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Boundary effects in a magnetized free electron gas: Green function approach

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Abstract. A Green function approach to the boundary effects of a free electron gas in a magnetic field is presented. It is shown that truncation of the multiple-reflection expansion for the Green function of a confined system is not justified if a magnetic field is present, not even for a system with flat boundaries. Using the full expansion we calculate the profiles for the particle density, the current density and the components of the pressure tensor near the boundary.

1 Introduction

The study of boundary effects and finite-size corrections in physical systems has a long history. A well-known example is the Landau orbital diamagnetism of a free electron gas in a magnetic field. Although in Landau's original derivation [1] only bulk properties are considered, the diamagnetism is actually caused by surface currents that are induced by the magnetic field. Unfortunately, it is difficult to get a hold on these surface effects, in particular for general systems with arbitrary shapes. A lot of work has been done on the subject, as can be seen from the rather extensive literature (see [2] - [14], and the references cited therein).

An interesting approach to the study of surface effects in finite systems is due to Balian and Bloch [15]. They present an equation for the Green function of a free-particle system in a finite volume in terms of the Green function for the infinite domain. This equation, which is valid for arbitrary domain shapes, is a so-called multiple-reflection expansion. Higher-order terms in this expansion become increasingly more important when the local curvature radii of the wall diminish. For (nearly) flat surfaces the leading term in the expansion is already sufficient to determine the first-order finite-size corrections. Later on, Robnik [10] generalized this method so as to include the influence of an external magnetic field on the motion of charged particles without mutual interaction. In deriving explicit results for the boundary effects he took into account only the first term in the multiple-reflection expansion, as was done before by Balian and Bloch. Whereas that approximation is justified for an unmagnetized free-particle system in which the particle trajectories are straight lines, it is not clear whether it still makes sense if the trajectories become curved under the influence of the magnetic field.

In this paper we will investigate the validity of the truncation of the multiple-reflection expansion for a magnetized free-particle system in a finite enclosure. In a similar way as in [10] the formalism of [15] will be generalized to account for the presence of a magnetic field. The resulting expansion will be analyzed for the special case of a slab geometry in order to determine whether a truncation is indeed allowed for flat boundaries. Subsequently, it will be shown how the multiple-reflection expansion for the temperature-dependent Green function can be rearranged to yield an expansion in the cyclotron frequency. Finally, it will be demonstrated how the latter can be used to obtain explicit expressions for the finite-size correction to the partition function of a non-degenerate electron gas and for the profiles of some local physical quantities, such as the particle density or the electric current density. The results will be compared to expressions derived recently by using standard perturbation theory [16].

2 Green functions

We consider a free electron gas in a uniform magnetic field. The electron gas is confined to a three-dimensional cylinder-shaped domain D with hard walls. The base of the cylinder is arbitrary and the direction of the magnetic field is perpendicular to the base manifold. The Hamiltonian for a single particle in a magnetic field is given by

$$H = \frac{1}{2m}(\mathbf{p} - \frac{e}{c}\mathbf{A})^2 \equiv H_\perp + H_{||}, \tag{1}$$

where

$$H_\perp = -\frac{\hbar^2}{2m}\Delta_\perp + i\hbar\omega_c x\frac{\partial}{\partial y} + \tfrac{1}{2}m\omega_c^2 x^2. \tag{2}$$

We have taken the vector potential for the magnetic field $\mathbf{B} = (0, 0, B)$ to be in the Landau gauge so that $\mathbf{A} = (0, Bx, 0)$. The associated cyclotron frequency is $\omega_c = eB/mc$. Since we can split off the z-dependent part in the Hamiltonian, the motion in the z direction is trivial. Therefore, we will only deal with the transverse (x, y) part in the following. Accordingly, we shall write $\mathbf{r}$ to denote (x, y). The eigenvalue equation of the transverse problem can be written as

$$H_\perp\psi_n(\mathbf{r}) = E_n\psi_n(\mathbf{r}). \tag{3}$$

The eigenfunction must vanish at the boundary

$$\psi_n(\mathbf{r}) = 0, \quad \mathbf{r} \in \partial D. \tag{4}$$

The Green function corresponding to the eigenvalue equation is defined as

$$G_z(\mathbf{r}, \mathbf{r}') = \sum_n \psi_n(\mathbf{r})\psi_n^*(\mathbf{r}')\frac{1}{z - E_n}, \tag{5}$$

for arbitrary complex z. The Green function satisfies the equation

$$(H_\perp - z)G_z(\mathbf{r}, \mathbf{r}') = -\delta(\mathbf{r} - \mathbf{r}'), \tag{6}$$

with Dirichlet boundary conditions

$$G_z(\mathbf{r}, \mathbf{r}') = 0, \quad \mathbf{r} \in \partial D \quad \text{and/or} \quad \mathbf{r}' \in \partial D. \tag{7}$$

The relation with the energy and the temperature Green functions is

$$G_E(\mathbf{r},\mathbf{r}') = \frac{i}{2\pi}[G_{z=E+i0}(\mathbf{r},\mathbf{r}') - G_{z=E-i0}(\mathbf{r},\mathbf{r}')], \tag{8}$$

$$G_\beta(\mathbf{r},\mathbf{r}') = \int_0^\infty dE\, e^{-\beta E} G_E(\mathbf{r},\mathbf{r}'), \tag{9}$$

respectively.

We split the Green function in a part G_z^0, which is the Green function for the system without confinement, and a correction part G_z^c, so that $G_z = G_z^0 + G_z^c$. We will now derive an equation for this correction part in terms of G_z^0. The equation which the correction part satisfies is

$$(H_\perp - z)G_z^c(\mathbf{r},\mathbf{r}') = 0, \tag{10}$$

for all $\mathbf{r},\mathbf{r}' \in D/\partial D$, with boundary condition

$$G_z^c(\mathbf{r},\mathbf{r}') = -G_z^0(\mathbf{r},\mathbf{r}'), \quad \mathbf{r} \in \partial D \quad \text{and/or} \quad \mathbf{r}' \in \partial D. \tag{11}$$

From (10), (11) and the Green equality one finds

$$G_z^c(\mathbf{r},\mathbf{r}') = -\frac{\hbar^2}{2m}\int_{\partial D} d\sigma''^W \mathbf{n}'' \cdot \left[\nabla_{\mathbf{r}''} G_z(\mathbf{r},\mathbf{r}'')\right]_{\mathbf{r}''\to\mathbf{r}''^W} G_z^0(\mathbf{r}''^W,\mathbf{r}'), \tag{12}$$

where $\mathbf{n}''$ is the normal vector, directed outwards, at the point r'' of the boundary. The symbol W in (12) means that the coordinate is located at the boundary. Furthermore, one should interpret $G_z^0(\mathbf{r}''^W,\mathbf{r}')$ as $\left[G_z^0(\mathbf{r}'',\mathbf{r}')\right]_{\mathbf{r}''\to\mathbf{r}''^W}$. Next, we differentiate (12) with respect to $\mathbf{r}'$, take the limit $\mathbf{r}' \to \mathbf{r}'^W$ and write it in the following form

$$\begin{aligned}
&\mathbf{n}'\cdot\left[\nabla_{\mathbf{r}'} G_z^c(\mathbf{r},\mathbf{r}')\right]_{\mathbf{r}'\to\mathbf{r}'^W} = \\
&= -\frac{\hbar^2}{2m}\int_{\partial D} d\sigma''^W \mathbf{n}'' \cdot \left[\nabla_{\mathbf{r}''} G_z(\mathbf{r},\mathbf{r}'')\right]_{\mathbf{r}''\to\mathbf{r}''^W} \mathbf{n}' \cdot \left[\nabla_{\mathbf{r}'} G_z^0(\mathbf{r}''^W,\mathbf{r}')\right]_{\mathbf{r}'\uparrow\downarrow\mathbf{r}'^W} \\
&\quad - \frac{\hbar^2}{2m}\left\{\int_{\partial D} d\sigma''^W \mathbf{n}'' \cdot \left[\nabla_{\mathbf{r}''} G_z(\mathbf{r},\mathbf{r}'')\right]_{\mathbf{r}''\to\mathbf{r}''^W} \mathbf{n}' \cdot \left[\nabla_{\mathbf{r}'} G_z^0(\mathbf{r}''^W,\mathbf{r}')\right]_{\mathbf{r}'\to\mathbf{r}'^W}\right. \\
&\quad \left. - \int_{\partial D} d\sigma''^W\, \mathbf{n}'' \cdot \left[\nabla_{\mathbf{r}''} G_z(\mathbf{r},\mathbf{r}'')\right]_{\mathbf{r}''\to\mathbf{r}''^W} \mathbf{n}' \cdot \left[\nabla_{\mathbf{r}'} G_z^0(\mathbf{r}''^W,\mathbf{r}')\right]_{\mathbf{r}'\uparrow\downarrow\mathbf{r}'^W}\right\}.
\end{aligned} \tag{13}$$

In (13) we defined the following limiting procedure

$$\left[\nabla_{\mathbf{r}'} G_z^0(\mathbf{r}''^W,\mathbf{r}')\right]_{\mathbf{r}'\uparrow\downarrow\mathbf{r}'^W} = \tfrac{1}{2}\left[\nabla_{\mathbf{r}'} G_z^0(\mathbf{r}''^W,\mathbf{r}')\right]_{\mathbf{r}'\to\mathbf{r}'^W} + \tfrac{1}{2}\left[\nabla_{\mathbf{r}'} G_z^0(\mathbf{r}''^W,\mathbf{r}')\right]_{\mathbf{r}'\to\mathbf{r}'^{W\,\mathrm{ex}}}, \tag{14}$$

that is, an average of two limits: one coming from the inside and one coming from the outside of the system. The piece between curly brackets in (13) only contributes if $\mathbf{r}''^W \simeq \mathbf{r}'^W$, because the two terms cancel otherwise. Therefore, we can take the factors with derivatives of G_z out of the integral. Subsequently, one may use the asymptotic formula

$$G_z^0(\mathbf{r},\mathbf{r}') \simeq \frac{m}{\pi\hbar^2}\log|\mathbf{r}-\mathbf{r}'| \tag{15}$$

for the infinite-domain Green function for small $|\mathbf{r}-\mathbf{r}'|$, which follows from (6). In this way one finds that the piece between brackets reduces to $-(m/\hbar^2)\mathbf{n}'\cdot\left[\nabla_{\mathbf{r}'}G_z(\mathbf{r},\mathbf{r}')\right]_{\mathbf{r}'\to\mathbf{r}'^W}$. Consequently, (13) reduces to

$$\mathbf{n}'\cdot\left[\nabla_{\mathbf{r}'}G_z(\mathbf{r},\mathbf{r}')\right]_{\mathbf{r}'\to\mathbf{r}'^W}=2\mathbf{n}'\cdot\left[\nabla_{\mathbf{r}'}G^0_z(\mathbf{r},\mathbf{r}')\right]_{\mathbf{r}'\to\mathbf{r}'^W}$$
$$-\frac{\hbar^2}{m}\int_{\partial D}d\sigma''^W\mathbf{n}''\cdot\left[\nabla_{\mathbf{r}''}G_z(\mathbf{r},\mathbf{r}'')\right]_{\mathbf{r}''\to\mathbf{r}''^W}\mathbf{n}'\cdot\left[\nabla_{\mathbf{r}'}G^0_z(\mathbf{r}''^W,\mathbf{r}')\right]_{\mathbf{r}'\uparrow\downarrow\mathbf{r}'^W}. \qquad (16)$$

One can solve this equation iteratively for $\mathbf{n}'\cdot\left[\nabla_{\mathbf{r}'}G_z(\mathbf{r},\mathbf{r}')\right]_{\mathbf{r}'\to\mathbf{r}'^W}$. The solution in its turn can be substituted in (12) so as to get a (formal) expression for the Green function of the confined system in terms of the infinite-domain Green function. The expression found in this way can be understood as a multiple-reflection expansion for the Green function of the confined system.

The multiple-reflection expansion for the Green function has been discussed extensively in [15] for the case of a free-particle system without a magnetic field. In particular, both the leading term and the higher-order terms of the multiple-reflection expansion are analyzed in detail in that paper. It is shown that for a (nearly) planar boundary the leading term is by far the most important, whereas the higher-order terms contribute for curved boundaries only. These findings are taken over as such in [10], where a magnetized free-particle system is considered. Once again only the first term in the iteration is taken into account, while the higher-order terms are assumed to be negligible for almost planar boundaries. However, as mentioned already in the introduction of the present paper, it is not obvious that these higher-order terms can be thrown away for a magnetized system as well. Indeed, because the particles follow curved trajectories, they can scatter several times off the same boundary, so that the multiple-reflection argument in [10] may break down. For that reason we will keep all terms in the expansion for the time being.

Let us consider the correction part G^c_z of the Green function for the case of a half-space geometry $x\geq 0$ with a boundary located at $x=0$. In this geometry (12) can be written as

$$G^c_z(\mathbf{r},\mathbf{r}')=\frac{\hbar^2}{2m}\int_{-\infty}^{\infty}dy''\left[\frac{\partial G_z(\mathbf{r},\mathbf{r}'')}{\partial x''}\right]_{x''\to 0}G^0_z(\mathbf{r}''^W,\mathbf{r}'), \qquad (17)$$

with $\mathbf{r}''^W=(0,y'')$. Furthermore, one can write (16) as

$$\left[\frac{\partial G_z(\mathbf{r},\mathbf{r}')}{\partial x'}\right]_{x'\to 0}=2\left[\frac{\partial G^0_z(\mathbf{r},\mathbf{r}')}{\partial x'}\right]_{x'\to 0}+\frac{\hbar^2}{m}\int_{-\infty}^{\infty}dy''\left[\frac{\partial G_z(\mathbf{r},\mathbf{r}'')}{\partial x''}\right]_{x''\to 0}\left[\frac{\partial G^0_z(\mathbf{r}''^W,\mathbf{r}')}{\partial x'}\right]_{x'\uparrow\downarrow 0}. \qquad (18)$$

We may now use the fact that the Green functions are all translation invariant in the y-direction and introduce the Fourier representation

$$G_z(\mathbf{r},\mathbf{r}')=\int_{-\infty}^{\infty}dk\,e^{ik(y-y')}G_z(k,x,x'). \qquad (19)$$

In this representation we can solve (17) and (18) algebraically. The result is

$$G^c_z(k,x,x')=\frac{2\pi\hbar^2}{m}\left[\frac{\partial G^0_z(k,x,x'')}{\partial x''}\right]_{x''\to 0}\left\{1-\frac{2\pi\hbar^2}{m}\left[\frac{\partial G^0_z(k,0,x'')}{\partial x''}\right]_{x''\uparrow\downarrow 0}\right\}^{-1}G^0_z(k,0,x'). \quad (20)$$

To evaluate (20) we have to insert an explicit expression for $G_z^0(k,x,x')$. It can be found either by solving (6) directly, or by using (5). In both ways we find that the infinite-domain Green function can be expressed in terms of parabolic cylinder functions [5], [17]

$$G_z^0(k,x,x') = -\sqrt{\frac{m}{4\pi^3\hbar^3\omega_c}}\Gamma(-\bar{z}+\tfrac{1}{2})D_{\bar{z}-1/2}(\sqrt{2}(\bar{x}-\bar{k}))D_{\bar{z}-1/2}(-\sqrt{2}(\bar{x}'-\bar{k})), \tag{21}$$

for $x > x'$, and

$$G_z^0(k,x,x') = -\sqrt{\frac{m}{4\pi^3\hbar^3\omega_c}}\Gamma(-\bar{z}+\tfrac{1}{2})D_{\bar{z}-1/2}(-\sqrt{2}(\bar{x}-\bar{k}))D_{\bar{z}-1/2}(\sqrt{2}(\bar{x}'-\bar{k})), \tag{22}$$

for $x < x'$. Here we introduced the abbreviations $\bar{z} = z/\hbar\omega_c$, $\bar{x} = (m\omega_c/\hbar)^{1/2}x$ and $\bar{k} = (\hbar/m\omega_c)^{1/2}k$.

If we substitute these formulae into (20) we arrive at the following expression for the correction part of the Green function

$$G_z^c(k,x,x') = \sqrt{\frac{m}{4\pi^3\hbar^3\omega_c}}\Gamma(-\bar{z}+\tfrac{1}{2})\frac{D_{\bar{z}-1/2}(\sqrt{2}\bar{k})}{D_{\bar{z}-1/2}(-\sqrt{2}\bar{k})}D_{\bar{z}-1/2}(\sqrt{2}(\bar{x}-\bar{k}))D_{\bar{z}-1/2}(\sqrt{2}(\bar{x}'-\bar{k})), \tag{23}$$

which is valid for all non-negative x and x'. Adding this result to either (21) or (22) one obtains the complete Green function for the confined system.

The complete Green function for the confined system can also be found directly by solving (6) with the appropriate boundary conditions for the half-space geometry [5]. In this way one arrives at the same result as above, so that (23) is checked independently. This check is useful in assessing the validity of a truncated version of the multiple-reflection expansion for a system with a planar boundary. Indeed, in deriving (23) from (20) it was essential to take into account the full expression between the curly brackets in (20). Using a truncated form, for instance by throwing away the partial derivative (which amounts to using the leading order in the multiple-reflection expansion), would have led to a completely different result for the correction part of the Green function. Hence, it must be concluded that the use of a truncated version of the multiple-reflection expansion for a magnetized free-particle system is not justified, not even for a planar-boundary geometry.

3 The finite-domain correction to the temperature Green function

If the temperature is sufficiently high, degeneracy effects play no role. In that case all space-dependent properties of the system, like the profiles of the particle density or the electric current density, follow directly from the temperature Green function. In this section we shall derive the general form of the finite-domain correction to the temperature Green function.

The infinite-domain temperature Green function is [2]

$$G_\beta^0(\mathbf{r},\mathbf{r}') = \frac{m\omega_c}{4\pi\hbar\sinh(\beta\hbar\omega_c/2)}\exp\Big[-\frac{m\omega_c}{4\hbar}(\mathbf{r}-\mathbf{r}')^2\coth(\beta\hbar\omega_c/2)+\frac{im\omega_c}{2\hbar}(x+x')(y-y')\Big]. \tag{24}$$

Using (8) and (9) we can write (20) as:

$$G^c_\beta(k,x,x') = -\frac{2\pi\hbar^2}{m}\int_0^\beta d\tau\int_0^\tau d\tau'\left[\frac{\partial G^0_\tau(k,x,x'')}{\partial x''}\right]_{x''=0} T_{\tau'}(k)G^0_{\beta-\tau-\tau'}(k,0,x'), \tag{25}$$

where $T_\tau(k)$ is given by

$$\begin{aligned} T_\tau(k) &= 2\delta(\tau) - \frac{2\pi\hbar^2}{m}\left[\frac{\partial G^0_\tau(k,0,x')}{\partial x'}\right]_{x'=0} \\ &+ \left(\frac{2\pi\hbar^2}{m}\right)^2\int_0^\tau d\tau'\left[\frac{\partial G^0_{\tau'}(k,0,x')}{\partial x'}\right]_{x'=0}\left[\frac{\partial G^0_{\tau-\tau'}(k,0,x')}{\partial x'}\right]_{x'=0} - \cdots . \end{aligned} \tag{26}$$

The delta function is multiplied by a factor 2 to compensate for the fact that it is non-zero precisely at the edge of the integration area.

Inserting (24) and transforming back to real space we find the correction part of the temperature Green function as a multiple-reflection series

$$G^c_\beta(\mathbf{r},\mathbf{r}') = \sum_{n=1}^\infty G^{(n)}_\beta(\mathbf{r},\mathbf{r}'), \tag{27}$$

where $G^{(n)}_\beta(\mathbf{r},\mathbf{r}')$ is a multiple integral over τ's:

$$\begin{aligned} G^{(n)}_\beta(\mathbf{r},\mathbf{r}') &= (-1)^n\frac{m\omega_c^2}{16\pi^{3/2}}\Big(\frac{\hbar\omega_c}{2\pi^{1/2}}\Big)^{n-1}\int_0^\beta d\tau_1\cdots\int_0^\beta d\tau_n\,\Theta(\tau_{n+1}) \\ &\times f^{(n)}_{\beta,\tau_1,\ldots,\tau_{n+1}}(\mathbf{r},\mathbf{r}')\exp\Big[g^{(n)}_{\beta,\tau_1,\ldots,\tau_{n+1}}(\mathbf{r},\mathbf{r}')\Big]. \end{aligned} \tag{28}$$

We defined $\tau_{n+1}\equiv\beta-\tau_1-\cdots-\tau_n$. Moreover, Θ denotes the Heaviside step function. The functions f and g are given by

$$\begin{aligned} f^{(n)}_{\beta,\tau_1,\ldots,\tau_{n+1}}(\mathbf{r},\mathbf{r}') &= \frac{1}{t_1}\Big(\prod_{i=1}^{n+1}\frac{t_i^{3/2}}{s_i}\Big)\Big(\sum_{i=1}^{n+1}t_i\Big)^{-(n+1)/2} \\ &\times\Bigg\{2(\tfrac12)_{n/2}\delta_{n,\mathrm{even}} + \sum_{p=0}^{[(n-1)/2]}\frac{(\frac12)_p}{2^{n-2p-1}}\Big(\sum_{i=1}^{n+1}t_i\Big)^{p-n/2}\Big(\frac{m\omega_c}{\hbar}\Big)^{n/2-p} \\ &\times(t_2x+t_1x'+i(y-y'))^{n-2p-1}\Bigg[(t_2^{-2}-1)\Big(\sum_{i=1}^{n+1}t_i\Big)\binom{n-1}{2p}x \\ &+\binom{n}{2p}(t_2x+t_1x'+i(y-y'))\Bigg]\Bigg\}, \end{aligned} \tag{29}$$

and

$$\begin{aligned} g^{(n)}_{\beta,\tau_1,\ldots,\tau_{n+1}}(\mathbf{r},\mathbf{r}') &= \frac{m\omega_c}{4\hbar}\Bigg\{\Big(\sum_{i=1}^{n+1}t_i\Big)^{-1}[t_2x+t_1x'+i(y-y')]^2 \\ &-\Big[(t_2+t_2^{-1})x^2+(t_1+t_1^{-1})x'^2\Big]\Bigg\}, \end{aligned} \tag{30}$$

where we defined $t_i \equiv \tanh(\tau_i \hbar\omega_c/2)$ and $s_i \equiv \sinh(\tau_i \hbar\omega_c/2)$. Furthermore, $(a)_n$ denotes the Pochhammer symbol and $[x]$ is the entier function.

One way to look at the series (27) with (28) is to interpret it as an expansion of the correction part of the temperature Green function in powers of the cyclotron frequency. Indeed, for increasing n the terms $G_\beta^{(n)}(\mathbf{r},\mathbf{r}')$ in the expansion are of growing order in ω_c. For $\mathbf{r}=\mathbf{r}'$ one has for example

$$G_\beta^{(n)}(\mathbf{r},\mathbf{r}) = \begin{cases} \mathcal{O}(\omega_c^{n-1}), & n \text{ odd;} \\ \mathcal{O}(\omega_c^{n}), & n \text{ even.} \end{cases} \tag{31}$$

4 Calculation of profiles for the nondegenerate case

As already stated in the previous section, we can use the temperature Green function to calculate the spatial dependence of physical properties near the boundary of the system. In fact, we can derive a series expansion in the cyclotron frequency for the profiles of physical observables, like the particle density, the electric current density or the pressure tensor.

We start with the density profile, which is obtained from the temperature Green function as

$$n(x) = \frac{n}{Z_\perp^{(0)}} G_\beta(\mathbf{r},\mathbf{r}), \tag{32}$$

where $Z_\perp^{(0)}$ is the transverse part of the partition function per unit of surface for the non-confined system

$$Z_\perp^{(0)} = \frac{m}{2\pi\beta\hbar^2} \frac{\beta\hbar\omega_c/2}{\sinh(\beta\hbar\omega_c/2)}. \tag{33}$$

In order to calculate the density profile up to second order in the cyclotron frequency, we have to evaluate, according to (31), the terms of first, second and third order in the multiple-reflection expansion (27). By expanding the first-order term up to ω_c^2 we get

$$n^{(1)}(x) = -\frac{n\beta^2\xi}{4\sqrt{\pi}} \int_0^\beta d\tau \, \frac{1}{[\tau(\beta-\tau)]^{3/2}} \left[1 + \tfrac{1}{8}\hbar^2\omega_c^2\tau(\beta-\tau) - \tfrac{1}{48}\beta^2\hbar^2\omega_c^2\xi^2\right] \exp\left[-\tfrac{1}{4}\frac{\beta^2}{\tau(\beta-\tau)}\xi^2\right], \tag{34}$$

with $\xi^2 := 2mx^2/(\beta\hbar^2)$. This is a sum of integrals of type (A1), which can be expressed in terms of Whittaker functions, as is explained in the appendix. In this way we get

$$n^{(1)}(x) = -\frac{n}{\sqrt{\xi}}(1 - \tfrac{1}{48}\beta^2\hbar^2\omega_c^2\xi^2)e^{-\xi^2/2}W_{\frac{1}{4},\frac{1}{4}}(\xi^2) - \tfrac{1}{32}n\beta^2\hbar^2\omega_c^2\sqrt{\xi}e^{-\xi^2/2}W_{-\frac{1}{4},\frac{1}{4}}(\xi^2). \tag{35}$$

Note that we find contributions of order ω_c^0 and order ω_c^2.

The $n=2$ and $n=3$ terms in the multiple-reflection expansion (27) are both of order ω_c^2, as follows from (31). Hence, in evaluating these terms by starting from (29) and (30) only the leading terms of s_i and t_i in powers of the cyclotron frequency have to be retained. For $n=2$ we find

$$n^{(2)}(x) = \frac{n\hbar^2\omega_c^2}{16\pi\sqrt{\beta}} \int_0^\beta d\tau_1 \int_0^{\beta-\tau_1} d\tau_2 \, \frac{(\beta-\tau_1-\tau_2)^{1/2}(\tau_1+\tau_2)}{(\tau_1\tau_2)^{1/2}} \left(1 + \tfrac{1}{2}\beta\frac{\tau_1+\tau_2}{\tau_1\tau_2}\xi^2\right) \times \exp\left(-\tfrac{1}{4}\beta\frac{\tau_1+\tau_2}{\tau_1\tau_2}\xi^2\right). \tag{36}$$

The integration over τ_2, at fixed $\tau_1 + \tau_2$, can be performed with the use of (A1)–(A6). The result contains an error function, which can be eliminated by partial integration. The ensuing integral can be carried out with the help of (A7), with the result

$$n^{(2)}(x) = \frac{n\beta^2\hbar^2\omega_c^2}{32\sqrt{\xi}} e^{-\xi^2/2}\Big[6W_{-\frac{11}{4},\frac{1}{4}}(\xi^2) - 5W_{-\frac{7}{4},\frac{1}{4}}(\xi^2) + 2W_{-\frac{3}{4},\frac{1}{4}}(\xi^2)\Big]. \tag{37}$$

Finally, we consider the $n = 3$ term. In order ω_c^2 we find

$$n^{(3)}(x) = -\frac{n\hbar^2\omega_c^2\xi}{16\pi^{3/2}} \int_0^\beta d\tau_1 \int_0^{\beta-\tau_1} d\tau_2 \int_0^{\beta-\tau_1-\tau_2} d\tau_3\, \frac{\sqrt{\tau_3}(\beta - \tau_1 - \tau_2 - \tau_3)^{1/2}}{\sqrt{\tau_1}\tau_2^{3/2}} \times \exp\!\left(-\tfrac{1}{4}\beta\frac{\tau_1 + \tau_2}{\tau_1\tau_2}\xi^2\right). \tag{38}$$

The integration over τ_3 is trivial, and the rest of the steps are similar to the $n = 2$ case. We end up with

$$n^{(3)}(x) = -\frac{n\beta^2\hbar^2\omega_c^2}{32\sqrt{\xi}} e^{-\xi^2/2} W_{-\frac{11}{4},\frac{1}{4}}(\xi^2). \tag{39}$$

If we now collect all the terms, and evaluate the Whittaker functions using their recursion relations, we get the following expression for the density profile up to second order in the cyclotron frequency

$$n(x) = n(1 - e^{-\xi^2}) + \tfrac{1}{24} n\beta^2\hbar^2\omega_c^2\xi^4\Big[e^{-\xi^2} - \sqrt{\pi}\,\xi \mathrm{Erfc}(\xi)\Big]. \tag{40}$$

In the same manner we can calculate the y-component of the current profile

$$J^y(x) = \frac{n}{Z_\perp^{(0)}}\frac{e\hbar}{2mi}\left[\frac{\partial}{\partial y}G_\beta(\mathbf{r},\mathbf{r}') - \frac{\partial}{\partial y'}G_\beta(\mathbf{r},\mathbf{r}')\right]_{\mathbf{r}=\mathbf{r}'} - \frac{e^2}{mc}n(x)A^y(\mathbf{r}). \tag{41}$$

Up to first order we get

$$J^y(x) = \frac{en\omega_c\sqrt{\pi}}{4k}\xi^2\mathrm{Erfc}(\xi), \tag{42}$$

where $k \equiv [m/(2\hbar^2\beta)]^{1/2}$.

Finally, the profiles of the components of the pressure tensor follow from

$$P^{ii}(x) = \frac{n}{4mZ_\perp^{(0)}}\Big[(\pi^i - \pi'^i)^2 G_\beta(\mathbf{r},\mathbf{r}')\Big]_{\mathbf{r}=\mathbf{r}'}, \tag{43}$$

(no summation), where we wrote $\boldsymbol{\pi} = \mathbf{p} - (e/c)\mathbf{A}(\mathbf{r})$. After some algebra (43) yields

$$P^{ii}(x) = \frac{n}{\beta}\Big[1 - (1 - \delta_{i,x})e^{-\xi^2}\Big] + \frac{1}{12}n\beta\hbar^2\omega_c^2 F^i(\xi), \tag{44}$$

with

$$F^x(\xi) = 1 - (1 + \xi^2)e^{-\xi^2} + \sqrt{\pi}\,\xi^3\mathrm{Erfc}(\xi), \tag{45}$$

$$F^y(\xi) = 1 - (1 - 4\xi^2 - \tfrac{3}{2}\xi^4)e^{-\xi^2} - 6\sqrt{\pi}\,\xi^3(1 + \tfrac{1}{4}\xi^2)\mathrm{Erfc}(\xi), \tag{46}$$

$$F^z(\xi) = \tfrac{1}{2}\xi^4 e^{-\xi^2} - \tfrac{1}{2}\sqrt{\pi}\,\xi^5\mathrm{Erfc}(\xi). \tag{47}$$

The results (40), (42) and (44) agree with those obtained before via a direct perturbation method [16]. The present method is less complicated in the technical details. Moreover, it can be generalized easily to include higher-order terms in the cyclotron frequency and to describe systems with other geometries.

From the present formalism it is straightforward to analyze the finite-size corrections to the transverse partition function for a system in a slab geometry, that is, for a system which is confined between two walls at $x = 0$ and $x = L$. The transverse part of the partition function can be found from the temperature Green function $G_\beta(\mathbf{r}, \mathbf{r})$ by integration:

$$Z_\perp = \frac{1}{L} \int_0^L dx \, G_\beta(\mathbf{r}, \mathbf{r}), \tag{48}$$

where $G_\beta(\mathbf{r}, \mathbf{r})$ is now the temperature Green function for the system in a slab geometry. This Green function follows from the half-space Green function by adding terms with x replaced by $L - x$. The $n = 1$ contribution to $Z_\perp$ can be found from (28)–(30). One gets after integration over x:

$$Z_\perp^{(1)} = -\frac{k}{2^{5/2}\pi^{3/2}\beta L} \frac{(\beta\hbar\omega_c)^{3/2}}{[\sinh(\beta\hbar\omega_c/2)]^{1/2}} \int_0^\beta d\tau \, \frac{1}{[\sinh(\tau\hbar\omega_c/2)\sinh((\beta - \tau)\hbar\omega_c/2)]^{1/2}}. \tag{49}$$

By introducing the variable $z = \tanh(\tau\hbar\omega_c/4)$, we can write the integrand in an algebraic form. One gets

$$Z_\perp^{(1)} = -\frac{k}{2\pi^{3/2}L} (\beta\hbar\omega_c)^{1/2} \frac{(1 - t^2)K(t)}{\sqrt{t}}, \tag{50}$$

where $K(t)$ is the complete elliptic integral of the first kind [17], and where we introduced the variable $t = \tanh(\beta\hbar\omega_c/4)$. The result (50) differs from that in [10], where the lowest-order term (with $n = 1$) in the multiple-reflection expansion of the transverse partition function is approximated by making some additional assumptions about its behaviour.

After expanding in terms of ω_c one finds from (33) and (50) that up to second order in ω_c the sum of the $n = 0$ and the $n = 1$ parts of the partition function can be written as

$$Z_\perp^{(0+1)} = Z_\perp^{(0)} \Big[1 - \frac{\sqrt{\pi}}{2kL} (1 + \tfrac{1}{192}\beta^2\hbar^2\omega_c^2) \Big] + \mathcal{O}(\omega_c^4/L). \tag{51}$$

As we have seen above, the $n = 1$ term is not sufficient to evaluate the finite-system correction to the Green function and to the partition function, if a magnetic field is present. Indeed, to obtain the complete finite-size correction of the partition function in second order in the cyclotron frequency one has to calculate the $n = 2$ and $n = 3$ contributions as well. The fastest way to arrive at the result is by substituting (32), (37) and (39) in (48). One finds

$$Z_\perp = Z_\perp^{(0)} \Big[1 - \frac{\sqrt{\pi}}{2kL} (1 - \tfrac{1}{192}\beta^2\hbar^2\omega_c^2) \Big] + \mathcal{O}(\omega_c^4/L). \tag{52}$$

This agrees with the results found in [6], [7] and [16]. However, it differs from (51). Thus, it becomes obvious once again that it is essential to take the higher-order terms in the multiple-reflection expansion into account, even if the boundaries are flat.

Appendix

In order to calculate the profiles we need to evaluate integrals of the form

$$I_{\mu,\nu} = \int_0^\beta d\tau\, \tau^\mu (\beta-\tau)^\nu \exp\Big(-\frac{a^2}{\tau(\beta-\tau)}\Big), \tag{A1}$$

where μ and ν are half-integral. Introducing $x = \beta^2/4\tau(\beta-\tau)$ and using the relation

$$\Big(1-\sqrt{\frac{x-1}{x}}\Big)^n + \Big(1+\sqrt{\frac{x-1}{x}}\Big)^n = 2\,x^{-n/2}T_{|n|}(\sqrt{x}), \tag{A2}$$

where T_n are the Chebyshev polynomials of the first kind, we can rewrite the integral (A1) as

$$I_{\mu,\nu} = \Big(\frac{\beta}{2}\Big)^{\mu+\nu+1} \int_1^\infty dx\, \frac{1}{(x-1)^{1/2} x^{(\mu+\nu+3)/2}} T_{|\mu-\nu|}(\sqrt{x}) \exp\Big(-\frac{4a^2}{\beta^2}x\Big). \tag{A3}$$

This integral can be written in terms of Whittaker functions by employing the identity [18]

$$\int_1^\infty dx\, \frac{x^{\alpha-1}}{\sqrt{x-1}} \exp(-zx) = z^{-\alpha/2-1/4}\Gamma(\tfrac{1}{2}) \exp(-z/2)\, W_{\alpha/2-1/4,\alpha/2-1/4}(z), \tag{A4}$$

for $z > 0$ and α real. For integer α the Whittaker functions can be expressed in terms of algebraic functions, exponentials and error functions by using their recursion relations [19]. Special cases of the Whittaker functions are

$$W_{\frac{1}{4},\frac{1}{4}}(x) = x^{1/4} e^{-x/2}, \tag{A5}$$

$$W_{-\frac{1}{4},\frac{1}{4}}(x) = \sqrt{\pi}\, x^{1/4} e^{x/2} \mathrm{Erfc}(\sqrt{x}). \tag{A6}$$

These formulae can be used as a starting point for the recursion relations.

Another type of integral that we encounter in the calculation of the profiles can also be written in terms of Whittaker functions [18]:

$$\int_0^\beta d\tau\, \tau^{\mu-1}(\beta-\tau)^{\nu-1} \exp\Big(-\frac{a}{\tau}\Big) = a^{(\mu-1)/2} \beta^{(\mu+2\nu-1)/2} \exp\Big(-\frac{a}{2\beta}\Big)\, \Gamma(\nu)\, W_{(1-\mu-2\nu)/2,\mu/2}(a/\beta), \tag{A7}$$

where β, ν and a are positive. These Whittaker functions can likewise be reduced to algebraic functions, exponentials and error functions, if μ and ν are half-integral.

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