

# Electron Wind on a Metal Surface with a Finite Work Function

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## Abstract

The current density distribution  $J(x, W)$  in Landau diamagnetism for a finite step function potential of the height  $W$  is solved in a form of superposition of partial waves. Exact value of  $J(0, W)$  is given. The divergence caused by the non-uniform displacements of divergent partial waves in  $J(x, \infty)$  is exactly canceled by the additional waves due to the deviation from symmetry in  $E - \alpha$  relation. Thus  $J(x, W)$  is similar to  $J(x - \eta/k_F, \infty)$ , where  $\eta^2 \equiv \mu/(\mu + W)$ .

The apparent contradiction between the singularity<sup>4-5)</sup> and the linearity<sup>2,3)</sup> in Landau diamagnetism has been comprehensively clarified by the author<sup>1)</sup> by the concept of uniform convergence. In the nearest region  $R_F(R_F k_F)^{-2/3} \gg |x| > 0$ , the current density  $J(x)$  is linear in the magnetic field  $H$  and oscillates in  $x$  with a wavelength  $\pi/k_F$  ( $R_F, k_F$ ; orbit radius and wave number at Fermi level), while in the region  $2R_F > |x| > R_F(R_F k_F)^{-2/3}$  it varies slowly in  $x$  and strongly oscillates in  $H$ , giving rise to de Haas-van Alphen effect.

The linear current density of which the integral over  $x$  gives the exact magnitude corresponding to the bulk Landau diamagnetism is concentrated over a few wavelengths. It is therefore by no means small (with  $10^4$  gauß,  $\sim 10^6$  [A/cm<sup>2</sup>] for normal metal and  $\sim 2 \times 10^7$  [A/cm<sup>2</sup>] for Bi) in spite of its small integral. The current near a clean surface of metal or semimetal with a low work function is an interesting subject. This paper treats the current density distribution  $J(x, W)$  with a finite step function surface potential of the height  $W$ . It treats the free electrons in a large box  $LL_y L_z (-L < x < 0)$  in a weak  $z$ -direction field, i.e.  $k_F^{-1} \ll R_F < L/2$ . The calculation for  $J(x, W)$  will give an exact lowest order ( $\propto H^1$ ) asymptotic term in  $H$ , which is exact in any  $W$ . Since the current at a finite temperature  $T$  is merely a superposition of that at  $T=0$ , hereafter  $T=0$  is assumed.<sup>1)</sup>

The current density with an infinite  $W$ ;  $J(x, \infty)$  has been given as a function of  $X \equiv 2k_F x$ , in terms of the Bessel function of order  $5/2$ ;  $J_{5/2}(t)$ , namely,

$$F(X, \infty) \equiv \left( \frac{e^2 k_F^2 H}{64 \pi m c} \right)^{-1} J(x, \infty) = -X^2 \left[ 1 + \frac{2}{\sqrt{\pi}} \int_0^X (t/2)^{-5/2} J_{5/2}(t) dt \right] + \text{H.O.} \quad (1)$$

where H.O. means higher order terms. The main (linear) term was given for the first time by K. Ohtaka and T. Moriya<sup>2)</sup> by a linear response theory. Its validity in the nearest region has been clarified by the author,<sup>1)</sup> whose success depends essentially on three situations: 1s) The wave functions  $\phi(x, a)$  of which the centers of orbits  $a$  lie near  $x = \pm$  (orbit radius) give only higher order contributions in the nearest region. 2s) The  $r - a$  relation for  $W = \infty$  (Fig.

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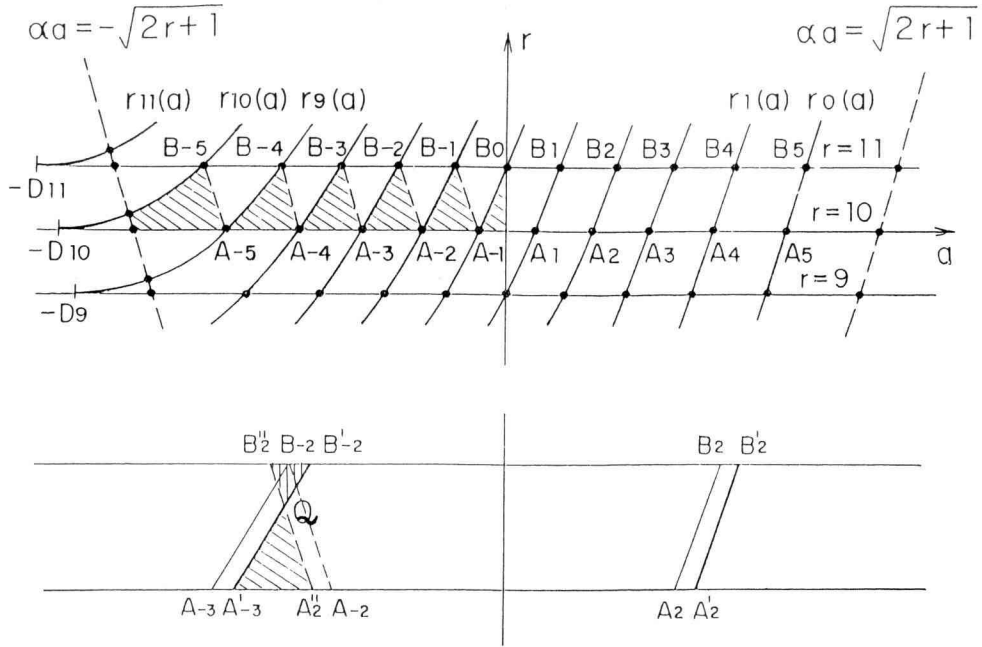


Fig. 1. UPPER;  $r$ - $a$  relation for  $W = \infty$ :  $a$ ; center of orbit,  $(r+1/2)\hbar\omega = E - (\hbar k_z)^2/2m$ ,  $E$ ; energy,  $\alpha^2 \equiv m\omega/\hbar$ .  
BELOW; Enlarged (2 times) curved triangle  $B_{-2}A_{-3}A_{-2}$ : When  $W$  becomes finite,  $B_{-2}A_{-3}$  is displaced to  $B'_{-2}A'_{-3}$  and  $B_2A_2$  to  $B'_2A'_2$ .  
The area  $B_{-2}A_{-3}A_{-2}$  is changed into  $QA'_{-3}A''_2$  minus  $QB''_2B'_{-2}$ , where  $B''_2A''_2$  is the mirror image of  $B'_2A'_2$ .

1) keeps complete symmetry at  $r = m$  ( $m$ ; integer). 3s) An exact relation  $a^{-2}[\phi'(0)]^2 = 2(\partial r/\partial a)$  holds.

While 1s) valid also for a finite  $W$ , both 2s) and 3s) break. Therefore the generalization of the method for  $W = \infty$  to a finite  $W$  is not straightforward. Furthermore, the convergent function  $[F(X \rightarrow -\infty, \infty) - \text{H.O.}] \sim (16/\pi)X^{-1} \cos(X)$  will take a form of superposition of divergent partial waves. Therefore, it is not at first sight evident whether  $J(x \rightarrow -\infty, W)$  is appreciably changed from  $J(k \rightarrow -\infty, \infty)$  or not.

Nevertheless, this paper will show three results: 1r) The form of  $J(x, W)$  as a superposition of partial waves. 2r) No appreciable change in  $J(x \rightarrow -\infty, W)$  from  $J(x \rightarrow -\infty, \infty)$ . 3r) Exact value of  $J(x=0, W)$ .

$J(x, W)$  is written in terms of the wave function;  $\phi(x, E, a) \exp(ik_y y + ik_z z)/(L_y L_z)^{1/2}$ , ( $E$ ; energy,  $\omega = eH/mc$ ; cyclotron frequency),

$$J(x, W) \equiv \sum -e\omega(x-a) |\phi(x, E, a)|^2 / L_y L_z \quad (2)$$

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

$$\phi(x, E, a) = a^{1/2} u(t, r) / \left[ \int_{-\infty}^{+\infty} [u(t, r)]^2 dt \right]^{1/2} \quad (3)$$

with

$$a^2 \equiv \frac{m\omega}{\hbar}, \quad t \equiv a(x-a), \quad \left(r + \frac{1}{2}\right)\hbar\omega \equiv E \frac{(\hbar k_z)^2}{2m}, \quad (4)$$

and

$$\left[ -\frac{\partial^2}{\partial t^2} - t^2 + (2\zeta + 1) \right] u(t, r) = 0, \quad [\zeta = r, t < b \text{ and } \zeta = r - B, b < t] \quad (5)$$

where  $B \equiv (W + \mu)/\hbar\omega$  ( $\mu$ ; Fermi energy), and  $b \equiv -aa$ .

We can readily verify by direct differentiation that

$$2 \int t u^2 dt = [t^2 - (2\zeta + 1)] u^2 - \left( \frac{\partial u}{\partial t} \right)^2 \quad (6)$$

The sum of eq. (6) in both regions  $\zeta = r, t < b$  and  $\zeta = r - B, b < t$  yields

$$\int_{-\infty}^{+\infty} t u^2 dt = -B [u(b)]^2 \quad (7)$$

Since the adiabatic relation:  $(\partial r / \partial a) - \alpha \int t u^2 dt / \int u^2 dt$ ,<sup>1)</sup> holds for an arbitrary potential, its combination with eqs. (7) and (3) yields,

$$\frac{\partial r}{\partial a} = \alpha B [u(b)]^2 / \int_{-\infty}^{+\infty} u^2 dt = B [\phi(0)]^2 \quad (8)$$

With  $W \rightarrow \infty$ , eq. (8) is reduced to the previously mentioned 3s).

Hereafter we omit to write H.O..  $J(x, \infty)$  in eq. (1) has been derived from the Taylor coefficients at  $x=0$ .<sup>1)</sup>

$$\begin{aligned} & -(L_y L_z / e\omega) J^{(2q+1)}(0) \\ & = \sum 16 \alpha^{2q} (2q+1) [(q-1)b^2 - K] (-4K)^{q-2} (\partial r / \partial a) \\ & -(L_y L_z / e\omega) J^{(2q)}(0) = \sum 4 \alpha^{2q-1} b (-4K)^{q-1} (\partial r / \partial a) \end{aligned} \quad (9)$$

$$(10)$$

where  $K \equiv (2r+1) - b^2$ .  $J^{(2q+1)}(0)$  is a sum of even function of  $b$ :  $\sum f(b)$ ,  $f(b)$  being  $\propto H^1$ . The sum is substituted by  $\propto \alpha^2 \int dk_z dr \int f(b) (2/\pi) K^{1/2} db$ . Any higher order terms in  $f(b)$  give no contributions to the lowest order term ( $\propto H^0$ ) in the sum. On the other hand,  $J^{(2q)}(0)$  is a sum of odd function of  $b$ :  $\sum g(b)$ ,  $g(b)$  being  $\propto H^0$ . The sum takes an apparent form to be  $\propto H^{-1}$ . However, because of the symmetry in  $r-a$  relation at  $r=m$ , the sum is substituted by  $\propto \alpha^2 \int dk_z dr \int 1/2 (\partial g / \partial b) db$ , which is  $\propto H^0$ . If  $g(b)$  includes some higher order ( $\propto H^1$ ) even terms, they also give some contributions to the lowest order term in the sum.

Transforming the integral in eqs. (9) and (10) over  $b, r$  and  $k_z$  into that over  $r, k_z$  and  $s \equiv (\alpha/k_F) K^{1/2}$ , we get,

$$F^{(2q)} = 4(-1)^q \int_0^1 s^{2q} [(1-s^4) - q(1-s^2)^2] s^{-3} ds \quad (11)$$

$$F^{(2q+1)} = \frac{4}{\pi} (-1)^q \int_0^1 s^{2q+1} (2q+1) [(1-s^2)(1+3s^2) - q(1-s^2)^2] s^{-3} ds$$

The function corresponding to these Taylor coefficients is,

$$F(X, \infty) = \int_0^1 [f_e(X, s) + f_0(X, s)] ds \quad (12)$$

where

$$f_e(X, s) = -4(s^{-3} - s)[1 - \cos(sX)] + 2s^{-2}(1-s^2)^2 X \sin(sX) \quad (13)$$

and

$$f_0(X, s) = -(4/\pi)s^{-2}(1-s^2)(1+3s^2)X[1 - \cos(sX)] \\ + (2/\pi)s^{-1}(1-s^2)^2 X^2 \sin(sX) \quad (14)$$

What alteration in eqs. (12, 13) and (14) will occur when  $W$  becomes finite? Let us assume that  $\phi(x < 0)$  be extended into  $0 < x$ , with the surface potential virtually removed, till the nearest node. The lowest order term in the position of the node  $\Delta a$  as well as the one in  $[\phi'(\Delta a)]^2$  are obtained by assuming  $\phi$  to be a plane wave, which gives the first term of,

$$\Delta a(s) = (k_F s)^{-1} \arcsin(\eta s) + O(H^2), \text{ where } \eta^2 \equiv \mu/(\mu + W) \quad (15)$$

and makes eq. (8) to be identical to 3s).

By choosing suitable  $k(t)$  and  $K(t)$ , it holds exactly that  $u(t) \propto k^{-1/2} \sin\left(\int k dt\right)$ ;  $\zeta = r$  and  $u(t) \propto x^{-1/2} \exp\left(-\int x dt\right)$ ;  $\zeta = r - B$ . We can show  $(k^2 + x^2)/2B = 1 + o(H^2)$ . From this reason and from 1s) we can prove that W.K.B. gives exact results at least for  $H^1$  higher order terms both in  $\Delta a(s)$  and in  $[\phi'(\Delta a)]^2$ . The combination of eq. (8) and W.K.B. yields,

$$\frac{[\phi'(\Delta a(s))]^2}{[(2/\alpha)(\partial r/\partial a)]} = 1 + \left(\frac{\eta}{2B}\right) \left(\frac{bs}{K^{1/2}}\right) \frac{(\tan \theta - \theta)}{(\sin \theta)^3}, \quad (16)$$

where  $\sin \theta = \eta s$

as well as the second term in eq. (15).

The right hand sides in eqs. (9) and (10) excluding the factor  $2\alpha^2(\partial r/\partial a)$  are the ratios of each contribution to  $[\phi'(O)]^2$ , which have been derived from the differential equation (5). These ratios remain unchanged for a finite  $W$  only by replacing  $b \equiv -\alpha a$  by  $-\alpha[a - \Delta a(s)]$ . Thus we get a correct result by multiplying the right hand side of eq. (16) to the right hand sides of eqs. (9) and (10).

As stated previously, the higher order terms in eq. (9) give no contributions to the result. The effect of a finite  $W$  is only to displace  $f_0(X, s)$  into  $f_0(X - \Delta X, s)$ , where  $\Delta X \equiv 2k_F \Delta a(s)$ . On the other hand, the higher order terms in eq. (10) give rise to an additional integral, namely,

$$\int f_1^{(2q)}(\Delta X(s)) ds = 2\eta^3 \frac{4}{\pi} (-1)^q \int_0^1 s^{2q} (1-s^2)^2 \frac{(\tan \theta - \theta)}{(\sin \theta)^3} ds$$

which corresponds to,

$$F_1(X, W) = -2\eta^3 \frac{4}{\pi} \int_0^1 (1-s^2)^2 (1 - \cos(s[X - \Delta x(s)])) \cdot \frac{(\tan \theta - \theta)}{(\sin \theta)^3} ds \quad (17)$$

Thus we get the form of a superposition of the partial waves: 1r) that

$$F(X, W) = \int_0^1 [f_e(X - \Delta X(s), s) + f_o(X - \Delta X(s), s)] ds + F_1(X, W) \quad (18)$$

Now let us evaluate  $F(X \rightarrow -\infty, W)$ . We can write,

$$F(X, W) = F(X - \Delta X(0), \infty) - \int_0^1 \left[ \frac{\partial f_o}{\partial X} + \frac{\partial f_e}{\partial X} \right] [\Delta X(s) - \Delta X(0)] ds \\ + F_1(X, W) + \text{residual} \quad (19)$$

where  $\Delta X(s) - \Delta X(0) = 2[s^{-1} \arcsin(\eta s) - \eta] = \eta^3 s^2/3 + 3\eta^5 s^5/20 + \dots$ . All the oscillating terms in the integrand have factors  $[Xs(1-s)]^n$ ;  $n=0, 1$  or  $2$ . Hence, they give only  $O(X^{-1})$  by integrating by parts. The steady terms from  $(\partial f_o/\partial z)$  and from  $F_1$  give terms  $O(X^0)$ . Therefore, the sum of the original two integrals;  $\int [f_e + f_o] ds$ , suffers an appreciable change caused by the non-uniform displacements of partial waves with a finite  $W$ . However, the sum of two steady terms exactly vanishes by direct calculation. The residual is from  $[\partial^2 f_e/\partial X^2 + \partial^2 f_o/\partial X^2]$ , which gives only small  $O(X^{-1})$ . We therefore get the result: 2r) that  $F(X \rightarrow -\infty, W)$  suffers no appreciable change when  $W$  becomes finite, namely,

$$F(X \rightarrow -\infty, W) = F(X - 2\eta, \infty) + (\eta^3/3) |F(X, \infty)| [\pi/4 - \sin(X)] \quad (20)$$

where  $|F(X, \infty)| = -(16/\pi)X^{-1}$  denotes its amplitude.

Finally let us evaluate  $F(0, W)$ . We can do it from eq. (18) of course. However, we use here eqs. (2) and (8). Their combination yields,

$$-(L_y L_z / e\omega) BJ(0, W) = \Sigma - a(\partial r / \partial a) \quad (21)$$

In the limit  $W \rightarrow \infty$ , the right hand side becomes the sum of the shaded areas in Fig. 1<sup>1)</sup>, and eq. (21) becomes identical to the expression for  $J''(0, \infty)$  in eq. (10) with  $J''(0, \infty)$  replaced by  $(4a^2)BJ(0, W)$ . By the loss of symmetry the contribution from the area of a curved triangle, e.g.  $B_{-2}A_{-3}A_{-2}$  in Fig. 1 is changed to the area  $QA'_{-3}A'_{-2}$  minus  $QB'_2B'_{-2}$ . The exact result is obtained by multiplying a reduction factor  $[1 - 4\theta(s)/\pi]$  to each curved triangle. Hence, the expression for  $F''(0, \infty)$  in eq. (11) is replaced by,

$$-(2\eta^2)^{-1} F(0, W) = 8 \int s(1-s^2) [1 - 4\theta(s)/\pi] ds$$

By integrating by parts we get the result: 3r) that

$$F(0, W) = -4\eta^2 + (16/\pi)\eta^3 \times \{[\eta^{-1} - \eta^{-3} + (3/8)\eta^{-5}] \arcsin \eta \\ + [3/4\eta^{-2} - (3/8)\eta^{-4}](1 - \eta^2)^{1/2}\} \quad (22)$$

In the limit  $W \rightarrow \infty$  or  $W \rightarrow 0$ , ( $\varepsilon^2 \equiv 1 - \eta^2$ )

$$F(0, W \rightarrow \infty) \rightarrow -4\eta^2 + (128/15\pi)\eta^3 + (64/105\pi)\eta^5 + \dots \\ F(0, W \rightarrow 0) \rightarrow -1 + (12/\pi)\varepsilon - \varepsilon^2 + (15/\pi)\varepsilon^3 + \dots,$$

We have the conclusion that  $J(x, W)$  is similar to the uniformly displaced  $J(x, \infty)$ , namely to  $J(x - \eta/k_F, \infty)$ . An “electron wind” existing on a clean surface with a low work function is an interesting subject.

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### References

- 1) F. Shishido : Phys. Lett. **A152** (1991) 437.
- 2) K. Ohtaka and T. Moriya : J. Phys. Soc. Jpn. **34** (1973) 1203.
- 3) M. Robnik : J. Phys. **A19** (1986) 3619.
- 4) L.A. Falkovskii : Sov. Phys. -JETP Lett. **11** (1971) 111.
- 5) R. Peierls : Quantum Theory of Solids (Oxford 1955).
- 6) F. Shishido : Phys. Lett. **A152** (1991) 443.