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# DIAMAGNETISM OF AN ELECTRON GAS AND SURFACE CURRENTS

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When an electron gas is submitted to a uniform magnetic field, the diamagnetic part of its magnetization is associated with amperian surface currents. In the weak-field limit, explicit expressions are found for the current density near an infinitely steep wall, and near a soft wall, for both Boltzmann and Fermi statistics. The Wigner distribution function in presence of a magnetic field is a convenient tool.

## 1. Introduction

The conventional way[1, 2]) of studying the diamagnetism of an electron gas is based on the calculation of the partition function in a large volume. The detail of what happens near the boundaries is not needed for computing the net magnetization, a fortunate simplifying feature for practical calculations.

Yet, it is well known that the magnetization can be ascribed to amperian currents, which are localized at the surface in the case of a uniformly magnetized body; sending away to infinity these currents is somewhat unsatisfactory. Although the structure of the surface currents might not be directly observable, it is at least an amusing exercise to investigate that structure, and this is the aim of this paper.

The current density has already been calculated for the simple model of a magnetized electron gas confined by a harmonic oscillator potential well[3]). This model has the immense advantage of being exactly soluble for an arbitrary field strength, but is does not represent even schematically a large system with a surface region of finite depth; the harmonic oscillator well model rather represents a small system[4,5]), in which the "surface" region occupies the whole volume. The present paper deals with large systems and studies surface regions described by potential walls of more realistic shapes. Unfortunately, it is then no longer possible to obtain a simple exact solution for an arbitrary strength of the applied magnetic field, and the current will be

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computed only in the linear-response regime, i.e. in the weak-field limit. Of course, the de Haas–van Alphen oscillations of the magnetization as a function of the magnetic field are beyond the scope of this approach.

Two extreme cases for the shape of the potential wall which bounds the electron gas will be considered: an infinitely steep wall (in section 2) and a soft wall (in section 3). Both cases of Boltzmann statistics (valid at high temperature) and Fermi statistics (in the zero-temperature limit) will be treated; the results for the Fermi case will be derived from the results for the Boltzmann case by the inverse Laplace transform method[6]). In the special case of a soft wall with Boltzmann statistics, the interactions are taken into account; they are not, in all other cases.

## 2. Steep wall

We consider an ideal electron gas, in a semi-infinite geometry. The gas is confined in the region $x > 0$ by an infinitely steep plane potential wall $V(x)$;

$$V(x) = 0 \text{ if } x > 0, \quad V(x) = \infty \text{ if } x < 0. \tag{2.1}$$

The gas is submitted to a weak uniform magnetic field $\boldsymbol{B}$ directed along the $z$ axis. It is convenient to choose for the vector potential the gauge

$$\boldsymbol{A} = (0, Bx, 0). \tag{2.2}$$

Therefore, for an electron of mass $m$ and charge $e$, the one-body hamiltonian is

$$H = \frac{1}{2m}\left(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}\right)^2 + V(x), \tag{2.3}$$

where $\boldsymbol{p}$ stands for the operator $-i\hbar\boldsymbol{\nabla}$.

We want to compute the electrical current density $j(\boldsymbol{r}_0)$ at some point $\boldsymbol{r}_0 = (x_0, y_0, z_0)$. This current density is directed along the $y$ axis, as it can be shown by a symmetry argument. Indeed, the hamiltonian is invariant under a time reversal followed by a symmetry with respect to the plane $y = y_0$. The $x$ and $z$ components of the current density operator are reversed by the above transformation, while the $y$ component is unchanged. Therefore, only the $y$ component can have a non-vanishing thermal average. Furthermore, the current density does not depend on $y_0$ and $z_0$, since the hamiltonian is invariant under translations along the $y$ and $z$ axes.

### 2.1. *Boltzmann statistics*

For a system of $N$ independent electrons with Boltzmann statistics, the current density is given by

$$j_y(x_0) = \frac{N}{Z}\left\langle r_0 \left| \mathrm{e}^{-\beta H} \frac{e}{m}\left(p_y - \frac{eB}{c}x_0\right)\right| r_0\right\rangle, \tag{2.4}$$

where $\beta$ is related to the temperature $T$ and Boltzmann's constant $k$ by $\beta = 1/kT$, and where $Z$ is the one-body partition function (since $\exp(-\beta H)$ and $p_y$ commute, their order is irrelevant).

We are interested in the linear response, i.e. in the part of the current density which is proportional to $B$. Since the partition function $Z$ has no term of first order in $B$ (it must be an even function of $B$), it can be replaced by its zero-field value

$$Z = \Omega/\lambda^3, \tag{2.5}$$

where $\Omega$ is some large normalization volume and $\lambda = (2\pi\hbar^2\beta/m)^{1/2}$ is the thermal de Broglie wavelength. To first order in $B$, the hamiltonian can be written as

$$H = H_0 - \frac{eB}{mc}p_y x, \tag{2.6}$$

where $H_0$ is the zero-field hamiltonian

$$H_0 = \frac{p^2}{2m} + V(x), \tag{2.7}$$

and the density operator can be expanded as

$$\mathrm{e}^{-\beta H} = \mathrm{e}^{-\beta H_0} + \frac{eB}{mc}\int_0^\beta \mathrm{d}\tau\, \mathrm{e}^{-(\beta-\tau)H_0} p_y x\, \mathrm{e}^{-\tau H_0}. \tag{2.8}$$

Using (2.5) and (2.8) in (2.4), we find, to first order in $B$,

$$j_y(x_0) = n\lambda^3\left[\frac{e}{m}\left\langle r_0\left| \mathrm{e}^{-\beta H_0} p_y \right| r_0\right\rangle + \frac{e^2 B}{m^2 c}\int_0^\beta \mathrm{d}\tau \left\langle r_0 \left| \mathrm{e}^{-(\beta-\tau)H_0} p_y x\, \mathrm{e}^{-\tau H_0} p_y \right| r_0\right\rangle \right.$$
$$\left. - \frac{e^2 B}{mc} x_0 \left\langle r_0 \left| \mathrm{e}^{-\beta H_0} \right| r_0\right\rangle\right], \tag{2.9}$$

where $n = N/\Omega$ is the number density. The first term of (2.9) vanishes for symmetry reasons. In the other terms, the contributions from the $y$ and $z$ degrees of freedom can be easily computed and factorized out ($p_y$ commutes with $H_0$, and the $p_y^2$ which appears in the second term of (2.9) gives the simple contribution $m/\beta$).

Calling

$$H_{0x} = \frac{p_x^2}{2m} + V(x) \tag{2.10}$$

the $x$ part of $H_0$, and using the closure property

$$\langle x_0 | \, e^{-\beta H_{0x}} \, | x_0 \rangle = \int dx \langle x_0 | \, e^{-(\beta-\tau)H_{0x}} \, | x \rangle \langle x | \, e^{-\tau H_{0x}} \, | x_0 \rangle, \tag{2.11}$$

we recast (2.9) as

$$j_y(x_0) = \frac{n\lambda e^2 B}{\beta mc} \int_0^\beta d\tau \int dx \langle x_0 | \, e^{-(\beta-\tau)H_{0x}} \, | x \rangle (x - x_0) \langle x | \, e^{-\tau H_{0x}} \, | x_0 \rangle. \tag{2.12}$$

With $V(x)$ given by (2.1), the thermal propagator which appears in (2.12) has the simple form

$$\langle x_0 | \, e^{-\beta H_{0x}} \, | x \rangle = \left( \frac{m}{2\pi \hbar^2 \beta} \right)^{1/2} \left\{ \exp\left[ -\frac{m(x-x_0)^2}{2\beta\hbar^2} \right] - \exp\left[ -\frac{m(x+x_0)^2}{2\beta\hbar^2} \right] \right\} \theta(x)\, \theta(x_0), \tag{2.13}$$

where $\theta$ is the step function (the first term in (2.13) is the free-particle propagator, and the second one is the image term which accounts for the infinite potential wall). Using (2.13) in (2.12), and performing the integral on $x$, one obtains

$$j_y(x_0) = \frac{ne^2 B}{\beta mc} x_0 \int_0^\beta d\tau \left\{ \mathrm{Erf}\left[ \left( \frac{m\beta}{2\hbar^2(\beta-\tau)\tau} \right)^{1/2} x_0 \right] + \exp\left( -\frac{2m}{\beta\hbar^2} x_0^2 \right) - 1 + \frac{2\tau - \beta}{\beta} \exp\left( -\frac{2m}{\beta\hbar^2} x_0^2 \right) \mathrm{Erf}\left[ \left( \frac{m}{2\hbar^2 \beta(\beta-\tau)\tau} \right)^{1/2} (\beta - 2\tau) x_0 \right] \right\}, \tag{2.14}$$

where Erf is the error function. Then, the integral on $\tau$ is performed by integration by parts and using $u^2 = \beta^2/4(\beta-\tau)\tau$ as a new variable.

The final result is (the variable $x_0$ has been renamed $x$ for simplicity)

$$j_y(x) = \frac{\pi ne^2 B}{mc\lambda} x^2 \left[ 1 - \mathrm{Erf}\left( 2\pi^{1/2} \frac{x}{\lambda} \right) \right]. \tag{2.15}$$

This current-density profile is plotted in fig. 1. As expected, the current density is localized near the surface, actually within a depth of the order of the de Broglie wavelength $\lambda$. The total surface current is

$$J_y = \int_0^\infty j_y(x) dx = \frac{n\beta e^2 \hbar^2 B}{12 m^2 c}. \tag{2.16}$$

If the body, far away from its surface, has a uniform magnetization density $\boldsymbol{M}$ along the $z$ axis, the surface current should be

$$J_y = -cM_z. \tag{2.17}$$

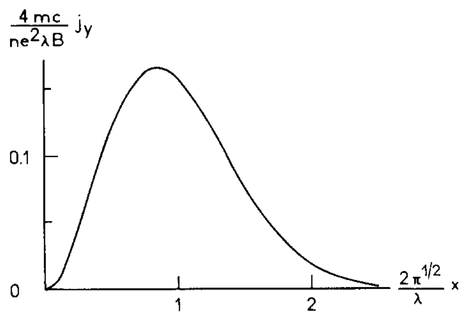


Fig. 1. The current-density profile near an infinitely steep wall, with Boltzmann statistics.

The magnetization $M_z$ which is obtained from (2.16) and (2.17) is indeed the Landau result for an extended electron gas. Of course, for obtaining the total magnetization density, one must add to the present diamagnetic contribution the paramagnetic one from the spins, which has the opposite sign and is three times larger.

### 2.2. *Fermi statistics* (*zero temperature*)

*For a system of independent particles*, it is possible to obtain the current density with Fermi statistics at zero temperature from the current density with Boltzmann statistics by an inverse Laplace transform[6]). Indeed, the current density with Boltzmann statistics is

$$j_B = \frac{N}{Z} \sum_n e^{-\beta E_n} j_n, \tag{2.18}$$

where $j_n$ is the current density in the $n$th one-particle orbital quantum state and $E_n$ is the energy of that state. The current density at zero temperature with Fermi statistics is

$$j_F = 2 \sum_n \theta(\mu - E_n) j_n, \tag{2.19}$$

where $\mu$ is the Fermi energy and $\theta$ the step function (the factor 2 in (2.19) accounts for the spin). Since the Laplace transform of this step function is

$$\int_0^\infty e^{-\beta\mu} \theta(\mu - E_n) d\mu = \frac{1}{\beta} e^{-\beta E_n}, \tag{2.20}$$

it is readily seen that

$$j_F = \mathscr{L}_\mu^{-1} \left( \frac{2 Z j_B}{N\beta} \right), \tag{2.21}$$

where $\mathscr{L}_\mu^{-1}$ is the inverse Laplace transform from the variable $\beta$ to the variable $\mu$.

When (2.15) is used for $j_B$, the inverse Laplace transform (2.21) is easily computed. Indeed, since[7])

$$\mathscr{L}_\mu^{-1}\{\mathrm{Erf}[(2mx^2/\hbar^2)^{1/2}\,\beta^{-1/2}]\} = \frac{1}{\pi\mu}\sin[(2mx^2/\hbar^2)^{1/2}\,\mu^{1/2}], \tag{2.22}$$

the current density with Fermi statistics is

$$\begin{aligned} j_y(x) &= \frac{me^2B}{2\pi\hbar^4c}\,x^2\,\mathscr{L}_\mu^{-1}\left\{\frac{1}{\beta^3}-\frac{1}{\beta^3}\,\mathrm{Erf}[(2mx^2/\hbar^2)^{1/2}\,\beta^{-1/2}]\right\} \\ &= \frac{me^2B}{2\pi\hbar^4c}\,x^2\left\{\frac{1}{2}\mu^2-\int_0^\mu \mathrm{d}\mu\int_0^\mu \mathrm{d}\mu\int_0^\mu \mathrm{d}\mu\,\sin[(2mx^2/\hbar^2)^{1/2}\,\mu^{1/2}]\right\} \\ &= \frac{e^2f^2B}{32\pi^2mc}\left\{4f^2x^2\left[\frac{\pi}{2}-\mathrm{Si}(2fx)\right]+\left(\frac{6}{4f^2x^2}-1\right)\sin 2fx \right. \\ &\quad \left. -\left(\frac{6}{2fx}+2fx\right)\cos 2fx\right\}, \end{aligned} \tag{2.23}$$

where the Fermi wave number $f$ is defined by $\mu=\hbar^2f^2/2m$ and Si is the sine-integral function. The limiting behaviours are

$$\begin{aligned} j_y(x) &\sim \frac{e^2f^4B}{16\pi mc}\,x^2 \quad \text{if } x\to 0, \\ j_y(x) &\sim -\frac{e^2f^2B}{4\pi^2mc}\,\frac{\cos 2fx}{2fx} \quad \text{if } x\to\infty; \end{aligned} \tag{2.24}$$

it is seen that $j_y(x)$ has Friedel-type oscillations on a length scale of the order of $f^{-1}$. This current-density profile is plotted in fig. 2. The total surface current

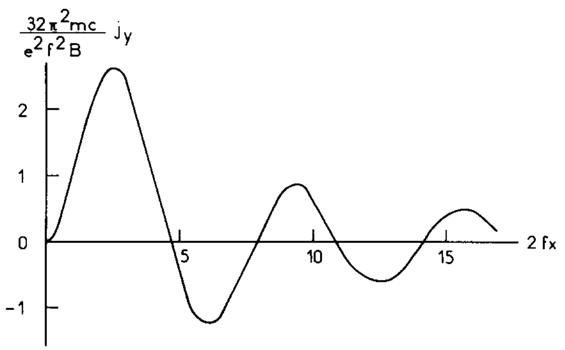


Fig. 2. The current-density profile near an infinitely steep wall, with Fermi statistics.

is obtained either by integration of (2.23) or by using (2.16) in the inverse Laplace transform (2.21); it is

$$J_y = \int_0^\infty j_y(x)\mathrm{d}x = \frac{e^2 fB}{12\pi^2 mc}, \tag{2.25}$$

and $-(1/c)J_y$ is the Landau value for the diamagnetic magnetization density in an extended degenerate electron gas, as it should.

An alternative calculation of the current densities (2.15) and (2.23) is given in appendix I.

## 3. Soft wall

### 3.1. *Boltzmann statistics*

We now turn to the case of a "soft" potential wall, i.e. we assume that the de Broglie wavelength $\lambda$ is small compared to some characteristic length scale of the potential. In that case, the interactions between the electrons can be included in the formalism provided they are also soft enough; this condition is fulfilled if $\lambda$ is small compared to the classical distance of closest approach $\beta e^2$ and to the average interparticle distance $a$. A weak uniform magnetic field $\boldsymbol{B}$ is applied.

A convenient tool for dealing with this nearly classical situation is the Wigner distribution function[8,9]. For describing a $N$-particle system with interactions, with a total hamiltonian $H$, we use $3N$-dimensional position or momentum vectors such as $r$, $p$, etc.... From the density matrix in configuration space, one obtains another representation of this matrix, called the Wigner distribution $f(r, p, \beta)$, through the definition*

$$f(r, p, \beta) = \int \mathrm{d}s\ \mathrm{e}^{(\mathrm{i}/\hbar)p\cdot s}\left\langle r - \frac{s}{2} \,\middle|\, \mathrm{e}^{-\beta H} \,\middle|\, r + \frac{s}{2}\right\rangle. \tag{3.1}$$

The density matrix obeys Bloch's equation. In the Wigner representation, this equation becomes[11])

$$\frac{\partial f(r, p, \beta)}{\partial \beta} = -H(r, p)\cos\left[\frac{\hbar}{2}(\overleftarrow{\nabla}_p \cdot \overrightarrow{\nabla}_r - \overleftarrow{\nabla}_r \cdot \overrightarrow{\nabla}_p)\right] f(r, p, \beta), \tag{3.2}$$

where $H(r, p)$ is the classical hamiltonian; the gradient operators operate either to the right or to the left, as indicated by the arrows.

* In eq. (2.2) of a previous paper[10]) we have defined as the "Wigner distribution" a slightly different function. The present definition, which is the original one[8]), is more symmetrical and more convenient.

The hamiltonian of concern here is

$$H=\frac{1}{2m}\left(p-\frac{e}{c}A\right)^2+V(r), \tag{3.3}$$

where $A$ is the $3N$-dimensional vector potential, the components of which are $\boldsymbol{A}(\boldsymbol{r}_1)$, $\boldsymbol{A}(\boldsymbol{r}_2), \ldots, \boldsymbol{A}(\boldsymbol{r}_N)$ ($\boldsymbol{r}_i$ is the position of the $i$th particle, and $\boldsymbol{A}(\boldsymbol{r}_i)$ is the 3-dimensional vector potential at this point); the potential $V(r)$ includes the walls as well as the interactions between the particles. In this magnetic case, it is more convenient to use the "physical" momentum (mass times velocity) $\pi=p-(e/c)A$, rather than the canonical one $p$. With the variables $(r, \pi)$, after the gradient operations to the left have been performed, (3.2) becomes

$$\frac{\partial f(r,\pi,\beta)}{\partial\beta}=-\left[\frac{\pi^2}{2m}+\cos\left(\frac{1}{2}\hbar\nabla_r\cdot\nabla_\pi\right)V(r)-\frac{\hbar^2}{8m}\left(\nabla_r+\frac{e}{c}\boldsymbol{B}\wedge\nabla_\pi\right)^2\right]f(r,\pi,\beta). \tag{3.4}$$

In this equation, the gradient $\nabla_r$ in the argument of the cosine operates only on $V(r)$; the vector product $\boldsymbol{B}\wedge\nabla_\pi$ is the $3N$-dimensional vector operator, the components of which are $\boldsymbol{B}\wedge\nabla_{\pi_1}, \boldsymbol{B}\wedge\nabla_{\pi_2}, \ldots, \boldsymbol{B}\wedge\nabla_{\pi_N}$. A remarkable feature of eq. (3.4) is that it contains the magnetic field $\boldsymbol{B}=\operatorname{curl}\boldsymbol{A}$ itself rather than $\boldsymbol{A}$, and therefore it is explicitly gauge invariant. It may also be noted that the field-dependent term in (3.4) vanishes in the classical limit $\hbar\to 0$, in agreement with the well-known Bohr–van Leeuwen theorem which states that magnetism does not exist in classical physics.

Under the nearly classical conditions which are considered here, the solution of (3.4) can be computed as an expansion in powers of $\hbar^2$; this expansion will then be used for computing the electrical-current density. In the limit $\hbar=0$, the solution of (3.4) (with the initial condition $f=1$ at $\beta=0$) is the classical distribution

$$f_{\mathrm{cl}}=\exp\left[-\beta\left(\frac{\pi^2}{2m}+V\right)\right]. \tag{3.5}$$

Therefore, we look for a solution of (3.4) of the form

$$f=f_{\mathrm{cl}}(1+\hbar^2\Phi_1+\hbar^4\Phi_2+\ldots). \tag{3.6}$$

Using (3.6) in (3.4), we can obtain $\Phi_1$, $\Phi_2$, etc... by succesive iterations. For a linear response calculation, it is enough to keep the $B$-dependent terms only up to first order in $B$. The results up to order $\hbar^4$ are

$$\Phi_1=-\frac{\beta^2}{8m}\nabla^2V+\frac{\beta^3}{24m}(\nabla V)^2+\frac{\beta^3}{24m^2}(\pi\cdot\nabla)^2V-\frac{e\beta^3}{12m^2c}(\boldsymbol{B}\wedge\nabla V)\cdot\pi \tag{3.7}$$

(from now on, $\nabla$ means $\nabla_r$ and $\boldsymbol{B}\wedge\nabla$ is the $3N$-dimensional vector operator the components of which are $\boldsymbol{B} \wedge \nabla_1, \boldsymbol{B} \wedge \nabla_2, \ldots, \boldsymbol{B} \wedge \nabla_N$) and

$$\begin{aligned}\Phi_2 = \Phi_2^{(0)} &+ \frac{e\beta^5}{96m^3c}[(\boldsymbol{B} \wedge \nabla V)\cdot\pi]\left[\nabla^2 V - \frac{\beta}{3}(\nabla V)^2 - \frac{\beta}{3m}(\pi\cdot\nabla)^2 V\right] \\ &+ \frac{e\beta^5}{120m^3c}(\boldsymbol{B} \wedge \nabla V)\cdot\nabla(\pi\cdot\nabla)V \\ &+ \frac{e\beta^4}{96m^3c}\pi\cdot(\boldsymbol{B}\wedge\nabla)\left[-\nabla^2 V + \frac{2\beta}{5}(\nabla V)^2 + \frac{\beta}{5m}(\pi\cdot\nabla)^2 V\right], \end{aligned} \tag{3.8}$$

where $\Phi_2^{(0)}$ is independent of $\boldsymbol{B}$ and even in $\pi$; $\Phi_2^{(0)}$, which is not needed here, has been computed in ref. 9.

We can now use the above expansion of the distribution function $f$ for computing the electrical current density. In the Wigner representation, the current-density operator at some point $\boldsymbol{r}$ is

$$\frac{e}{m}\sum_{i=1}^{N} \boldsymbol{\pi}_i\,\delta(\boldsymbol{r}-\boldsymbol{r}_i).$$

Since all particles are equivalent, the current density at $\boldsymbol{r}_1$ is

$$\boldsymbol{j}(\boldsymbol{r}_1) = \frac{e}{m}\frac{N\int f\boldsymbol{\pi}_1\,\mathrm{d}\pi\,\mathrm{d}\boldsymbol{r}_2\ldots\mathrm{d}\boldsymbol{r}_N}{\int f\,\mathrm{d}\pi\,\mathrm{d}\boldsymbol{r}}. \tag{3.9}$$

Using in (3.9) the expansion (3.6), one easily performs the integrations on $\pi$. For expressing the result in a simpler form, it is convenient to introduce the number density

$$n(\boldsymbol{r}_1) = \frac{N\int f\,\mathrm{d}\pi\,\mathrm{d}\boldsymbol{r}_2\ldots\mathrm{d}\boldsymbol{r}_N}{\int f\,\mathrm{d}\pi\,\mathrm{d}\boldsymbol{r}} = \frac{N\int \varphi(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r}_2\ldots\mathrm{d}\boldsymbol{r}_N}{\int\varphi(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r}}, \tag{3.10}$$

where, to order $\hbar^2$,

$$\varphi(\boldsymbol{r}) = \mathrm{e}^{-\beta V}\left[1 - \frac{\hbar^2\beta^2}{12m}\nabla^2 V + \frac{\hbar^2\beta^3}{24m}(\nabla V)^2\right]. \tag{3.11}$$

Then, after some manipulations, one finds

$$\boldsymbol{j}(\boldsymbol{r}_1) = c\,\mathrm{curl}\,\boldsymbol{M}(\boldsymbol{r}_1), \tag{3.12}$$

where, to order $\hbar^4$,

$$\boldsymbol{M}(\boldsymbol{r}_1) = -\frac{\beta e^2\hbar^2 n(\boldsymbol{r}_1)}{12m^2c^2}\left[\boldsymbol{B} - \frac{\hbar^2\beta^2}{60m}\boldsymbol{B}\langle\nabla_1^2 V\rangle_1 + \frac{\hbar^2\beta^2}{60m}\langle(\boldsymbol{B}\cdot\nabla_1)\nabla_1 V\rangle_1\right]. \tag{3.13}$$

In this equation, $\nabla_1$ is the gradient with respect to $\boldsymbol{r}_1$, and an average on all positions except $\boldsymbol{r}_1$ is defined by

$$\langle F(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N)\rangle_1 = \frac{\int \mathrm{e}^{-\beta V} F\,\mathrm{d}\boldsymbol{r}_2\ldots\mathrm{d}\boldsymbol{r}_N}{\int \mathrm{e}^{-\beta V}\,\mathrm{d}\boldsymbol{r}_2\ldots\mathrm{d}\boldsymbol{r}_N} \tag{3.14}$$

for any function $F(\boldsymbol{r})$.

Eq. (3.12) indicates that $M(r)$ plays the role of a magnetization density. However, in the present problem, there are no microscopic magnetic dipoles, and $M(r)$ is only a convenient aid for expressing the current density $j(r)$. Current conservation imposes that $j(r)$ be a curl, but of course $M(r)$ is not uniquely defined by (3.12) and an arbitrary gradient could have been added to (3.13). On the other hand, the total magnetic moment of the sample is uniquely defined and has the value

$$\frac{1}{2c}\int \boldsymbol{r}\wedge \boldsymbol{j}(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r}=\int \boldsymbol{M}(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r}. \tag{3.15}$$

For a large system, the number density $n(r)$, and the magnetization density $M(r)$ as defined by (3.13), have constant values except near the walls. The resulting magnetization per unit volume is identical to the one which had been obtained in another paper[10]). For a small sample, (3.13) is a generalization of a previously derived formula[12]).

For a system of interacting particles, our formalism expresses the current density $j(r)$ to order $\hbar^4$ in terms of classical averages, which in principle can be computed if the distribution functions of the classical system are known. Within order $\hbar^2$, $j(r)$ is simply proportional to the curl of the classical one-body density $n(r)$. It is clear that, for a large system, $j(r)$ is localized near the walls; it extends on the whole region where $n(r)$ varies.

A simple special case is a large system of non-interacting particles bounded by a soft plane potential wall $V(x)$. It is assumed that $V$ is infinite at $x=0$, and goes to zero as $x$ increases. Then, the density $n(x)$ is

$$n(x)=n\,\mathrm{e}^{-\beta V}\left[1-\frac{\hbar^2\beta^2}{12m}\frac{\mathrm{d}^2V}{\mathrm{d}x^2}+\frac{\hbar^2\beta^3}{24m}\left(\frac{\mathrm{d}V}{\mathrm{d}x}\right)^2\right], \tag{3.16}$$

where $n$ is the bulk density far away from the wall.

When a uniform magnetic field $B$ is applied along the $z$ axis, the electrical-current density is

$$j_y(x)=\frac{\beta e^2\hbar^2 B}{12m^2c}\frac{\mathrm{d}}{\mathrm{d}x}\left\{n(x)\left[1-\frac{\hbar^2\beta^2}{60m}\frac{\mathrm{d}^2V}{\mathrm{d}x^2}\right]\right\}. \tag{3.17}$$

Only the leading term of order $\hbar^2$ in (3.17) contributes to the total surface current which is given by the same expression (2.16) as in the case of an infinitely steep wall. A general proof that the total surface current is independent of the shape of the potential wall $V(x)$ is given in appendix II.

### 3.2. *Fermi statistics (zero temperature)*

For a system of independent particles, we can again go from Boltzmann to Fermi statistics by an inverse Laplace transform. We consider a large system of $N$ particles in a volume $\Omega$, confined by a potential $V(\boldsymbol{r})$ which is zero inside the system far away from the walls, and goes to infinity in the walls. We work at order $\hbar^2$. With Boltzmann statistics, the magnetization density is

$$\boldsymbol{M}_{\mathrm{B}}(\boldsymbol{r}) = -\frac{\beta e^2\hbar^2\boldsymbol{B}}{12m^2c^2}\frac{N}{\Omega}\,\mathrm{e}^{-\beta V(\boldsymbol{r})}; \tag{3.18}$$

The one-body partition function is again given by (2.5). By the same kind of argument as the one leading to (2.21), one finds for the magnetization density with Fermi statistics

$$\boldsymbol{M}_{\mathrm{F}}(\boldsymbol{r}) = \mathscr{L}_{\mu}^{-1}\left(\frac{2Z\boldsymbol{M}_{\mathrm{B}}}{N\beta}\right) = -\frac{e^2\boldsymbol{B}}{12\pi^2mc^2}\left\{\frac{2m[\mu - V(\boldsymbol{r})]}{\hbar^2}\right\}^{1/2}. \tag{3.19}$$

Not unexpectedly, at this order of approximation, we obtain a result à la Thomas–Fermi, since, for a constant potential, (3.19) is just the Landau result. The current density $c$ curl $\boldsymbol{M}_{\mathrm{F}}$ behaves like $(\mu - V)^{-1/2}$, and therefore diverges at the turning points where $V(\boldsymbol{r}) = \mu$; the distributions of density, magnetization, current, etc. . . . , have no tail beyond the turning points.

This behaviour near and beyond the turning points is a well-known spurious effect. Similar divergences arise in the calculation of the density near the surface of a nucleus when expansions in powers of $\hbar^2$ are used[13]). Here, a current density behaving like $(\mu - V)^{-1/2}$ gives at least a finite correct total surface current when integrated on $\boldsymbol{r}$. But higher order terms in the $\hbar^2$ expansion would generate worse divergences, which would not even be integrable. These divergences can be avoided by partial resummations of the $\hbar^2$ expansions[14]), a program which will be carried on in a future publication. Here, we shall content ourselves with (3.19), noting that this expression ceases to be valid near and beyond the turning points.

In the simple special case of the soft plane potential wall $V(x)$, one finds from (3.12) and (3.19) a current density

$$j_{y\mathrm{F}}(x) = \frac{e^2B}{12\pi^2mc}\frac{\mathrm{d}}{\mathrm{d}x}\left\{\frac{2m[\mu - V(x)]}{\hbar^2}\right\}^{1/2}, \tag{3.20}$$

for $x > x_0$, where $x_0$ is the turning point defined by $V(x_0) = \mu$. The total surface current is

$$J_{y\mathrm{F}} = \int_{x_0}^{\infty} j_{y\mathrm{F}}\,\mathrm{d}x = \frac{e^2B}{12\pi^2mc}\left(\frac{2m\mu}{\hbar^2}\right)^{1/2}, \tag{3.21}$$

and therefore has the same value as the one found in (2.25) for the case of an infinitely steep wall.

## 4. Conclusion

We have explicitly computed the electrical-current density associated with the diamagnetism of an electron gas, in the weak-field limit. As expected, the current is localized near the surface of the sample. The detail of the current-density distribution depends on the profile of the confining potential wall. The total surface current, however, does not depend on this profile, as expected, since the total surface current is related to the bulk magnetization inside the sample, a quantity which should not be sensitive to surface features.

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## Appendix I

An alternative derivation of the current density near an infinitely steep wall can be obtained by using the eigenfunctions of the potential (2.1) as a basis. When normalized in a large cube of volume $\Omega = L^3$, these eigenfunctions are

$$\psi_{klq} = \left(\frac{2}{L^3}\right)^{1/2} \sin kx \, e^{i(ly+qz)}. \tag{I.1}$$

The summation prescriptions are

$$\sum_k \ldots = \frac{L}{\pi}\int_0^\infty dk \ldots, \quad \sum_l \ldots = \frac{L}{2\pi}\int_{-\infty}^\infty dl \ldots, \quad \sum_q \ldots = \frac{L}{2\pi}\int_{-\infty}^\infty dq \ldots. \tag{I.2}$$

With the gauge (2.2), the many-body current density operator at some point $\boldsymbol{r}_0 = (x_0, y_0, z_0)$ is

$$j_{yop} = j_1 + j_2, \tag{I.3}$$

where

$$j_1 = \frac{e}{2m}\sum_i [p_{yi}\,\delta(\boldsymbol{r}_i - \boldsymbol{r}_0) + \delta(\boldsymbol{r}_i - \boldsymbol{r}_0)p_{yi}], \quad j_2 = -\frac{e^2 B}{mc}x_0 \sum_i \delta(\boldsymbol{r}_i - \boldsymbol{r}_0). \tag{I.4}$$

In the second quantization representation, these operators become

$$j_1 = \frac{e}{2m}\frac{2}{L^3}\sum_{\substack{klq\\k'l'q'}} \hbar(l+l')\exp[\mathrm{i}(l-l')y_0+\mathrm{i}(q-q')z_0]$$
$$\times \sin k'x_0 \sin kx_0\, a^+_{k'l'q'}\, a_{klq},$$
$$j_2 = -\frac{e^2B}{mc}x_0\frac{2}{L^3}\sum_{\substack{klq\\k'l'q'}} \exp[\mathrm{i}(l-l')y_0+\mathrm{i}(q-q')z_0]$$
$$\times \sin k'x_0 \sin kx_0\, a^+_{k'l'q'}\, a_{klq}, \tag{I.5}$$

where $a(a^+)$ are annihilation (creation) operators. To first order in $\boldsymbol{B}$, the interaction hamiltonian is

$$H' = -\frac{eB}{mc}\sum_i p_{yi}x_i; \tag{I.6}$$

it becomes, in the second quantization representation,

$$H' = -\frac{eB}{mc}\frac{2}{L}\sum_{kk'lq} \hbar l \int_0^\infty \mathrm{d}x\, x \sin k'x \sin kx\, a^+_{k'lq}\, a_{klq}. \tag{I.7}$$

A straightforward use of the linear response theory[15]) gives an expression for the expectation value of $j_1$; since the operator $j_2$ already contains $B$, its expectation value can be simply computed with the zero-field wavefunctions. The total current density is

$$j_y(x_0) = -\frac{1}{\mathfrak{z}}\sum_{\substack{nn'\\n\neq n'}} \mathrm{e}^{-\beta E_n}\frac{H'_{nn'}(j_1)_{n'n}+(j_1)_{nn'}H'_{n'n}}{E_{n'}-E_n} + \frac{1}{\mathfrak{z}}\sum_n \mathrm{e}^{-\beta E_n}(j_2)_{nn}, \tag{I.8}$$

where $n$ and $E_n$ label quantum states and energies of the zero-field $N$-body system; $\mathfrak{z}$ is the partition function

$$\mathfrak{z} = \sum_n \mathrm{e}^{-\beta E_n}. \tag{I.9}$$

When (I.5) and (I.7) are used in (I.8), the current density becomes

$$j_y(x_0) = \frac{2e^2B}{m^2c}\frac{2}{L^3}\sum_{klq}\frac{2}{L}\sum_{\substack{k'\\k'\neq k}} \hbar^2 l^2 \frac{n_{klq}(1-n_{k'lq})}{(\hbar^2/2m)(k'^2-k^2)} \sin k'x_0 \sin kx_0$$
$$\times\int_0^\infty \mathrm{d}x x \sin k'x \sin kx - \frac{e^2B}{mc}\frac{2}{L^3}\sum_{klq} n_{klq}x_0 \sin^2 kx_0, \tag{I.10}$$

where $n_{klq}$ is the occupation number of the one-particle state $(klq)$.

In (I.10), $1-n_{k'lq}$ can be replaced by 1, since the contribution involving $n_{k'lq}$

vanishes, by symmetry. The sum on $k'$ is then

$$\frac{2}{L}\sum_{\substack{k' \\ k'\neq k}} \frac{\sin k'x_0 \sin k'x}{k'^2-k^2} = \frac{2}{\pi}\,\mathrm{P}\int_0^\infty \mathrm{d}k'\,\frac{\sin k'x_0 \sin k'x}{k'^2-k^2} = \frac{1}{k}\cos kx_> \sin kx_<, \tag{I.11}$$

where P means principal part; $x_>$ is $\max(x, x_0)$ and $x_<$ is $\min(x, x_0)$. Using (I.11) in (I.10) and performing the integral on $x$, one finds

$$j_y(x_0) = \frac{e^2B}{mc}\frac{2}{L^3}\sum_{klq} n_{klq}\left\{\frac{l^2}{k}[x_0^2 \sin kx_0 \cos kx_0 - \frac{x_0}{k}\sin^2 kx_0 - \frac{\pi}{2}\,\delta'(k)\sin^2 kx_0] - x_0 \sin^2 kx_0\right\}. \tag{I.12}$$

The integrand in this equation will be an even function of $k$; in order to avoid difficulties with the $\delta'(k)$, we change the summation prescription for $k$ from (I.2) to

$$\sum_k \ldots = \frac{L}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}k \ldots. \tag{I.2'}$$

With Boltzmann statistics, the occupation number is

$$n_{klq} = n\lambda^3 \exp\left[-\frac{\beta\hbar^2}{2m}(k^2+l^2+q^2)\right]; \tag{I.13}$$

the spin degree of freedom is taken into account by using for $n_{klq}$ the total occupation number of the orbital state ($klq$), including both spin states. When (I.13) is used in (I.12) and the summation performed, one recovers the Boltzmann current (2.15).

With Fermi statistics, at zero temperature, the occupation number is

$$n_{klq} = 2\theta(f^2 - k^2 - l^2 - q^2), \tag{I.14}$$

where $f$ is the Fermi wave number and $\theta$ the step function; the factor 2 accounts for the two spin states. When (I.14) is used in (I.12), one recovers the Fermi current (2.23).

**Appendix II**

For a system of independent particles near a plane potential wall, we prove in this Appendix that the *total* surface current does not depend on the profile $V(x)$ of the potential. It is enough to give the proof for Boltzmann statistics, since the results for Fermi statistics can be obtained afterwards by the inverse Laplace transform method described in section 2.2.

For an arbitrary shape of $V(x)$, the current density is given by (2.10) and (2.12), and the total surface current is

$$J_y = \frac{n\lambda e^2 B}{\beta mc} \int_0^\beta \mathrm{d}\tau \int \mathrm{d}x_0 \int \mathrm{d}x \langle x_0 | \mathrm{e}^{-(\beta-\tau)H_{0x}} | x \rangle (x - x_0) \langle x | \mathrm{e}^{-\tau H_{0x}} | x_0 \rangle. \qquad \text{(II.1)}$$

In this equation, the order of the integrations on $x$ and $x_0$ cannot be freely interchanged, because the integral is not an absolutely convergent one (the propagators do not go to zero when $x, x_0 \to +\infty$ for a fixed difference $x - x_0$). We can, however, split the integration domain in the $(x, x_0)$ plane into a domain $D$ defined by $(x > a, x_0 > a)$ and the complementary domain $D^*$. We choose for $a$ some large value, well inside the sample, far away from the wall, and therefore, in $D$, the propagators can be replaced by their free particle values, since $V(x)$ is assumed to be negligible inside the sample. In $D^*$, the integral is absolutely convergent, and since the integrand is odd under the permutation of $x$ and $x_0$, the contribution from $D^*$ vanishes. The contribution from $D$ is

$$J_y = \frac{n\lambda e^2 B}{\beta mc} \int_0^\beta \mathrm{d}\tau \int_a^\infty \mathrm{d}x_0 \int_a^\infty \mathrm{d}x \left[\frac{m}{2\pi\hbar^2(\beta-\tau)}\right]^{1/2} \exp\left[-\frac{m(x-x_0)^2}{2\hbar^2(\beta-\tau)}\right]$$
$$\times (x - x_0)\left[\frac{m}{2\pi\hbar^2\tau}\right]^{1/2} \exp\left[-\frac{m(x-x_0)^2}{2\hbar^2\tau}\right]. \qquad \text{(II.2)}$$

When the integrations are performed in the indicated order, one finds

$$J_y = \frac{n\beta e^2\hbar^2 B}{12 m^2 c}, \qquad \text{(II.3)}$$

independently of the shape of $V(x)$.

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