{aligned} \tag{3}$$

where ρ denotes the state density. This formula shows that any $M(H, \mu, T)$ at a finite temperature is expressed as a superposition of $M(H, \nu, 0)$ at 0°K integrated over ν. Hereafter we discuss $M(H, \mu, 0)$ and its superposition.

Let us consider a free electron in a uniform magnetic field in the z-direction, confined in a box $LL_yL_z(-L<x<0)$. With the vector potential $[0, (L+x)H, 0]$, the Hamiltonian and the current operator in the y-direction j are written as,

$$\mathscr{H} = \frac{1}{2m} p_x^2 + \frac{1}{2} m\omega^2 (x-a)^2 + \frac{1}{2m} p_z^2 + V(x) \tag{4}$$

$$j = -e\omega(x-a) \tag{5}$$

with

$$\omega = \frac{eH}{mc}, \quad a = -L - \left(\frac{ch}{eH}\right) k_y \tag{6}$$

The surface potential $V(x)$ is of general form near $x=0$ and of its mirror image near $x=-L$. Writing the derivatives of the energy levels $E[k_z, n, \omega(H), a(H, k_y)]$ with constant k_z and n, such that,

$$\left[\frac{\partial E}{\partial H}\right]_{k_y} = \left[\frac{\partial E}{\partial \omega}\right]_a \frac{d\omega}{dH} + \left[\frac{\partial E}{\partial a}\right]_\omega \left[\frac{\partial a}{\partial H}\right]$$

these are also written in terms of the expectation value of the current $\langle j\rangle$ as,

$$\left[\frac{\partial E}{\partial H}\right]_{k_y} = \left\langle \left[\frac{\partial \mathscr{H}}{\partial H}\right]_{k_y} \right\rangle = -\frac{1}{c}(\langle jx\rangle + L\langle j\rangle) \tag{7}$$

$$\left[\frac{\partial E}{\partial \omega}\right]_a \frac{d\omega}{dH} = \frac{\omega}{H}\left[\frac{\partial E}{\partial \omega}\right]_a = -\frac{1}{c}(\langle jx\rangle - a\langle j\rangle) \tag{8}$$

$$\left[\frac{\partial E}{\partial a}\right]_\omega \left[\frac{\partial a}{\partial H}\right]_{k_y} = -\frac{L+a}{H}\left[\frac{\partial E}{\partial a}\right]_\omega = -\frac{1}{c}(L+a)\langle j\rangle \tag{9}$$

we define by $\sum^x\langle j\rangle$ the sum of the current expectation value in half volume $(-L/2<x<0)$, as to wave functions in this region, which yields macroscopic current. And by $\sum^a$ the sum as to electrons centered in this region, which yields, in addition, edge current near $x=-L/2$.

From eqs. (1, 2, 7),

$$-M=\Sigma\left[\frac{\partial E}{\partial H}\right]_{ky}=\Sigma-\frac{1}{c}(\langle jx\rangle+L\langle j\rangle) \tag{10}$$

Since $\Sigma(\langle jx\rangle+L\langle j\rangle)=L\,\Sigma^{x}\langle j\rangle+\Sigma^{x}\langle jx\rangle+\sum^{x}_{x<-L/2}\langle(L+x)j\rangle$, and the sum of the second and the third term is independent of L, the total current I is,

$$L_yI\equiv\Sigma^{x}\langle j\rangle=c(\partial M/\partial L) \tag{11}$$

From eqs. (7, 8, 9), the next two relations are derived.

$$H\left[\frac{\partial E}{\partial H}\right]_{ky}=\omega\left[\frac{\partial E}{\partial\omega}\right]_{a}-(L+a)\left[\frac{\partial E}{\partial a}\right]_{\omega} \tag{12}$$

$$\omega\left[\frac{\partial E}{\partial\omega}\right]_{a}-a\left[\frac{\partial E}{\partial a}\right]_{\omega}=-\frac{H}{c}\langle jx\rangle,\ \text{and}\ \left[\frac{\partial E}{\partial a}\right]_{\omega}=\frac{H}{c}\langle j\rangle \tag{13}$$

If I is concentrated at the boundary like δ-function, it yields a moment M_L without size effect. From eqs. (7-13), substituting the integral by k_y by the integral by a, and counting the spin factor 2, we obtain,

$$\begin{aligned}-M_L&\equiv-\frac{1}{c}LL_yI=-L\frac{\partial M}{\partial L}\\&=\int dk_z 2\frac{L_yL_z}{(2\pi)^2}\left(\frac{e}{c\hbar}\right)L\frac{\partial}{\partial L}\left[\sum_n\left[\int\left[\omega\frac{\partial E}{\partial\omega}-(L+a)\frac{\partial E}{\partial a}\right]da\right]\right]\end{aligned} \tag{14}$$

By symmetry,

$$\int\left[\omega\frac{\partial E}{\partial\omega}-(L+a)\frac{\partial E}{\partial a}\right]da=2\int_{-L/2}\left[\omega\frac{\partial E}{\partial\omega}-a\frac{\partial E}{\partial a}\right]da-L\int_{-L/2}\frac{\partial E}{\partial a}da \tag{15}$$

So that the left of eq. (15) differentiated by L is,

$$\frac{\partial}{\partial L}\left[\int[\quad]da\right]=\left(n+\frac{1}{2}\right)\hbar\omega-\int_{-L/2}\frac{\partial E}{\partial a}da=\left(2n-R+\frac{1}{2}\right)\hbar\omega \tag{16}$$

where R is definded such that,

$$\left(R+\frac{1}{2}\right)\hbar\omega=\mu-\frac{(\hbar k_z)^2}{2m} \tag{17}$$

From eqs. (14, 16) we obtain,

$$-M_L/(LL_yL_z)=\int dk_z\frac{1}{2\pi^2}\left(\frac{e}{c\hbar}\right)\sum_n\left(2n-R+\frac{1}{2}\right)\hbar\omega \tag{18}$$

Averaged over $(N-1/2+\delta)\leqq R<(N+1/2+\delta)$, ($N$; integer, $0\leqq\delta<1$,)

$$\sum_n(\quad)=\frac{1}{2}\delta(1-\delta)\hbar\omega$$

Again averaged over $0\leqq\delta<1$ then $\Sigma(\quad)=(1/12)\hbar\omega$, and next integrated over $-k_F\leqq k_z\leqq k_F$ (k_F ; Fermi wave number),

$$-\overline{M_L}/(LL_yL_z) \equiv -\frac{1}{c}\overline{I}\Big/L_y = \frac{e^2}{12\pi^2 mc^2}k_F H \tag{19}$$

This is just the Landau diamagnetism independent of the form of surface potential.

Now let us consider about the current distribution near the boundary and the size effect of the moment ΔM.

From eqs. (12, 13),

$$\Delta M \equiv M - L\frac{\partial M}{\partial L} = \frac{2}{c}\Sigma^x \langle jx\rangle \tag{20}$$

Substituting eqs. (14, 15, 16) into eq. (20), we obtain,

$$\Delta M = -\int dk_z \frac{2L_yL_z}{(2\pi)^2}\left(\frac{e}{c\hbar}\right)\sum_n\left[2\int_{-L/2}\left[\omega\frac{\partial E}{\partial\omega} - a\frac{\partial E}{\partial a}\right]da - L\left(n+\frac{1}{2}\right)\hbar\omega\right] \tag{21}$$

The integrand is rewritten by eqs. (6, 13),

$$\omega\frac{\partial E}{\partial\omega} - a\frac{\partial E}{\partial a} = -\frac{m\omega}{e}\langle jx\rangle \tag{22}$$

Substituting eq. (22) into eq. (21) and taking into account that the integrand in bulk is just $(n+1/2)\hbar\omega$, we obtain,

$$\frac{c}{2}\Delta M = \Sigma^x \langle jx\rangle = \int dk_z \frac{2L_yL_z}{(2\pi)^2}\left(\frac{e}{\hbar}\right)\sum_n\left[\left(\frac{m\omega}{e}\right)\int_{-D_n}\langle jx\rangle da + D_n\left(n+\frac{1}{2}\right)\hbar\omega\right] \tag{23}$$

where D_n denotes a length a little larger than orbit radius such that the wave amplitude is exponentially negligible. The first term in the right corresponds to $\Sigma^a\langle jx\rangle$, yielding the moments of the edge current near $x=-D_n$, which is just subtracted by the second term. This relation (23), rigorous for a potential of general shape is the main result of this paper which will be powerful to derive some integral theorems in the specified potential in the succeeding paper.

Conclusions

Any magnetic moment $M(H, \mu, T)$ is expressed as a superposition of $M(H, \nu, 0)$ integrated over ν, so that we can give a general argument from $M(H, \mu, 0)$ as a function of μ. The rigorous formula of eq. (23) valid for a potential of general shape shows the relation among ΔM, $\Sigma^x\langle jx\rangle$, and $\Sigma^a\langle jx\rangle$, which will be powerful for the derivation of some rigorous integral theorems. The quasi-static drift of orbits is the clear explanation of the equivalence between Landau's approach and Teller's. The explanation of diamagnetism by the smaller state density in E-space near the surface is erroneous.

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