Surface corrections to the Landau diamagnetic susceptibility*

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(Received 15 March 1976)

Surface effects on the steady value of the diamagnetic susceptibility of a noninteracting electron gas are investigated. Expressions for the susceptibility are obtained, in the presence of an arbitrary surface potential, for both the zero- and high-temperature limits. By constructing explicit examples, it is shown that surface corrections to the usual Landau value of the susceptibility vanish at high temperatures, while at zero temperature small correction terms may persist.

I. INTRODUCTION

By considering a system of free electrons confined in a large box and neglecting surface effects due to the walls of the box, Landau[1] obtained the diamagnetic susceptibility of the electron gas. In the weak-field limit, simple expressions for this quantity are obtained for a zero-temperature degenerate gas, or a high-temperature classical gas, and these are often referred to as the Landau values. These are the so-called steady values, and we are not concerned here about that part of the orbital susceptibility that oscillates with a varying field and shows up at low temperatures as the de Haas–van Alphen effect. One may then ask as to how the steady value of the susceptibility is affected due to surface effects. Since the electrons are confined by some sort of a potential barrier, one may expect changes from the Landau values as the classical radius of gyration of the electrons becomes comparable to the confinement size, or the "radius" of the potential barrier. Since the radius of gyration of an electron is inversely proportional to the applied magnetic field strength, one may expect the surface effects to be of importance in the weak-field limit for electrons in a potential barrier of small radius. The answer to the above question has been sought by a large number of authors[2] within the past 40 years and we shall pay particular attention to the more recent papers by Friedman[3] and Thomas.[4] Both these authors consider some simple specific models for the potential barrier to answer the question posed earlier. Friedman[3] considered two types of one-dimensional potential barriers in a direction perpendicular to the applied field — an infinite wall, and a harmonic barrier. For the infinite wall, he obtained the Landau susceptibility for the degenerate gas at zero temperature,[5] as well as for the classical gas at high temperatures. For the harmonic barrier, he considered only the high-temperature behavior and obtained the Landau result. Thomas[4] added a small fourth-order anharmonic term to the one-dimensional harmonic barrier, and under certain restrictions on the anharmonic term, showed that the high-temperature Landau value is reproduced. Since the two model potential barriers are of very different shapes, it was argued that the Landau susceptibility should remain unaltered in any surface potential, even when the classical radius of gyration of the electron is much larger than the spatial dimension of the potential barrier.

In this paper, we consider the same problem that was posed earlier, and answered by Friedman[3] and Thomas[4] for the cases of specific model potential barriers. We are able to obtain the general expression for the diamagnetic susceptibility of the electrons moving in a *smooth* potential barrier of arbitrary shape. Explicit expressions for the susceptibility are derived both in the high-temperature limit of a classical gas and the zero-temperature limit of the degenerate gas. Our expressions yield the Landau values for both cases as the leading term, plus a correction term which is smaller by a factor of $\hbar^2$, and dependent on the shape of the potential.[6] In the high-temperature limit, this correction term goes to zero faster than T^{-1}, and one gets the Landau value exactly. Applying our formulation to electrons at high temperature moving in the same potential barrier as that of Thomas,[4] a thorough analysis of the problem is made, and it is shown that the Landau result is obtained under more general conditions than imposed by Thomas. For the degenerate gas, when the specific example of one-dimensional harmonic barrier is taken, we again obtain the Landau result, since our correction term in this case vanishes identically. We show, however, that in the degenerate gas it is possible to have a small nonzero correction to the Landau zero-temperature susceptibility when more general shapes of potentials are considered.

In Sec. II, we develop the formalism that is employed to derive the expressions for diamagnetic susceptibility of the classical and degenerate gas in the weak-field limit. In Sec. II, the formal expressions for the susceptibility are derived assuming the potential barrier to be symmetric about the axis of the applied magnetic field. This assumption is made solely for algebraic simplicity, and the final expression that is obtained is valid even in the absence of such symmetry, as is indicated in the Appendix. In Sec. III, we evaluate the susceptibility expression for specific potential shapes, including the ones considered by Friedman[3] and Thomas.[4] Implications of these results are discussed in the same section.

II. DERIVATION OF THE RESULT

A. Diamagnetic susceptibility in terms of the one-body electronic partition function

Consider an electron gas, in which each electron moves independently of the others, but in a one-body potential $U(\vec{r})$, whose form need not be specified. A magnetic field $\vec{B}$ will couple with the orbital as well as the spin angular momentum of the electron. The spin coupling will give rise to paramagnetism, and is irrelevant in the present context. We shall therefore regard the electrons as spinless in what follows, although it can be included in the formalism easily. The orbital Hamiltonian of an electron in a magnetic field $\vec{B}$ is

$$\hat{H}_B = (1/2m)[\hat{p} + (e/c)\vec{A}]^2 + U(\vec{r}),$$

where $-e$ is the charge, m is the mass of the electron, and $\hat{p} = -i\hbar\vec{\nabla}$. For a uniform magnetic field, the vector potential $\vec{A} = \frac{1}{2}(\vec{B}\times\vec{r})$. The above Hamiltonian may be simplified by taking the z axis along the direction of the magnetic field, and we get

$$\hat{H}_B = \hat{H}_0 + \frac{e^2B^2}{8mc^2}r_\perp^2 + \frac{eB}{2mc}\hat{l}_z, \quad (1)$$

with

$$\hat{H}_0 = \frac{\hat{p}^2}{2m} + U(\vec{r}), \quad r_\perp^2 = (x^2+y^2)$$

and

$$\hat{l}_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right).$$

We now define the one-body partition function

$$Z_B(\beta) = \mathrm{Tr}\, e^{-\beta\hat{H}_B} = \sum_i e^{-\beta\epsilon_i}, \quad (2)$$

where ϵ_i's are the single-particle eigenenergies of $\hat{H}_B$. By defining $g(\epsilon) = \sum_i \delta(\epsilon - \epsilon_i)$ as the density of states of an electron in the presence of the magnetic field, we may rewrite Eq. (2) as

$$Z_B(\beta) = \int_0^\infty g(\epsilon)e^{-\beta\epsilon}d\epsilon. \quad (3)$$

It is easy to show that the diamagnetic susceptibility is completely determined in terms of Z_B, both in the zero- and high-temperature limits. For a classical gas at high temperature, the magnetization per electron is given by

$$\frac{M}{N} = (kT)\frac{1}{Z_B}\frac{\partial Z_B}{\partial B}, \quad (4)$$

where N is the number of electrons is a given volume V. In the weak-field limit it is only necessary to evaluate Z_B to order B^2, and the field-independent susceptibility per particle is

$$\frac{1}{N}\chi(T\to\infty) = (kT)\frac{1}{Z_{B=0}}\left(\frac{\partial^2 Z_B}{\partial B^2}\right)_{B=0}. \quad (5)$$

To express the zero-temperature susceptibility of a degenerate gas in terms of Z_B, note that the magnetization M in a volume V at a temperature T is

$$M = kT\left(\frac{\partial}{\partial B}\ln Q\right)_{\mu, V, T}, \quad (6)$$

where Q is the grand-canonical partition function and μ is the chemical potential. In our model,

$$\ln Q = \int_0^\infty g(\epsilon)\ln(1+e^{(\mu-\epsilon)/kT})\,d\epsilon.$$

For a degenerate gas, in the limit of $T\to 0$, this reduces to

$$\ln Q = \frac{1}{kT}\int_0^\mu g(\epsilon)(\mu-\epsilon)\,d\epsilon$$

or

$$\lim_{T\to 0}(kT\ln Q) = \mu N - E. \quad (7)$$

Here we have used the zero-temperature relations

$$\int_0^\mu g(\epsilon)\,d\epsilon = N$$

and

$$\int_0^\mu \epsilon g(\epsilon)\,d\epsilon = E.$$

From Eq. (3), we see that $g(\epsilon)$ is the inverse Laplace transform of Z_B, i.e.,

$$g(\epsilon) \equiv L^{-1}Z_B(\beta) = \frac{1}{2\pi i}\int_{-i\infty}^{i\infty} Z_B(\beta)e^{\beta\epsilon}d\beta. \quad (8)$$

Note that β here becomes just a dummy integration variable. Using standard properties of Laplace transforms,[7] we get

$$N = L_\mu^{-1}\frac{Z_B(\beta)}{\beta} \quad \text{and} \quad E = \mu N - L_\mu^{-1}\frac{Z_B(\beta)}{\beta^2}.$$

Substituting these in Eq. (7), and using Eq. (6), we get the zero-temperature magnetization

$$M = L_\mu^{-1} \frac{1}{\beta^2}\left(\frac{\partial Z_B}{\partial B}\right). \qquad (9)$$

The weak-field susceptibility χ of a degenerate gas at zero temperature in a volume V is thus

$$\chi(T\to 0) = \frac{1}{B} L_\mu^{-1} \frac{1}{\beta^2}\left(\frac{\partial Z_B}{\partial B}\right) = \frac{1}{2\pi i}\frac{1}{B}\int_{-i\infty}^{i\infty} \frac{1}{\beta^2}\left(\frac{\partial Z_B}{\partial B}\right) e^{\beta\mu} d\beta. \qquad (10)$$

Note again that β here is just an integration variable. To examine the behavior of χ in the zero- or high-temperature limits, it is therefore necessary to evaluate the one-body partition function Z_B to order B^2.

B. Wigner-Kirkwood expansion of the partition function

A straightforward calculation of Z_B by Eq. (2) would require a knowledge of the single-particle eigenenergy spectrum of the Hamiltonian $\hat{H}_B$, and this has forced most previous authors to assume a simple potential $U(\vec{r})$, like the harmonic oscillator or infinite wall. It is also known[3] that taking the approximate Wentzel-Kramers-Brillouin (WKB) energies for the eigenspectrum yields a spurious result for Z_B. There exists, however, the well-known expansion of the partition function itself in powers of $\hbar^2$, which is due to Wigner[8] and Kirkwood,[9] and is ideally suited for the present problem. It is quite straightforward, as we now show, to adapt this formalism to the presence of a magnetic field.

The basic problem is the calculation, to order B^2, of the partition function

$$Z_B = \mathrm{Tr}\exp\left[-\beta\left(\hat{H}_0 + \frac{e^2B^2}{8mc^2} r_\perp^2 + \frac{eB}{2mc}\hat{l}_z\right)\right], \qquad (11)$$

where the quantities in the exponent have been defined following Eq. (1). For simplicity in algebra, we shall assume here that the potential $U(\vec{r})$ is axially symmetric, so that $\hat{H}_0$ and $\hat{l}_z$ commute. This restriction will be relaxed in the appendix, and the final expression would remain unaltered. Note that even if $\hat{l}_z$ and $\hat{H}_0$ commute, $r_\perp^2$ and $\hat{H}_0$ do not. If two operators $\hat{O}_1$ and $\hat{O}_2$ do not commute, one cannot write $\mathrm{Tr}\exp[-\beta(\hat{O}_1+\hat{O}_2)]$ as equal to $\mathrm{Tr}\exp(-\beta\hat{O}_1)\exp(-\beta\hat{O}_2)$. The correct form is

$$\mathrm{Tr}e^{-\beta(\hat{O}_1+\hat{O}_2)} = \mathrm{Tr}e^{-\beta\hat{O}_1}e^{-\beta\hat{O}_2} + \frac{\beta^3}{3!}\mathrm{Tr}e^{-\beta\hat{O}_1}[\hat{O}_1,\hat{O}_2]\hat{O}_2 + \cdots. \qquad (12)$$

In Eq. (11), the noncommuting part $\hat{O}_2$ is $(e^2B^2/8mc^2)r_\perp^2$, proportional to B^2, so the correction terms in Eq. (12), which all involve $\hat{O}_2$ twice or more, are at least of order B^4. We may therefore neglect these and write

$$Z_B = \mathrm{Tr}e^{-\beta\hat{H}_0}\exp\left[-\beta\left(\frac{e^2B^2}{8mc^2}r_\perp^2 + \frac{eB}{2mc}\hat{l}_z\right)\right]. \qquad (13)$$

By expanding the second exponential in the right to order B^2, and noting that $\mathrm{Tr}\exp(-\beta\hat{H}_0)\hat{l}_z = 0$, we get

$$Z_B(\beta) = Z_0(\beta) + \frac{\beta^2e^2B^2}{8m^2c^2}\mathrm{Tr}e^{-\beta\hat{H}_0}\left(\hat{l}_z^2 - \frac{1}{\beta}mr_\perp^2\right), \qquad (14)$$

with $Z_0(\beta)$ being the field-independent partition function

$$Z_0(\beta) = \mathrm{Tr}e^{-\beta\hat{H}_0}, \qquad (15)$$

which does not contribute to the magnetization. The trace of the operator $\exp(-\beta\hat{H}_0)[\hat{l}_z^2 - (1/\beta)mr_\perp^2]$ may be expressed in any complete basis, and it is most convenient to take the plane-wave basis. Then we get[9]

$$\mathrm{Tr}e^{-\beta\hat{H}_0}\left(\hat{l}_z^2 - \frac{m}{\beta}r_\perp^2\right) = \frac{1}{h^3}\int e^{-i\vec{p}\cdot\vec{r}/\hbar} \times e^{-\beta\hat{H}_0}\left(\hat{l}_z^2 - \frac{1}{\beta}mr_\perp^2\right) \times e^{i\vec{p}\cdot\vec{r}/\hbar} d^3p\, d^3r.$$

Since $\hat{H}_0$ is Hermitian, the right-hand side may be written

$$= \frac{1}{h^3}\int (e^{-\beta\hat{H}_0}e^{i\vec{p}\cdot\vec{r}/\hbar})^*\left(\hat{l}_z^2 - \frac{1}{\beta}mr_\perp^2\right)e^{i\vec{p}\cdot\vec{r}/\hbar}d^3p\, d^3r. \qquad (16)$$

In the Wigner-Kirkwood expansion, one writes[9]

$$e^{-\beta\hat{H}_0}e^{i\vec{p}\cdot\vec{r}/\hbar} = e^{i\vec{p}\cdot\vec{r}/\hbar}e^{-\beta H_0}(1 + \hbar w_1 + \hbar^2 w_2 + \hbar^3 w_3 + \hbar^4 w_4 + \cdots), \qquad (17)$$

where, on the right-hand side, $H_0 = p^2/2m + U(\vec{r})$ is the *classical* Hamiltonian, and w_1, w_2, etc., are functions of the derivatives of the potential $U(\vec{r})$ and contain the classical variables $\vec{p}$, $\vec{r}$ and the parameter β. Obviously, the formalism is only valid for smooth potentials whose spatial derivatives exist. In the above expansion, if we retained terms up to $\hbar^2 w_2$, we shall obtain the usual Landau values of the susceptibility. By retaining terms up to $\hbar^4 w_4$, we shall find the next order correction term to the Landau value. Expressions for w_1 and w_2 are[9]

$$w_1 = -(i\beta^2/2m)\vec{p}\cdot\vec{\nabla}U,$$
$$w_2 = (\beta^3/6m^2)(\vec{p}\cdot\vec{\nabla})^2U - (\beta^4/8m^2)(\vec{p}\cdot\vec{\nabla}U)^2 - (\beta^2/4m)\nabla^2U + (\beta^3/6m)(\vec{\nabla}U)^2. \qquad (18)$$

In our calculation, the expressions for w_3, w_4 are also required. These are very lengthy, but may be obtained directly from the recursion formula given by Kirkwood,[9] and will not be written here. It is found that w_1, w_3, are imaginary and contain only odd powers of the classical variable $\vec{p}$, while w_2, w_4 are real and involve only even powers of $\vec{p}$. To evaluate the relevant trace from Eq. (16), we use expansion (17) with the appropriate w's up to w_4, and the identity

$$\hat{l}_z^2 e^{i\vec{p}\cdot\vec{r}/\hbar} = [i\hbar(xp_x + yp_y) + (xp_y - yp_x)^2]e^{i\vec{p}\cdot\vec{r}/\hbar}. \tag{19}$$

Then we get

$$\mathrm{Tr}e^{-\beta\hat{H}_0}\left(\hat{l}_z^2 - \frac{m}{\beta}r_\perp^2\right) = \frac{1}{h^3}\int e^{-\beta[p^2/2m + U(\vec{r})]} \times\left[\left((xp_y - yp_x)^2 - \frac{m}{\beta}r_\perp^2\right)(1 + \hbar^2 w_2 + \hbar^4 w_4) + i\hbar(xp_x + yp_y)(\hbar w_1^* + \hbar^3 w_3^*)\right]d^3r\, d^3p. \tag{20}$$

In Eq. (20), we have dropped the terms that are linear in $\vec{p}$ and vanish on $\vec{p}$ integration, and the resulting expression (20) is real. This expression, apart from the overall factor of h^3, has terms of order $\hbar^0$, which are purely classical and vanish identically,[10] terms of order $\hbar^2$ which give rise to Landau susceptibility, and terms of order $\hbar^4$ which are the corrections that we are seeking. Since the $\vec{p}$ dependence of w_1 to w_4 are known, all the p integrations in Eq. (20) may be done analytically. This is a very tedious but straightforward job, and we do not think it worthwhile to give the extensive details here.

Before presenting the final result, however, it is useful to write down the Kirkwood expansion of the field-free partition function (15) to order $\hbar^4$. This is given by[11]

$$Z_0^{(4)}(\beta) = \frac{1}{8\pi^{3/2}\beta^{3/2}}\left(\frac{2m}{\hbar^2}\right)^{3/2} \times\int d^3r\, e^{-\beta U(\vec{r})} \left[1 - \frac{\beta^2}{12}\frac{\hbar^2}{2m}\nabla^2 U + \frac{\beta^3}{1440}\left(\frac{\hbar^2}{2m}\right)^2 \times[-7\nabla^4 U + 5\beta(\nabla^2 U)^2 + \beta\nabla^2(\nabla U)^2]\right], \tag{21}$$

where the superscript 4 in parentheses in $Z_0^{(4)}$ indicates that it is a semiclassical expansion containing terms up to order $\hbar^4$, apart from the overall phase-space factor of $\hbar^{-3}$ in front. In similar notation,

$$Z_0^{(2)}(\beta) = \frac{1}{8\pi^{3/2}\beta^{3/2}}\left(\frac{2m}{\hbar^2}\right)^{3/2} \times\int d^3r\, e^{-\beta U(\vec{r})}\left(1 - \frac{\beta^2}{12}\frac{\hbar^2}{2m}\nabla^2 U\right),$$

$$Z_0^{(0)}(\beta) = \frac{1}{8\pi^{3/2}\beta^{3/2}}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int d^3r\, e^{-\beta U(\vec{r})}.$$

On doing the $\vec{p}$ integrations in Eq. (20), we get

$$\mathrm{Tr}e^{-\beta\hat{H}_0}\left(\hat{l}_z^2 - \frac{m}{\beta}r_\perp^2\right) = -\frac{\hbar^2}{3}Z_0^{(2)}(\beta) + \frac{\beta^2\hbar^4}{180m}\left\langle\left(\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2}\right)\right\rangle Z_0^{(0)}(\beta), \tag{22}$$

where

$$\left\langle\left(\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2}\right)\right\rangle = \int d^3r\, e^{-\beta U}\left(\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2}\right)\left(\int d^3r e^{-\beta U}\right)^{-1}.$$

This expression may now be substituted in Eq. (14) to obtain a semiclassical expression for Z_B to the desired order in $\hbar$. Using the same superscript notation in Z_B to indicate this order as in Z_0, we get

$$Z_B^{(4)}(\beta) = Z_0^{(4)}(\beta) - \frac{e^2B^2\hbar^2}{24m^2c^2}\beta^2 Z_0^{(2)}(\beta) + \frac{e^2B^2\hbar^2}{24m^2c^2}\beta^4\frac{\hbar^2}{60m}\left\langle\left(\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2}\right)\right\rangle Z_0^{(0)}(\beta). \tag{23}$$

Expression (23) is correct only to power B^2, and up to order $\hbar^4$ in the Kirkwood expansion. We may therefore replace $Z_0^{(2)}$ and $Z_0^{(0)}$ in the right-hand side of Eq. (23) by $Z_0^{(4)}$, incurring only errors of higher order in $\hbar$. This expression for $Z_B(\beta)$ may be directly used in Eqs. (5) and (10) to obtain the final expressions for the susceptibility. From Eqs. (5) and (23), we get the high-temperature susceptibility per particle of a classical gas as

$$\frac{1}{N}\chi(T\to\infty) = -\frac{e^2\hbar^2}{12m^2c^2}\frac{1}{kT} + \frac{e^2\hbar^2}{12m^2c^2}\frac{1}{(kT)^3}\frac{\hbar^2}{60m}\left\langle\left(\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2}\right)\right\rangle, \tag{24}$$

where the first term is just the Landau value, and the second the sought after correction term.[12]

Equations (10) and (23) may be used to obtain the zero-temperature susceptibility of the degenerate gas. Note from Eq. (23) that

$$\frac{1}{B}\frac{1}{\beta^2}\left(\frac{\partial Z_B}{\partial B}\right) = -\frac{e^2\hbar^2}{12m^2c^2}\left[Z_0(\beta) - \frac{\beta^{1/2}}{8\pi^{3/2}}\left(\frac{2m}{\hbar^2}\right)^{1/2}\frac{1}{30}\int e^{-\beta U}\left(\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2}\right)d^3r\right].$$

Using Eq. (10), and some properties[13] of the Laplace transform, we get

$$\chi(T=0)=-\frac{e^2\hbar^2}{12m^2c^2}\left[g_0(\mu)-\frac{1}{8\pi^2}\left(\frac{2m}{\hbar^2}\right)^{1/2}\frac{1}{30}\frac{\partial}{\partial\mu}\int d^3r\left(\frac{\partial^2U}{\partial x^2}+\frac{\partial^2U}{\partial y^2}\right)\frac{\Theta(\mu-U)}{(\mu-U)^{1/2}}\right], \tag{25}$$

where $g_0(\mu)$ is the density of states of an electron at the Fermi energy μ in the absence of any magnetic field, and $\Theta(x)$ is the unit step function, zero for $x\leq 0$, and unity for $x>0$. Again, the first term in Eq. (25) is the well-known Landau term, while the next term is the sought-after correction term.

III. SPECIFIC EXAMPLES

In this section, we shall apply formulas (24) and (25) to evaluate the diamagnetic susceptibility for some potential barriers of simple shape.

A. One-dimensional harmonic barrier

In this case, $U=\frac{1}{2}m\Omega^2y^2$, where Ω is the oscillator "frequency." Then $\partial^2U/\partial x^2=0$, $\partial^2U/\partial y^2=m\Omega^2$, and $\langle(\partial^2U/\partial x^2+\partial^2U/\partial y^2)\rangle=m\Omega^2$. Substituting this into Eq. (24), we get, for the classical gas,

$$\frac{1}{N}\chi(T\to\infty)=\chi_L\left(1-\frac{\hbar^2\Omega^2}{60(kT)^2}\right), \tag{26}$$

where $\chi_L=-(e^2\hbar^2/12m^2c^2)(1/kT)$ is the classical Landau value. Hence the correction term to the Landau value goes to zero at high temperatures irrespective of the parameter Ω. This is in agreement with Eq. (4.10) of Thomas.[4]

To calculate the zero-temperature susceptibility of a degenerate gas for the same potential, we use Eq. (25). In this case it is necessary to evaluate the integral

$$I=\int dy\,\frac{\partial^2U}{\partial y^2}\frac{\Theta(\mu-U)}{(\mu-U)^{1/2}},$$

and then take its derivative with respect to μ. Because of the step function $\Theta(\mu-U)$, the y integration is cut off at $y=\pm y_0=(2\mu/m\Omega^2)^{1/2}$. Thus

$$I=m\Omega^2\int_{-y_0}^{y_0}dy\,(\mu-\tfrac{1}{2}m\Omega^2y^2)^{-1/2}=\pi(2m\Omega^2)^{1/2}.$$

Since this is independent of μ, $\partial I/\partial\mu=0$, and the correction to the Landau value of susceptibility at zero temperature vanishes identically to this order.

B. Isotropic Harmonic-oscillator potential

Now we choose $U=\frac{1}{2}m\Omega^2r^2$, isotropic in three dimensions. Using Eq. (24) again, it is straightforward to show that

$$\frac{1}{N}\chi(T\to\infty)=\chi_L\left(1-\frac{\hbar^2\Omega^2}{30(kT)^2}\right). \tag{27}$$

To evaluate the correction at zero temperature, note that $\partial^2U/\partial x^2+\partial^2U/\partial y^2=2m\Omega^2$, so we have to evaluate the integral

$$I=2m\Omega^2\int d^3r\,(\mu-\tfrac{1}{2}m\Omega^2r^2)^{-1/2}\Theta(\mu-\tfrac{1}{2}m\Omega^2r^2)$$
$$=2^{5/2}\pi^2\mu/(m\Omega^2)^{1/2}.$$

Substituting this in Eq. (25), we get

$$\chi(T=0)=-\frac{e^2\hbar^2}{12m^2c^2}\left(g_0(\mu)-\frac{1}{30\hbar\Omega}\right). \tag{28}$$

Remembering that the smooth density of states for a harmonic oscillator potential (without spin degeneracy) is[14]

$$g_0(\mu)=\frac{\mu^2}{2(\hbar\Omega)^3}-\frac{1}{8\hbar\Omega}, \tag{29}$$

we see that the correction to Landau term is very small.

C. Thomas (Ref. 4) potential $U(y)=\frac{1}{2}m\Omega^2y^2+V_0b_4y^4$

We shall evaluate the high-temperature susceptibility for this potential. Here

$$\left\langle\frac{\partial^2U}{\partial y^2}\right\rangle=m\Omega^2+12V_0b_4I, \tag{30}$$

with

$$I=\int_{-\infty}^{+\infty}y^2e^{-\beta(m\Omega^2y^2/2+V_0b_4y^4)}dy\times\left(\int_{-\infty}^{+\infty}e^{-\beta(m\Omega^2y^2/2+V_0b_4y^4)}dy\right)^{-1}$$
$$=-\frac{2}{\beta\Omega^2}\frac{\partial}{\partial m}\ln\int_{-\infty}^{+\infty}\left(e^{-\beta(m\Omega^2y^2/2+V_0b_4y^4)}dy\right).$$

Using the relation[15]

$$\int_{-\infty}^{+\infty}e^{-\beta(m\Omega^2y^2/2+V_0b_4y^4)}dy=\frac{1}{2}\left(\frac{m\Omega^2}{2V_0b_4}\right)^{1/2}\exp\left(\frac{1}{32}\beta\frac{m^2\Omega^4}{V_0b_4}\right)K_{1/4}\left(\frac{1}{32}\beta\frac{m^2\Omega^4}{V_0b_4}\right).$$

where $K_{1/4}$ is defined[16] in terms of a Hankel's function of imaginary argument, and the identity[16]

$$\frac{d}{dz}K_\nu(z)=-\frac{\nu}{z}K_\nu(z)-K_{\nu-1}(z),$$

we immediately obtain

$$I=\frac{m\Omega^2}{8V_0b_4}\left\{-1+K_{3/4}\left(\frac{1}{32}\beta\frac{m^2\Omega^4}{V_0b_4}\right)\times\left[K_{1/4}\left(\frac{1}{32}\beta\frac{m^2\Omega^4}{V_0b_4}\right)\right]^{-1}\right\}. \quad (31)$$

To take the proper high-temperature limit of this, we assume the parameters of the potential $U(y)$ to be fixed, and let $\beta\to 0$. In this limit,

$$z=\tfrac{1}{32}\beta\, m^2\Omega^4/V_0b_4\ll 1, \quad (32)$$

and we may write[17]

$$\frac{K_{3/4}(z)}{K_{1/4}(z)}\sim\frac{\Gamma(\frac{3}{4})}{\Gamma(\frac{1}{4})}(\tfrac{1}{2}z)^{-1/2}+\frac{[\Gamma(\frac{3}{4})]^2}{\Gamma(\frac{1}{4})\Gamma(\frac{5}{4})}. \quad (33)$$

Using relation (33) in Eq. (31), we obtain I in the high-temperature limit; and substituting this value of I in Eq. (30), we get

$$\left\langle\frac{\partial^2 U}{\partial y^2}\right\rangle\approx\frac{12(V_0b_4)^{1/2}}{\beta^{1/2}}\frac{\Gamma(\frac{3}{4})}{\Gamma(\frac{1}{4})}+\frac{m\Omega^2}{2}\left(\frac{3[\Gamma(\frac{3}{4})]^2}{\Gamma(\frac{1}{4})\Gamma(\frac{5}{4})}-1\right).$$

Putting this into Eq. (24), the high-temperature susceptibility is

$$\frac{1}{B}\chi(T\to\infty)=\chi_L\left[1-\frac{1}{(kT)^{3/2}}\frac{\hbar^2}{5m}(V_0b_4)^{1/2}\frac{\Gamma(\frac{3}{4})}{\Gamma(\frac{1}{4})}-\frac{\hbar^2\Omega^2}{120(kT)^2}\left(\frac{3[\Gamma(\frac{3}{4})]^2}{\Gamma(\frac{1}{4})\Gamma(\frac{5}{4})}-1\right)\right], \quad (34)$$

which shows that it again reduces to the Landau value at high temperatures. We emphasize that relation (34) was *not* obtained by Thomas, since he did not evaluate χ in the high-temperature limit (32). Rather, he used a perturbation formalism, and assumed that the strength of the y^4 term in $U(y)$ to be adjustable at high temperatures, so that the condition[18]

$$V_0b_4/m^2\Omega^4\ll\beta \quad (35)$$

is satisfied, which is really the opposite of condition (32). Using the asymptotic relation[19] for z in Eq. (31),

$$K_\nu(z)\sim\left(\frac{\pi}{2z}\right)^{1/2}e^{-z}\left(1+\frac{4\nu^2-1}{8z}\right),$$

where $z=\frac{1}{32}\beta m^2\Omega^4/V_0b_4$, the expression for I now reduces to

$$I\sim 1/\beta m\Omega^2.$$

Substituting this into Eq. (30),

$$\left\langle\frac{\partial^2 U}{\partial y^2}\right\rangle=m\Omega^2+\frac{12V_0b_4}{\beta m\Omega^2}.$$

From Eq. (24), we now get

$$\frac{1}{N}\chi=\chi_L\left(1-\frac{\hbar^2\Omega^2}{60(kT)^2}-\frac{\hbar^2\Omega^2}{5(kT)}\frac{V_0b_4}{m^2\Omega^4}\right), \quad (36)$$

which is the result under the restriction (35). This is the same result as obtained by Thomas,[4] after minor algebraic errors[20] in his paper are corrected.

To summarize, we have derived the *weak-field* susceptibility expressions for the classical and degenerate electron gas subject to a smooth potential barrier of arbitrary shape. These expressions are given by Eqs. (24) and (25), and the main advantage of our method is that no knowledge of the eigenspectrum of the potential in the presence of the magnetic field is required. The disadvantage of our method is that we cannot handle discontinuous potential barriers, or even barriers that are very steep, since then the higher-order terms in powers of $\hbar$ containing higher derivatives may contribute significantly. Even in this weak-field limit, when surface effects should be most effective, we find that the corrections to the Landau levels of susceptibility are unimportant.

APPENDIX

We will here indicate the procedure for obtaining the partition function when $\hat{H}_0$ and $\hat{l}_z$ do not commute. The exponential in Eq. (11) can no longer be written as the product of two exponentials as in Eq. (13). However we can still write

$$\exp\left[-\beta\left(\hat{H}_0+\frac{e^2B^2}{8mc^2}r_\perp^2+\frac{eB}{2mc}\hat{l}_z\right)\right]=e^{-\beta\hat{H}_0}\hat{S}(\beta),$$

where $\hat{S}(\beta)$ can be written

$$\hat{S}(\beta)=1-\int_0^\beta\hat{R}(\beta')\,d\beta'+\int_0^\beta\hat{R}(\beta')\int_0^{\beta'}\hat{R}(\beta'')d\beta''d\beta'+\cdots, \quad (A1)$$

with $\hat{R}(\beta)$ given by

$$\hat{R}(\beta)=e^{\beta\hat{H}_0}\left(\frac{e^2B^2}{8mc^2}r_\perp^2+\frac{eB}{2mc}\hat{l}_z\right)e^{-\beta H_0}=\left(\frac{e^2B^2}{8mc^2}r_\perp^2+\frac{eB}{2mc}\hat{l}_z\right)+\beta\left[\hat{H}_0,\left(\frac{e^2B^2}{8mc^2}r_\perp^2+\frac{eB}{2mc}\hat{l}_z\right)\right]+\frac{\beta^2}{2!}\left[\hat{H}_0,\left[\hat{H}_0,\left(\frac{e^2B^2}{8mc^2}r_\perp^2+\frac{eB}{2mc}\hat{l}_z\right)\right]\right]+\cdots. \quad (A2)$$

The partition function can now be written

$$Z_B(\beta)=\mathrm{Tr}\,e^{-\beta\hat{H}_0}\hat{S}(\beta),$$

or in analogy with Eq. (16),

$$Z_B(\beta)=\frac{1}{h^3}\int(e^{-\beta\hat{H}_0}e^{i\vec{p}\cdot\vec{r}/\hbar})^*\,\hat{S}(\beta)e^{i\vec{p}\cdot\vec{r}/\hbar}d^3p\,d^3r.$$

The effect of the operator $\hat{S}(\beta)$ acting on the plane wave can be determined to any desired order in $\hbar$

by using Eqs. (A1) and (A2). The result can be formally written

$$\hat{S}(\beta)e^{i\vec{p}\cdot\vec{r}/\hbar}=e^{i\vec{p}\cdot\vec{r}/\hbar}[1+BI_1(\vec{r},\vec{p},\beta)+B^2I_2(\vec{r},\vec{p},\beta)+\cdots],$$

where $I_1(\vec{r},\vec{p},\beta)$ and $I_2(\vec{r},\vec{p},\beta)$ are lengthy expressions involving $\vec{r},\vec{p},\beta$ and derivatives of the potential. The partition function now becomes

$$Z_B(\beta)=\frac{1}{h^3}\int e^{-\beta[p^2/2m+U(\vec{r})]}\times(1+\hbar w_1^*+\hbar^2w_2+\hbar^3w_3^*+\hbar^4w_4+\cdots)\times[1+BI_1(\vec{r},\vec{p},\beta)+B^2I_2(\vec{r},\vec{p},\beta)+\cdots]\times d^3r\,d^3p.$$

Upon doing the p integrations, a straightforward but lengthy procedure, the same expression (23) as derived in the text for the axially symmetric case, is, obtained.

*Work supported by National Research Council of Canada.

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[2]Earlier references may be found in the papers by Friedman (Ref. 3) and Thomas (Ref. 4).

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[6]R. Kubo had suggested earlier that the orbital susceptibility may be expanded in a power series of $\hbar$, with the leading term given by the Landau value. See *Lectures in Theoretical Physics* (University of Colorado Press, Boulder, 1966), Vol. III-A, p. 239.

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[16]I. S. Gradshteyn and I. M. Ryzhik, in Ref. 15, pp. 952 and 970.

[17]See Ref. 7, p. 375.

[18]This is obtained from Thomas (Ref. 4) when his Eqs. (3.9), (4.3), and (4.9) are combined. For the physical implications of this restriction, see his paper.

[19]See Ref. 7, p. 378.

[20]In Ref. 4, there are algebraic errors in Eqs. (4.13) and (4.14). Using Thomas's equation (4.6) and (4.12), it is easy to verify that the overall multiplying factor in Eq. (4.13) should be $-18\chi_L$ in place of $\frac{9}{2}\chi_L$, and that the last term in the square bracket in the same equation should be multiplied by $\operatorname{csch}\frac{1}{2}\hbar\Omega\beta$. When these changes are made, the first term in his equation (4.14), in which we are interested, increases by a factor of 4, in agreement with our result