

A Theory of Surface Landau Diamagnetism in exact formalism

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An exact proof is given that such a steady term in surface Landau diamagnetism $\langle \Delta M(\mu, H) \rangle = f(\mu) H^{1-\gamma}$ ($f(\mu)$; of definite sign, $\gamma > 0$) for $H \rightarrow 0$, is non-existent in any region $a < \mu < b$, so long as an infinite square potential is assumed. It is based on the similarity that an electron with H, E, a , (a ; the distance of the center of orbit from the surface) and the one with $NH, NE, a/\sqrt{N}$, have exactly similar wave functions. The region of β for which the partition function $Z(\beta, H)$ is uniformly convergent enlarges $\propto H^{-1}$ for $H \rightarrow 0$, so that the contribution of the Fourier component outside the uniformly convergent region to $\langle \Delta M(\mu, H) \rangle$ vanishes.

Key Words: Non-existence of singular $\langle \Delta M(\mu, H) \rangle = f(\mu) H^{1-\gamma}$, exact similarity of an wave function.

1. Introduction

If surface Landau diamagnetism of an enormous magnitude is found, it will be of great interest theoretically as well as from practical point of view, because it implies large Nernst-Ettinghausen effect, expected to realize efficient thermoelectric conversion.

Studies in the early period predicted an enormous moment $\langle \Delta M \rangle \propto H^{-1/3}$ for $H \rightarrow 0$, where $\langle \Delta M \rangle$ denotes the steady term in surface magnetic moment, provided the sample size L becomes still larger than the orbit radius. The result derived by the typical calculation happens to be a minute difference between an included enormous diamagnetic term and an enormous paramagnetic one. The effect brought about by the approximation far exceeds the result [1]. Later studies led to the conclusions that such an enormous term is non-existent or a higher order singular term $\langle \Delta M \rangle \propto H^{1/2}$ appears [1-6]. However, the exact conclusion is not yet clear to the author, because some approximations are still included in the process before reaching some exact expression of an integrand of definite sign. Furthermore, since an infinite square surface potential is assumed in most cases the calculations strongly depend on some special formulas such as of $\zeta(z)$, so that no prospect is expected for the case of a more general potential.

This letter investigates the relation between surface Landau diamagnetism and the partition function $Z(\beta)$ for an infinite square potential. From the relation that the uniform convergent region of β increases $\propto H^{-1}$ for $H \rightarrow 0$, an exact conclusion is given that such a singular term $\langle \Delta M \rangle \propto H^{1-\gamma}$ ($\gamma > 0$) is non-existent. The proof includes the generality which makes possible the discussion for a more general potential.

An essential requirement in this field is exactness. For example, no reliability is expected to the result derived by a self-consistent field approximation which contradicts the first principle from the beginning, because such an approximation in principle breaks the delicate balance between an enormous diamagnetic magnitude and a paramagnetic one. On the contrary, even the simplest model such as a free electron, if the calculation is exact, will give us a significant insight for the actual object.

2. Restriction on function form

This letter treats a free electron. In a free electron model the magnetic moment $M(\mu, H, T)$ (μ ; chemical potential, T ; temperature) is merely a superposition of $M(\mu, H, 0)$ [4, 7]. Besides, the 3-dimensional $M(\mu, H, 0)$ is a superposition of 2-dimensional $M(\mu - p_z^2/2m, H, 0) dp_z$. From these two reasons discussion is hereafter confined to the 2-dimensional $M(\mu, H)$ at $T=0$.

The magnetic moment is the derivative of the potential $\Omega = \sum E_i(H) - N(\mu, H)\mu$ (E_i ; energy level, N ; number of electrons) by H .

$$-M(\mu, H) = \frac{\partial}{\partial H} [\sum E_i(H) - N\mu] = \frac{\partial}{\partial H} \sum [E_i(H) - \mu] = \sum \frac{\partial}{\partial H} E_i(H), \quad \text{where } E_i(H) \leq \mu. \quad (1)$$

The partition function $Z(\beta, H)$ is defined by,

$$Z(\beta, H) = \sum \exp[-\beta E_i(H)]. \quad (2)$$

This is also rewritten in terms of the state density $\rho(E, H) = \sum \delta[E - E_i(H)]$,

$$Z(\beta, H) = \int \rho(E, H) \exp(-\beta E) dE. \quad (3)$$

Comparison of (1) and (2) yields,

$$\frac{1}{\beta^2} \frac{\partial}{\partial H} Z(\beta, H) = - \int M(\mu, H) \exp(-\beta \mu) d\mu. \quad (4)$$

Some restriction is imposed on the function form of $Z(\beta, H)$. Since $\rho(E, H) \propto F_1(E/H)$, provided the contribution from near the surface is neglected [4, 8], substitution of this form into (3) and its further substitution into (4) yields,

$$Z(\beta, H) \propto \beta^{-1} F_2(\beta H), \quad \text{hence } M(\mu, H) \propto H F_3(\mu/H).$$

Note that the contribution from near the surface is only a small correction in (2), while it is enormous in the expression of (1).

Concerning the surface effect $\Delta M(\mu, H)$, an exact restriction is derived for the case of an infinite square potential. Since an electron with H, E, a , (a ; the distance of the center of orbit from the surface) and the one with $NH, NE, a/\sqrt{N}$,

have exactly similar wave functions, the latter being $1/\sqrt{N}$ contracted [4], we have,

$$\Delta M(\mu, H) \propto H^{1/2} F_4(\mu/H), \text{ hence } \Delta Z(\beta, H) \propto \beta^{-1/2} F_5(\beta H). \quad (5)$$

This exact restriction (5) is of central importance for the final conclusion of this letter. The absolute value of the strongly oscillating function $F_4(\mu/H)$ is known to be estimated from the E_0 trajectories [4],

$$|\Delta M(\mu, H)| < C_1 H^{-1} \mu^{3/2}. \quad (6)$$

3. Density Matrix

To find out the form of $F_5(\beta H)$, the method of density matrix is used. Consider a free electron confined in a large rectangle in a uniform z -direction magnetic field. With the vector potential $\mathbf{A}=(0, Hx)$, the Hamiltonian is,

$$\mathbf{H} = -\frac{1}{2} \frac{\partial^2}{\partial x^2} + \frac{1}{2} \left[\frac{\partial}{\partial y} + eHx \right]^2 + U(x).$$

where we set $h=1, c=1, m=1$, and $U(x)$ denotes the surface potential.

The density matrix G is defined by

$$G(x, y; X, Y; \beta) = \langle x, y | \exp(-\beta \mathbf{H}) | X, Y \rangle.$$

The partition function is related to $G(x, y; X, Y; \beta)$ by,

$$\int dx dy G(x \rightarrow X, y \rightarrow Y; X, Y; \beta) = \sum \exp(-\beta E_i) = Z(\beta). \quad (7)$$

The solution for $H=0$ and $U(x)=0$ is,

$$G_0(x, y; X, Y; \beta) = G_0(x; X; \beta) G_0(y; Y; \beta), \quad G_0(x; X; \beta) = (2\pi\beta)^{-1/2} \exp[-(x-X)^2/2\beta].$$

An exact solution for $H \neq 0$ and $U(x)=0$ is known to be [8],

$$G(x \rightarrow X, y \rightarrow Y; X, Y; \beta) = (1/2\pi\beta) (\beta eH/2) / \sinh(\beta eH/2). \quad (8)$$

The solution for $H \neq 0$ and $U(x) \neq 0$ is investigated by perturbation.

An infinite square potential is assumed.

$$U(x)=0, \quad -L < x < L. \quad U(x)=\infty, \quad |x| > L.$$

When $H=0$, the solution for $L \rightarrow \infty$ is given by the mirror image method,

$$\begin{aligned} G_s(x; X; \beta) &= G_0(x; X; \beta) - G_0(x; -2L-X; \beta) & -L < x < 0, \\ G_s(x; X; \beta) &= G_0(x; X; \beta) - G_0(x; 2L-X; \beta) & 0 < x < L. \end{aligned} \quad (9)$$

The lowest order perturbation consists of two terms of the second order,

$$I: \quad -\frac{1}{2} \frac{1}{(2\pi\beta)^{1/2}} \int_0^\beta dt \int dx G_s(X; x; t) x^2 G_s(x; X; \beta-t), \quad (10a)$$

and

$$II: \quad \frac{1}{(2\pi\beta^3)^{1/2}} \int_0^\beta ds \int_0^{\beta-s} dt \int dx du G_s(X; x; s) x G_s(x; u; t) u G_s(u; X; \beta-s-t). \quad (10b)$$

Direct calculation of (10b) is lengthy and difficult, which was carried out for a semi-infinite boundary condition [9]. Here is shown a concise and gauge-invariant method. Since the region of x and X is limited, the order of integral by X in (7) and that by x, u in (10b) can be exchanged, while it is wrong in a semi-infinite case.

By adding three terms: The integral of \mathbb{I} ; (10b) by X ,
 Half of the integral of I ; (10a) by X ,
 and Substitution of half of I ; (10a) into (7),
 the following symmetric and gauge-invariant expression is obtained,

$$\int [I + \mathbb{I}] dX = -\frac{1}{4(2\pi\beta)^{1/2}} \int_0^\beta dt \int dx dX G_s(X; x; t) (x-X)^2 G_s(x; X; \beta-t). \quad (11)$$

This calculation is far easier than the direct calculation of (10b). The result is, (L_y ; y -direction size of the rectangle)

$$\frac{Z(\beta)}{L_y} = \frac{2L}{(2\pi\beta)} - \frac{1}{2} \frac{1}{(2\pi\beta)^{1/2}} + \left[-\frac{1}{24} \frac{2L}{(2\pi\beta)} + \frac{3}{128} \frac{1}{(2\pi\beta)^{1/2}} \right] (\beta eH)^2 + O(H^4). \quad (12)$$

Since the mirror image method in (9) becomes exact for $L \rightarrow \infty$, the surface effect of $Z(\beta)$ is defined by,

$$\Delta Z(\beta) = \lim \{ Z(\beta) - 2L [\partial Z(\beta) / \partial (2L)] \}. \quad (13)$$

4. Uniform Convergence

We prove the conclusion of this letter by the combination of eq. (12), the restriction (5) and the estimate (6). We see from (8) that for any given small H , if we choose $\beta \sim i2\pi/eH$, it diverges. It means that near $\beta \sim i2\pi/eH$ the higher order terms become dominant in (12). On the other hand, for any given ε and K_0 , we can choose a sufficiently small H_0 such that (12) is uniformly convergent in the region $|\beta| = |a + ik| \leq K_0$, $0 < a$, namely,

$$\text{for } H \leq H_0 \text{ and } |\beta| \leq K_0 \text{ } 0 < a, \quad |\text{higher order}| / |\propto H^2 \text{ term}| < \varepsilon.$$

Then we see from the restriction (5) it still holds that,

$$\text{for } H \leq H_0/N \text{ and } |\beta| \leq NK_0 \text{ } 0 < a, \quad |\text{higher order}| / |\propto H^2 \text{ term}| < \varepsilon. \quad (14)$$

Let us assume that in the region of μ ; $a < \mu < b = a + d$, the steady term

$$\langle \Delta M(\mu, H) \rangle = f(\mu) H^{1-\gamma} \quad (f(\mu); \text{of definite sign}, \gamma > 0) \quad (15)$$

appears, in order to show that one is thereby led to a contradiction.

5. Proof

To do this we begin with defining the n -th averaged surface moment $\Delta M(n, \mu, H)$ by,

$$\Delta M(0, \mu, H) = \Delta M(\mu, H), \quad \Delta M(n, \mu, H) = \frac{1}{eH} \int_{-eH/2}^{+eH/2} \Delta M(n-1, \mu+t, H) dt. \quad (16)$$

If the same definition is given on the volume moment $M(n, \mu, H)$, it becomes a constant for $n \geq 2$, which is just the steady term of Landau diamagnetism [4]. On the other hand, there still remains a minute oscillation in $\Delta M(2, \mu, H)$, though it rapidly diminishes with increasing n . When it becomes almost steady at some value of n , say 4, it is regarded as $\langle \Delta M(\mu, H) \rangle$. Then (15) is rewritten as,

$$\Delta M(4, \mu, H) = \langle \Delta M(\mu, H) \rangle = f(\mu) H^{1-\gamma} \quad (f(\mu); \text{of definite sign}, \gamma > 0). \quad (17)$$

We see from the definition (16) that $\Delta M(n+4, \mu, H)$ is determined by the value of $\Delta M(\mu, H)$ in the region between $(\mu - neH/2)$ and $(\mu + neH/2)$. So that, if we choose

$n = [d/(2eH)]$, then,

$$\text{for } (a+d/4) < \mu < (b-d/4), \quad |\Delta M(n, \mu, H)| \geq \text{Min} |f(\mu)| H^{1-\tau}. \quad (18)$$

Noting $\Delta M(n, \mu, H) = 0$ for $\mu < -n(eH/2)$, we define the integral $g(n, E, H)$ by,

$$g(n, E, H) = \int_{-d/4}^E \Delta M(n, \mu, H) d\mu. \quad (19)$$

Since the definition (16) is rewritten in a form of convolution with rectangle function, its Laplace transform (in the following extended definition) takes a form of simple multiplication,

$$G(n, \beta, H) = \int_{-d/4}^{\infty} g(n, E, H) \exp(-\beta E) dE = \frac{1}{\beta} \left[\frac{\sinh(eH\beta/2)}{(eH\beta/2)} \right] L[\Delta M(E, H)]. \quad (20)$$

where $L[\Delta M(E, H)]$ is given by (4). We see from (20) that the order of the averaging (16) and the integral (19) can be exchanged.

The relation between $g(n, E, H)$ and $G(n, \beta, H)$ is expressed in a form of inverse Fourier transform.

$$g(n, E, H) \exp(-aE) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} G(n, a+ik, H) \exp(ikE) dk.$$

$G(0, \beta, H)$ is related to $\Delta Z(\beta, H)$ by (4), of which the function form is given by (5) and (12).

$$-G(0, \beta, H) = \frac{1}{\beta^3} \frac{\partial}{\partial H} \Delta Z(\beta, H) = C_2 \beta^{-3/2} H [1 + F_6(\beta H)]. \quad (21)$$

By Parseval's theorem,

$$\int_{-d/4}^{+\infty} |g(n, E, H) \exp(-aE)|^2 dE = \frac{1}{2\pi} \int_{-\infty}^{+\infty} |G(n, a+ik, H)|^2 dk. \quad (22)$$

Let us prove that one is led to a contradiction by the comparison of lower bound of the left hand side of (22) and the upper bound of the right. We consider the limit $H \rightarrow 0$ hence $n \rightarrow \infty$, with $a = \text{constant}$.

Firstly the lower bound of the left is evaluated. Let $|g(n, E, H)| = \text{Minimum}$ at $E = E_0$ in the region $(a+d/4) < E < (b-d/4)$, then from (18) and (19),

$$\text{for } |E - E_0| > d/8 \text{ and } (a+d/4) < E < (b-d/4), \quad |g(n, E, H)| > (d/8) [\text{Min} |f(\mu)|] H^{1-\tau}.$$

So that the evaluation of the integral over $(a+d/4) < E < (b-d/4)$ yields,

$$\text{left of (22)} > (d/16)^2 [\text{Min} |f(\mu)|]^2 \exp(-2ab) H^{2-2\tau}. \quad (23)$$

Secondly the upper bound of the right is evaluated. Our first step to do this is the evaluation of (22) for $n=0$. The estimate (6) of $|\Delta M(\mu, H)|$, together with the definition (19), gives the evaluation of $|g(0, E, H)|$,

$$|g(0, E, H)| < (2/5) C_1 H^{-1} E^{5/2}.$$

This evaluation gives the upper evaluation of (22) for $n=0$,

$$\text{for } n=0, \quad (22) < (3/10) C_1^2 H^{-2} a^{-6}. \quad (24)$$

With the aid of (24), let us consider how the right of (22) varies with increasing n .

As stated concerning (14) and (5), G is uniformly convergent in the region $|\beta| \leq NK_0$ for $H \leq (H_0/N)$. On the boundary of the region, $|k| = k_N = [(NK_0)^2 - a^2]^{1/2}$.

The factor [] appearing in the right hand side of (20) should be examined.

$$\left[\frac{\sinh(eH\beta/2)}{(eH\beta/2)}\right]^2 = \frac{[\sin(eH_0k/2N)]^2 + [\sinh(eH_0a/2N)]^2}{(eH_0k/2N)^2 + (eH_0a/2N)^2}. \quad (25)$$

Near $k=0$, (25) >1 and in the distance, (25) <1 . The integral in the right of (22) should be divided into three regions;

$$\text{I}; |k| < \sim a \quad (25) \geq 1, \quad \text{II}; \sim a < |k| < k_N \quad (25) < 1, \quad \text{III}; k_N < |k| \quad (25) < 1,$$

First we show that the contribution from III vanishes exponentially for $N \rightarrow \infty$.

Since $(eH_0k/2N) \sim eH_0K_0/2 \ll 1$ at the boundary, the factor (25) is smaller in III than at the boundary. Substitution of $n = [Nd/(2eH_0)]$ together with the evaluation (24) yields,

$$\text{III}; \int |G(n, a+ik, H)|^2 dk < \left[\frac{\sin(eH_0K_0/2)}{(eH_0K_0/2)}\right]^{[Nd/(2eH_0)]} N^2 \left(\frac{3}{5}\right) C_1^2 H_0^{-2} a^{-6}. \quad (26)$$

The right hand side vanishes exponentially for $N \rightarrow \infty$. Next we evaluate the contribution from I and II. In the region I the factor (25) becomes maximum at $k=0$, hence,

$$\left[\frac{\sinh(eH\beta/2)}{(eH\beta/2)}\right]^n \leq \left[\frac{\sinh(eH_0a/2N)}{(eH_0a/2N)}\right]^n \sim \left[1 + \frac{1}{6}(eH_0a/2N)^2\right]^{[Nd/(2eH_0)]} \rightarrow 1.$$

So that we can estimate that

$$\text{in I and II, } (25) < 2, \quad \text{for } N \rightarrow \infty \quad (27)$$

The combination of (21), (20) and (14) gives,

$$\text{in I and II, } -G(n, \beta, H) = \left[\frac{\sinh(eH\beta/2)}{(eH\beta/2)}\right]^n C_2 \beta^{-3/2} H(1+\epsilon).$$

Its substitution into (22) together with the estimate (27) yields,

$$\text{I and II}; \int |G(n, a+ik, H)|^2 dk < C_2^2 H^2 \int_{-\infty}^{+\infty} [a^2 + k^2]^{-3/2} dk = 4C_2^2 H^2 a^{-2} \quad (28)$$

We see from (28) and (26) that the right hand side of (22) is at most $\propto H^2$ for $H \rightarrow 0$. On the other hand we see from (23) that the left hand side of (22) is at least $\propto H^{2-2\gamma}$ for $H \rightarrow 0$. Thus one is led to a contradiction.

So that we have reached our final conclusion that such a steady term in surface Landau diamagnetism $\langle \Delta M(\mu, H) \rangle = f(\mu) H^{1-\gamma}$ ($f(\mu)$; of definite sign, $\gamma > 0$) for $H \rightarrow 0$ is non-existent in any region $a < \mu < b = a+d$, so long as an infinite square potential is assumed.

6. Conclusion

The restriction (5), which is of central importance for the conclusion, is exact only for infinite square potential. However, the conclusion holds if only the uniform convergent region of β enlarges $\sim H^{-1}$ for $H \rightarrow 0$. So that the same conclusion seems to hold for some of more general potentials of semi-infinite type. At first sight it seems rather disappointing for workers who have been searching for some types of singularities.

Still the author believes that the exactness and generality in this letter suggests the way for searching singularities for such cases of shallow

potential, double square potential or intermediate strength in H such that the orbit radius becomes comparable to some size in the structure.

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