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Boundary Effects in the Pressure of a Confined Magnetized Electron Gas

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The role of boundary effects in the pressure of a magnetized quantum plasma is determined by evaluating the spatial dependence of the mechanical pressure tensor for several simplified model systems, namely for a non-interacting magnetized electron gas in either a slab geometry or in a harmonic confining potential. From the pressure profiles it is shown that the bulk and surface values of the pressure are related in such a way that an earlier result on the difference between the thermodynamic and the mechanical pressure in a magnetized quantum plasma is confirmed.

Key Words: Electron gas, Pressure, Magnetization, Boundary effects

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1 Introduction

In an earlier paper [1] we established a relation between the thermodynamic pressure and the mechanical pressure in a quantum plasma via a scaling technique. It turned out that the thermodynamic pressure, which is defined as the volume derivative of the free energy, and the mechanical pressure, which is the ensemble average of the microscopic pressure tensor, are no longer equivalent for a quantum plasma in the presence of a magnetic field. In particular, the mechanical pressure is no longer isotropic in a magnetic field. This is in contrast to what one expects for fluid systems in general.

In this paper we shall elucidate this result by an explicit evaluation of the local mechanical pressure tensor for a quantum plasma in a magnetic field. In general, this is too complicated a task. Therefore, one has to look for some simplified model system, in which the essential features of the pressure tensor are still present. Since the anisotropy in the mechanical pressure is solely due to its kinetic part we will consider an ideal electron gas, that is, the electrons do not interact with each other. Even then the task we have set ourselves is a tricky one. The anisotropy in the pressure is related to the total magnetization in the system. As is well known one should be very careful when calculating the magnetization in a confined electron gas [2]-[4]. It should be clear beforehand that boundary effects are important, since an overall magnetization can only exist because of surface currents.

The first system we investigate is the ideal non-degenerate magnetized electron gas in a slab. The slab is confined in a direction orthogonal to the magnetic field. The boundary effects near the surfaces of the slab will be calculated via perturbation theory with respect to the strength of the magnetic field. This calculation is similar to that in [5] and [6], although the technical details are considerably more involved. In section 3 we will consider the volume-averaged mechanical pressure and show that it is indeed of the form predicted in [1]. Then we will proceed with the partition function of the confined system. From the partition function one can explicitly find the magnetization. Moreover, a knowledge of the partition function is needed in section 5, where we will calculate the profile of the mechanical pressure near the wall in order to obtain more insight in the boundary effects. In this way one can see the effects of surface currents and obtain a better understanding of how the thermodynamic and mechanical pressure can differ.

The second system we look at is the ideal non-degenerate electron gas in a harmonic confining potential. This system was first considered by Darwin [7] and studied later by Papadopoulos [8] and by Felderhof and Raval [9], among others. The nice feature of this system is that it is exactly solvable. In section 6 it is shown that the volume-averaged pressure again satisfies the predicted relation. Finally, in section 7, we consider the profiles of the mechanical pressure, which are, of course, modified by the harmonic potential.

2 Ideal non-degenerate magnetized electron gas

We consider an ideal electron gas which is confined in a slab by an infinite wall potential of the form

$$V(x) = \begin{cases} 0 & 0 < x < L; \\ \infty & \text{elsewhere.} \end{cases} \tag{1}$$

Periodic boundary conditions will be imposed in the y- and the z-direction. The single-particle Hamiltonian reads

$$H = \frac{\boldsymbol{\pi}^2}{2m} + V(x), \tag{2}$$

with $\boldsymbol{\pi} = \mathbf{p} - (e/c)\mathbf{A}(\mathbf{r})$ the mechanical momentum. We take the magnetic field in the z-direction. It is convenient to use the Landau gauge

$$\mathbf{A}(\mathbf{r}) = (0, Bx, 0). \tag{3}$$

We will consider a gas of non-degenerate electrons, that is, we will use Boltzmann statistics.

The partition function for a single particle is

$$Z = \mathrm{tr}(e^{-\beta H}), \tag{4}$$

where β is the inverse temperature. We will evaluate Z through perturbation theory with respect to the magnetic field [6]. The Hamiltonian can be written as a sum of terms of zeroth, first and second order in the following way

$$H = H_0 + H_1 + H_2, \tag{5}$$

with

$$H_0 = \frac{\mathbf{p}^2}{2m} + V(x), \tag{6}$$

$$H_1 = -\omega_c x p_y, \tag{7}$$

$$H_2 = \tfrac{1}{2} m\omega_c^2 x^2, \tag{8}$$

in which we used the cyclotron frequency $\omega_c = eB/mc$. We can now write the Boltzmann factor up to second order in the cyclotron frequency as

$$e^{-\beta H} = e^{-\beta H_0} - \int_0^\beta d\tau\, e^{-(\beta-\tau)H_0} H_1 e^{-\tau H_0} - \int_0^\beta d\tau\, e^{-(\beta-\tau)H_0} H_2 e^{-\tau H_0} + \int_0^\beta d\tau \int_0^\tau d\tau'\, e^{-(\beta-\tau)H_0} H_1 e^{-(\tau-\tau')H_0} H_1 e^{-\tau' H_0}. \tag{9}$$

The partition function up to second order is

$$Z = Z_0 + Z_2 \tag{10}$$

(note there is no first-order term). The zeroth-order term is trivially calculated to be

$$Z_0 = V\left(\frac{k^2}{\pi}\right)^{\frac{3}{2}}, \tag{11}$$

with V the volume and where we defined $k := (m/2\hbar^2\beta)^{\frac{1}{2}}$. The second-order term can be written as a sum of two contributions

$$Z_2 = Z_{2a} + Z_{2b}, \tag{12}$$

with

$$Z_{2a} = -m\omega_c^2 V \frac{\beta k^2}{2\pi L} \int_0^L dx\, G_\beta(x,x) x^2, \tag{13}$$

$$Z_{2b} = m\omega_c^2 V \frac{k^2}{2\pi L} \int_0^\beta d\tau \int_0^L dx \int_0^L dx'\, G_{\beta-\tau}(x,x') G_\tau(x',x) x x'. \tag{14}$$

In (13) and (14) we already performed the momentum averages. The propagator (or the single-particle density matrix) for a free particle in the slab is

$$G_\beta(x,x') = \frac{k}{\sqrt{\pi}} \sum_{n=-\infty}^{\infty} \left\{ \exp\left[-k^2(x - x' + 2nL)^2\right] - \exp\left[-k^2(x + x' + 2nL)^2\right] \right\}, \tag{15}$$

where the sum over n is due to the repeated reflections from the hard walls.

From the partition function one can find the thermodynamic pressure p in the usual way by differentiation of the free energy with respect to the volume

$$p = \frac{N}{\beta} \frac{\partial}{\partial V} \log\left(\frac{Z}{N}\right). \tag{16}$$

In zeroth order the pressure follows the ideal gas law

$$p_0 = \frac{n}{\beta}. \tag{17}$$

The corrections due to the presence of the magnetic field will be calculated in section 4.

The mechanical pressure is defined as the average of the microscopic kinetic pressure tensor. The single-particle pressure tensor at position $\mathbf{r}_0$ is

$$T^{ij}(\mathbf{r}_0) = \frac{1}{2m}[\pi^i\pi^j\delta(\mathbf{r}_0 - \mathbf{r}) + \delta(\mathbf{r}_0 - \mathbf{r})\pi^j\pi^i]. \tag{18}$$

The mechanical pressure is the ensemble average

$$\mathbf{P}(\mathbf{r}_0) = N\langle\mathbf{T}(\mathbf{r}_0)\rangle. \tag{19}$$

We are not interested in the full dependence of the mechanical pressure on $\mathbf{r}_0$; basically, we are only interested in the dependence on the distance from the walls. Hence, we define the slice average of the mechanical pressure as

$$\tilde{\mathbf{P}}(x_0) = \frac{L}{V}\int dy_0\, dz_0\, \mathbf{P}(\mathbf{r}_0), \tag{20}$$

which in terms of an average over the microscopic pressure tensor reads as

$$\tilde{\mathbf{P}}(x_0) = \frac{nL}{Z}\,\mathrm{tr}\left[e^{-\beta H}\int dy_0\, dz_0\, \mathbf{T}(\mathbf{r}_0)\right], \tag{21}$$

with $n = N/V$. The slice average $\tilde{\mathbf{P}}$ is a diagonal tensor. In general, it will depend on the magnetic field. This dependence can stem from three different origins: the partition function, the Boltzmann factor or the microscopic pressure tensor itself. We will start with the zz-component, then continue with the yy-component and, finally, consider the xx-component.

The component in the direction of z can be written as

$$\tilde{P}^{zz}(x_0) = \frac{nL}{Z}\,\mathrm{tr}\left[e^{-\beta H}\frac{p_z^2}{m}\delta(x - x_0)\right]. \tag{22}$$

In zeroth order the average over the momenta is easily performed, resulting in

$$\tilde{P}_0^{zz}(x) = \frac{n\sqrt{\pi}}{\beta k}G_\beta(x, x). \tag{23}$$

We see that the pressure profile is determined by the propagator; in fact, if we consider L to be large compared to k^{-1}, we can write the pressure profile for small x as

$$\tilde{P}_0^{zz}(x) = \frac{n}{\beta}\left[1 - \exp(-4k^2x^2)\right]. \tag{24}$$

So, there is a rapid change of the pressure over a distance of the order of the thermal wavelength: at the wall one has $\tilde{P}_0^{zz}(x) = 0$, but in the bulk one has $\tilde{P}_0^{zz}(x) = p_0$.

In a non-zero magnetic field the slice-averaged pressure changes. This is due to the change in the partition function and due to the second-order terms in the Boltzmann factor. We can write the second-order term as

$$\tilde{P}_2^{zz} = \tilde{P}_{2a}^{zz} + \tilde{P}_{2b}^{zz} + \tilde{P}_{2c}^{zz}, \tag{25}$$

with

$$\tilde{P}_{2a}^{zz}(x) = -\frac{n\sqrt{\pi}}{\beta k}\frac{Z_2}{Z_0} G_\beta(x,x), \tag{26}$$

$$\tilde{P}_{2b}^{zz}(x) = -\frac{n\sqrt{\pi}}{2\beta k} m\omega_c^2 \int_0^\beta d\tau \int_0^L dx'\, G_{\beta-\tau}(x,x')G_\tau(x',x)x'^2, \tag{27}$$

$$\begin{aligned}\tilde{P}_{2c}^{zz}(x) = \frac{n\sqrt{\pi}}{\beta^2 k} m\omega_c^2 \int_0^\beta d\tau \int_0^\tau d\tau' \int_0^L dx' \int_0^L dx''\, G_{\beta-\tau}(x,x') \\ \times G_{\tau-\tau'}(x',x'')G_{\tau'}(x'',x)x'x''.\end{aligned} \tag{28}$$

The evaluation of these terms will be presented in section 5.

Next we consider the yy-component of the slice-averaged pressure tensor. In zeroth order the result is identical to the zz-component, i.e.,

$$\tilde{P}_0^{yy}(x) = \tilde{P}_0^{zz}(x). \tag{29}$$

Several of the second-order terms are (nearly) the same as (26)-(28), but there are also additional terms due to the fact that π_y depends on B. If we write the second-order contribution in a way analogous to (25), the result is

$$\tilde{P}_{2i}^{yy}(x) = \tilde{P}_{2i}^{zz}(x), \qquad (i = a, b), \tag{30}$$

$$\tilde{P}_{2c}^{yy}(x) = 3\tilde{P}_{2c}^{zz}(x), \tag{31}$$

$$\tilde{P}_{2d}^{yy}(x) = \frac{n\sqrt{\pi}}{k} m\omega_c^2 x^2 G_\beta(x,x), \tag{32}$$

$$\tilde{P}_{2e}^{yy}(x) = -\frac{2n\sqrt{\pi}}{\beta k} m\omega_c^2 x \int_0^\beta d\tau \int_0^L dx'\, G_{\beta-\tau}(x,x')G_\tau(x',x)x'. \tag{33}$$

Again, we will calculate these terms in section 5.

Finally, we will consider the xx-component of the slice-averaged pressure. It is more complicated to evaluate, because both p_x and $\delta(x - x_0)$ occur in the ensemble average. Therefore, we employ a different method. It makes use of the equation of motion, which yields

$$\nabla \cdot \mathbf{P}(\mathbf{r}) = c^{-1}\langle \mathbf{J}(\mathbf{r})\rangle \wedge \mathbf{B}, \tag{34}$$

where $\langle \mathbf{J}(\mathbf{r})\rangle$ is the ensemble average of the electric current density

$$\langle \mathbf{J}(\mathbf{r}_0)\rangle = \frac{Ne}{2m}\langle \boldsymbol{\pi}\delta(\mathbf{r}-\mathbf{r}_0) + \delta(\mathbf{r}-\mathbf{r}_0)\boldsymbol{\pi}\rangle. \tag{35}$$

Taking the slice average of (34), we get

$$\frac{\partial}{\partial x}\tilde{P}^{xx}(x) = c^{-1}\tilde{J}^{y}(x)B, \tag{36}$$

where $\tilde{J}$ is the slice average of the current density.

From (36) it follows that in zeroth order the pressure is independent of x. Since the pressure in the bulk in zeroth order is isotropic, one has

$$\tilde{P}_0^{xx} = \frac{n}{\beta}. \tag{37}$$

Note that there is no profile.

For non-zero magnetic field, one needs the slice-averaged current in first order. We write

$$\tilde{J}^{y}_{1}(x) = \tilde{J}^{y}_{1a}(x) + \tilde{J}^{y}_{1b}(x), \tag{38}$$

with

$$\tilde{J}^{y}_{1a}(x) = -\frac{n\sqrt{\pi}e}{k}\omega_c x G_\beta(x,x), \tag{39}$$

$$\tilde{J}^{y}_{1b}(x) = \frac{n\sqrt{\pi}e}{\beta k}\omega_c \int_0^\beta d\tau \int_0^L dx'\, G_{\beta-\tau}(x,x')G_\tau(x',x)x'. \tag{40}$$

Again, the evaluation of these expressions will be considered in section 5. By integrating (36) one gets $\tilde{P}_2^{xx}$. The integration constant is fixed, since in the *bulk* one has

$$\tilde{P}_2^{xx}(x) = \tilde{P}_2^{yy}(x), \tag{41}$$

as can be inferred from cylinder symmetry.

In view of the interpretation of the results in sections 3–5 it is useful to consider the density as well. The slice-averaged density is given by

$$\tilde{n}(x_0) = \frac{nL}{Z}\,\mathrm{tr}\left[e^{-\beta H}\delta(x-x_0)\right]. \tag{42}$$

Comparison with (22) yields, after momentum averaging, the simple relation

$$\tilde{P}^{zz}(x) = \frac{1}{\beta}\tilde{n}(x). \tag{43}$$

In particular, the zeroth-order term can be read off from (24):

$$\tilde{n}_0(x) = n\left[1 - \exp(-4k^2x^2)\right]. \tag{44}$$

For non-vanishing magnetic fields the density can be found from (26)-(28).

3 Bulk value of the mechanical pressure

In this section we will calculate the bulk value of the mechanical pressure. This follows from taking the volume average, or alternatively, from performing the integral over x (and dividing by L):

$$\overline{\mathbf{P}} = \frac{1}{L}\int_0^L dx\, \tilde{\mathbf{P}}(x). \tag{45}$$

The zz-component trivially follows from (22) to be

$$\overline{P}^{zz} = \frac{n}{\beta}, \tag{46}$$

and is independent of the field. Of course, the density can be found from (42) in the same manner, leading to the trivial statement $\overline{n} = n$.

The calculation of the yy-component is more complicated. One should use

$$\frac{1}{L}\int_0^L dx\, G_\beta(x,x) = \frac{k}{\sqrt{\pi}}, \tag{47}$$

$$\int_0^L dx'\, G_{\beta-\tau}(x,x')G_\tau(x',x'') = G_\beta(x,x''). \tag{48}$$

From (30)-(33) one then finds, up to second order in the magnetic field

$$\begin{aligned}\overline{P}^{yy} &= \frac{n}{\beta}\Big(1-\frac{Z_2}{Z_0}\Big) + m\omega_c^2\frac{n\sqrt{\pi}}{2k}\frac{1}{L}\int_0^L dx\, G_\beta(x,x)x^2 \\ &\quad - m\omega_c^2\frac{n\sqrt{\pi}}{2\beta k}\frac{1}{L}\int_0^\beta d\tau\int_0^L dx\int_0^L dx'\, G_{\beta-\tau}(x,x')G_\tau(x',x)xx'.\end{aligned} \tag{49}$$

Comparison with (13)-(14) yields

$$\overline{P}^{yy} = \frac{n}{\beta}\Big(1-\frac{2Z_2}{Z_0}\Big). \tag{50}$$

We can write $\overline{P}^{yy}$ in terms of $\overline{M}$, the average magnetization per unit of volume. The latter directly follows from the partition function by differentiation with respect to the magnetic field

$$\overline{M} = \frac{n}{\beta}\frac{\partial}{\partial B}\log Z = \frac{2n}{\beta B}\frac{Z_2}{Z_0}, \tag{51}$$

where the last equality is valid up to second order. Hence, by comparison to (50), we can write

$$\overline{P}^{yy} = \frac{n}{\beta} - B\overline{M}. \tag{52}$$

Finally, the xx-component of the pressure tensor can be found by using cylinder symmetry, so that one has $\overline{P}^{xx} = \overline{P}^{yy}$. Thus the bulk mechanical pressure tensor can be written as

$$\overline{\mathbf{P}} = p_0\mathbf{U} - B\overline{M}\,(\mathbf{U} - \hat{\mathbf{B}}\hat{\mathbf{B}}), \tag{53}$$

where we used (17). We see that the bulk value of the mechanical pressure tensor in second order of the magnetic field is anisotropic: it consists of an isotropic part which is related to the thermodynamic pressure in zeroth order, and an anisotropic part that is determined by the volume-averaged magnetization. Since the thermodynamic pressure up to second-order is given by the zeroth-order term, as we shall see in section 4, this confirms our earlier (general) result, found by scaling arguments [1]. For an infinite ideal non-degenerate magnetized electron gas similar results have been obtained before in [10] and [11]. More insight can be obtained by considering the pressure profiles near the wall. These will be evaluated in section 5. But first we will calculate the partition function, since it will be needed for the pressure profiles.

4 The partition function

In this section we will evaluate the partition function for the electron gas in a slab up to second order in the magnetic field. We will present the calculation in some detail, since the same method will be used in the next section for the evaluation of the pressure profiles.

The second-order terms were given in (13)-(14) as integrals over the propagator. The contribution from Z_{2a} is simple; if the thickness L of the slab is much larger than the thermal wavelength, we get

$$Z_{2a} = -m\omega_c^2 V \frac{\beta k^3}{2\pi^{\frac{3}{2}} L}\int_0^L dx\, x^2\left[1 - e^{-4k^2x^2} - e^{-4k^2(L-x)^2}\right]. \tag{54}$$

For Z_{2b} one needs to evaluate

$$\mathcal{I}_\beta(x,x') = \int_0^\beta d\tau \int_0^L dx''\, G_{\beta-\tau}(x,x'')G_\tau(x'',x')x'', \tag{55}$$

for $x = x'$. However, in view of (28) we will consider the integral for general $x \neq x'$. Inserting (15) and performing the (Gaussian) integral over x'' yields

$$\mathcal{I}_\beta(x,x') = \frac{\beta}{2\sqrt{\pi}} \sum_{\lambda,\lambda'=\pm 1}\ \sum_{n,n'=-\infty}^{\infty} (-1)^{\frac{1}{2}(\lambda+\lambda')+1}\, \overline{\mathcal{I}}_\beta(\zeta_{n\lambda},\zeta'_{n'\lambda'}), \tag{56}$$

with $\zeta_{n\lambda} = k(\lambda x + 2nL)$ and a similar definition for $\zeta'_{n\lambda}$, with x replaced by x'. Furthermore, we introduced the dimensionless integral

$$\overline{\mathcal{I}}_\beta(\zeta,\zeta') = e^{-(\zeta-\zeta')^2}\beta^{-2}\int_0^\beta d\tau\,[\zeta(\beta-\tau)+\zeta'\tau]$$
$$\times\left\{\mathrm{Erf}\left(\frac{[\zeta(\beta-\tau)+\zeta'\tau]}{[\tau(\beta-\tau)]^{\frac{1}{2}}}\right) - \mathrm{Erf}\left(\frac{[(\zeta+kL)(\beta-\tau)+(\zeta'+kL)\tau]}{[\tau(\beta-\tau)]^{\frac{1}{2}}}\right)\right\}. \tag{57}$$

The sums over n and n' in (56) converge fast, since $\overline{\mathcal{I}}_\beta(\zeta,\zeta')$ quickly goes to 0 if $|\zeta|$ and/or $|\zeta'|$ go to infinity. We can evaluate $\overline{\mathcal{I}}_\beta(\zeta,\zeta')$ by partial integration; we write

$$[\zeta(\beta-\tau)+\zeta'\tau]d\tau = d[\tfrac{1}{2}\tau^2(-\zeta+\zeta')+\zeta\beta\tau-\tfrac{1}{4}(\zeta+\zeta')\beta^2], \tag{58}$$

where we have chosen the integration constant such that the right-hand side of (58) is antisymmetric for $\tau\leftrightarrow\beta-\tau$ and $\zeta\leftrightarrow\zeta'$. Only a few values of n and n' contribute to the sum in (56) for a thick slab with $kL\gg 1$. As a result we get

$$\begin{aligned}\mathcal{I}_\beta(x,x') = {} & \frac{\beta}{2\sqrt{\pi}}k(x+x')\left[e^{-k^2(x-x')^2}-e^{-k^2(x+x')^2}-e^{-k^2((L-x)+(L-x'))^2}\right]\\ & +\frac{\beta}{\pi}k^2xx'\int_0^\beta d\tau\,\frac{1}{[\tau(\beta-\tau)]^{\frac{1}{2}}}\exp\Big\{-\frac{\beta k^2}{\tau(\beta-\tau)}[\tau x^2+(\beta-\tau)x'^2]\Big\}\\ & -\frac{\beta}{\pi}k^2(L-x)(L-x')\int_0^\beta d\tau\,\frac{1}{[\tau(\beta-\tau)]^{\frac{1}{2}}}\\ & \qquad\times\exp\Big\{-\frac{\beta k^2}{\tau(\beta-\tau)}[\tau(L-x)^2+(\beta-\tau)(L-x')^2]\Big\}.\end{aligned} \tag{59}$$

We can use the integrals in the appendix to express (59) in error functions. The result is

$$\begin{aligned}\mathcal{I}_\beta(x,x') = {} & \frac{\beta}{2\sqrt{\pi}}k(x+x')\left[e^{-k^2(x-x')^2}-e^{-k^2(x+x')^2}-e^{-k^2((L-x)+(L-x'))^2}\right]\\ & +\beta k^2xx'\mathrm{Erfc}(k(x+x'))-\beta k^2(L-x)(L-x')\mathrm{Erfc}(k(2L-x-x')).\end{aligned} \tag{60}$$

Substituting this in (14) and adding the result to (54) yields

$$Z_2 = m\omega_c^2V\frac{\beta k^4}{2\pi L}\int_0^L dx\,x\Big[x^2\mathrm{Erfc}(2kx)-(L-x)^2\mathrm{Erfc}(2k(L-x))\Big]. \tag{61}$$

Finally, we perform the integration over x. For $kL\gg 1$ we end up with

$$Z_2 = -\tfrac{1}{24}\hbar^2\beta^2\omega_c^2Z_0. \tag{62}$$

This result agrees with the second-order term in the expression for the partition function of a magnetized electron gas without confining walls [12], as it should. The method of calculation chosen here enables us to find the finite-size corrections to the partition function as well. Up to terms of first order in $(kL)^{-1}$ one gets from (61)

$$Z_2 = -\tfrac{1}{24}\hbar^2\beta^2\omega_c^2Z_0\Big(1-\frac{\sqrt{\pi}}{16kL}\Big), \tag{63}$$

where Z_0 now stands for the zeroth-order partition function with a first finite-size correction included:

$$Z_0 = V\left(\frac{k^2}{\pi}\right)^{\frac{3}{2}}\left(1 - \frac{\sqrt{\pi}}{2kL}\right). \tag{64}$$

The finite-size correction in (63) agrees with that of [5], [13] which was also obtained from perturbation theory for small magnetic field. However, it disagrees with the result in [14] which was found via a different method; even after correcting for an inconsistent calculation, the result of that paper still differs from ours.

The result for the partition function allows us to find expressions for the field-dependent terms in the thermodynamic pressure and the magnetization. Since the thermodynamic pressure p is defined as a logarithmic derivative of the partition function, we find that there is no second-order term in p, so that we have

$$p = \frac{n}{\beta}, \tag{65}$$

up to second order in the field. Furthermore, we can calculate the average magnetization:

$$\bar{M} = -\frac{ne\beta\hbar^2\omega_c}{12mc}, \tag{66}$$

up to first order in the field. As is well-known the response is diamagnetic [12]. Insertion of $\bar{M}$ in (53) leads to

$$\bar{P}^{xx} = \bar{P}^{yy} = \frac{n}{\beta} + \tfrac{1}{12}n\beta\hbar^2\omega_c^2, \tag{67}$$

$$\bar{P}^{zz} = \frac{n}{\beta}, \tag{68}$$

up to second order in the field. We see that in the bulk the pressure in the direction of the field is lower than the transverse pressure [10,11].

5 Profiles of the mechanical pressure

In this section we will determine the pressure profile functions near the wall. We start with the zz-component. The second-order terms are given in (26)-(28). The first of these is already known from (62).

For (27) one has to calculate the double integral

$$\mathcal{J}_\beta(x) = \int_0^\beta d\tau \int_0^L dx'\, G_{\beta-\tau}(x,x')G_\tau(x',x)x'^2. \tag{69}$$

The evaluation of this integral goes similar to that of $\mathcal{I}_\beta(x,x)$. The result is

$$\begin{aligned}\mathcal{J}_\beta(x) = {} & \frac{\beta}{\sqrt{\pi}k}(k^2x^2 + \tfrac{1}{12})\left[1 - e^{-4k^2x^2} - e^{-4k^2(L-x)^2}\right] \\ & + \frac{2\beta k}{3\sqrt{\pi}}\left[x^2e^{-4k^2x^2} + (L-x)^2e^{-4k^2(L-x)^2}\right] \\ & - 2\beta k^2L(L-x)^2\mathrm{Erfc}(2k(L-x)).\end{aligned} \tag{70}$$

The expression (28) contains the integral

$$\mathcal{K}_\beta(x) = \int_0^\beta d\tau \int_0^L dx'\, G_{\beta-\tau}(x,x')\mathcal{J}_\tau(x',x)x', \tag{71}$$

where one has to insert (59). The integrand then consists of two kinds of terms, containing either exponential functions or products of exponentials with integrals. The contribution from the former type of terms follows from (60) and (70), since the sum of exponentials in (59) is proportional to $G_\beta(x,x')$ for $kL \gg 1$. So one is left with the contributions from the integrals in (59). The calculation of these contributions is carried out by first integrating over x'. Subsequently, the formulas in the appendix can be used to evaluate the integral over τ. In the end one gets

$$\begin{aligned}\mathcal{K}_\beta(x) = &\frac{\beta^2}{2\sqrt{\pi}k}(k^2x^2 + \tfrac{1}{24})\Big[1 - e^{-4k^2x^2} - e^{-4k^2(L-x)^2}\Big]\\
&+ \frac{\beta^2}{3\sqrt{\pi}k}\Big[k^2x^2(1+k^2x^2)e^{-4k^2x^2} + k^2(L-x)^2(1+k^2(L-x)^2)e^{-4k^2(L-x)^2}\Big]\\
&- \beta^2k^2L(L-x)^2\mathrm{Erfc}(2k(L-x))\\
&- \tfrac{2}{3}\beta^2k^4\Big[x^5\mathrm{Erfc}(2kx) + (L-x)^5\mathrm{Erfc}(2k(L-x))\Big].\end{aligned} \tag{72}$$

We can now give the expressions for the profile functions of the yy- and zz-components of the mechanical pressure tensor. Insertion of (15), (60), (62), (70), and (72) into (26)-(28) and (30)-(33) yields for the pressure components in second order of the magnetic field

$$\tilde{P}_2^{ii}(x) = \tfrac{1}{12}n\beta\hbar^2\omega_c^2\Big[F^i(2kx) + F^i(2k(L-x))\Big], \tag{73}$$

with

$$\begin{aligned}F^y(\xi) &= 1 - (1 - 4\xi^2 - \tfrac{3}{2}\xi^4)e^{-\xi^2} - 6\sqrt{\pi}\xi^3(1 + \tfrac{1}{4}\xi^2)\mathrm{Erfc}(\xi),\\
F^z(\xi) &= \tfrac{1}{2}\xi^4e^{-\xi^2} - \tfrac{1}{2}\sqrt{\pi}\xi^5\mathrm{Erfc}(\xi).\end{aligned} \tag{74}$$

The profile function for the xx-component of the pressure follows from (36). From (39)-(40) with (15) and (60) one gets for the current profile function [6]

$$\tilde{J}_1^y(x) = \frac{en\omega_c\sqrt{\pi}}{4k}\Big[G(2kx) - G(2k(L-x))\Big], \tag{75}$$

where

$$G(\xi) = \xi^2\mathrm{Erfc}(\xi). \tag{76}$$

By integration one finds for $\tilde{P}_2^{xx}(x)$ a profile like (73), where

$$F^x(\xi) = 1 - (1+\xi^2)e^{-\xi^2} + \sqrt{\pi}\xi^3\mathrm{Erfc}(\xi). \tag{77}$$

For the sake of completeness we also give the density profile function

$$\tilde{n}_2(x) = \tfrac{1}{12} n \beta^2 \hbar^2 \omega_c^2 \left[F^z(2kx) + F^z(2k(L - x)) \right], \qquad (78)$$

which follows from $\tilde{P}_2^{zz}(x)$. The pressure profile functions are plotted in figure 1.

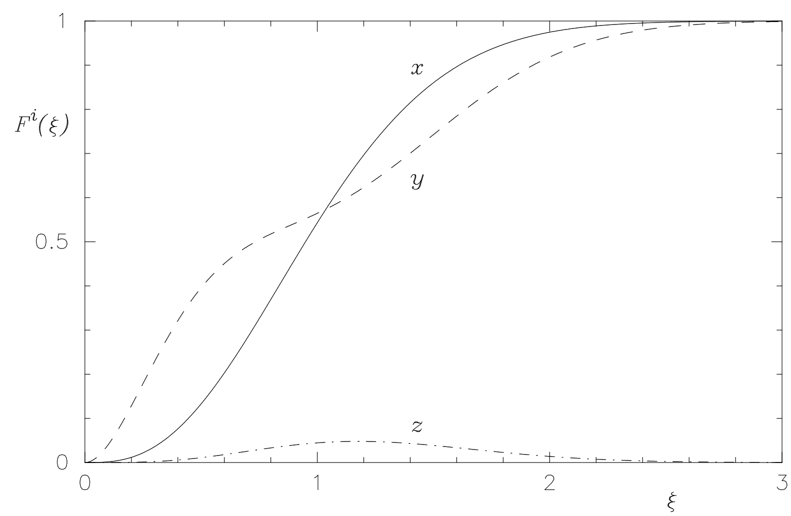

Figure 1: The profile functions for the xx-, yy- and zz-components of the field-dependent part of the mechanical pressure tensor near the wall.

One should note that the second-order terms of all components of the pressure tensor vanish at the wall. However, away from the wall, in the bulk, the various components have a different behaviour. The xx- and yy-component have a finite value, but the zz-component vanishes in the bulk. It now becomes clear why the thermodynamic and the volume-averaged mechanical pressure can have a different value. The thermodynamic pressure measures the change in the free energy due to a change in the position of the boundary. Hence, it is determined by the pressure just at the wall. The volume-averaged mechanical pressure, however, is essentially a bulk value. The two pressures can be different when the mechanical pressure drastically changes near the wall; and indeed this is the case, as one can see in the picture. In its turn, such a change in the pressure can occur only, if the forces associated with the pressure drop are compensated properly. In the present case this compensation is furnished by the Lorentz forces, which act on the electric currents that circulate near the wall (see Figure 2). Since these currents cause the diamagnetic response of the system, a direct relation between the anisotropy in the mechanical pressure tensor and the magnetization is established.

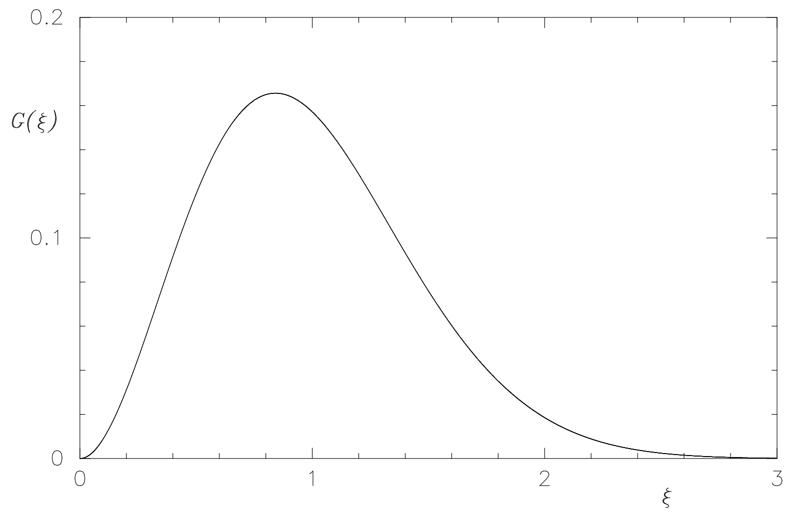

Figure 2: The profile function for the y-component of the current density near the wall.

6 Electron gas in a harmonic confinement potential

In the next two sections we will consider a magnetized electron gas in a harmonic confinement potential. The nice thing about this way of confining the system is that it is possible to evaluate its equilibrium properties exactly [7]-[9].

The harmonic potential is taken to be

$$V(\mathbf{r}) = \tfrac{1}{2}K_\perp(x^2+y^2) + \tfrac{1}{2}K_{||}z^2. \tag{79}$$

Note that the elastic constant in the z-direction differs from the elastic constant in the x- and y-direction. The magnetic field will be chosen in the z-direction, as before, but we will adopt the symmetric gauge $\mathbf{A} = (-\frac{1}{2}By, \frac{1}{2}Bx, 0)$ instead of the Landau gauge. The single-particle Hamiltonian reads

$$H = \frac{\boldsymbol{\pi}^2}{2m} + V(\mathbf{r}), \tag{80}$$

with the mechanical momentum $\boldsymbol{\pi} = \mathbf{p} - (e/2c)\mathbf{B}\wedge\mathbf{r}$. The Hamiltonian is quadratic in the coordinates and the momenta and is thus exactly solvable. Introduce the following (annihilation) operators [9]

$$a_\pm = \tfrac{1}{2}\Big(\frac{m\Omega_L}{\hbar}\Big)^{\frac{1}{2}}(x \mp iy) + \tfrac{1}{2}i(\hbar m\Omega_L)^{-\frac{1}{2}}(p_x \mp ip_y), \tag{81}$$

$$a_{||} = \Big(\frac{m\omega_{||}}{2\hbar}\Big)^{\frac{1}{2}}z + i(2\hbar m\omega_{||})^{-\frac{1}{2}}p_z, \tag{82}$$

and the corresponding adjoints, which satisfy the standard commutation relations. In (81)-(82) we defined $\Omega_L^2 = \omega_L^2 + \omega_\perp^2$, with $\omega_\perp^2 = K_\perp/m$ and likewise $\omega_{||}^2 = K_{||}/m$, and with the Larmor frequency $\omega_L = eB/2mc$. The Hamiltonian can be written in terms of these operators as

$$H = \hbar\omega_+(a_+^\dagger a_+ + \tfrac{1}{2}) + \hbar\omega_-(a_-^\dagger a_- + \tfrac{1}{2}) + \hbar\omega_{||}(a_{||}^\dagger a_{||} + \tfrac{1}{2}), \tag{83}$$

with $\omega_\pm = \Omega_L \mp \omega_L$. The energy eigenvalues follow by using the standard 'step' operator formalism.

Since we do not have a clear-cut volume to which the system is confined, we cannot define the thermodynamic pressure in the usual way, i.e. through differentiation of the free energy with respect to the volume. The analogon of volume differentiation for the present case is differentiation with respect to the elastic constants, since these provide the scale of the system. Therefore, we define the 'thermodynamic' pressure as

$$p_\perp = \langle K_\perp \frac{\partial H}{\partial K_\perp}\rangle, \tag{84}$$

$$p_{||} = 2\langle K_{||} \frac{\partial H}{\partial K_{||}}\rangle. \tag{85}$$

In fact, this is the analogon of pV/N of the earlier part of the paper. Mark that a change of $K_\perp$ gives rise to a change of effective dimension in both the x- and the y-direction, so that the reason for the factor 2 in the definition of $p_{||}$ is clear. In terms of the creation and annihilation operators the 'thermodynamic' pressure can be written as

$$p_\perp = \frac{\hbar\omega_\perp^2}{2\Omega_L}\langle a_+^\dagger a_+ + a_-^\dagger a_- + 1\rangle, \tag{86}$$

$$p_{||} = \hbar\omega_{||}\langle a_{||}^\dagger a_{||} + \tfrac{1}{2}\rangle. \tag{87}$$

The microscopic single-particle pressure is defined as in (18). Substitution of the inverse of (81)-(82) gives

$$\int d\mathbf{r}\, T^{xx}(\mathbf{r}) = -\frac{\hbar}{4\Omega_L}\left[\omega_+(a_+^\dagger - a_+) + \omega_-(a_-^\dagger - a_-)\right]^2, \tag{88}$$

$$\int d\mathbf{r}\, T^{yy}(\mathbf{r}) = \frac{\hbar}{4\Omega_L}\left[\omega_+(a_+^\dagger + a_+) - \omega_-(a_-^\dagger + a_-)\right]^2, \tag{89}$$

$$\int d\mathbf{r}\, T^{zz}(\mathbf{r}) = -\tfrac{1}{2}\hbar\omega_{||}(a_{||}^\dagger - a_{||})^2. \tag{90}$$

The ensemble average yields the (integrated) mechanical pressure tensor $\overline{\mathbf{P}} = \int d\mathbf{r}\langle \mathbf{T}(\mathbf{r})\rangle$ (again this differs by a factor V/N from the earlier part of the paper). The formal result is

$$\overline{P}^{xx} = \overline{P}^{yy} = \frac{\hbar}{2\Omega_L}\langle\left[\omega_+^2(a_+^\dagger a_+ + \tfrac{1}{2}) + \omega_-^2(a_-^\dagger a_- + \tfrac{1}{2})\right]\rangle, \tag{91}$$

$$\overline{P}^{zz} = \hbar\omega_{||}\langle a_{||}^\dagger a_{||} + \tfrac{1}{2}\rangle. \tag{92}$$

Only the diagonal components are non-vanishing.

The microscopic magnetization density per particle is defined in terms of the microscopic current density per particle $\mathbf{J}(\mathbf{r})$ as $\mathbf{M}(\mathbf{r}) = (1/2c)\mathbf{r} \wedge \mathbf{J}(\mathbf{r})$. The integral over the volume can be written as

$$\int d\mathbf{r}\, M^z(\mathbf{r}) = \frac{e\hbar}{2mc\Omega_L}\Big[\omega_+(a_+^\dagger a_+ + \tfrac{1}{2}) - \omega_-(a_-^\dagger a_- + \tfrac{1}{2}) - \omega_L(a_+^\dagger a_-^\dagger + a_- a_+)\Big]. \quad (93)$$

Taking the ensemble average yields for $\bar{M} = \int d\mathbf{r}\langle M^z(\mathbf{r})\rangle$ the formal result

$$\bar{M} = \frac{e\hbar}{2mc\Omega_L}\Big\langle\Big[\omega_+(a_+^\dagger a_+ + \tfrac{1}{2}) - \omega_-(a_-^\dagger a_- + \tfrac{1}{2})\Big]\Big\rangle. \quad (94)$$

By comparing (86)-(87), (91)-(92) and (94) one gets

$$\bar{P}^{xx} = \bar{P}^{yy} = p_\perp - B\bar{M}\,, \quad (95)$$

$$\bar{P}^{zz} = p_{||}. \quad (96)$$

These relations are closely analogous to those expressed by (53). Again it is found that in the direction parallel to the field the mechanical and thermodynamic pressure agree, whereas in the directions orthogonal to the field they differ by an amount determined by the magnetization. Once again the result that was established via scaling methods in [1] is recovered. Indeed, one can give an alternative derivation of (95) and (96) via a scaling technique. To that end one scales the elastic constants as $K_\perp \to K_\perp + \delta K_\perp$, and $K_{||} \to K_{||} + \delta K_{||}$, while the coordinates are simultaneously scaled as $x \to x' = x(1 + \frac{1}{2}\delta K_\perp/K_\perp)$, $y \to y' = y(1 + \frac{1}{2}\delta K_\perp/K_\perp)$, and $z \to z' = z(1 + \frac{1}{2}\delta K_{||}/K_{||})$, so that the confinement potential is unchanged. Evaluation of the change δH of the Hamiltonian leads to the same result as (95)-(96).

All the results derived up to now are found without specifying the way in which the ensemble average is performed. In order to obtain explicit results for the pressure and the magnetization we now assume the system to be non-degenerate, so it may be described by the canonical ensemble with Boltzmann statistics. The single-particle partition function is then [7]

$$Z = \tfrac{1}{4}[\cosh(\beta\hbar\Omega_L) - \cosh(\beta\hbar\omega_L)]^{-1}[\sinh(\tfrac{1}{2}\beta\hbar\omega_{||})]^{-1}. \quad (97)$$

The thermodynamic pressure can be calculated from (84)-(85) to be

$$\begin{aligned} p_\perp &= -\beta^{-1}K_\perp\frac{\partial}{\partial K_\perp}\log Z \\ &= \tfrac{1}{2}\hbar\frac{\omega_\perp^2}{\Omega_L}\frac{\sinh(\beta\hbar\Omega_L)}{\cosh(\beta\hbar\Omega_L) - \cosh(\beta\hbar\omega_L)}, \end{aligned} \quad (98)$$

and

$$\begin{aligned} p_{\|} &= -2\beta^{-1} K_{\|} \frac{\partial}{\partial K_{\|}} \log Z \\ &= \tfrac{1}{2}\hbar\omega_{\|} \coth(\tfrac{1}{2}\beta\hbar\omega_{\|}). \end{aligned} \tag{99}$$

The mechanical pressure follows by evaluating the ensemble averages in (91)-(92)

$$\begin{aligned} \overline{P}^{xx} = \overline{P}^{yy} &= \frac{\hbar\omega_L}{\Omega_L} \frac{\omega_L \sinh(\beta\hbar\Omega_L) - \Omega_L \sinh(\beta\hbar\omega_L)}{\cosh(\beta\hbar\Omega_L) - \cosh(\beta\hbar\omega_L)} \\ &\quad + \frac{\hbar\omega_\perp^2}{2\Omega_L} \frac{\sinh(\beta\hbar\Omega_L)}{\cosh(\beta\hbar\Omega_L) - \cosh(\beta\hbar\omega_L)}, \end{aligned} \tag{100}$$

$$\overline{P}^{zz} = \tfrac{1}{2}\hbar\omega_{\|} \coth(\tfrac{1}{2}\beta\hbar\omega_{\|}). \tag{101}$$

Finally, the magnetization per particle is obtained by differentiation with respect to the magnetic field

$$B\overline{M} = \beta^{-1} B \frac{\partial}{\partial B} \log Z \tag{102}$$

$$= -\frac{\hbar\omega_L}{\Omega_L} \frac{\omega_L \sinh(\beta\hbar\Omega_L) - \Omega_L \sinh(\beta\hbar\omega_L)}{\cosh(\beta\hbar\Omega_L) - \cosh(\beta\hbar\omega_L)}. \tag{103}$$

If we now take the limit of vanishing potential $K_\perp \to 0$, $K_{\|} \to 0$, we find

$$p_\perp = p_{\|} = \beta^{-1}, \tag{104}$$

$$\overline{P}^{xx} = \overline{P}^{yy} = \hbar\omega_L \coth(\beta\hbar\omega_L), \tag{105}$$

$$\overline{P}^{zz} = \beta^{-1}, \tag{106}$$

$$B\overline{M} = -\hbar\omega_L \left[\coth(\beta\hbar\omega_L) - \frac{1}{\beta\hbar\omega_L}\right]. \tag{107}$$

Hence, the anisotropy in the mechanical pressure remains present even in the limit $K_\perp, K_{\|} \to 0$. Both the difference between the mechanical pressure components and their relation to the thermodynamic pressure agree completely with (53).

7 Pressure profiles for the electron gas in a harmonic potential

To obtain the spatial dependence of the mechanical pressure for the electron gas in a harmonic potential the representation in terms of creation and annihilation operators is not useful. Instead, one has to start from the propagator in the presence of the harmonic potential and the magnetic field. The latter has been determined in [8]. It can be written as

$$G_\beta(\mathbf{r}, \mathbf{r}') = G_{\beta,\|}(z, z') G_{\beta,\perp}(\mathbf{r}_\perp, \mathbf{r}'_\perp), \tag{108}$$

with $\mathbf{r}_\perp = \mathbf{r} - \mathbf{r}\cdot\hat{\mathbf{B}}\hat{\mathbf{B}}$. The longitudinal and transverse propagators are

$$\begin{aligned} G_{\beta,||}(z,z') &= \left[\frac{m\omega_{||}}{2\pi\hbar\sinh(\beta\hbar\omega_{||})}\right]^{\frac{1}{2}} \\ &\times \exp\left\{-\frac{m\omega_{||}}{2\hbar\sinh(\beta\hbar\omega_{||})}\left[(z^2+z'^2)\cosh(\beta\hbar\omega_{||}) - 2zz'\right]\right\}, \end{aligned} \tag{109}$$

$$\begin{aligned} G_{\beta,\perp}(\mathbf{r}_\perp,\mathbf{r}'_\perp) &= \frac{m\Omega_L}{2\pi\hbar\sinh(\beta\hbar\Omega_L)} \\ &\times \exp\left\{-\frac{m\Omega_L}{2\hbar\sinh(\beta\hbar\Omega_L)}\left[(\mathbf{r}_\perp^2+\mathbf{r}'^2_\perp)\cosh(\beta\hbar\Omega_L)\right.\right. \\ &\left.\left. - 2\mathbf{r}_\perp\cdot\mathbf{r}'_\perp\cosh(\beta\hbar\omega_L) + 2i(\mathbf{r}_\perp\wedge\mathbf{r}'_\perp)\cdot\hat{\mathbf{B}}\sinh(\beta\hbar\omega_L)\right]\right\}. \end{aligned} \tag{110}$$

From the propagator one finds for the mechanical pressure tensor $\mathsf{P}(\mathbf{r}) = \langle\mathsf{T}(\mathbf{r})\rangle$

$$P^{xx}(\mathbf{r}) = n(\mathbf{r})\left[m\omega_{\mathrm{rot}}^2y^2 + \tfrac{1}{2}\hbar\Omega_L\frac{\cosh(\beta\hbar\Omega_L)+\cosh(\beta\hbar\omega_L)}{\sinh(\beta\hbar\Omega_L)}\right], \tag{111}$$

$$P^{yy}(\mathbf{r}) = n(\mathbf{r})\left[m\omega_{\mathrm{rot}}^2x^2 + \tfrac{1}{2}\hbar\Omega_L\frac{\cosh(\beta\hbar\Omega_L)+\cosh(\beta\hbar\omega_L)}{\sinh(\beta\hbar\Omega_L)}\right], \tag{112}$$

$$P^{xy}(\mathbf{r}) = -n(\mathbf{r})m\omega_{\mathrm{rot}}^2xy, \tag{113}$$

$$P^{zz}(\mathbf{r}) = n(\mathbf{r})\tfrac{1}{2}\hbar\omega_{||}\coth(\tfrac{1}{2}\beta\hbar\omega_{||}). \tag{114}$$

In these expressions for the pressure profile functions the density $n(\mathbf{r})$ appears as a multiplicative factor. It has the form [9]

$$n(\mathbf{r}) = n_{||}(z)n_\perp(\mathbf{r}_\perp), \tag{115}$$

with

$$n_{||}(z) = \left[\frac{m\omega_{||}\tanh(\frac{1}{2}\beta\hbar\omega_{||})}{\pi\hbar}\right]^{\frac{1}{2}}\exp\left[-\frac{m\omega_{||}}{\hbar}z^2\tanh(\tfrac{1}{2}\beta\hbar\omega_{||})\right], \tag{116}$$

$$n_\perp(\mathbf{r}_\perp) = \frac{\lambda}{\pi}\exp(-\lambda r_\perp^2), \tag{117}$$

with the abbreviation

$$\lambda = \frac{m\Omega_L}{\hbar}\frac{\cosh(\beta\hbar\Omega_L)-\cosh(\beta\hbar\omega_L)}{\sinh(\beta\hbar\Omega_L)}. \tag{118}$$

Furthermore, we defined in (111)-(113) the rotation velocity as

$$\omega_{\mathrm{rot}} := \omega_L - \Omega_L\frac{\sinh(\beta\hbar\omega_L)}{\sinh(\beta\hbar\Omega_L)}. \tag{119}$$

Integration of (111)-(114) yields (100)-(101) again.

The interpretation of the pressure profile function becomes clear by considering the current-density profile, just as for the electron gas in a slab. The current density is found to be [9]

$$\langle \mathbf{J}(\mathbf{r})\rangle = e\omega_{\mathrm{rot}} n(\mathbf{r})\mathbf{r}\wedge\hat{\mathbf{B}}. \tag{120}$$

So, the plasma rotates with a frequency ω_{rot} around the field. Using this form for the current-density profile one can check the validity of the equation of motion

$$-\nabla\cdot\mathbf{P}(\mathbf{r}) + c^{-1}\langle\mathbf{J}(\mathbf{r})\rangle\wedge\mathbf{B} + n(\mathbf{r})\mathbf{F}(\mathbf{r}) = 0, \tag{121}$$

with $\mathbf{F}(\mathbf{r}) = -\nabla V(\mathbf{r})$ the confining force.

The contributions depending on ω_{rot} in (111)-(113) are due to the bulk motion. This bulk motion gives rise to a centrifugal potential $\frac{1}{2}m\omega_{\mathrm{rot}}^2\mathbf{r}_\perp^2$ and to a corresponding centrifugal force $-\nabla(\frac{1}{2}m\omega_{\mathrm{rot}}^2\mathbf{r}_\perp^2)$.

Appendix

In this appendix we give some integrals which are useful in the integration of the propagators. In the main text we repeatedly use the following representation of the error function

$$\int_0^\beta d\tau\,\frac{1}{[\tau(\beta-\tau)]^{\frac{1}{2}}}\exp\Big[-\frac{a^2}{\tau(\beta-\tau)}\Big] = \pi\,\mathrm{Erfc}\Big(\frac{2a}{\beta}\Big). \tag{A1}$$

By differentiation with respect to a one finds

$$\int_0^\beta d\tau\,\frac{1}{[\tau(\beta-\tau)]^{\frac{3}{2}}}\exp\Big[-\frac{a^2}{\tau(\beta-\tau)}\Big] = \frac{2\sqrt{\pi}}{\beta a}\exp\Big(-\frac{4a^2}{\beta^2}\Big). \tag{A2}$$

We do not need any higher derivatives.

Furthermore, we need information on

$$K_n(a,\beta) := \int_0^\beta d\tau\,\tau^{-n+\frac{1}{2}}\exp\Big(-\frac{a^2}{\beta\tau}\Big)\mathrm{Erfc}\Big(\frac{a}{[\beta(\beta-\tau)]^{\frac{1}{2}}}\Big), \tag{A3}$$

for non-negative integer n. Partial integration yields a recurrence relation for $n\geq 0$

$$K_{n+1}(a,\beta) = \frac{2n-3}{2a^2}\beta K_n(a,\beta) + \frac{1}{2a}\sqrt{\frac{\beta}{\pi}}\int_0^\beta d\tau\,\frac{\tau^{-n+3}+(\beta-\tau)^{-n+3}}{[\tau(\beta-\tau)]^{\frac{3}{2}}}\exp\Big[-\frac{a^2}{\tau(\beta-\tau)}\Big]. \tag{A4}$$

For the evaluation of the last term, use [15]

$$\tau^p + (\beta-\tau)^p = 2[\tau(\beta-\tau)]^{\frac{p}{2}}\,T_{|p|}\Big(\frac{\beta}{2[\tau(\beta-\tau)]^{\frac{1}{2}}}\Big), \tag{A5}$$

where $T_n(x)$ are the Chebyshev polynomials of the first kind; hence, the last term in (A4) is known in terms of derivatives of (A1).

Differentiation with respect to a gives

$$\frac{\partial K_n(a,\beta)}{\partial a} = -\frac{2n-3}{a}K_n(a,\beta) - \sqrt{\frac{\beta}{\pi}}\int_0^\beta d\tau\,\frac{\tau^{-n+2}+(\beta-\tau)^{-n+2}}{[\beta(\beta-\tau)]^{\frac{3}{2}}}\exp\Big[-\frac{a^2}{\tau(\beta-\tau)}\Big]. \tag{A6}$$

The solution of this equation is the simplest for $n = 2$; one gets

$$K_2(a,\beta) = \frac{\sqrt{\pi\beta}}{a}\mathrm{Erfc}\Big(\frac{2a}{\beta}\Big) + \frac{c(\beta)}{a}, \tag{A7}$$

with an as yet unknown constant $c(\beta)$. To fix this constant, put $\tau = a^2x/\beta$. Then

$$K_2(a,\beta) = \frac{\sqrt{\beta}}{a}\int_0^{(\beta/a)^2} dx\, x^{-\frac{3}{2}}\exp\Big(-\frac{1}{x}\Big)\mathrm{Erfc}\Big(\frac{1}{[\beta^2/a^2-x]^{\frac{1}{2}}}\Big). \tag{A8}$$

For $a \to 0$, the function $aK_2(a,\beta)$ goes to $\sqrt{\beta}\int_0^\infty dy\, y^{-\frac{3}{2}}\exp(-1/y) = \sqrt{\beta\pi}$, so one finds $c(\beta) = 0$.

Using the recursion relations we can write

$$K_1(a,\beta) = -4a\sqrt{\frac{\pi}{\beta}}\mathrm{Erfc}\Big(\frac{2a}{\beta}\Big) + 2\sqrt{\beta}\exp\Big(-\frac{4a^2}{\beta^2}\Big), \tag{A9}$$

$$\begin{aligned} K_0(a,\beta) &= a\sqrt{\beta}\Big[\tfrac{2}{3}\Big(\frac{2a}{\beta}\Big)^2 - 1\Big]\sqrt{\pi}\,\mathrm{Erfc}\Big(\frac{2a}{\beta}\Big) \\ &\quad + \beta^{\frac{3}{2}}\Big[-\tfrac{1}{3}\Big(\frac{2a}{\beta}\Big)^2 + \tfrac{2}{3}\Big]\exp\Big(-\frac{4a^2}{\beta^2}\Big). \end{aligned} \tag{A10}$$

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