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Surface Orbital Magnetism

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We compute the surface correction to the density of states of a particle in a convex box subjected to a magnetic field. Applying these results to orbital magnetism, we find that at high temperatures or weak magnetic fields the surface magnetization is always paramagnetic, but oscillations appear at low temperatures. In two dimensions they can give very large paramagnetic contributions near integer values of the filling factor. Explicit formulas are given for the zero-field susceptibility and for samples with a cylindrical shape in arbitrary magnetic field.

KEY WORDS: Density of states; surface effects; diamagnetism; susceptibility.

1. INTRODUCTION

There is presently a renewed interest in size effects on the physical properties of small metallic or semiconductor systems. In the ballistic regime, it is a reasonable approximation to ignore the interaction of particles between themselves or with impurities and to consider collisions with the walls as the dominant effect. If the particles are subjected to a magnetic field, their motion in the box leads to the formation of a magnetic moment, resulting in the so-called orbital magnetism. In the bulk limit, the systems shows a diamagnetic behavior at low magnetic fields, as was first discovered by Landau in his classic work. An interesting question is to investigate the possible change in this behavior when the size of the system is reduced. The first correction expected is a surface one, which one can reasonably expect to be able to compute analytically. At still smaller sizes, in the mesoscopic range, we enter into a regime where the system is a quantum billiard and the system could only be analyzed numerically, at least presently, and properties characteristic of quantum "chaotic" systems should appear.

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In this article, we will be concerned with the problem of computing the surface correction to the bulk behavior. Since the 1930 paper of Landau, up to the present day, many authors have made an attempt at this tricky problem. A brief summary of the history of the problem and many references can be found in a 1975 paper of Angelescu *et al.*(1) and in a very recent review by Ruitenbeeck and van Leeuwen.(2) The Roumanian authors were the first to compute the surface susceptibility in zero field of a parallelepiped in a magnetic field perpendicular to some faces. The other problem on which exact results are available is that of a thin plate parallel to the field.(2) More recently, various approximate treatments have indicated a paramagnetic contribution of the surface term in more general cases.(3, 4)

In this work, we first derive a general expression for the surface density of states of a convex body. Following Kac's strategy in his famous article(5) on the same problem without a magnetic field, we analyze the partition function: This allows us to compute the surface magnetization. In the two-dimensional case, it can be expressed in terms of zeros of the Weber cylinder function. In this case also we can find a relationship between both the bulk and surface magnetization and the surface current of a semiinfinite system. Such relations should hold even in the presence of interactions. At a very low temperature, when the filling factor is near an integer, the surface magnetization is paramagnetic and grows with the square root of the logarithm of the temperature.

In the usual three-dimensional case we give an explicit expression for the surface magnetization for samples with a cylindrical shape in a magnetic field directed along the axis of the cylinder or perpendicular. The zero-field surface susceptibility is computed for arbitrary convex samples. It is paramagnetic. We show that at high temperatures (Maxwell–Boltzmann statistics) the surface magnetization is paramagnetic for any value of the magnetic field and any convex shape. However, at low temperatures, at least for cylindrical shapes, the surface magnetization shows de Haas–van Alphen-type oscillations.

2. DENSITY OF STATES

We want to consider the motion of a quantum particle of charge e and mass m in a box Λ_L subjected to a constant magnetic field B in the z axis. We choose as unit of energy $\epsilon = \hbar eB/mc$ and of length $l = (\hbar c/eB)^{1/2}$. In these units the Hamiltonian is given by

$$H_{\Lambda_L} = -\frac{1}{2}\partial_x^2 + \frac{1}{2}\left(\frac{1}{i}\partial_y - x\right)^2 - \frac{1}{2}\partial_z^2 \tag{2.1}$$

with Dirichlet boundary conditions on the surface $\partial\Lambda_L$. The boxes Λ_L are all obtained from the box Λ by a dilating factor L, i.e.,

$$\Lambda_L = \left\{ x \,\middle|\, \frac{x}{L} \in \Lambda \right\} \tag{2.2}$$

When we will discuss the two-dimensional problem, the term $-\frac{1}{2}\partial_z^2$ will be absent from the Hamiltonian and the motion will be restricted to the x–y plane. We are interested by the integrated density of states $N_{\Lambda_L}(\lambda)$ of this system

$$N_{\Lambda_L}(\lambda) = \sum_{n:\varepsilon_n \leqslant \lambda} \tag{2.3}$$

where ε_n are the eigenvalues of the Hamiltonian. Our purpose is to compute the asymptotic behavior of this quantity for large boxes Λ_L, i.e., when $L \to \infty$. On physical grounds one expects a contribution proportional to the volume $|\Lambda_L| = L^d |\Lambda|$ of the box and one of the order of the surface $|\partial\Lambda_L|$ of this box. We will show that, when $d = 2, 3$,

$$N_{\Lambda_L}(\lambda) \sim L^d |\Lambda| \, n(\lambda) + L^{d-1} s_{\partial_\Lambda}(\lambda) \tag{2.4}$$

It turns out, however, that whereas in two dimensions the surface contribution is indeed proportional to the perimeter of the box, i.e., $s_{\partial_\Lambda}(\lambda) = |\partial\Lambda| \, s(\lambda)$, in three dimensions $s_{\partial_\Lambda}(\lambda)$ depends on the specific shape and of the orientation of the box with respect to the magnetic field.

Instead of considering directly N_{Λ_L}, we will analyze the behavior of its Laplace transform or in more physical terms of the partition function

$$Z_{\Lambda_L} = \operatorname{tr} \exp - tH_{\Lambda_L} = \int_{-\infty}^{\infty} \exp(-t\lambda) \, dN_{\Lambda_L}(\lambda) \tag{2.5}$$

We will then essentially follow Kac's strategy when he analyzed the same problem in the absence of a magnetic field. The partition function can be expressed by means of the fundamental solution $P_{\Lambda_L}(x \mid y; t)$ of the heat equation

$$\frac{\partial}{\partial t} P_{\Lambda_L} = -H_{\Lambda_L} P_{\Lambda_L} \tag{2.6}$$

The partition function is given by

$$Z_{\Lambda_L} = \int_{\Lambda_L} dx \, P_{\Lambda_L}(x \mid x; t) \tag{2.7}$$

From now on, we will assume that Λ is compact and *convex*. If $x \in \Lambda$, let $q(x)$ be the point of the boundary $\partial\Lambda$ closest to x (for Lebesgue almost all x it is unique). If we denote by $\Lambda(x)$ the half-space bounded by the plane $l(x)$ tangent at $\partial\Lambda$ in $q(x)$, then $\Lambda \subset \Lambda(x)$. We can then introduce the fundamental solution of the heat equation

$$\frac{\partial}{\partial t} P_{\Lambda_L(x)} = -H_{\Lambda_L(x)} P_{\Lambda_L(x)} \tag{2.8}$$

where $H_{\Lambda_L(x)}$ is the same Hamiltonian as the one defined in Eq. (2.1), except that now it is defined on the half-space $\Lambda_L(x)$ and Dirichlet boundary conditions are imposed on the plane $l(x)$.

Consider now the fundamental solutions of the usual heat equations

$$\partial_t Q_{\Lambda_L} = \tfrac{1}{2} \Delta_{\Lambda_L} Q_{\Lambda_L} \tag{2.9}$$

$$\partial_t Q_{\Lambda_L(x)} = \tfrac{1}{2} \Delta_{\Lambda_L(x)} Q_{\Lambda_L(x)} \tag{2.10}$$

where Δ_Λ is the Laplacian with Dirichlet boundary conditions on $\partial\Lambda$. We have the basic inequality, if $x \in \Lambda$,

$$|P_{\Lambda_L}(x \mid x; t) - P_{\Lambda_L(x)}(x \mid x; t)| \leqslant Q_{\Lambda_L(x)}(x \mid x; t) - Q_{\Lambda_L}(x \mid x; t) \tag{2.11}$$

This inequality follows easily from the following functional integral representations of P_Λ and Q_Λ,[6]

$$P_\Lambda(x \mid x; t) = \int d\mu^{\Lambda}_{0x;\, tx}(\omega) \exp -i \int_0^t \omega_1(s)\, d\omega_2(s) \tag{2.12}$$

$$Q_\Lambda(x \mid x; t) = \int d\mu^{\Lambda}_{0x;\, tx}(\omega) \tag{2.13}$$

$d\mu^{\Lambda}_{0x;\, tx}$ is the conditional Wiener measure for paths starting from x at time 0 and ending at x at time t, but remaining in Λ.

The inequality follows from the fact that the magnetic field contribution in P_Λ is of modulus one, and $\Lambda \subset \Lambda(x)$ as a consequence of the convexity of Λ.

From this inequality we can see that

$$Z_{\Lambda_L}(t) = \int_{\Lambda_L} dx\, P_{\Lambda_L(x)}(x \mid x; t) + r_{\Lambda_L}(t) \tag{2.14}$$

and

$$0 \leqslant r_{\Lambda_L}(t) \leqslant \int_\Lambda dx\, [Q_{\Lambda_L(x)}(x \mid x; t) - Q_{\Lambda_L}(x \mid x; t)] \tag{2.15}$$

But we have the scaling relationship

$$Q_{\Lambda_L}(x \mid x; t) = L^{-d} Q_\Lambda \left(\frac{x}{L} \,\middle|\, \frac{x}{L}; \frac{t}{L^2} \right) \tag{2.16}$$

and we can see that it follows from Kac's result that

$$r_{\Lambda_L}(t) = O(L^{d-2}) \tag{2.17}$$

In this way we have reduced the computation of the partition function (with an L^{d-2} accuracy) to the problem of computing $P_{\Lambda_{L(x)}}(x \mid x; t)$. This amounts essentially to replacing the boundary locally by its tangent plane. We will show that

$$P_{\Lambda_{L(x)}}(x \mid x; t) = \rho t(u; n^3(x)) \tag{2.18}$$

where u denotes the distance of x to the boundary $\partial \Lambda_L$ and $n^3(x)$ denotes the z component (i.e., along the direction of the magnetic field) of the inward normal $\mathbf{n}(x)$ at the point x of the boundary closest to x. One can interpret $\rho_t(u; n^3(x))$ as the density of particles constrained to move in the half-space $\Lambda_L(x)$ at distance u from the boundary. One expects on physical grounds that $\lim_{u \to \infty} \rho_t(u; n^3(x)) = \rho_t(\infty)$, where $\rho_t(\infty)$ is the density in the infinite system. The approach of $\rho_t(u; n^3(x))$ to its limit $\rho_t(\infty)$ is rapid enough so that

$$\int_0^\infty du\, u \left| \frac{\partial}{\partial u} \rho_t(u; n^3(x)) \right| < \infty \tag{2.19}$$

We can therefore write

$$Z_{\Lambda_L}(t) = L^d \, |\Lambda| \, \rho_t(\infty) - L^{d-1} \int_0^\infty dz \int_{\substack{\Lambda \\ \operatorname{dist}(r,\, \partial\Lambda) \leqslant z/L}} dr \frac{\partial}{\partial z} \rho_t(z; n^3(r)) + r_{\Lambda_L}(t) \tag{2.20}$$

so that we get

$$Z_{\Lambda_L}(t) = L^d \, |\Lambda| \, \rho_t(\infty) - L^{d-1} \int_0^\infty dz \int_{\partial\Lambda} d\sigma \, z \frac{\partial}{\partial z} \rho_t(z; n^3(\sigma)) + O(L^{d-2}) \tag{2.21}$$

We have thus shown that if we can find the representations

$$\rho^t(\infty) = t \int_0^\infty e^{-t\lambda} n(\lambda) \, d\lambda \tag{2.22}$$

and

$$\int_0^\infty du\,[\rho_t(u; n^3(\sigma)) - \rho_t(\infty)] = t\int_0^\infty e^{-t\lambda} s(\lambda; n^3(\sigma))\,d\lambda \qquad (2.23)$$

then

$$\int_0^\infty e^{-t\lambda} N_{\Lambda_L}(\lambda)\,d\lambda$$

$$= L^d\,|\Lambda| \int_0^\infty e^{-t\lambda} n(\lambda) + L^{d-1}\int_0^\infty e^{-t\lambda} s_{\partial\Lambda}(\lambda)\,d\lambda + O(L^{d-2}) \qquad (2.24)$$

with

$$s_{\partial\Lambda}(\lambda) = \int_{\partial\Lambda} d\sigma\, s(\lambda; n^3(\sigma)) \qquad (2.25)$$

From Eq. (2.24) it should follow that

$$N_{\Lambda_L}(\lambda) \sim L^d\,|\Lambda|\, n(\lambda) + L^{d-1} s_{\partial\Lambda}(\lambda) \qquad (2.26)$$

This result, however, is stronger than (2.24), and more information is needed to derive it. We discuss this point in the Appendix. It can be proved that quite generally

$$\lim_{L\to\infty} \frac{N_{\Lambda_L}}{L^d}(\lambda) = n(\lambda)$$

For the surface term, one can only prove that

$$\lim_{L\to\infty} \frac{1}{L^{d-1}}\,[N_{\Lambda_L}(\lambda) - |\Lambda|\, L^d n(\lambda)] = s_{\partial\Lambda}(\lambda)$$

when Λ is a parallelepiped. The convergence is the so-called weak convergence of measures, appropriate for the thermodynamics.

To proceed further, we need to analyze the density $\rho_t(u)$ of a half-infinite system.

In the two-dimensional case, if we choose the origin on the line delimiting the allowed domain, the Hamiltonian becomes

$$h_+ = -\frac{1}{2}\partial_u^2 + \frac{1}{2}\left(\frac{1}{i}\partial_v - u\right)^2 \qquad (2.27)$$

defined on the half-space $u \geqslant 0$, and with Dirichlet boundary conditions at $u=0$. We therefore have

$$\rho_t(u)=\int_{-\infty}^{+\infty} \frac{dk}{2\pi}\,(u|\exp -th_+(k)\,|u) \tag{2.28}$$

where

$$h_+(k)= -\tfrac{1}{2}\partial_u^2+\tfrac{1}{2}(k+u)^2 \tag{2.29}$$

is now defined on the half-line $u \geqslant 0$. If we call $h(k)$ the same operator as the one in (2.29), but defined on the full line, then we claim that

$$\rho_t(\infty)=\int_{-\infty}^{+\infty} \frac{dk}{2\pi}\,(u|\exp -th(k)\,|u) \tag{2.30}$$

$\rho_t(\infty)$ is easily computed:

$$\rho_t(\infty)=\frac{1}{2\pi}\sum_{n=0}^{\infty}\exp -t\left(n+\frac{1}{2}\right) \tag{2.31}$$

we have $\rho_t(u) \leqslant \rho_t(\infty)$ and if we write

$$\rho_t(u)-\rho_t(\infty)=\int_{-\infty}^{+\infty} \frac{dk}{2\pi}\,(u|\exp -th_+(k)-\chi\exp -th(k)\chi\,|u) \tag{2.32}$$

with

$$\chi(u)=\begin{cases}1 & \text{if } u \geqslant 0\\ 0 & \text{if } u<0\end{cases} \tag{2.33}$$

we should have

$$\int_0^{\infty} du\,[\rho_t(u)-\rho_t(\infty)]$$

$$=\frac{1}{2\pi}\int_{-\infty}^{+\infty} dk\,[\operatorname{tr}\exp -th_+(k)-\operatorname{tr}\chi\exp -th(k)\chi] \tag{2.34}$$

if the trace of the operator on the right-hand side is finite and integrable, as can be checked, indeed. If we call $E_\lambda^+(k)$ and $E_\lambda(k)$ the spectral projectors of $h_+(k)$ and $h(k)$, in the energy range $(-\infty, \lambda)$, then we can write

$$\int_0^{\infty} du\,[\rho_t(u)-\rho_t(\infty)]=\frac{t}{2\pi}\int_0^{\infty} d\lambda\, e^{-t\lambda}\int_{-\infty}^{+\infty} dk\,\operatorname{tr}[E_\lambda^+(k)-\chi E(k)\chi] \tag{2.35}$$

We can therefore summarize the results in two dimensions by the following equations. The bulk density of states $n(\lambda)$ is given by

$$n(\lambda)=\frac{1}{2\pi}\sum_{n=0}^{\infty}\theta\left(\lambda-n-\frac{1}{2}\right) \tag{2.36}$$

and the surface density of states is given by

$$s(\lambda)=\frac{1}{2\pi}\int_{-\infty}^{+\infty} dk\,\mathrm{tr}[E_\lambda^+(k)-\chi E(k)\chi] \tag{2.37}$$

We will give later a more explicit expression for this quantity in terms of zeros of cylinder functions. In three dimensions, we proceed in the same way. Choosing the origin on the plane, with normal **n**, and calling **b** the unit vector in the direction of the magnetic field and θ the angle between the magnetic field and the normal **n**, we choose the axes as follows (if $\sin\theta\neq 0$):

$$\mathbf{e}_1=\frac{\mathbf{b}-\cos\theta\,\mathbf{n}}{\sin\theta},\qquad \mathbf{e}_2=\frac{\mathbf{n}\wedge\mathbf{b}}{\sin\theta},\qquad \mathbf{e}_3=\mathbf{n} \tag{2.38}$$

Since the density is gauge independent, we choose the useful gauge

$$A_1=A_3=0,\qquad A_2=-\sin\theta x_3+\cos\theta x_1$$

The appropriate Hamiltonian is therefore

$$H_+=-\frac{1}{2}\partial_u^2+\frac{1}{2}\left(\frac{1}{i}\partial_w+\sin\theta u-\cos\theta v\right)^2-\frac{1}{2}\partial_v^2 \tag{2.39}$$

in the half-space $u\geqslant 0$, with Dirichlet boundary conditions on the plane $u=0$.

If we call $x_1=u$, $x_2=w$, $x_3=v$, the density $\rho_t(u)$ is given by

$$\rho_t(u)=\int_{-\infty}^{+\infty}\frac{dk}{2\pi}(uv|\exp -tH_+(k)\,|uv) \tag{2.40}$$

$H_+(k)$ is the same operator as the one in (2.39), but where $(1/i)\partial_w$ is replaced by k.

$\rho_t(u)$ does not depend on v, because if $V_+^k(uv\mid u'v')$ designates the kernel of $\exp -tH_+(k)$, we have, for any b,

$$V_+^{k+b\cos\theta}(u\,v+b\mid u'v'+b)=V_+^k(uv\mid u'v') \tag{2.41}$$

Hence when $\cos\theta \neq 0$ we can rewrite (2.40) as

$$\rho_t(u) = \frac{|\cos\theta|}{2\pi} \int_{-\infty}^{+\infty} dv\, (uv|\exp -tH_+(0)\,|uv) \tag{2.42}$$

Introducing the operator $H(0)$, which is the same as $H_+(0)$ but defined on the whole space, we will have

$$\rho_\infty(u) = \frac{|\cos\theta|}{2\pi} \int_{-\infty}^{+\infty} dv\, (uv|\exp -tH(0)\,|uv) \tag{2.43}$$

In fact,

$$\rho_t(\infty) = \frac{1}{(2\pi t)^{1/2}} \frac{1}{2\pi} \sum_{n=0}^{\infty} \exp -t\left(n+\frac{1}{2}\right) \tag{2.44}$$

From (2.42) and (2.43), we see that we can write

$$\int_0^\infty du\, [\rho_t(u) - \rho_t(\infty)] = \frac{|\cos\theta|}{2\pi} \operatorname{tr}[\exp -tH_+(0) - \chi \exp -tH(0)\chi] \tag{2.45}$$

There are two special cases where this expression simplifies. If $\cos\theta = 0$, we are essentially in the two-dimensional case; then

$$\int_0^\infty du\, [\rho_t(u) - \rho_t(\infty)]$$
$$= \frac{1}{(2\pi t)^{1/2}} \frac{1}{2\pi} \int_{-\infty}^{+\infty} dk \operatorname{tr}[\exp -th_+(k) - \chi \exp -th(k)\chi] \tag{2.46}$$

as can be seen by using (2.40) and (2.34).

If $\cos\theta = \pm 1$, the problem is that of a free particle in half-space and a harmonic oscillator in the whole space. Therefore

$$\int_0^\infty du\, [\rho_t(u) - \rho_t(\infty)] = \frac{-1}{(2\pi t)^{1/2}} \frac{1}{2} \left(\frac{\pi t}{2}\right)^{1/2} \frac{1}{2\pi} \sum_{n=0}^{\infty} \exp -t\left(n+\frac{1}{2}\right) \tag{2.47}$$

To summarize, in the general case we have for the bulk density of states the familiar Landau formula

$$n(\lambda) = \frac{1}{\sqrt{2}} \frac{1}{\pi^2} \sum_{n=0}^{[\lambda-1/2]} \left(\lambda - n - \frac{1}{2}\right)^{1/2} \tag{2.48}$$

and for the surface density of states

$$s_{\partial\Lambda}(\lambda) = \int_{\partial\Lambda} d\sigma\, s(\lambda, \theta(\sigma)) \tag{2.49}$$

where

$$s(\lambda, \theta) = \frac{|\cos\theta|}{2\pi} \operatorname{tr}[E_\lambda^+(\theta) - \chi E_\lambda(\theta)\chi] \tag{2.50}$$

$E_\lambda^+(\theta)$ and $E_\lambda(\theta)$ are the spectral projectors in the energy range $(-\infty, \lambda)$ of the Hamiltonian

$$H_+ = -\tfrac{1}{2}\Delta_+ + \tfrac{1}{2}(\sin\theta u - \cos\theta v)^2 \tag{2.51}$$

defined on $u \geqslant 0$, with Dirichlet boundary conditions on $u = 0$ and

$$H = -\tfrac{1}{2}\Delta + \tfrac{1}{2}(\sin\theta u - \cos\theta v)^2 \tag{2.52}$$

defined on the whole space $\mathbb{R}^2$.

Apart from the special cases $\theta = 0$, $\pi/2$, π, we have not succeeded in finding a more explicit expression for $s(\lambda, \theta)$. There may be some hope to solve this problem, however, because at the classical level the Hamiltonian H_+ describing a harmonic oscillator with a wall is integrable, although not separable.

The special cases $\theta = 0$, $\pi/2$, π will allow us, however, to find expressions for the density of states when the volume has a cylindrical shape and the magnetic field is directed along the axis of the cylinder or perpendicular to it. The general formula (2.50) can be used to compute the density of states in small magnetic fields.

3. THE TWO-DIMENSIONAL CASE. MAGNETIZATION AND SURFACE CURRENT

In order to analyze more thoroughly the two-dimensional case, we need to look at the spectral properties of the Hamiltonian

$$h_+(k) = -\tfrac{1}{2}\partial_x^2 + \tfrac{1}{2}(k + x)^2 \tag{3.1}$$

defined on the half-line $x \geqslant 0$, with Dirichlet boundary condition at $x = 0$. We denote the ordered eigenvalues by $\varepsilon_n(k)$, $n = 0, 1, 2,\ldots$, and $\varepsilon_n(k) < \varepsilon_{n+1}(k)$. To the eigenvalue $\varepsilon_n(k)$ corresponds the unnormalized eigenfunction

$$\psi_{n,k}(x) = D_{\varepsilon_n - 1/2}(\sqrt{2}\,(x + k)) \tag{3.2}$$

where $D_\nu(x)$ is the usual Weber cylinder function. The equation for the eigenvalue is

$$D_{\varepsilon_n - 1/2}(\sqrt{2}\, k) = 0 \tag{3.3}$$

The following properties of the eigenvalues can be established: $\varepsilon_n(k)$ is strictly increasing in k.

We have $\varepsilon_n(-\infty) = n + 1/2$ and more precisely

$$\varepsilon_n(k) - \varepsilon_n(-\infty) \sim \frac{(\sqrt{2}\, k)^{2n+1}}{n!\,(2\pi)^{1/2}} \exp -k^2 \tag{3.4}$$

when $k \to -\infty$.

When $k \to +\infty$, $\varepsilon_n(k)$ grows quadratically in k. Finally

$$\varepsilon_n(0) = 2n + \tfrac{3}{2} \tag{3.5}$$

We can uniquely define the function $k_n(\lambda)$ by the relation $\varepsilon_n(k) = \lambda$. Now, $\sqrt{2}\, k_n(\lambda) = x_n(\lambda)$ is a zero of $D_{\lambda - 1/2}(x)$. If $\lambda - 1/2 = N + \theta$, where $\theta \in (0, 1)$ and N a positive integer, then $D_{\lambda - 1/2}$ has $N+1$ finite zeros, ordered as $x_0 > x_1 > \cdots > x_n$. When $\lambda - 1/2 \to N^+$, $x_N(\lambda) \to -\infty$, and when $\lambda - 1/2 \to (N+1)^-$, all the zeros tend to the $N+1$ finite zeros of D_{N+1}, which is proportional to a Hermite polynomial. With these preliminaries we can analyze the density $s(\lambda)$. Equation (2.37) tells us that it is given by

$$s(\lambda) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dk \left[\sum_n \theta(\lambda - \varepsilon_n(k)) - \sum_n \theta\left(\lambda - \frac{1}{2} - n\right) c_n(k) \right] \tag{3.6}$$

θ is the usual Heaviside function and

$$c_n(k) = \int_k^{+\infty} dy\, \varphi_n^2(y) \tag{3.7}$$

$\varphi_n(y)$ is the normalized eigenfunction of the usual harmonic oscillator

$$h = -\tfrac{1}{2}\partial_x^2 + \tfrac{1}{2}x^2 \tag{3.8}$$

Since $\varepsilon_n(k) \geqslant n + 1/2$, we can rewrite (3.6) as

$$s(\lambda) = \frac{1}{2\pi} \sum_{n=0}^{[\lambda - 1/2]} \int_{-\infty}^{+\infty} dk\, [\theta(k_n(\lambda) - k) - c_n(k)] \tag{3.9}$$

Using the fact that $\varphi_n^2(y)$ is even, we have

$$\int_{-\infty}^{+\infty} dk\, [\theta(k_n(\lambda) - k) - c_n(k)] = k_n(\lambda) \tag{3.10}$$

Thus we get the desired expression

$$s(\lambda)=\frac{1}{\sqrt{2}}\frac{1}{2\pi}\sum_{n=0}^{[\lambda-1/2]} x_n\left(\lambda-\frac{1}{2}\right) \tag{3.11}$$

where $x_n(v)$ is the nth zero of $D_v(x)$, the zeros decreasing when the index n increases.

It is clear that the index n is nothing else than the Landau level index.

When $\lambda-1/2$ is not an integer, the zeros $x_n(\lambda-1/2)$ are increasing in λ, therefore $s(\lambda)$ is increasing. Since if we start from the value of $\lambda-1/2=N$ and increase it until it reaches the value $\lambda-1/2=N+1$, the zeros tend to those of $D_{N+1}(x)$, whose sum vanishes because of the parity of $D_{N+1}(x)$; we conclude that $s(\lambda)\leqslant 0$. Thus we conclude that when $\lambda-1/2$ is between the integers N and $N+1$, $s(\lambda)$ is a negative increasing function which diverges to $-\infty$ near N as

$$s(\lambda)\sim -\frac{1}{2\pi}\left[\sqrt{\delta}-\frac{N+1/2}{2}\frac{\ln\delta}{\sqrt{\delta}}\right] \tag{3.12}$$

where

$$\delta=\ln\frac{1}{\lambda-N-1/2} \tag{3.13}$$

This result follows from the asymptotic behavior of $\varepsilon_n(k)$ as expressed in (3.4).

When λ approaches $N+3/2$, $s(\lambda)$ vanishes.

The complicated asymptotic behavior revealed by (3.12) indicates that the energy levels are packed in a very intricate way near the Landau levels in a large but finite system. Let us discuss now the thermodynamic properties. We consider an assembly of fermions of chemical potential μ in a convex box of volume V and area A. The pressure of the finite system is given by

$$\beta pV=2\int_0^\infty \ln[1+ze^{-tx}]\,dN_A(x)=2t\int_0^\infty \frac{ze^{-tx}}{1+ze^{-tx}}N_A(x) \tag{3.14}$$

The factor 2 comes from the spin degeneracy, since we neglect the Zeeman energy. $t=\beta\hbar eB/mc$ is the inverse temperature in magnetic units, and $z=e^{\beta\mu}$ is the fugacity. For a large sample, we have shown that

$$\beta pV=\frac{2V}{\lambda^2}t\sum_{n=0}^{\infty}\ln[1+ze^{-t(n+1/2)}]$$
$$+\frac{2A}{\lambda}(2\pi t^3)^{1/2}\int_0^\infty \frac{ze^{-tx}}{1+ze^{-tx}}s(x)\,dx \tag{3.15}$$

where $\lambda=(2\pi\hbar^2\beta/m)^{1/2}$ is the thermal wavelength.

The magnetization measured in the Bohr unit $\mu_B = \hbar e/2mc$ will therefore decompose into a bulk contribution

$$\frac{M_b}{\mu_B} = \frac{4V}{\lambda^2} \partial_t \sum_{n=0}^{\infty} \ln[1 + ze^{-t(n+1/2)}] \tag{3.16}$$

and a surface contribution

$$\frac{M_s}{\mu_B} = \frac{4A}{\lambda} \partial_t (2\pi t^3)^{1/2} \int_0^{\infty} \frac{ze^{-tx}}{1 + ze^{-tx}} s(x)\, dx \tag{3.17}$$

We will see that in the small magnetic field limit, $t \ll 1$, the surface magnetization is positive (paramagnetism), whereas the bulk magnetization is of course negative (diamagnetism), as is well known. The same result holds quite generally at high temperatures, where we can use Boltzmann statistics, namely replace $ze^{-tx}/(1 + ze^{-tx})$ by ze^{-tx}.

We will also prove an identity relating both the bulk magnetization and the surface one to the surface current of a semiinfinite system. This identity indicates that the bulk and surface magnetization tend to have opposite signs.

It is interesting, however, to analyze the expression for the surface magnetization in the zero-temperature limit. It can be expressed as

$$\frac{M_s}{\mu_B} = \frac{4A(2\pi)^{1/2}}{l_F} v^{-1/2} \left[\frac{3}{2} \int_0^v s(x)\, dx - vs(v) \right] \tag{3.18}$$

where $v = \mu/\epsilon$ is essentially the ratio of the Fermi energy to the magnetic one, and

$$l_F = \left(\frac{2\pi\hbar^2}{\mu m} \right)^{1/2}$$

is the Fermi wavelength. We can see that

$$f(v) = \tfrac{3}{2} \int_0^v s(x)\, dx - vs(v)$$

is a decreasing function of v when v is between $N + 1/2$ and $N + 3/2$, since $s(v)$ is negative and increasing in this range of v for any integer N.

On the other hand, each time v approaches $N + 1/2$ from above, $f(v)$ diverges like

$$\frac{N + 1/2}{2\pi} \left(\ln \frac{1}{v - N - 1/2} \right)^{1/2}$$

according to (3.12), but when v approaches $N+3/2$ from below, $f(v)$ tends to $\frac{2}{3}\int_0^{N+3/2} s(x)\,dx$, which is negative. Thus we see that the surface magnetization will be positive (paramagnetic) when $v \sim N+1/2$ and even divergent like

$$\frac{M_s}{\mu_B} \sim \frac{4A}{l_F}\left(\frac{N+1/2}{2\pi}\ln\frac{1}{v-N-1/2}\right)^{1/2} \tag{3.19}$$

and decrease to a negative value (diamagnetism) when v approaches $N+3/2$ from below.

At very low temperatures, the singularity will be washed out and

$$\frac{M_s}{\mu_B} \sim \frac{4A}{l_F}\left(\frac{N+1/2}{2\pi}\ln t\right)^{1/2}$$

but one will see very strong oscillations opposite in sign to those of the bulk magnetization. These oscillations, like the de Haas–van Alphen one, are the remnants of the Landau level structure.

Let us finally look at the relation between the magnetization and surface currents.

Consider the semiinfinite system $x \geqslant 0$ and a particle subjected to a magnetic field, whose dynamics is described by the Hamiltonian

$$h_+ = -\frac{1}{2}\partial_x^2 + \frac{1}{2}\left(\frac{1}{i}\partial_y - x\right)^2 \tag{3.20}$$

There will be a current $j(x)$ flowing along the y axis, induced by the magnetic field. This current will be given by

$$j(x) = -z\int_{-\infty}^{+\infty} dk\,(k+x)(x|\exp -th_+(k)\,|x) \tag{3.21}$$

where the Hamiltonian $h_+(k)$ is given in Eq. (3.1). We have used the Boltzmann distribution. In the more interesting case of Fermi statistics the operator on the right-hand side of (3.21) should be replaced by

$$\frac{z\exp -th_+(k)}{1+z\exp -th_+(k)}$$

If we write

$$L_k = \exp -th_+(k) - \chi\exp -th(k)\chi \tag{3.22}$$

then we can see that

$$j(x) = \frac{-z}{2\pi} \int_{-\infty}^{+\infty} dk\ (k+x)\, L_k(x\,|\,x) \tag{3.23}$$

and we have

$$\int_0^{\infty} dx\ j(x) = -\frac{z}{2\pi} \int_{-\infty}^{+\infty} dk\ \mathrm{tr}(x+k) L_k \tag{3.24}$$

and

$$\int_0^{\infty} dx\ xj(x) = -\frac{z}{2\pi} \int_{-\infty}^{+\infty} dk\ \mathrm{tr}\ x(x+k) L_k \tag{3.25}$$

On the other hand,

$$\partial_k\ \mathrm{tr}\ L_k = -t\ \mathrm{tr}(k+x) L_k - t\ \mathrm{tr}(k+x)\chi V_k \chi - \partial_k\ \mathrm{tr}\ \chi V_k \chi \tag{3.26}$$

where

$$V_k = \exp -th(k) \tag{3.27}$$

but

$$\int_{-\infty}^{+\infty} dk\ \partial_k\ \mathrm{tr}\ L_k = 0 \tag{3.28}$$

and

$$\begin{aligned} \int_{-\infty}^{+\infty} dk\ \partial_k\ \mathrm{tr}\ \chi V_k \chi &= \sum_{n=0}^{\infty} e^{-t(n+1/2)} \int_k^{+\infty} dy\ \varphi_n^2(y) \Big|_{-\infty}^{+\infty} \\ &= -\sum_{n=0}^{\infty} e^{-t(n+1/2)} \end{aligned} \tag{3.29}$$

$$\begin{aligned} \int_{-\infty}^{+\infty} dk\ \mathrm{tr}(k+x)\chi V_k \chi &= \sum_{n=0}^{\infty} e^{-t(n+1/2)} \int_{-\infty}^{+\infty} dk \int_k^{+\infty} \varphi_n^2(y) \\ &= \sum_{n=0}^{\infty} (n+\tfrac{1}{2}) e^{-t(n+1/2)} \end{aligned} \tag{3.30}$$

Thus we see that integrating Eq. (3.26) and using Eqs. (3.28)–(3.30) and the definition (3.23), we get

$$t \int_0^{\infty} j(x)\, dx = \frac{z}{2\pi} \sum_{n=0}^{\infty} \left[-1 + t\left(n+\frac{1}{2}\right)\right] \exp -t\left(n+\frac{1}{2}\right) \tag{3.31}$$

or

$$t\int_0^\infty j(x)\,dx = -\frac{z}{2\pi}\partial_t t\sum_{n=0}^\infty \exp -t\left(n+\frac{1}{2}\right) \tag{3.32}$$

It can be seen from Eq. (3.16) that the right-hand side of this equality is $(-\lambda^2/4V)M_b/\mu_B$, where M_b is the bulk magnetization with Boltzmann statistics (first order in z).

The case of Fermi statistics can be treated by expanding the Fermi operator in z when $|z|<1$,

$$\frac{z\exp -th}{1+z\exp -th} = -\sum_{j=1}^\infty (-z)^j \exp -tjh$$

using the identity (3.32) for each term in the sum, we get

$$\frac{M_b}{\mu_B} = -\frac{4V}{\lambda^2} t\int_0^\infty j(x)\,dx \tag{3.33}$$

The result remains valid when $z>1$ by analytic continuation. Such a result was first obtained by Macris *et al.*[7] by a different technique and generalized to some interacting situations. Let us write

$$q(t) = t\int_0^\infty e^{-tx}s(x) \tag{3.34}$$

We have

$$q(t) = \int_{-\infty}^{+\infty}\frac{dk}{2\pi}\operatorname{tr} L_k \tag{3.35}$$

We rewrite this as

$$\sqrt{t}\,q(t) = \int_{-\infty}^{+\infty}\frac{dk}{2\pi}\operatorname{tr}[U_k^+(1) - \chi U_k(1)\chi] \tag{3.36}$$

where

$$U_k^+(s) = \exp -\frac{s}{2}[-\partial_x^2 + (k+xt)^2] \tag{3.37}$$

the operator in the exponential being defined on the half-line $x \geqslant 0$. $U_k(s)$ is the same operator, but defined on the whole line.

From this equation it follows that

$$\partial_t \sqrt{t}\, q(t) = \int_{-\infty}^{+\infty} \frac{dk}{2\pi} \{ -\mathrm{tr}\, x(x+k)[U_k^+(1) - \chi U_k(1)\chi] + a(k)\} \quad (3.38)$$

where

$$a(k) = \int_0^1 ds\, \mathrm{tr}\, \chi [U_k(1-s), x(k+x)]\, U_k(s)\chi$$

It is easily seen that $a(k)$ is integrable and odd in k. Thus we have the identity

$$\partial_t \sqrt{t}\, q(t) = -\sqrt{t} \int_{-\infty}^{+\infty} \frac{dk}{2\pi} \mathrm{tr}\, x(x+k) L_k \quad (3.39)$$

and therefore, from (3.29) and (3.17) it follows that

$$\frac{M_s}{\mu_B} = \frac{4A(2\pi t)^{1/2}}{\lambda} \int_0^\infty xj(x)\, dx \quad (3.40)$$

for the Boltzmann distribution. The case of Fermi statistics can be handled similarly and the identity (3.40) still holds. Equations (3.33) and (3.40) giving the bulk magnetization as $M_b \sim -\int_0^\infty j(x)\, dx$ and the surface magnetization as $M_s \sim \int_0^\infty xj(x)\, dx$ should remain valid even in the interacting case, at least when the system does not show a phase transition. It would be particularly interesting to see if they keep their validity in the quantum Hall regime, when the filling factor is a fraction associated with plateau in the Hall conductivity. If not, they could characterize the nature of these incompressible states. We can also remark that these identities explain qualitatively that the surface magnetization tends to be opposite to the bulk magnetization, favoring paramagnetism at low fields. We have been unable to generalize the identity for the surface magnetization to the three-dimensional case. There is a term proportional to $\sin\theta \int_0^\infty xj(x)\, dx$, but to which is added another one, whose physical interpretation remains elusive.

4. SAMPLES WITH A CYLINDRICAL SHAPE

For a large sample of volume V and area A, the pressure of a three-dimensional system is given by

$$\beta p V = \frac{2V}{\lambda^3} (2\pi t)^{3/2}\, t \int_0^\infty \frac{ze^{-tx}}{1+ze^{-tx}} n(x)\, dx$$
$$+ \frac{2A}{\lambda^2} 2\pi t^2 \int_0^\infty \frac{ze^{-tx}}{1+ze^{-tx}} \bar{s}_{\partial A}(x)\, dx \quad (4.1)$$

where

$$n(x) = \frac{1}{\sqrt{2}\,\pi^2} \sum_{n=0}^{[x-1/2]} \left(x - n - \frac{1}{2}\right)^{1/2} \tag{4.2}$$

and

$$\bar{s}_{\partial\Lambda}(x) = \frac{1}{|\partial\Lambda|} \int_{\partial\Lambda} d\sigma\, s(x, \theta(\sigma)) \tag{4.3}$$

The bulk pressure is of course the familiar Landau expression.

The surface magnetization is given by

$$\frac{M_s}{\mu_B} = \frac{4A\,2\pi}{\lambda^2}\, \partial_t t^2 \int_0^\infty \frac{ze^{-tx}}{1+ze^{-tx}}\, \bar{s}_{\partial\Lambda}(x)\, dx \tag{4.4}$$

Since we can compute explicitly $s(x, \theta)$ only for special values of θ, we need to turn to special types of shapes in order to get an explicit expression for the magnetization for arbitrary magnetic fields.

Let us assume therefore from now on that the sample has the shape of a cylinder with an arbitrary convex base. The magnetic field will be assumed to be either parallel or perpendicular to the axis of the cylinder.

The surface of the sample parallel to the magnetic field, of area $A^{\|}$, will give a contribution to the magnetization given by

$$\frac{M_s^{\|}}{\mu_B} = \frac{4A^{\|} \cdot 2\pi}{\lambda^2}\, \partial_t t^2 \int_0^\infty \frac{ze^{-tx}}{1+ze^{-tx}}\, s_{\|}(x)\, dx \tag{4.5}$$

and the part perpendicular to the magnetic field, of area $A^{\perp}$, will give another contribution,

$$\frac{M_s^{\perp}}{\mu_B} = \frac{4A^{\perp} \cdot 2\pi}{\lambda^2}\, \partial_t t^2 \int_0^\infty \frac{ze^{-tx}}{1+ze^{-tx}}\, s_{\perp}(x)\, dx \tag{4.6}$$

and the surface magnetization will be

$$M_s = M_s^{\|} + M_s^{\perp} \tag{4.7}$$

According to Eq. (2.47), $s_{\perp}(x)$ will be such that

$$t \int_0^\infty s_{\perp}(x) \exp -tx = -\frac{1}{8\pi} \sum_{n=0}^{\infty} \exp -t\left(n + \frac{1}{2}\right) \tag{4.8}$$

which gives

$$s_{\perp}(x) = -\frac{1}{8\pi}\left[x + \frac{1}{2}\right] \tag{4.9}$$

Therefore

$$\frac{M_s^{\perp}}{\mu_B} = -\frac{A^{\perp}}{\lambda^2}\partial_t t \sum_{n=0}^{\infty} \ln[1 + ze^{-t(n+1/2)}] \tag{4.10}$$

This expression shows that

$$M_s^{\perp} = -\tfrac{1}{4}M_b(2d) \tag{4.11}$$

where $M_b(2d)$ is the bulk magnetization of a two-dimensional system of volume $A^{\perp}$. The presence of the minus sign shows that at weak field or high temperatures this contribution is paramagnetic. It also indicates that at low temperatures $M_s^{\perp}$ will show anti-de Haas–van Alphen-type oscillations.

Equation (2.46) gives for $s_{||}(x)$

$$t\int_0^{\infty} dx\, e^{-tx} s_{||}(x) = \frac{t}{(2\pi t)^{1/2}}\int_0^{\infty} dx\, e^{-tx} s(x)$$

and therefore

$$s_{||}(x) = \frac{1}{\sqrt{2}\,\pi}\int_0^{x} dy\, \frac{1}{(x-y)^{1/2}}\, s(y) \tag{4.12}$$

We see that $s_{||}(x)$ is negative. Thus both surface contributions give a negative surface pressure. Equation (4.12) shows that, contrary to the two-dimensional case, the density of states $s_{||}(x)$ does not diverge at a Landau level, but rather vanishes like $[\varepsilon \ln(1/\varepsilon)]^{1/2}$, where $\varepsilon = x - N - 1/2$.

The precise dependence of $M_s^{||}$ in the magnetic field is not very easy to analyze from Eqs. (4.6) and (4.12), even at zero temperature. It should, however, be possible to compute numerically this function from the expression we derived for $s(x)$. We would expect oscillations, as in the case $M_s^{\perp}$.

Finally, we would like to remark that often the magnetization is needed for a system in which the density and not the chemical potential is fixed. One should in this case study surface corrections in the canonical ensemble. But one expects equivalence of ensembles to hold with an $L^{3/2}$ accuracy in three dimensions. Since in this case the surface term is of order L^2, it is possible to express the magnetization in the canonical ensemble M_ρ as

$$M_\rho = M_\mu(\rho, B) + \left(\frac{\partial \mu}{\partial B}\right)_\rho \rho_s(\rho, B) \tag{4.13}$$

where $M_\mu(\rho, B)$ is the grand-canonical magnetization that we computed, in which the chemical potential μ has been expressed in terms of the density

ρ by using the bulk relationship between them. $\rho_s(\rho, B)$ is the surface contribution to the density in the grand-canonical ensemble, but with μ expressed in terms of ρ.

5. WEAK MAGNETIC FIELDS

In the general case, it is possible to compute the zero-field susceptibility, defined as

$$\chi_s = \lim_{B \to 0} \frac{M_s}{B} \tag{5.1}$$

From Eq. (4.4) we see that this quantity is given by

$$\chi_s = \frac{2e^2}{mc^2} \frac{z}{z+1} \frac{A}{|\partial \Lambda|} \int_{\partial \Lambda} d\sigma\, a(\theta(\sigma)) \tag{5.2}$$

where

$$a(\theta) = \lim_{t \to 0} \frac{1}{t} \partial_t t \gamma_\theta(t) \tag{5.3}$$

with

$$\gamma_\theta(t) = t \int_0^\infty e^{-tx} s(x, \theta)\, dx \tag{5.4}$$

From Eq. (2.50), we have

$$\gamma_\theta(t) = \frac{|\cos \theta|}{2\pi} \operatorname{tr}[\exp -tH_+ - \chi \exp -tH\chi] \tag{5.5}$$

It appears useful to express this quantity as a path integral[7]

$$\gamma_\theta(t) = \frac{|\cos \theta|}{(2\pi)^2} \int_0^\infty dx \int_{-\infty}^{+\infty} dy \int D\alpha\, F_x(\alpha) \exp -\frac{t^2}{2} \int_0^1 (X + R(s))^2\, ds \tag{5.6}$$

In this expression

$$\begin{aligned} X &= \sin \theta x + \cos \theta y \\ R(s) &= \sin \theta \alpha_x(s) + \cos \theta \alpha_y(s) \end{aligned} \tag{5.7}$$

and

$$F_x(\alpha) = \begin{cases} -1 & \text{if } \; x + \alpha_x(s) \leqslant 0 \text{ for some } s \\ 0 & \text{otherwise} \end{cases} \tag{5.8}$$

expressing the fact that the paths are constrained to the half-space $x \geqslant 0$. The $\alpha_x(s)$ and $\alpha_y(s)$ are independent Brownian bridges, i.e., Gaussian processes with covariance

$$\overline{\alpha(s)\,\alpha(s')} = s(1-s') \qquad (0 \leqslant s \leqslant s' \leqslant 1) \tag{5.9}$$

and zero mean.

The introduction of these processes is a useful way to extract the spatial dependence of the paths in the Wiener integral.

If we integrate over the y coordinate, we get

$$t\gamma_\theta(t) = \left(\frac{1}{2\pi}\right)^{3/2} \int_0^\infty dx \int D\alpha\, F_x(\alpha) \exp -\frac{t^2}{2} \int_0^1 (R(s) - \bar{R})^2\, ds \tag{5.10}$$

where

$$\bar{R} = \int_0^1 ds\, R(s) \tag{5.11}$$

We can deduce an interesting consequence of this representation, namely

$$\partial_t t\gamma_\theta(t) \geqslant 0 \tag{5.12}$$

The meaning of this inequality is the following. If we were using the Boltzmann distribution instead of the Fermi one, the surface magnetization would be given by

$$\frac{M_s}{\mu_B} = \frac{4A}{\lambda^2}\, 2\pi z \partial_t t \int_{\partial A} \gamma_{\theta(\sigma)}(t)\, \frac{d\sigma}{|\partial A|} \tag{5.13}$$

We can therefore conclude that in the case of the *Boltzmann distribution* (i.e., at high temperatures in the Fermi case), *the surface magnetization is paramagnetic* for all fields, i.e., $M_s \geqslant 0$.

We can also use the path integral to simplify the computation at weak fields. Indeed, from (5.10) it follows that

$$a(\theta) = -\int_0^\infty \frac{dx}{(2\pi)^{3/2}} \int D\alpha\, F_x(\alpha) \int_0^1 (R(s) - \bar{R})^2\, ds \tag{5.14}$$

an expression which shows immediately that the weak-field magnetization will be also paramagnetic.

But in fact, (5.14) shows that

$$a(\theta) = a(0)\cos^2\theta + a\left(\frac{\pi}{2}\right)\sin^2\theta \tag{5.15}$$

because the mixed term $\int D\alpha\,(\alpha_x(s)-\bar{\alpha}_x)(\alpha_y(s)-\bar{\alpha}_y)=0$ in Eq. (5.14). We are left to compute only $a(0)$ and $a(\pi/2)$. We have seen in Eq. (2.47) that

$$\gamma_0(t) = -\frac{1}{8\pi}\sum_{n=0}^{\infty} \exp -t\left(n+\frac{1}{2}\right) \tag{5.16}$$

This gives easily

$$a(0) = \frac{1}{8\pi}\cdot\frac{1}{12} \tag{5.17}$$

From Eqs. (2.46) and (3.34) it follows that

$$\gamma_{\pi/2}(t) = \frac{1}{(2\pi t)^{1/2}}\, q(t) \tag{5.18}$$

and therefore

$$a\left(\frac{\pi}{2}\right) = \frac{1}{(2\pi)^{1/2}} \lim_{t\to 0} \frac{1}{t}\,\partial_t \sqrt{t}\, q(t) \tag{5.19}$$

The computation of this quantity is a bit more tricky. We will use the relationship between surface magnetization and the surface current established in Section 3. After some rescaling of the variables, Eq. (3.39) can be written as

$$\frac{1}{t}\,\partial_t \sqrt{t}\, q(t) = -\int_{-\infty}^{+\infty} \frac{dk}{2\pi}\, \mathrm{tr}\, x\left(x+\frac{k}{t}\right) \bar{L}_k(1) \tag{5.20}$$

where

$$\bar{L}_k(s) = V_k^+(s) - \chi V_k(s)\chi \tag{5.21}$$

with

$$V_k^+(s) = \exp -\frac{s}{2}\left[-\partial_x^2 + (k+xt)^2\right] \tag{5.22}$$

the operator being defined on the half-line with Dirichlet boundary conditions. $V_k(s)$ is the same operator, but defined on the whole line. If in the second term of the expression appearing on the right-hand side of Eq. (5.20) we make an integration by parts on the k variable, we can put Eq. (5.20) in the more useful form

$$\frac{1}{t}\,\partial_t \sqrt{t}\, q(t) = -\int_{-\infty}^{+\infty} \frac{dk}{2\pi}\, ds\, \mathrm{tr}\, x[x, V_k^+(1-s)]\, V_k^+(s) \tag{5.23}$$

the term corresponding to V_k disappearing because it gives a contribution odd in k.

In this form, it is possible to take the limit $t \to 0$. In the limit the kernel of $V_k^+(s)$ becomes $e^{-k^2/2}U_s(x \mid y)$, with

$$U_s(x \mid y) = \frac{1}{(2\pi s)^{1/2}} \left[\exp -\frac{(x-y)^2}{2s} - \exp -\frac{(x+y)^2}{2s} \right] \tag{5.24}$$

Inserting this expression into (5.23), we get after a lengthy computation

$$\lim_{t \to 0} \frac{1}{t} \partial_t \sqrt{t}\, q(t) = \frac{1}{(2\pi)^{1/2}} \frac{3}{2^7} \tag{5.25}$$

and therefore

$$a\left(\frac{\pi}{2}\right) = \frac{1}{2\pi} \frac{3}{2^7} \tag{5.26}$$

Grouping all these results, we get finally

$$\chi_s = \frac{Ae^2}{mc^2} \frac{z}{z+1} \frac{1}{\pi 2^7} \left[3 - \frac{1}{3\,|\partial A|} \int_{\partial A} d\sigma (\mathbf{n}(\sigma) \cdot \mathbf{b})^2 \right] \tag{5.27}$$

where we have denoted by $\mathbf{b}$ the unit vector directed along the magnetic field, and we recall that $\mathbf{n}(\sigma)$ is the normal at the boundary point σ. In the case of a cylindrical shape, this formula becomes

$$\chi_s = \frac{e^2}{mc^2} \frac{z}{z+1} \frac{1}{\pi 2^7} \left[2A_1 \left(3 - \frac{\cos^2 \theta_1}{3} \right) + A_2 \left(3 - \frac{\cos^2 \theta_2}{3} \right) \right] \tag{5.28}$$

where A_1 and A_2 are the areas respectively of the base and of the lateral face of the cylinder, and θ_1 and θ_2 designate the angles made by the magnetic field with the respective normals to these faces. This formula reproduces the result of Angelescu *et al.*[1] in the case of a parallelepiped. In the case of a sphere, Eq. (5.27) gives

$$\chi_s = \frac{Ae^2}{mc^2} \frac{z}{z+1} \frac{13}{9\pi \cdot 2^6} \tag{5.29}$$

We note that the zero-field limit is a subtle one and quite probably the development in a magnetic field is only asymptotic.

6. CONCLUSION

We can briefly summarize the new results we have obtained. First, the computation of the surface density of states for convex bodies is reduced to the solution of the Schrödinger equation for a particle confined to a tilted half-plane and subjected to a harmonic potential in the x direction. An explicit solution of this last problem in special cases allows us to determine completely the surface density of states in two dimensions and for cylindrical shapes in three dimensions for arbitrary magnetic fields. In the most general case, the best we could do was to compute the zero-field magnetic susceptibility.

A more explicit solution of the Schrödinger equation alluded to would allow a complete determination of the surface density of states for arbitrary magnetic fields in the three-dimensional case. This is the most important remaining problem to be solved in our opinion.

APPENDIX

We briefly discuss the problem of the asymptotic behavior of the density of states.

If we consider a box made up of the disjoint union of two boxes Λ_1 and Λ_2, then for Dirichlet boundary conditions the density of states $N_\Lambda(x)$ satisfies the inequality

$$N_{\Lambda_1 \cup \Lambda_2}(x) \geqslant N_{\Lambda_1}(x) + N_{\Lambda_2}(x) \tag{A.1}$$

On the other hand, Colin de Verdière[8] has proven that for a cube

$$N_\Lambda(x) \leqslant |\Lambda| \, n(x) \tag{A.2}$$

where $n(x)$ is the bulk density of states (2.48). This inequality can be extended to parallelepipeds. From these two sets of inequalities it can be proven by standard techniques that

$$\lim_{\Lambda \nearrow R^d} \frac{N_\Lambda(x)}{|\Lambda|} = n(x)$$

for a large class of boxes.

The problem of the surface correction is, however, much more subtle. It is known in the case of the Laplacian, i.e., for the problem without a magnetic field, that convergence of the difference

$$s_\Lambda(x) = \frac{N_\Lambda(x) - |\Lambda| \, n(x)}{|\partial \Lambda|}$$

cannot hold pointwise, generally. Some assumptions must be made about the density of periodic orbits of the corresponding classical system.[9] But in statistical mechanics a much weaker kind of convergence is needed at positive temperatures, the so-called weak convergence of measures. It guarantees, for example, that the pressure

$$p = z \int_0^\infty \frac{e^{-\beta\lambda}}{1 + ze^{-\beta\lambda}} \frac{N_\Lambda(\lambda)}{|\Lambda|} \, d\lambda \tag{A.3}$$

will have the asymptotic behavior that we derived. Indeed Theorem 2a, XIII 1, of Feller[10] guarantees that this will hold provided $s_\Lambda(x)$ is negative or positive, so that the convergence of its Laplace transform (which we proved) will imply convergence of the measure $s_\Lambda(x)\,dx$. In our case the Colin de Verdière inequality (A.2) guarantees that $s_\Lambda(x)$ is negative for parallelepipeds. We would expect such a result for large enough convex boxes, but have not proved it.

The pointwise type of convergence would be needed if we were to consider the problem at zero temperature and then look at the asymptotic behavior for large samples. Fortunately, from the physical point of view, in most situations one needs to consider the other order of limits, first large samples and then low temperatures.

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