The Origin of Essential Singularity in Landau Diamagnetism

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Abstract

The current density distribution $J(x)$ in Landau diamagnetism, for any given x, converges to be linear to the magnetic field H with $H \to 0$. However, it never converges uniformly for all x. For $|x| \ll R_F$ (R_F; orbit radius), $J(x)$ is linear to H and has been solved completely. Linear response theory happens to give a correct result only for it, however, it fails for $J(|x| \sim R_F)$ or for the size effect ΔM.

1. Introduction

In a number of papers concerning the size effect of the moment ΔM in Landau diamagnetism, several different conclusions by a few different methods were given[1~6]. Among them, only Ohtaka and Moriya's laborious work gave, in addition to a value for ΔM, a solution for the current density distribution $J(x)$[1]. Green's function method was used there with no approximation required, while in most of others some approximation such as W.K.B. was required[3~6]. However, the theoretical basis as to whether such a linear response theory is applicable or not, is not clear. The moment at $T=0$°K is known to have an essential singularity at $H=0$ as a function of H[7]. It happens to be linear at a finite temperature or in an inhomogeneous field, as a result of smoothing effect. However, it doesn't mean that other quantity such as ΔM or $J(x)$ must be linear at a finite temperature. An a priori assumption that a linear response theory is applicable, led to a logical result that both ΔM and the amplitude of $J(x)$ are $\propto H^1$, whereas several of others predicted that ΔM is $\propto H^{-1/3}$ and far larger. The conclusion that the result has no memory of cyclotron orbit radius at Fermi level R_F, which is important in the results of other several, seems rather unconvincing to insight.

This paper will show an exact treatment without an a priori linear theory nor any approximation more than free electron assumption. It will clarify that Ohtaka and Moriya's linear solution is correct only in the region nearest to the boundary and that the apparent paradox is comprehensibly explained by the concept of uniform convergence in mathematics. The same surface potential as theirs (an infinite step function) is assumed, however, most of the argument keeps the generality applicable also to a finite work function in a further study. It treats the case of a sufficiently weak field and still sufficiently large system size: $k_F^{-1} \ll R_F < L/2$ (k_F; wave number at Fermi level, L; system size), i.e. $2k_F L^{-1} < eH/c\hbar \ll k_F^2$.

Received September 28, 1990

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Let us begin with the above-mentioned smoothing effect. The current density distribution at $T°K$;

$J(x, T, \mu)=\int[\Sigma j_i(x)\delta(E-E_i)] f((E-\mu)/kT)dE$ is expressed as an average of $J(x, 0, \mu)=\int^{\mu}[\Sigma j(x, E_i)\delta(E-E_i)]\, dE$ with a slowly varying weight function of ν, namely,

$$J(x, T, \mu)=\int J(x, 0, \nu)[-f'((\nu-\mu)/kT)/kT]\, d\nu \tag{1}$$

We can verify this relation by integrating by parts. Here, E_i and $j_i(x)$ denote the energy and the current density distribution respectively of one electron state i, and f the Fermi distribution function. Hence we shall hereafter concern ourselves with $J(x, 0, \mu)$ denoted by $J(x)$.

2. Wave Function

Consider a free electron confined in a large box $LL_yL_z(-L<x<0)$ of infinite step function surface potential in a uniform z-direction magnetic field. With the vector potential $[0, (L+x)H, 0]$, the wave function of an electron takes the form $\phi(x, E, a)\exp(ik_yy+ik_zz)(L_yL_z)^{-1/2}$, where $a\equiv-L-(c\hbar/eH)k_y$ denotes the x-coordinate of the center of orbit [7,9].

The current (y-direction) expectation value $\langle j\rangle$ of an electron and the current density created by all electrons $J(x)$ are defined from the current operator $j\equiv-e\omega(x-a)$,[1,7,9]

$$\langle j\rangle\equiv-e\omega\int(x-a)|\phi|^2dx,\quad J(x)\equiv\Sigma -e\omega(x-a)|\phi(x, E, a)|^2L_yL_z \tag{2}$$

where $\omega\equiv eH/mc$ denotes the cyclotron frequency. The adiabatic principle leads to the relation that[7,9]

$$\frac{\partial E}{\partial a}=\frac{m\omega}{e}\langle j\rangle \tag{3}$$

$\phi(x, E, a)$ for $a\ll-D_n$ is a well-known harmonic oscillator wave function. Here, D_n denotes a distance slightly larger than the radius R_n of complete orbit of a state with a guantum number n, such that the wave function is exponentially negligible at $x-a=D_n$. That for $-D_n<a$ also satisfies, in the region $x<0$, the harmonic oscillator wave equation generalized to non-integer eigenvalues. Both even and odd solutions diverge at $x=-\infty$ as well as, if extended to $0<x$ with the surface removed, at $x=+\infty$. Some suitable linear combinations converge at $x=-\infty$. The boundary condition $\phi(0, E, a)=0$ requires E to be a dependent variable of a.

With a real phase factor, $\phi(x, E, a)$ is

$$\phi(x, E, a)=\alpha^{1/2}u(t, r)\Big/[\int_{-\infty}^{b}[u(t, r)]^2dt]^{1/2} \tag{4}$$

with

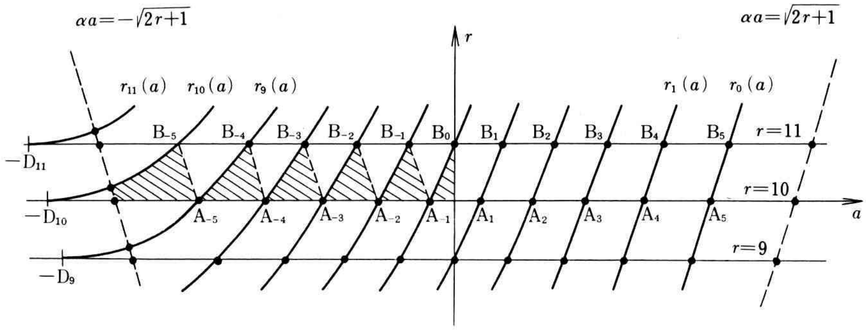

Fig. 1. Curves $r_n\ (a)$: a: center of orbit. $(r+1/2)\hbar_\omega=E-(\hbar k_z)^2/2m$, E; energy. $\alpha^2=m\omega/\hbar$. These curves are the trajectories of nodes of wave functions centered at $x=0$ and convergent at $x=+\infty$.

$$\alpha^2\equiv\frac{m\omega}{\hbar},\ t\equiv\alpha(x-a),\ \left(r+\frac{1}{2}\right)\hbar\omega\equiv E-\frac{(\hbar k_z)^2}{2m},\ b\equiv-\alpha a, \tag{5}$$

and

$$\left[\frac{\partial^2}{\partial t^2}-t^2+(2r+1)\right]u(t,\ r)=0\ [u(-\infty,\ r)=u(b,\ r)=0] \tag{6}$$

For $a\ll-D_n$, r is an integer: $r=n$. For $-D_n<a$ it deviates from n, which we write as $r_n(a)$. Its inverse function is represented by $a_n(r)$. Fig. 1 shows curves of $r_n(a)$ (or $a_n(r)$) which start from the points $(a=-D_n,\ r=n)$ and extend to $r=R$ $[(R+1/2)\hbar\omega\equiv\mu-(\hbar k_z)^2/2m]$. We can also regard these curves as the trajectories of the nodes of wave functions centered at $x=0(a=0)$ and convergent at $x=+\infty$.

It is readily verified by direct differentiation and from eq. (6) that

$$2\int tu^2dt=[t^2-(2r+1)]\ u^2-\left(\frac{\partial u}{\partial t}\right)^2 \tag{7}$$

Insertion of eqs. (4) and (5) into eq. (2) yields

$$\langle j\rangle=-\left(\frac{e\hbar}{m}\right)\alpha\int_{-\infty}^{b}tu^2dt\Big/\int_{-\infty}^{b}u^2dt \tag{8}$$

Inserting eq. (7) into eq. (8), combining it with eq. (3) and taking into account that $u(-\infty,\ r)=u(b,\ r)=0$, we get

$$2\frac{\partial r}{\partial a}=\alpha\,[u'(b)]^2/\int_{-\infty}^{b}u^2dt=\alpha^{-2}\,[\phi'(0)]^2 \tag{9}$$

3. Current $J(x)$

Let us consider the Taylor series for $J(x<0)$ at $x=0$. From its definition in eq. (2), both $J(0)\propto\Sigma a\,[\phi(0)]^2$ and $J'(0)\propto\Sigma\,[2a\phi'(0)-\phi(0)]\,\phi(0)$ vanish. In the second derivative $J''(x)\propto\Sigma[-\{4\phi'+2(x-a)\phi''\}\phi-2(x-a)\phi'^2]$, all terms except the last $\propto\phi'^2$ vanish at $x=0$.

Hence $L_yL_zJ''(0)=e\omega\sum 2a\,[\phi'(0)]^2$. According to eq. (9) we can rewrite $L_yL_zJ''(0)=e\omega\sum 4a\alpha^2(\partial r/\partial a)$.

Let us carry out the summation over states, namely, over k_z, k_y and n. The statistical factor for summation; $2L_yL_z(2\pi)^{-2}\iint dk_z dk_y\sum_n$ is transformed into $2L_yL_z(2\pi)^{-2}\int dk_z\sum_n \int(eH/c\hbar)da$, by transforming the integral by k_y into that by a[7,9]. Then we can write

$$-(L_yL_z)J''(0)=\int dk_z 2\frac{L_yL_z}{(2\pi)^2}\left(\frac{eH}{c\hbar}\right)4e\omega\alpha^2\sum_n\int -a\left(\frac{\partial r}{\partial a}\right)da \tag{10}$$

Rewriting $F(R)\equiv\sum_n\int -a(\partial r/\partial a)da=\int^R[\sum_n - a_n(r)]\,dr$, let us consider what is represented by $\sum_n - a_n(r)$ in Fig. 1. The solid curves on the right half plane represented by positive a's are just the mirror image of the dotted curves. Hence $\sum_n - a_n(r)$ corresponds to the sum of a-coordinates of the dotted curves minus the sum of a-coordinates of the solid curves on the left half. Its integral over $10<r<11$ just equals the area with virgules denoted by S_{10}. The lowest order term in the asymptotic expansion of S_m for $m\to\infty$ is $(2m+1)^{1/2}/2\alpha$ [10].

Since the integrand is positive or zero, $F(R)$ is a monotonically increasing function. Hence, substitution of $F(R=N+\delta)$ [N; integer, $0\leqq\delta<1$] by $F(N)$ creates only an error of higher order. We can therefore carry out the calculation for eq. (10) firstly summing the lowest order asymptotic term in S_m over $0\leqq m\leqq N$ and secondly integrating over $-k_F<k_z<k_F$.

$$-J''(0)=\frac{e^2}{8\pi mc}k_F^4H+\text{H.O. (; higher order terms)} \tag{11}$$

Hereafter H.O. denotes higher order terms. The ratio of H.O. to the lowest order term is of $O(N^{-\gamma})$ i.e. of $O(H^{\gamma})$ $(\gamma>0)$. Similarly as in the derivation of $J''(0)\propto\alpha\sum -4b(\partial r/\partial a)$, succesive differentiation of eq. (2) together with $\phi(0)=\phi'(0)=0$ and also eq. (9) yields that $J^{(3)}(0)\propto\alpha^2\sum -12(\partial r/\partial a)$, $J^{(4)}(0)\propto\alpha^3\sum 16b[(2r+1)-b^2](\partial r/\partial a)$ and $J^{(5)}(0)\propto\alpha^4\sum 80[\{(2r+1)-b^2\}-b^2](\partial r/\partial a)$. Odd order derivative has a factor of even function of b, while even order one has a factor of odd function. The calculation for $J^{(3)}(0)$ is carried out exactly, since the contribution over $m<r<m+1$ is $\propto\sum_n\int(\partial r/\partial a)da=\sum_{n=0}^{m}\left(\int_m^{m+1}dr\right)=m+1$.

In order to investigate the calculation for $J^{(4)}(0)$, let us consider the contribution over $10<r<11$, denoted by $dJ^{(4)}(0)$, in the example in Fig. 1. It takes the form $dJ^{(4)}(0)=\sum_n\int_{10}^{11}f(b,r)(\partial r/\partial a)da=\int_{10}^{11}\left[\sum_{n=0}^{10}f(b,r)\right]dr$. Since f is odd, $\sum f$ is the sum at the solid curves on the left half minus the sum at the dotted curves. Hence $\sum_n f(b.\,11)=0$ and $\sum_n f(b,10+\varepsilon)\to f(-\alpha a_{10}(r),10+\varepsilon)$ for $\varepsilon\to 0$. By interpolation we can evaluate, for an intermediate value of r $(r=10+\delta)$, that $\sum_n f(b,10+\delta)=(1-\delta)f(-\alpha a_{10}(10+\delta),10+\delta)$ with an error of only higher order. Besides, substitution of $f(-\alpha a_{10}(r),r)$ by $f((2r+1)^{1/2},r)=0$ creates an error of only higher order in $dJ^{(4)}(0)$ [10]. We therefore conclude that the lowest order term $\propto m^{3/2}$

in $dJ^{(4)}(0)$ vanishes.

On the other hand, the situation is quite different in the calculation for $J^{(5)}(0)$. Since it is a sum of even function of b; $g(b, r)$, $\sum_n g(b, r)$ is the sum at the solid curves on the left half plus that at the dotted curves. It is therefore approximated by an integral by a, of $g(b, r)$ multiplied by a weight function describing the distribution density of nodes. This approximation creates an error of only higher order. This weight function is approximated by theW.K.B. factor $\rho(b)$, which also creates an error of only higher order,

$$\rho(b)\equiv(2/\pi)[(2r+1)-b^2]^{1/2},\ \left[\int\rho(b)db=r+1/2\right] \tag{12}$$

Since all approximations create errors of only higher order, we will obtain an exact result for the lowest order asymptotic term in $J^{(5)}(0)$.

Let us try to find out general expressions for higher order derivatives. Differentiating eq. (2) p times and using eq. (4), we can write the p-th derivative in terms of $v(t)\equiv u^2$,

$$\begin{aligned}-(L_yL_z/e\omega)J^{(p)}(0)&=\sum\left[-a(\phi^2)^{(p)}+p(\phi^2)^{(p-1)}\right]_{x=0}\\&=\sum 4a^{p-1}[\{bv^{(p)}(b)+pv^{(p-1)}(b)\}/2\{u'(b)\}^2][\{\phi'(0)^2/2a^2]\end{aligned} \tag{13}$$

Let us try to find out some differential equation which v satisfies. Succesive differentiation of $v(t)\equiv u^2$ yields that $v'=2uu'$, $v''=-2K(t)u^2+2u'^2$ and $v^{(3)}=-8K(t)uu'+4tu^2$, where $K(t)\equiv(2r+1)-t^2$. We therefore get a third order differential equation in v,

$$v^{(3)}+4K(t)v'-4tv=0,\ \text{with}\ K(t)\equiv(2r+1)-t^2 \tag{14}$$

Its p times differentiation yields that

$$v^{(p+3)}+4K(t)v^{(p+1)}-4(2p+1)tv^{(p)}-4p^2v^{(p-1)}=0 \tag{15}$$

By induction, it is proved that

$$v^{(2q)}(b)=[-4K(b)]^{q-1}v''(b)+\text{H.O.}$$

and

$$v^{(2q+1)}(b)=4(2q+1)(q-1)[-4K(b)]^{q-2}bv''(b)+\text{H.O.} \tag{16}$$

Inserting eq. (16) into eq. (13), using $v''(b)=2\{u'(b)\}^2$ shown above and also using $\{\phi'(0)\}^2=2a^2(\partial r/\partial a)$ in eq. (9),

$$-(L_yL_z/e\omega)J^{(2q+1)}(0)=\sum 16a^{2q}(2q+1)[(q-1)b^2-K(b)][-4K(b)]^{q-2}(\partial r/\partial a)+\text{H.O.} \tag{17}$$

On the other hand, $J^{(2q)}(0)$ is a sum of an odd function $\propto b[K(b)]^{q-1}$ which vanishes at $b=(2r+1)^{1/2}$. Therefore, the lowest order term$\propto m^{q-1/2}$ in the contribution over $m<r<m+1$, which yields a term$\propto H^1$, vanishes similarly as in $dJ^{(4)}(0)$.

We can carry out the summation for $J^{(2q+1)}(0)$ in eq. (17) similarly as for $J^{(5)}(0)$. Firstly we multiply $\rho(b)$, secondly we integrate by a over $0<b<(2r+1)^{1/2}$, next by r over $0<r<R$, and finally by k_z over $|k_z|<k_F$. The final result is

$$J^{(2q+1)}(0)=\left(\frac{e^2k_F^2}{4\pi^2mc}\right)(-1)^q(2k_F)^{2q+1}\frac{2q}{(2q+3)(2q-1)}H+\text{H.O.} \tag{18}$$

The Taylor series with these coefficients is rewritten in the comprehensible form, in terms of Bessel's function of order 5/2 denoted by $J_{5/2}(z)$ (not the current $J(x)$), that

$$-J(x<0)=\frac{e^2}{64\pi mc}k_F^2(2k_Fx)^2[1+f(2k_Fx)]H+\text{H.O.} \tag{19}$$

with

$$f(z)\equiv\frac{2}{\sqrt{\pi}}\int_0^z\left(\frac{t}{2}\right)^{-5/2}J_{5/2}(t)dt,\ \left[1+f(z\to-\infty)\sim\frac{16}{\pi}z^{-3}\cos(z)\right]$$

The lowest order term in $J(x)$ is linear to H. It is an oscillating function of x with a wavelength $\sim\pi/k_F$ and with a diminishing amplitude $\sim x^{-1}$ in the distance. According to it and to eq. (1) it is estimated that the linear term in $J(x)$ is a good aproximation for a linear term in $J(x,\ T,\ \mu)$ in the region $-(\mu/kT)k_F^{-1}\ll x\leqq 0$.

4. Discussions

We see from eq. (19) that for any given x, with a sufficiently small H, $J(x)$ becomes linear to H. However, it doesn't mean that it is linear everywhere if H is sufficiently small.

It is known that when R increases from $N-0$ to $N+0$ an enormous diamagnetic current (de Haas current) appears, which corresponds to the contribution along the horizontal line $-\infty<a<-D_N$ in Fig. 1[7,8]. This contribution $dJ_N(x)$ is easily evaluated since it consists of merely a chain of complete orbits. We can therefore readily show that it has the factor $\int_{a(D_N+x)}^{+\infty}tu^2dt$. Since this factor is just the left hand side of eq. (7), the estimate of its right hand side by W.K.B. gives a rough evaluation that for $|x+D_N|<R_N$

$$dJ_N(x)\fallingdotseq-dk_z(e^2/2\pi^3mc)aNH[1+(x-D_N)^2/R_N^2]^{1/2}$$

and for $|x+D_N|>R_N$ (it includes $x\sim 0$) $dJ_N(x)$ becomes an exponentially vanishing tail. Since this tail is negligibly small at $x\sim 0$, its Tailor coefficients are negligibly small. Still the set of these small coefficients keep the complete information of $dJ_N(x)$ having a large amplitude in the distance $x\sim-R_N$, where it is a singular function of H.

Note that even if a given function is convergent in the distance, each Taylor term is divergent. Hence, for the function to converge at $x=-\infty$, each Taylor coefficient must not have even a smallest error. Let us examine the example in $J''(0)$. The contribution to it over $k_z\to k_z+dk_z$ is proportional to a monotonic function of R which we write as $G(R)$: $-dJ''(0)/dk_z\propto\int bdr\equiv G(R)$. It has a small oscillating component: $G(R=N)\propto R^{3/2}-(3/16)R^{1/2}$, $G(R=N+1/4)\propto R^{3/2}$, and $G(R=N+1/2)\propto R^{3/2}+(3/16)R^{1/2}$. The main term $\propto R^{3/2}$ yields the exact Tailor coefficient for the convergent function. The second term $\propto\pm(3/16)R^{1/2}$ is too small to break the property of monotonic increase in $G(R)$. Still it creates in $1/2J''(0)x^2$ a component which exceeds the convergent function in the distance and strongly oscillates with H.

We state again that for any given x, $J(x)$ converges to be linear with $H\to 0$. However, with some small value of H fixed, the term H.O. in eq. (19) may exceed the linear term in the distance. We see from the previous argument that for $|x| \ll R_F$, $J(x)$ is linear to H, while for $|x| \sim R_F$ (say $x=-B$) it is not. If we set H to be still sufficiently smaller to make $J(x)$ linear at $x=-B$, then $R_F \propto H^{-1}$ becomes still far larger such that $R_F \ll B$. Thus a linear theory never gives a correct description of $J(x)$ for $|x| \sim R_F$.

The situation just corresponds to the concept for $J(x)$ to be convergent but not to be uniformly convergent in mathematics. Since $J(x)$ is convergent at any given x, the formalism of linear response[11,12] is formally applicable although we are not sure whether it will give a description of the essential feature of the system for $H \to 0$. Therefore Ohtaka and Moriya's calculation, of which the result is in agreement with the linear term in eq. (19), gave a correct result for a linear term [1], although in general a linear theory may not always give a correct answer even to a linear term at an essential singular point [7].

Since it is not uniformly convergent, theformalism of linear response never gives a correct description of $J(x)$ for $|x| \sim R_F$, nor of $\varDelta M$ which is proportional to the integral of $xJ(x)$ over all x, and their calculation therefore failed for $\varDelta M$[1,2].

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