Path-decomposition expansion and edge effects in a confined magnetized free-electron gas

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Abstract. Path-integral methods can be used to derive a ‘path-decomposition expansion’ for the temperature Green function of a magnetized free-electron gas confined by a hard wall. With the help of this expansion the asymptotic behaviour of the profiles for the excess particle density and the electric current density far from the edge is determined for arbitrary values of the magnetic field strength. The asymptotics are found to depend sensitively on the degree of degeneracy. For a non-degenerate electron gas the asymptotic profiles are essentially Gaussian (albeit modulated by a Bessel function), on a length scale that is a function of the magnetic field strength and the temperature. For a completely degenerate electron gas the asymptotic behaviour is again proportional to a Gaussian, with a scale that is the magnetic length in this case. The prefactors are polynomial and logarithmic functions of the distance from the wall, which depend on the number of filled Landau levels \( n \). As a consequence, the Gaussian asymptotic decay sets in at distances that are large compared with the magnetic length multiplied by \( \sqrt{n} \).

1. Introduction

In a magnetized charged-particle system edge effects are of paramount importance. An illustration of this fact is furnished by the phenomenon of Landau diamagnetism [1], which is due to electric currents flowing near the boundaries of the sample. As a further example one may mention quantum Hall systems for which the relevance of edge effects has been amply shown.

The analysis of the influence of the boundary on the properties of a quantum many-body system is a difficult mathematical problem. Even if the bulk properties of the unconfined system are understood, the presence of the edge leads to a boundary-value problem that is often difficult to solve analytically. Leaving out the interparticle interaction simplifies this problem quite a lot, although even in that case the analysis remains complicated. A physical system that is particularly relevant in this context is the non-interacting electron gas in a uniform magnetic field in the presence of a confining hard wall. In fact, this is the system in which Landau diamagnetism, with currents flowing near the edge, can be studied in its purest form.

Several methods have been devised to analyse edge effects in the confined magnetized free-electron gas. At zero temperature one may try to solve the eigenvalue problem in terms of distorted Landau levels and determine the edge currents by summing the contributions of the lowest-lying eigenfunctions. Even for a simple flat geometry this leads to a rather involved mathematical analysis in terms of parabolic cylinder functions [2, 3]. Recently, we studied the profiles of the particle density and the electric current density along these lines [4].
An alternative approach starts by focusing on the high-temperature regime, where Maxwell–Boltzmann statistics applies. In that case a convenient tool is furnished by the one-particle temperature-dependent Green function. As shown by Balian and Bloch [5], the Green function for the confined system can be related to that of the corresponding system without boundaries by making a systematic expansion that accounts for an increasing number of reflections of the particles against the confining wall. The ensuing multiple-reflection expansion was used in recent years [6, 7] to determine the profiles of the particle density and the (electric) current density for small values of the magnetic field. These small-field profiles had been found before from perturbation theory [8, 9]. It turns out to be difficult to generalize these results for the profiles to arbitrary field strength and to relate them to those obtained by means of the eigenvalue method.

Some time ago Auerbach and Kivelson [10] invented a path-integral method to analyse boundary effects in Green functions. By suitably decomposing the relevant paths near the edge they derived a so-called ’path-decomposition expansion’ (PDX) for the one-particle Green function. The aim of this paper is to see whether the use of the PDX may shed light on the difficulties mentioned above and whether it may lead to new results on the profiles of physical quantities for arbitrary field strength, both for the high-temperature region and in the regime of high degeneracy.

The plan of the paper is as follows. We start by a review of the PDX and its derivation from the Feynman–Kac path integral. Particular attention will be given to the convergence of the PDX series. It will be shown that a suitable resummation can greatly enhance that convergence. The connection with the multiple-reflection expansion will be established. Subsequently, the extension of the method so as to include magnetic fields will be discussed by starting from the Feynman–Kac–Itô representation.

For the specific case of a non-interacting charged-particle system in a uniform magnetic field, confined by a hard wall parallel to the field, the general form of the terms in the PDX series can be established in detail. That result will be used to determine the first few terms of the asymptotic expansion for the profiles of the particle density and the current density. This asymptotic expansion is valid far from the edge and in the high-temperature regime. In contrast to earlier work we will not need to restrict ourselves to small field strengths, as we shall establish the full field dependence of the profiles. As it turns out, the precise knowledge of the asymptotic profiles for high temperatures and arbitrary fields is essential in determining how the profiles for the degenerate case depend on the filling of the Landau levels.

2. Path-decomposition expansion

Consider a particle in an external potential \( V(r) \), i.e. with the Hamiltonian

\[
H = \frac{p^2}{2} + V(r)
\]

where we have chosen units in such a way that the particle mass drops out. The equilibrium quantum statistical properties of a set of particles moving in the potential \( V \) is governed by the temperature Green function \( G_\beta(r', r) \), with \( \beta \) the inverse temperature. Its path-integral representation is given by the Feynman–Kac formula

\[
G_\beta(r', r) = \langle r'| e^{-\beta H} | r \rangle = \int d\mu^e_{r', 0} (\omega) \exp \left[-\int_0^\beta d\tau V(\omega(\tau)) \right]
\]

where \( \omega(\tau) \) describes the path and \( d\mu^e_{r', 0} \) is the conditional Wiener measure [11].

If a hard wall confines the particles to a region of space, the potential can be written as \( V(r) = V_0(r) + V_w(r) \), where \( V_w \) is a steep wall potential and \( V_0 \) is a smooth external
potential. Exact evaluation of (2) for the confined problem is, in general, not possible, even if the corresponding unconfined problem can be solved completely. In this section we will explore the use of the PDX, first introduced by Auerbach and Kivelson [10], to determine the Green function of the confined problem.

To simplify matters, consider the one-dimensional case, with a hard wall at $x = 0$, i.e. $V_w(x) = \infty$ for $x < 0$ and $V_w(x) = 0$ for $x > 0$. As a first step, we split the Green function into two parts

$$G_\beta(x', x) = G^0_\beta(x', x) + G^h_\beta(x', x).$$

Here $G^0_\beta$ is the Green function for the problem without a wall. In order to calculate it, one needs to specify the potential $V_0(x)$ for $x < 0$ as well. We will take the latter to be the analytical continuation of the potential for $x > 0$. We shall assume that the resulting $V_0(x)$ is such that $G^0_\beta$ can be evaluated in closed form.

The second term of (3) is the difficult part. It is a correction that contains contributions from all paths crossing the boundary at least once, with an additional minus sign so as to compensate the corresponding contributions in $G^0_\beta$. In order to calculate $G^h_\beta$, one discretizes the path integral in the usual way by introducing $n$ evenly spaced grid points at $\tau_m = m\epsilon_n$, with $\epsilon_n = \beta/(n + 1)$. Subsequently, one decomposes the paths at the boundary [10]. Here ‘decomposing’ means that the paths are split into two at the point $\tau$, where they cross the boundary for the last time. Choosing this ‘point of no return’ between $\tau_m$ and $\tau_{m+1}$, one writes the path integral for $G^h_\beta$ as

$$G^h_\beta(x', x) = -\lim_{n \to \infty} \lim_{x'' \downarrow 0} \sum_{m=1}^{n} \int_{-\infty}^{0} dx_m \int_{0}^{x''} dx_m+1 \times G_{\beta-(m+1)\epsilon_n}(x', x_m+1)G^0_{\epsilon_n}(x_m+1, x_m)G^0_{m\epsilon_n}(x_m, x).$$

for $x$ and $x'$ both positive.

In the small interval between $\tau_m$ and $\tau_{m+1}$ the potential $V_0$ can be ignored, since the error will vanish in the continuum limit. Hence, in this interval we may use the ‘free’ propagator $G^0_{f,\beta}(x', x) = (2\pi\beta)^{-1/2} \exp[-(x' - x)^2/2\beta]$, where we have put $\hbar = 1$. The free propagator satisfies the identity

$$G^0_{f,\beta}(|x'|, -|x|) = \text{sgn}(x') \lim_{x'' \downarrow 0} \int_{0}^{\beta} d\tau \frac{\partial}{\partial \tau} G^0_{f,\beta-\tau}(x', x'')G^0_{f,\tau}(0, x).$$

This identity, which is a generalization of that used in [10], follows directly by differentiation of the relation

$$\int_{0}^{1} d\tau (1 - \tau)^{-1/2} e^{-a^2/\beta + b^2/(1 - \tau)} = \pi \text{Erfc}(a + b) \quad (a > 0, b > 0)$$

with respect to $b$. Using (5) with $x < 0$ and $x' > 0$ in (4), we get

$$G^h_\beta(x', x) = -\lim_{n \to \infty} \lim_{x'' \downarrow 0} \sum_{m=1}^{n} \int_{-\infty}^{x''} d\tau \int_{0}^{x''} dx_m \times \frac{\partial}{\partial x''} G_{\beta-\tau-m\epsilon_n}(x'', x_m)G^0_t(0, x_m)G^0_{m\epsilon_n}(x_m, x).$$

The integral over $x_m$ can be extended to the interval $[-\infty, \infty]$, if a compensating factor $\frac{1}{2}$ is inserted. In fact, only small values of $x_m$ contribute anyway, at least in the continuum limit, owing to the presence of the second $G^0$ function. For these small values of $x_m$ the integrand
is approximately invariant under a change of sign of \(x_m\). Subsequently, we may join the two \(G^0\) into one, so that we get a closed integral relation

\[
G^c_\beta(x', x) = -\lim_{\gamma \to 0} \frac{1}{2} \int_0^\beta \frac{d\tau}{dx''} G_{\beta-\gamma}(x', x'') G^0_\tau(0, x)
\]  
(8)

for positive \(x\) and \(x'\). This integral relation is the PDX formula derived in [10]. Since the right-hand side contains the original Green function \(G\), we can iterate this integral equation by inserting (3). In this way we arrive at the PDX series

\[
G_\beta(x', x) = G^0_\beta(x', x) - \lim_{\gamma \to 0} \frac{1}{2} \int_0^\beta \frac{d\tau}{dx''} G^0_{\beta-\gamma}(x', x'') G^0_\tau(0, x)
\]

\[
+ \lim_{\gamma \to 0} \left( \frac{1}{2} \right) \int_0^\beta \frac{d\tau}{dx''} \lim_{\gamma \to 0} \int_0^{\beta-\tau} \frac{d\tau'}{dx'''} G^0_{\beta-\gamma}(x', x''') G^0_\tau(0, x''') G^0_\tau(0, x') \cdots.
\]
(9)

To study the convergence of the PDX series we look at the special case of a vanishing external potential \(V_0\). The Green function for a free particle in the presence of a hard wall can be calculated using a reflection principle. It reads

\[
G_{f,\beta}(x', x) = G^0_{f,\beta}(x', x) - G^0_{f,\beta}(-x', x)
\]
(10)

for \(x\) and \(x'\) positive. Since the first term is \(G^0_{f,\beta}\), the second term must be the correction \(G^c_\beta\).

To check the validity of (9) for the present case, we repeatedly employ (5), with the result

\[
G_{f,\beta}(x', x) = G^0_{f,\beta}(x', x) - \left( \sum_{n=1}^{\infty} 2^{-n} \right) G^0_{f,\beta}(-x', x).
\]
(11)

Indeed, this is identical to (10). It is clear that all terms in (9) are necessary to reproduce the correct result. In addition, we cannot change the order of integration and evaluation of the limit in (9). In fact, since one has \(\lim_{\gamma \to 0} \partial_{\gamma} G^0_{f,\tau}(0, x') = 0\), this would give an incorrect result. This suggests that (9) is not the most convenient form to use.

A slightly different series is obtained by modifying (8) as follows:

\[
G^c_\beta(x', x) = -\lim_{\gamma \to 0} \int_0^\beta \frac{d\tau}{dx''} G_{\beta-\gamma}(x', x'') G^0_\tau(0, x)
\]
(12)

where the limit \(x' \downarrow 0\) is the average of the limits \(x' \uparrow 0\) and \(x' \downarrow 0\). Since \(G_\tau(x', x)\) vanishes for \(x < 0\), at least for a hard wall, we have merely added zero to the right-hand side of (8). If we iterate (12), with (3) inserted, we get the resummed PDX series

\[
G_\beta(x', x) = G^0_\beta(x', x) - \lim_{\gamma \to 0} \int_0^\beta \frac{d\tau}{dx''} G^0_{\beta-\gamma}(x', x'') G^0_\tau(0, x)
\]

\[
+ \lim_{\gamma \to 0} \int_0^\beta \frac{d\tau}{dx''} \lim_{\gamma \to 0} \int_0^{\beta-\tau} \frac{d\tau'}{dx''' G^0_{\beta-\gamma}(x', x''') G^0_\tau(0, x''') G^0_\tau(0, x') \cdots.
\]
(13)

Let us again consider the case \(V_0(x) = 0\). One easily verifies that the correction \(G^c_\beta\) is given by the second term of (13) alone. The convergence of the resummed PDX series is thus found to be much better than that of of the original one. All higher-order terms in (13) vanish separately in the present case, since one may prove

\[
\lim_{\gamma \to 0} \frac{d}{dx''} \lim_{\gamma \to 0} \int_0^\tau \frac{d\tau'}{dx''' G^0_{f,\tau-\gamma}(x', x''') G^0_{f,\tau}(0, x''')} = 0.
\]
(14)
Note that here we are allowed to interchange the order of integration and evaluation of the limit. This property is an additional advantage of the series in (13). Returning to the general case with \( V_0(x) \neq 0 \), we expect that both favourable properties of the resummed PDX series (fast convergence and invariance under interchange of the order of integration and taking the limit) are conserved. Of course, in general the series will no longer terminate after the second term. Nevertheless, in some applications only a few terms in the expansion are relevant, as we shall see in the following.

The resummed PDX series (13) is of the general form

\[
G_\beta(x', x) = \sum_{n=0}^{\infty} G_\beta^{(n)}(x', x) \tag{15}
\]

where we put \( G_\beta^{(0)} = G_0^\beta \). The term of order \( n \) involves \( n \) positions at the boundary. It can be seen as arising from paths along which the particle hits the boundary \( n \) times. These multiple reflections at the boundary form the basis of the multiple-reflection expansion, which was derived by Balian and Bloch \[5\] quite some time before the PDX was written down. A close inspection shows that the two expansions are completely equivalent.

Note that in principle the PDX formula (8) and the PDX series (9) can be applied to any problem involving distinct spatial regions, for example to tunnelling problems \[10\]. In contrast, the modified PDX formula (12) depends on the presence of a hard wall. The application of the resummed PDX series (13) is likewise limited to hard-wall problems only.

3. Magnetic field

We will now apply the methods of the previous section to a confined free-electron gas in a uniform magnetic field. The Hamiltonian is given by

\[
H = \frac{1}{2} (p - A)^2 + V_w(r) \tag{16}
\]

where \( V_w \) is again a hard-wall potential. Because of the symmetry of the problem we will choose the Landau gauge \( A = (0, Bx, 0) \). The factor \( e/c \), with \( e \) the charge of the particles, has been absorbed in the constant \( B \).

The presence of the vector potential complicates matters. The Feynman–Kac representation (2) of the path integral is no longer valid. We have to use the Feynman–Kac–Itô formula instead, which in the special case of \( \nabla \cdot A = 0 \) reads \[11\]

\[
G_\beta(r', r) = \int d\mu_{r',r_0} \exp \left[ -\int_0^\beta d\tau V_w(\omega(\tau)) + i \int_0^\beta d\tau \dot{\omega}(\tau) \cdot A(\omega(\tau)) \right] \tag{17}
\]

If we let \( \omega_x \) denote the \( x \)-component of the path, we can replace the exponential factor containing \( V_w \) by \( \theta(\inf_\tau \omega_x(\tau)) \). Since the factor that contains the vector potential is independent of \( z \), the integral over the \( z \)-component of the path gives a trivial factor \((2\pi)^{1/2} \exp[-(z' - z)^2/2\beta]\). The part of the Green function that depends on \( x \) and \( y \) will be denoted by \( G_{\perp, \beta}(r', r) \) in the following.

The path integral over the \( y \)-component of the path can be evaluated by a Fourier-transform technique. In fact, discretizing the \( x \)- and \( y \)-components of the path, with \( n \) intermediate points, we write \( \omega(\tau_m) = r_m = (x_m, y_m) \), with \( r_0 = r \) and \( r_{n+1} = r' \). The integral in the exponent of (17) is then given by \( \int_0^\beta d\tau \omega(\tau) \cdot A(\omega(\tau)) = \sum_{m=0}^{n} (r_{m+1} - r_m) \cdot A(r_m) \) (in Itô’s convention). We get

\[
G_{\perp, \beta}(r', r) = \prod_{m=1}^{n+1} \int dr_m (2\pi \epsilon_n)^{-1} \exp \left[ -\frac{(r_m - r_{m-1})^2}{2\epsilon_n} \right] \theta(x_m) \times \exp[i(y_m - y_{m-1}) B x_m - r_{n+1} - r'] \tag{18}
\]
The integrals over $y_m$ can now be carried out by using the standard Fourier representation of the Dirac $\delta$-function. This introduces an integral over an additional variable $k$. Returning to the continuum limit for the path integral over the $x$-component of the path we arrive at

$$G_{\perp, \beta}(r', r) = (2\pi)^{-1} \int_{-\infty}^{\infty} dk \ e^{ik(y' - y)} \tilde{G}_\beta(x' - k/B, x - k/B, k)$$

with

$$\tilde{G}_\beta(x', x, k) = \int d\mu_{x, 0}(\omega_x) \theta(\inf_\tau \omega_x(\tau) + k/B) e^{-\frac{1}{2} B^2 \beta \omega_x(\tau)^2}.$$  \hspace{1cm} (20)

This function $\tilde{G}_\beta$ is the propagator for a particle in a one-dimensional harmonic potential with a wall at the position $-k/B$.

We are now in a position to use the PDX techniques from the previous section. The leading term in the PDX series is found by omitting the wall. In that case the propagator $\tilde{G}_\beta$ becomes [11]

$$\tilde{G}^{(0)}_{\beta}(x', x, k) = \left[ \frac{B}{2\pi \sinh(\beta B)} \right]^{1/2} \exp \left[ -\frac{B(x^2 + x'^2)}{2 \sinh(\beta B)} + \frac{B x' x}{2 \sinh(\beta B)} \right].$$

As a matter of fact, $\tilde{G}^{(0)}_{\beta}$ is independent of $k$, since the only $k$-dependence in (20) is in the position of the wall. After performing the integral over $k$, which is Gaussian, we find that the leading term in the PDX series is given by

$$G^{(0)}_{\perp, \beta}(r', r) = \frac{B}{4\pi \sinh(\beta B/2)} \exp \left[ -\frac{B}{4 \sinh(\beta B/2)} (r' - r)^2 + \frac{iB}{2} (x' + x)(y' - y) \right]$$

which is indeed the Green function in the Landau gauge for the unconfined system.

The next term in the resummed PDX series (13) (or (15)) is more complicated. The integral over $k$ is again Gaussian (in fact it is Gaussian for all terms), but the additional integral over $\tau$ is not. If we set $t_1 = \tanh(\tau B/2)$, $s_1 = \sinh(\tau B/2)$, $t_2 = \tanh((\beta - \tau) B/2)$ and $s_2 = \sinh((\beta - \tau) B/2)$, we can write

$$G^{(1)}_{\perp, \beta}(r', r) = -\frac{B^2}{16\pi^{3/2}} \int_0^\beta d\tau f^{(1)}_{\beta, \tau}(r', r) \exp[g^{(1)}_{\beta, \tau}(r', r)]$$

with

$$f^{(1)}_{\beta, \tau}(r', r) = \frac{1}{2} B^{1/2} \left( \frac{t_1 t_2}{s_1 s_2 (t_1 + t_2)} \right)^{1/2} \left[ \frac{x'}{t_1} + \frac{x}{t_2} + i(y' - y) \right]$$

and

$$g^{(1)}_{\beta, \tau}(r', r) = \frac{B}{4} \left\{ \frac{[x' t_1 + x t_2 + i(y' - y)]^2}{t_1 + t_2} - \left( t_1 + \frac{1}{t_1} \right)x'^2 - \left( t_2 + \frac{1}{t_2} \right)x^2 \right\}.$$

Similar expressions can be found in [7]. Note that the formulae in [7] differ slightly from those given above. We have made use of the property $G_{\beta}(r', r) = [G_{\beta}(r, r')]^{\tau}$ and of the possibility to change $\tau$ into $\beta - \tau$ to write $f^{(1)}$ and $g^{(1)}$ in a form that is more symmetric.

The higher-order terms in the resummed PDX series can be found along similar lines. For the special case $r' = r$ they have been collected in the appendix. They are found to agree with those derived in [7], after appropriate symmetrization.
4. Asymptotics (non-degenerate case)

The particle density and the (electric) current density can both be found from the Green function. In the absence of quantum degeneracy the particle density is directly related to $G_{\perp, \beta}$ via

$$\rho(x) = \frac{\rho_0}{Z_{\perp}} G_{\perp, \beta}(r, r)$$  \hspace{1cm} (26)

where $\rho_0$ is the bulk density and $Z_{\perp} = B/[4\pi \sinh(\beta B/2)]$ is the transverse one-particle partition function per unit area for the bulk. The expression for the current density is slightly more complicated, involving derivatives of $G_{\perp, \beta}$:

$$j_r(x) = \frac{\rho_0}{Z_{\perp}} \frac{1}{2i} \left[ \frac{\partial}{\partial y} G_{\perp, \beta}(r', r) - \frac{\partial}{\partial y} G_{\perp, \beta}(r', r') \right]_{r'=r} - Bx \rho(x).$$  \hspace{1cm} (27)

Using only the $n = 0$ term of the PDX series in the expression for $\rho(x)$ yields the bulk density $\rho_0$, as it should, since $G_{\perp, \beta}^{(0)}(r, r)$ equals $Z_{\perp}$. Therefore, we will consider the excess particle density $\delta \rho(x) = \rho(x) - \rho_0$ instead of $\rho(x)$ in the following. Since there is no bulk current, the $n = 0$ term of the PDX series does not contribute to the current density.

To determine the profiles of the excess particle density and the current density for arbitrary distances from the wall we need to evaluate all terms in the resummed PDX series. However, the $\tau$-integral in (23) cannot be carried out analytically. Likewise, evaluation of the multiple $\tau$-integrals in the higher-order terms given in the appendix is, in general, not possible.

For large distances from the wall (in units of the magnetic length $1/\sqrt{B}$) the leading contribution to the profiles comes from the $n = 1$ term in the resummed PDX series, as we will discuss presently. Moreover, the $\tau$-integral in (23) can be evaluated analytically in that limit. It is thus possible to derive asymptotic expressions for the profiles of the excess particle density and the current density that are valid for large $\sqrt{B}x$.

A change of variables $y = z^2/(z_0^2 - z^2)$, with $z = \tanh[B(2\tau - \beta)/4]$ and $z_0 = \tanh(B\beta/4)$, brings (23) into the form

$$G_{\perp, \beta}^{(1)}(r, r) = -\frac{B^{3/2}}{8\sqrt{2\pi}^{3/2}} \frac{1 - z_0^2}{z_0^{3/2}} \exp \left[ -\frac{Bx^2}{2z_0} \right] \int_0^\infty \frac{dy}{\sqrt{y(1+y)}} \sqrt{1 + (1 - z_0^2)y}$$

$$\times \exp \left[ -\frac{(1 - z_0^2)y}{2z_0} Bx^2 \right].$$  \hspace{1cm} (28)

Because of the presence of $Bx^2$ in the exponent, only small values of $(1 - z_0^2)y/z_0$ contribute to the integral for large $\sqrt{B}x$. Since one has $0 \leq z_0 < 1$, this implies small values of $(1 - z_0^2)y$. Note that this does not necessarily mean that $y$ itself is small, as $z_0$ may be close to 1. For large $\sqrt{B}x$ the factor $\sqrt{1 + (1 - z_0^2)y}$ in the integrand can be replaced by 1. Subsequently, we can use

$$\int_0^\infty \frac{dy}{\sqrt{y(1+y)}} e^{-ay} = e^{a^2/2} K_0(a/2)$$  \hspace{1cm} (29)

where $K_0$ is the modified Bessel function of the second kind. In this way we arrive at the following asymptotic expression for the transverse part of the Green function for large $\sqrt{B}x$:

$$G_{\perp, \beta}^{(1)}(r, r) \approx -\frac{B^{3/2}}{8\sqrt{2\pi}^{3/2}} \frac{1 - z_0^2}{z_0^{3/2}} \exp \left[ -\frac{1 + z_0^2}{4z_0} Bx^2 \right] K_0 \left( \frac{1 - z_0^2}{4z_0} Bx^2 \right).$$  \hspace{1cm} (30)

The next term in the asymptotic expansion of $G_{\perp, \beta}^{(1)}$ is

$$-\frac{B^{3/2}}{8\sqrt{2\pi}^{3/2}} \frac{(1 - z_0^2)^2}{4z_0^{3/2}} \exp \left[ -\frac{1 + z_0^2}{4z_0} Bx^2 \right] \left\{ K_1 \left( \frac{1 - z_0^2}{4z_0} Bx^2 \right) - K_0 \left( \frac{1 - z_0^2}{4z_0} Bx^2 \right) \right\}$$  \hspace{1cm} (31)
which can be derived by substituting $\sqrt{1 + (1 - z_0^2)y} \approx 1 + (1 - z_0^2)y/2$. Since $z[K_1(z) - K_0(z)]/K_0(z)$ is bounded for all positive $z$, we see that (31) is indeed of higher order in $1/(\sqrt{B}x)$.

Having investigated the $n = 1$ term in the resummed PDX series, we may turn to the higher orders. From a detailed analysis (see the appendix) it is found that all terms with $n > 1$ are of higher order in $1/(\sqrt{B}x)$ in comparison with (30). In figure 1 we have plotted $G^{(2)}_{\perp,\beta}/G^{(1)}_{\perp,\beta}$ as a function of $\xi = \sqrt{B}x$, for a representative value of $\beta B$. The decay is in good agreement with (A.10).

The asymptotic expression for the excess particle density at large $\sqrt{B}x$ follows by substituting (30) in (26):

$$
\delta \rho(x) \approx -\rho_0 \frac{B^{1/2}}{\sqrt{2\pi z_0}} x^{-1/2} \exp \left( -\frac{1 + z_0^2}{4z_0} B x^2 \right) K_0 \left( \frac{1 - z_0^2}{4z_0} B x^2 \right)
$$

(32)

where we have used that $Z_{\perp}$ is given by $Z_{\perp} = B(1 - z_0^2)/(8\pi z_0)$ in terms of $z_0$. In a similar way an asymptotic expression for the current density at large $\sqrt{B}x$ can be derived. In leading order it is found to be proportional to the asymptotic excess particle density

$$
j_y(x) \approx -\frac{1}{2} B x \delta \rho(x)
$$

(33)

with $\delta \rho(x)$ given in (32). This simple proportionality ceases to be valid, if higher-order terms are incorporated in the asymptotic expansion. Comparing (33) to (27) we see that there is a compensation between the term proportional to $\rho(x)$ and the term that contains the derivatives of the Green function. For the $n = 0$ contribution this compensation is complete, but for $n = 1$ only half of the second term in (27) is cancelled, at least in leading order in $1/(\sqrt{B}x)$.

It must be stressed that both (32) and (33) are valid for large $\sqrt{B}x$, whereas $\beta B$ may take arbitrary values. If, apart from $Bx^2$, $[(1 - z_0^2)/z_0]Bx^2$ is also large, we can simplify (30) to

$$
G^{(1)}_{\perp,\beta}(r, r) \approx -\frac{B}{8\pi} \frac{\sqrt{1 - z_0^2}}{z_0} \exp \left( -\frac{B x^2}{2z_0} \right)
$$

(34)
by using the asymptotic expansion for the modified Bessel function. In that case the excess particle density profile is asymptotically given by

\[
\delta \rho(x) \approx -\rho_0 \cosh(\beta B/4) \exp \left[ -\frac{B x^2}{2 \tanh(\beta B/4)} \right].
\]

(35)

Large \([1 - z_0^2]/z_0\)Bx² implies that the regime \(z_0 \to 1\) or \(\beta B \to \infty\) is not included, whereas no such limitation is imposed on the use of (32). For fixed \(B\) this is not a serious limitation in the present context of a non-degenerate electron gas, since for \(\beta \to \infty\) we have to use Fermi–Dirac statistics anyway. In the next section it will be shown that the Green function in the form (30) is crucial to obtain information on the asymptotic profiles for a degenerate electron gas with Fermi–Dirac statistics.

To investigate the validity of the asymptotic expressions for \(G^{(1)}\) mentioned above we have compared (30) and (34) with numerical results based on (23) or (28). The results are drawn in figure 2. It is clear that for \(\beta B = 4\) both asymptotic expressions are adequate, even for relatively small values of \(\xi\), whereas for \(\beta B = 16\) the performance of (30) is much better than that of (34).

Finally, for small \(B\), expression (35) for the excess particle density yields

\[
\rho(x) \approx \rho_0 (1 + \frac{1}{2} B^2 \beta^2 - \frac{1}{32} \beta B^2 x^2) e^{-2x^2/\beta}.
\]

(36)

Indeed, these terms correspond to the leading terms (for large \(x^2/\beta\)) in the expression for the density up to order \(B^2\), as given in [7].

In closing this section on the non-degenerate electron gas we remark that the path-integral representation can be used to derive a strict bound on the particle density for all values of \(x\). Upon setting \(k' = x - k/B\) we find from (19), (20) and (26)

\[
\delta \rho(x) = \frac{\rho_0 B}{2\pi Z} \int_{-\infty}^{\infty} dk' \int_{-\infty}^{k'} d\mu_{k',0} \theta(k' - x - \inf_{\tau} \omega_\tau(\tau)) e^{-\frac{1}{2} B^2 \beta^2 \int_{0}^{\tau} d\tau [\omega_\tau(\tau)]^2}.
\]

(37)

All paths that contribute to this integral must pass below the point \(k' = x\), while starting and finishing at \(k'\). Now look at paths that go via a point below \(k' = x\) precisely at \(\tau = \beta/2\). Since these form a subclass of all allowed paths, the corresponding path integral provides a lower bound on \(|\delta \rho(x)|\):

\[
|\delta \rho(x)| \geq \frac{\rho_0 B}{2\pi Z} \int_{-\infty}^{\infty} dk' \int_{-\infty}^{k'-x} dx' \int d\mu_{k',0} \theta(k' - x - \inf_{\tau} \omega_\tau(\tau)) e^{-\frac{1}{2} B^2 \beta^2 \int_{0}^{\tau} d\tau [\omega_\tau(\tau)]^2} \\
\times \int d\mu_{x',T} \theta(x' - \inf_{\tau} \omega_\tau(\tau)) e^{-\frac{1}{2} B^2 \beta^2 \int_{0}^{\tau} d\tau [\omega_\tau(\tau)]^2}.
\]

(38)

The path integrals in this expression are now unrestricted, so that they are given by \(\tilde{G}^0\) (see (21)). Integration over \(k'\) and \(x' = k'\) (in that order) gives

\[
|\delta \rho(x)| \geq \frac{1}{2} \rho_0 \operatorname{Erfc} \left( x \left[ \frac{B}{2 \tanh(\beta B/4) \beta} \right]^{1/2} \right)
\]

(39)

which is the bound for all \(x\) that we set out to derive. In the limit of large \(x\) this implies

\[
\lim_{x \to \infty} x \exp \left[ -\frac{B x^2}{2 \tanh(\beta B/4)} \right] |\delta \rho(x)| \geq \frac{\rho_0}{2\sqrt{\pi}} \left[ \frac{2 \tanh(\beta B/4)}{B} \right]^{1/2}.
\]

(40)

This inequality is consistent with (35), as it should be. In particular, the Gaussian decay of \(\delta \rho(x)\), with the same characteristic length as in (35), is corroborated.

As can be seen from the results (32) and (33) the decay towards the bulk value of both the excess particle density and the current density is Gaussian, modulated by a Bessel function.
and an algebraic factor. For not too large $\beta B$ the decay of the excess particle density, as given by (35), is strictly Gaussian far from the edge. The asymptotic decay of the current density is likewise Gaussian, albeit with an extra algebraic factor. The characteristic length on which the Gaussian decay manifests itself is proportional to $[\text{tanh}(\beta B/4)/B]^{1/2}$. As we have shown above, the Gaussian decay for the excess particle density is consistent with a lower bound that can be derived exactly. For the current density it is consistent with the upper bound on the absolute value of the current density that has been derived by Macris \textit{et al} [12]. However, it should be remarked that the upper bound obtained in that paper is rather wide. In fact, the characteristic length of the Gaussian function in their upper bound is the thermal wavelength, which is independent of the magnetic field. This characteristic length is larger than that in the Gaussian found here, at least for non-vanishing magnetic fields.
5. Asymptotics (degenerate case)

The particle density $\rho(x)_{FD}$ of a degenerate Fermi–Dirac system at temperature $T = 0$ and chemical potential $\mu$ is related to the density of the non-degenerate system by a Laplace transformation:

$$
\int_0^\infty d\mu \, e^{-\beta \mu} \rho(x)_{FD} = \frac{2Z}{\rho_0 \beta} \rho(x). \tag{41}
$$

Here, $Z = Z_1 Z_2$ is the total one-particle partition function per unit volume for the bulk, with $Z_1 = (2\pi \beta)^{-1/2}$; the factor 2 takes the spin degeneracy into account. The relation (41) implies that we can calculate the excess particle density $\delta \rho(x)_{FD}$ from $\delta \rho(x)$ via an inverse Laplace transform [13]:

$$
\delta \rho(x)_{FD} = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\beta \, e^{\beta \mu} \frac{2Z}{\rho_0 \beta} \delta \rho(x) \tag{42}
$$

with arbitrary $c > 0$. Hence, the asymptotic behaviour of the excess particle density of the degenerate system for large $\sqrt{B}x$ can be obtained on the basis of the results of the previous section.

Let $\xi = \sqrt{B}x$ and $\nu = \mu/B$, and introduce a new integration variable $t$ by writing $\beta = \xi (it + 1)/B$, so that $c$ is given by $\xi/B$. If we express the right-hand side of (32) in the variables $\xi$ and $\nu$, and substitute it into (42), we get

$$
\delta \rho(x)_{FD} \approx -\frac{B^{3/2} \xi^{1/2}}{16\pi^3} \int_\infty^{-\infty} \frac{dz_0}{(\nu + 1)^{3/2}} \left[ 1 - \frac{\nu}{2} \right] e^{\nu(it+1)/2} e^{z_0^2/4} e^{-z_0^2/4} K_0 \left( \frac{1}{4} \right) \tag{43}
$$

In the new variables we have $z_0 = \text{tanh}[\xi (it + 1)/4]$, so that large $\xi$ implies $z_0 \approx 1$ and $1 - z_0^2 \approx 4 \exp[-\xi (it + 1)/2]$. Consequently, the argument of $K_0$ in (43) is small in absolute value, so that we can use the series representation

$$
K_0(z) = \sum_{n=0}^\infty \left[ \sum_{m=1}^{\arcsinh(z/2)} \frac{1}{m} - \gamma - \log \left( \frac{z}{2} \right) \right] \frac{1}{2^{2n} (n!)^2} z^{2n} \tag{44}
$$

for the modified Bessel function. In this way we get

$$
\delta \rho(x)_{FD} \approx -\frac{B^{3/2} \xi^{1/2}}{4\pi^3} e^{-\xi^2/2} \sum_{n=0}^\infty \frac{\xi^{2n}}{2^{2n} (n!)^2} \int_\infty^{-\infty} dr \left[ (it + 1)^{\xi/2} + \sum_{m=1}^{\arcsinh(z/2)} \frac{1}{m} - \gamma - \log \left( \frac{\xi^2}{2} \right) \right] e^{(v-(n+1/2))\xi(it+1)/(\nu + 1)^{3/2}}. \tag{45}
$$

Upon using the identity†

$$
\int_{-\infty}^{\infty} dr \, \frac{e^{itx} \Gamma(\nu)}{(it + 1)^\nu} = \theta(x) \frac{2\pi x^{\nu-1}}{\Gamma(\nu)} \quad (\nu > 0) \tag{46}
$$

we arrive at the asymptotic expression for the excess particle density

$$
\delta \rho(x)_{FD} \approx -\frac{B^{3/2} \xi}{\pi^{5/2}} e^{-\xi^2/2} \sum_{n=0}^{\lfloor \nu^{1/2} \rfloor} \frac{\xi^{2n}}{2^{2n} (n!)^2} \left[ \frac{1}{4[n - (n + 1/2)]} + \sum_{m=1}^{\arcsinh(z/2)} \frac{1}{m} - \gamma - \log \left( \frac{\xi^2}{2} \right) \right] \tag{47}
$$

with $[x]$ the largest integer less than or equal to $x$. The asymptotic expression derived here is valid for large $\xi$ and fixed $\nu$.

† See formula 3.2.4 [14] in which the overall sign should be inverted.
The profile of the current density for large $\xi$ and fixed $\nu$ can likewise be obtained from the results of the previous section. In fact, because of the linearity of the inverse Laplace transform the asymptotic form of the current density is related to that of the excess particle density in the same way as in (33)

$$j_y(x)_{FD} \approx -\frac{1}{2} B x \delta \rho(x)_{FD}. \quad (48)$$

The expressions (47) and (48) for the asymptotic profiles of the excess particle density and the current density are identical to the leading terms of the asymptotic expansions in [4], which have been obtained by solving the eigenvalue problem and analysing the asymptotics of the eigenfunctions. It is also possible to recover the higher-order terms of [4] by inserting higher-order terms in the approximate expressions for the factors $z_0$ and $1 - z_0^2$ in the integrand in (43), taking into account corrections such as (31), and including more terms in the resummed PDX series as well.

The asymptotic behaviour of (47) (and of (48)) is Gaussian in $\xi$, so that the characteristic length is the magnetic length $1/\sqrt{B}$ for a completely degenerate electron gas. Furthermore, the Gaussian is multiplied by a prefactor that depends algebraically and logarithmically on $\xi$. For $\nu$ just above a half-odd integer, that is, for chemical potentials $\mu$ slightly above a Landau level, the profile of the excess particle density shows a singular behaviour that is a remnant of the de Haas–van Alphen effect. A numerical assessment of the convergence of this asymptotic expression can be found in [4].

The dominant term in the asymptotic behaviour comes from the highest Landau level with the label $[\nu - \frac{1}{2}]$. Since the prefactor of the Gaussian in this term is proportional to $\xi^{4[\nu - 1/2] + 1}$, the onset of the Gaussian decay shifts to larger and larger values of $\xi$, if $\nu$ increases. In fact, (47) is only useful for $\xi^2 \gg \nu$, or equivalently for $x$ large compared with the cyclotron radius $\sqrt{n}/B$ of particles at the Fermi level. If $\nu$ is large, a different behaviour can be expected in the regime $\xi^2 \approx \nu$, before the ultimate Gaussian decay sets in at $\xi^2 \gg \nu$.

In conclusion, we have studied the edge effects in the excess particle density and the current density of a magnetized free-electron gas, which is confined by a hard wall. In particular, we have investigated the long-range influence of the wall on these quantities, by determining their asymptotic profiles both for the non-degenerate case and for strong degeneracy. New results have been obtained for both these cases. In the former case the asymptotic spatial profiles were found to be Gaussian (or Gaussian modulated by a Bessel function), with a characteristic length that is proportional to $[\tanh(\beta B/4)]^{1/2}$. In the latter case the asymptotic behaviour depends on the number of filled Landau levels $n = [\mu/B - \frac{1}{2}]$. In fact, it is determined by a Gaussian with a characteristic length equal to the magnetic length $1/\sqrt{B}$, multiplied by a polynomial and a logarithmic prefactor. Since the degree of the polynomial prefactor grows with $n$, the Gaussian character of the asymptotics comes to the fore only for distances that are large compared with $\sqrt{n}$ times the magnetic length.

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Appendix. Higher-order terms in the PDX series

In this appendix we study the asymptotic behaviour of the terms with $n > 1$ in the resummed PDX series for the Green function, for large values of $\sqrt{B}x$. The general form of the term of
order $n$ in the resummed PDX series is

$$G_{\perp,\beta}(r', r) = (-)^n \frac{B_n^{n+1}}{2n+3} \int_0^1 \cdots \int_0^1 \, d\tau_1 \cdots d\tau_n \, \theta(\tau_{n+1})$$

$$\times f_{\beta, \tau_1, \ldots, \tau_n}^{(n)}(r', r) \exp[g_{\beta, \tau_1, \ldots, \tau_n}^{(n)}(r', r)]$$

(A.1)

with $\tau_{n+1} = \beta - \sum_{i=1}^n \tau_i$. The functions $f^{(n)}$ and $g^{(n)}$ can be found in [7]. Here we collect them for the case $r' = r$, which is relevant for the particle density. In that case we can symmetrize the expressions in $\tau_1$ and $\tau_2$. As a result they take the form

$$f_{\beta, \tau_1, \ldots, \tau_n}^{(n)}(r, r) = \left( \prod_{i=1}^{n+1} t_i^{3/2} \right) \left( \sum_{i=1}^{n+1} t_i \right)^{-n/2} \left[ 1 + \frac{1}{t_1 t_2} \right]$$

$$\times \left[ (t_1 + t_2) \left( \frac{n}{2} - 1 \right) - \delta_{n, \text{even}} \right]$$

$$+ \sum_{p=0}^{[n/2]} \frac{(t_1 + t_2)}{2} p \left( \frac{n}{2} - p \right) \left( \sum_{i=1}^{n+1} t_i \right)$$

$$\times \left[ (t_1 + t_2) \left( \frac{n}{2} - 1 \right) - \delta_{n, \text{even}} \right]$$

(A.2)

and

$$g_{\beta, \tau_1, \ldots, \tau_n}^{(n)}(r, r) = -\frac{Bx^2}{4} \left[ 1 + \frac{1}{t_1 t_2} \right]$$

$$- \frac{1}{t_1 t_2} \sum_{i=1}^{n+1} t_i$$

(A.3)

with $t_i = \tanh(B \tau_i/2)$, $s_i = \sinh(B \tau_i/2)$ and $(a)_n$ Pochhammer’s symbol $a(a+1) \ldots (a+n-1)$.

For large $\sqrt{Bx}$ the dominant contribution to the integral comes from the integrand region for which the factor multiplying $Bx^2$ in $|g^{(n)}|$ is minimal. This is the case for $\tau_1 = \tau_2 = \beta/2$ and $\tau_i = 0$ (with $3 \leq i \leq n+1$). Therefore, we introduce on a par with $z_0 = \tanh(B \beta/4)$ the new integration variables $z_+ = \tanh[B(\beta - \tau_1 - \tau_2)/4]$, $z_- = \tanh[B(\tau_1 - \tau_2)/4]$ and for $n > 1$ also $z_i = \tanh(B \tau_i/2) = t_i$ ($i = 3, \ldots, n$). If the integrations are carried out in the order $z_+, z_{-}$, the allowed intervals of these variables are $z_+ \in [z_0, z_+], z_- \in [0, (z_0 - z_-)/(1 - z_0 z_-)]$, and $z_i \in [0, 2z_i/(1 + z_i^2)]$, with an additional condition on $z_i$ resulting from the $\theta$-function in (A.1).

We now have to rewrite the integrand of (A.1) in terms of $z_+, z_-,$ and $z_i$. Let us consider small values of $z_+$ and $z_-$. The function $g^{(n)}$ then takes the form

$$g_{\beta, \tau_1, \ldots, \tau_n}^{(n)}(r, r) \approx -\frac{Bx^2}{2} \left[ \frac{z_0(1 - z_-^2)}{z_0^2 - z_-^2} + \frac{z_0^2 z_-^2}{z_0^2 - z_-^2} + \frac{4z_0^2 z_-^2 + z_0^2 - z_-^2}{(z_0^2 - z_-^2)^2} z_+ + \cdots \right].$$

(A.4)

From the right-hand side it is seen that it is indeed true that only small values of $z_+$ contribute to the integral in (A.1), as $Bx^2$ is large. In turn this implies that all $z_i$ have to be small as well, whereas no condition of smallness is imposed on $z_-$. In $f^{(n)}$ only the $p = 0$ terms are relevant for large $Bx^2$, since these give the terms with the highest power of $x$. As a consequence we can write $f^{(n)}$ as

$$f_{\beta, \tau_1, \ldots, \tau_n}^{(n)}(r, r) \approx (Bx^2)^{n/2} \frac{z_0^{1/2}(1 - z_0^2)}{2n^{1/2} n^{1/2}} \left( \frac{1 - z_-^2}{z_0^2 - z_-^2} \right)^{3/2} \left( 2z_+ - \sum_{i=1}^{n+1} z_i \right)^{1/2} \left( \prod_{i=3}^{n+1} z_i^{1/2} \right)$$

(A.5)
guarantees that only small values of $G(n)$ in the neighbourhood of $\approx$ asymptotic expression for $G(n)$ integral can then be carried out trivially.

we may use the fact that only small values of $\approx$ guarantees that only small values of $z_i$ contribute anyway. The subsequent integral over $z_s$ takes the following form:

$$
\int_0^{n-1} d\zeta_s (2\zeta_s)^{(3n-5)/2} \exp \left[ -\frac{Bx^2}{2} \frac{z_0^4 z_\perp^2 + z_0 z_\perp z_\parallel^4 - 4z_0 z_\perp z_\parallel^2 + z_\perp^2 + z_\parallel^2}{(z_0^2 - z_\perp^2)^2} z_s \right].
$$

Again we can choose $\approx$ for the upper limit, since only small values of $z_s$ are significant; the integral can then be carried out trivially.

We are left with the integral over $z_\perp$. Leaving it in its original form we arrive at

$$
G_{\perp,\beta}^{(n)}(r, r) \approx (-\alpha)^n \frac{2^{n-7/2}z_0^{1/2}}{\pi^{3/2}(Bx^2)^{n-5/2}x^2} (1 - z_0^2)
\times \int_0^{z_0} d\zeta_\perp \frac{(z_0^2 - z_\perp^2)^{3(n-3)/2}(1 - z_\perp^2)^{1/2}}{(z_0^2 - z_\perp^2)\perp^2 + z_\perp z_\parallel^4 + 4z_0 z_\perp z_\parallel^2 + z_\perp^2 + z_\parallel^2} \exp \left[ -\frac{Bx^2}{2} \frac{z_0(1 - z_\perp^2)}{z_\perp^2 - z_\parallel^2} \right].
$$

A final transformation of variables, by setting $z_\perp = \sqrt{\frac{\sqrt{1 + y}}{1 + z_0^2}}$, leads to the following asymptotic expression for $G_{\perp,\beta}^{(n)}$ in the regime of large $\sqrt{Bx}$:

$$
G_{\perp,\beta}^{(n)}(r, r) \approx (-\alpha)^n \frac{2^{n-9/2}z_0^{3n-9/2}(1 - z_0^2)}{\pi^{3/2}(Bx^2)^{n-5/2}x^2} \exp \left[ -\frac{Bx^2}{2z_0} \right] \int_0^{\frac{\sqrt{1 + (1 - z_0^2)y}}{1 + z_0^2}} dy \frac{1}{\sqrt{y(1 + y)}}
\times \frac{(1 - z_0^2)^2}{2z_0} Bx^2 \exp \left[ -\frac{(1 - z_0^2)^2}{2z_0} x \right].
$$

The expression found here looks very similar to (28), which is valid for $G_{\perp,\beta}^{(1)}$. As before, we may use the fact that only small values of $(1 - z_0^2)y$ contribute to the integral for large $\sqrt{Bx}$. As a result, one has the asymptotic relation

$$
G_{\perp,\beta}^{(n)}(r, r) \approx \left( -\frac{2z_0^3}{Bx^2} \right)^{n-1} G_{\perp,\beta}^{(1)}(r, r)
$$

for large $Bx^2$. A similar connection formula holds for the asymptotic forms of the excess particles density in various orders:

$$
\delta \rho^{(n)}(x) \approx \left( -\frac{2z_0^3}{Bx^2} \right)^{n-1} \delta \rho^{(1)}(x)
$$
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again for large $Bx^2$. Likewise, one derives for the asymptotic forms of the current density in various orders:

$$j_y^{(n)}(x) \approx \left( \frac{-2z_0^3}{Bx^2} \right)^{n-1} j_y^{(1)}(x).$$

(A.12)

We may draw the conclusion that for large $\sqrt{B}x$ the $n = 1$ term in the resummed PDX series yields the dominant contribution, both for the excess particle density and for the current density.

References

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