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Suttorp, L.G.

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Pressure and Compressibility of a Quantum Plasma in a Magnetic Field

L.G. Suttorp

Institute for Theoretical Physics, University of Amsterdam,
Valckenierstraat 65, 1018 XE Amsterdam, The Netherlands

Abstract

The equilibrium pressure tensor that occurs in the momentum balance equation for a quantum plasma in a magnetic field is shown to be anisotropic. Its relation to the pressure that follows from thermodynamics is elucidated. A general proof of the compressibility rule for a magnetized quantum plasma is presented.

1. Introduction

The pressure of a fluid in equilibrium can be defined in several alternative ways. One definition is based on the microscopic momentum balance equation in which the divergence of the microscopic pressure tensor appears. Taking the ensemble average of this pressure tensor one obtains the so-called mechanical pressure tensor. A different way to define the equilibrium pressure is to employ its well-known thermodynamic expression as a derivative of the free energy, which follows in the usual way from the canonical partition function. For classical systems it can be shown easily that both definitions lead to the same result. The virial theorem plays an essential role in establishing the equivalence. For quantum systems the proof of equivalence of the two definitions is less straightforward. Even for systems of neutral particles with short-range interactions the details of the proof of equivalence have led to some debate in the past; a further analysis has settled the matter completely [1],[2]. For the electron gas the presence of the uniform background needs to be taken into account [3]. If an external magnetic field is present in the electron gas, the precise relation between the two pressures is not so clear any more. A recent discussion of the two-dimensional case has shown that the standard virial theorem might lose its validity for magnetized systems [4]. Furthermore, it has been known for some time that the mechanical pressure tensor of a charged particle system could become anisotropic in a magnetic field [5]. An anisotropic pressure tensor implies an anisotropic compressibility. Hence, it is not obvious how the compressibility rule, which gives information on the density fluctuations, should be generalized to a magnetized electron gas.

The purpose of the present paper is to review some recent work [6] that has led to a better understanding of the pressure and the compressibility in a magnetized one-component plasma.

2. Mechanical pressure tensor

The Hamiltonian of a one-component quantum plasma in a uniform magnetic field is given by

$$
\begin{aligned}
H &= \frac{1}{2m}\sum_\alpha [\mathbf{p}_\alpha - \frac{e}{c}\mathbf{A}(\mathbf{r}_\alpha)]^2 + \frac{1}{2}\sum_{\alpha,\beta}{}' \; \frac{e^2}{4\pi|\mathbf{r}_\alpha - \mathbf{r}_\beta|} \\
&\quad -n\sum_\alpha \int^V d\mathbf{r}\; \frac{e^2}{4\pi|\mathbf{r}-\mathbf{r}_\alpha|} + \frac{1}{2}n^2 \int^V d\mathbf{r} \int^V d\mathbf{r}'\; \frac{e^2}{4\pi|\mathbf{r}-\mathbf{r}'|} \quad . \qquad (1)
\end{aligned}
$$

Here $\mathbf{r}_\alpha$ and $\mathbf{p}_\alpha$ are the positions and momenta of the plasma particles, which carry a charge e and a mass m. The particles move in an inert neutralizing background of charge density $-q_v = -en = -eN/V$, with N the number of particles and V the volume of the system. The vector potential $\mathbf{A}$ describes a uniform external magnetic field in the Coulomb gauge. The prime at the summation sign indicates that the self-terms are to be left out.

The charge density and the current density are given by

$$
\begin{aligned}
Q(\mathbf{r}) &= e\sum_\alpha \delta(\mathbf{r}-\mathbf{r}_\alpha) - q_v \quad , \qquad (2)\\
\mathbf{J}(\mathbf{r}) &= \frac{e}{2m}\sum_\alpha \{\boldsymbol{\pi}_\alpha, \delta(\mathbf{r}-\mathbf{r}_\alpha)\} \quad , \qquad (3)
\end{aligned}
$$

with $\boldsymbol{\pi}_\alpha = \mathbf{p}_\alpha - (e/c)\mathbf{A}(\mathbf{r}_\alpha)$ the mechanical momentum and with curly brackets denoting the anti-commutator.

The equation of motion has the form

$$
\frac{i}{\hbar}[H, \mathbf{J}(\mathbf{r})] = -\frac{e}{m}\nabla\cdot\mathsf{T}(\mathbf{r}) + \frac{e}{m}\mathbf{F}(\mathbf{r}) + \frac{e}{mc}\mathbf{J}(\mathbf{r})\wedge\mathbf{B} \quad . \qquad (4)
$$

Here T is the pressure tensor, which consists of a kinetic part $\mathsf{T}_{\rm kin}$ and a potential part $\mathsf{T}_{\rm pot}$. The components of the kinetic pressure tensor are defined as

$$
T^{ij}_{\rm kin}(\mathbf{r}) = \frac{1}{2m}\sum_\alpha [\pi^i_\alpha \pi^j_\alpha \delta(\mathbf{r}-\mathbf{r}_\alpha) + \delta(\mathbf{r}-\mathbf{r}_\alpha)\pi^j_\alpha \pi^i_\alpha] \quad . \qquad (5)
$$

The divergence of the potential pressure tensor is given by

$$
\nabla\cdot\mathsf{T}_{\rm pot}(\mathbf{r}) = \int^V d\mathbf{r}'\; \nabla_\mathbf{r} \frac{e^2}{4\pi|\mathbf{r}-\mathbf{r}'|} D(\mathbf{r},\mathbf{r}') \quad , \qquad (6)
$$

with the abbreviation

$$
D(\mathbf{r},\mathbf{r}') = \sum_{\alpha,\beta}{}' \; \delta(\mathbf{r}-\mathbf{r}_\alpha)\,\delta(\mathbf{r}'-\mathbf{r}_\beta) - n\sum_\alpha \delta(\mathbf{r}-\mathbf{r}_\alpha) - n\sum_\beta \delta(\mathbf{r}'-\mathbf{r}_\beta) + n^2 \quad . \qquad (7)
$$

Finally, the force density in (4) is defined as

$$
\mathbf{F}(\mathbf{r}) = -n\int^V d\mathbf{r}'\; \nabla_\mathbf{r} \frac{e}{4\pi|\mathbf{r}-\mathbf{r}'|}\, Q(\mathbf{r}') \quad . \qquad (8)
$$

The implicit definition (6) of the potential pressure tensor makes sense only if the right-hand side can be written as the divergence of a tensor. This is indeed the case owing to the symmetry of the factor $D(\mathbf{r},\mathbf{r}')$ in its two arguments. (In fact, to achieve this symmetry we had to split off the force density $\mathbf{F}(\mathbf{r})$ at the right-hand side of the equation of motion.) Using the symmetry properties of the integrand in (6) we may write [7]

$$\begin{aligned}\mathsf{T}_{\rm pot}(\mathbf{r}) &= -\frac{1}{2}\int_0^1 d\lambda \int d\mathbf{x}\, \left(\mathbf{x}\nabla_{\mathbf{x}}\frac{e^2}{4\pi x}\right)\theta_V(\mathbf{r}-\tfrac{1}{2}\lambda\mathbf{x})\theta_V(\mathbf{r}+(1-\tfrac{1}{2}\lambda)\mathbf{x}) \\ &\quad\times D(\mathbf{r}-\tfrac{1}{2}\lambda\mathbf{x},\mathbf{r}+(1-\tfrac{1}{2}\lambda)\mathbf{x}) \quad . \end{aligned} \tag{9}$$

The limits of integration over $\mathbf{x}$ have been fixed by incorporating in the integrand characteristic functions θ_V, which are 1 for arguments inside V and 0 elsewhere. We assume that the region occupied by the system is convex, so that the potential pressure tensor vanishes for $\mathbf{r}$ outside V.

The statistical average of the microscopic pressure tensor T, which is found above from the equation of motion, will be called the 'mechanical' pressure tensor in the following, to distinguish it from the 'thermodynamic' pressure that arises by differentiation of the free energy.

3. Thermodynamic pressure

In the canonical ensemble the thermodynamic equilibrium pressure $p_{\rm therm}$ follows by considering the free energy of the system for varying volume. For a system in a fluid phase, to which we shall confine the discussion, the thermodynamic pressure is isotropic. To determine it one may use a scaling argument as is well-known for systems of neutral particles [1],[2]. In fact, for neutral-particle systems in equilibrium this argument has been used to prove the equivalence of the thermodynamic pressure and the mechanical pressure tensor. As it turns out, this argument can not be taken over trivially to establish the equivalence of the two pressures in a magnetized quantum plasma, owing to the presence of the magnetic field.

Let us consider a variation of the volume of the system by deforming the boundary such that an arbitrary position $\mathbf{r}_w$ goes over to $\mathbf{r}_w+\delta\mathbf{r}_w=\mathbf{r}_w+\delta\boldsymbol{\epsilon}\cdot\mathbf{r}_w$, with a (uniform) deformation tensor $\delta\boldsymbol{\epsilon}$. At fixed temperature T and fixed magnetic field B the canonical partition function Z changes then as

$$\delta\log Z = -\frac{\beta}{Z}\sum_n \delta E_n e^{-\beta E_n} \quad , \tag{10}$$

with $\beta=1/k_BT$ and δE_n the change of the energy eigenvalue E_n. To determine δE_n as a function of $\delta\boldsymbol{\epsilon}$ one has to solve the Schrödinger equation for the Hamiltonian (1), with deformed boundary conditions. It is then useful to introduce deformed particle positions $\bar{\mathbf{r}}_\alpha=(\mathsf{U}-\delta\boldsymbol{\epsilon})\cdot\mathbf{r}_\alpha$ as well. Regarding the energy eigenfunction ψ_n as a function of $\bar{\mathbf{r}}_\alpha$ one finds immediately:

$$\delta E_n = <\psi_n|\delta H|\psi_n> \quad , \tag{11}$$

with δH the variation of H at fixed $\bar{\mathbf{r}}_\alpha$. Choosing for convenience the gauge $\mathbf{A}=\frac{1}{2}\mathbf{B}\wedge\mathbf{r}$ we get from the kinetic part of the Hamiltonian:

$$\delta H_{\rm kin} = -\tfrac{1}{2}\sum_\alpha \frac{1}{m}\boldsymbol{\pi}_\alpha\cdot(\delta\boldsymbol{\epsilon}+\delta\tilde{\boldsymbol{\epsilon}})\cdot\boldsymbol{\pi}_\alpha$$

$$+\frac{e}{2mc}\sum_{\alpha}\left[\mathbf{B}\cdot\delta\tilde{\boldsymbol{\epsilon}}\cdot(\mathbf{r}_\alpha\wedge\boldsymbol{\pi}_\alpha)-(\mathrm{tr}\,\delta\boldsymbol{\epsilon})(\mathbf{r}_\alpha\wedge\boldsymbol{\pi}_\alpha)\cdot\mathbf{B}\right] , \tag{12}$$

with $\delta\tilde{\boldsymbol{\epsilon}}$ the transpose of $\delta\boldsymbol{\epsilon}$. The right-hand side can be written in terms of the kinetic pressure tensor (5) and of the magnetization density

$$\mathbf{M}(\mathbf{r})=\frac{e}{4mc}\sum_{\alpha}\{\mathbf{r}_\alpha\wedge\boldsymbol{\pi}_\alpha,\delta(\mathbf{r}-\mathbf{r}_\alpha)\} \quad . \tag{13}$$

In fact, we get:

$$\delta H_{\mathrm{kin}}=-\delta\boldsymbol{\epsilon}:\int^{V}d\mathbf{r}\;\mathsf{T}_{\mathrm{kin}}(\mathbf{r})+\mathbf{B}\cdot\delta\tilde{\boldsymbol{\epsilon}}\cdot\int^{V}d\mathbf{r}\;\mathbf{M}(\mathbf{r})-(\mathrm{tr}\,\delta\boldsymbol{\epsilon})\;\mathbf{B}\cdot\int^{V}d\mathbf{r}\;\mathbf{M}(\mathbf{r}) . \tag{14}$$

Furthermore, we find for the variation of the potential part of the Hamiltonian

$$\delta H_{\mathrm{pot}}=-\delta\boldsymbol{\epsilon}:\int^{V}d\mathbf{r}\;\mathsf{T}_{\mathrm{pot}}(\mathbf{r}) \quad . \tag{15}$$

From (10), (11), (14) and (15) we obtain for the variation of the free energy f per particle at fixed temperature and magnetic field:

$$\delta f=-v\delta\boldsymbol{\epsilon}:\left[\frac{1}{V}\int^{V}d\mathbf{r}\;\langle\mathsf{T}(\mathbf{r})\rangle-\mathbf{B}\frac{1}{V}\int^{V}d\mathbf{r}\;\langle\mathbf{M}(\mathbf{r})\rangle+\mathbf{B}\cdot\frac{1}{V}\int^{V}d\mathbf{r}\;\langle\mathbf{M}(\mathbf{r})\rangle\;\mathsf{U}\right] \quad , \tag{16}$$

with v the volume per particle and U the unit tensor. For fluid systems the free energy per particle should depend only on the volume of the system and not on its shape. In fact, the 'thermodynamic' pressure p_{therm} is defined by writing $\delta f=-p_{\mathrm{therm}}\delta v$ at constant T and B. Since one has $\delta v=v\;\mathrm{tr}\,\delta\boldsymbol{\epsilon}$, the variation δf in (16) can depend only on the trace of the deformation tensor, so that the expression between square brackets should be isotropic:

$$\frac{1}{V}\int^{V}d\mathbf{r}\;\langle\mathsf{T}(\mathbf{r})\rangle-\mathbf{B}\frac{1}{V}\int^{V}d\mathbf{r}\;\langle\mathbf{M}(\mathbf{r})\rangle+\mathbf{B}\cdot\frac{1}{V}\int^{V}d\mathbf{r}\;\langle\mathbf{M}(\mathbf{r})\rangle\;\mathsf{U}=p_{\mathrm{therm}}\mathsf{U} \quad . \tag{17}$$

Since the terms with the magnetization are anisotropic the integral over the mechanical pressure is anisotropic as well. Writing

$$\frac{1}{V}\int^{V}d\mathbf{r}\;\langle\mathsf{T}(\mathbf{r})\rangle=p_B\mathsf{U}-\tfrac{3}{2}\delta p_B\,(\mathsf{U}-\hat{\mathbf{B}}\hat{\mathbf{B}}) \quad , \tag{18}$$

with $\hat{\mathbf{B}}$ a unit vector in the direction of the magnetic field, we get:

$$p_B = p_{\mathrm{therm}} \tag{19}$$

$$\delta p_B = \frac{2}{3V}\,\mathbf{B}\cdot\int^{V}d\mathbf{r}\;\langle\mathbf{M}(\mathbf{r})\rangle \quad . \tag{20}$$

For a diamagnetic response the anisotropic part δp_B of the pressure tensor is negative, so that the pressure in a direction transverse to the magnetic field is larger than that in a direction parallel to the field. It should be noted that it is essential to retain in the above the integral of the magnetization over the volume. In fact, in the bulk the average current density vanishes, and hence the local magnetization density is zero as well. The total magnetization is non-vanishing, however, owing to electrical currents flowing at the surface of the system.

4. Pressure of a confined magnetized free-particle system

It is instructive to study the pressure tensor of a simple model system, for which both the mechanical and the thermodynamic pressure can be evaluated explicitly. As we have seen in (14), the difference of the two pressures can be traced back to the behaviour of the kinetic pressure under a change of the boundary conditions; the potential pressure does not contribute to the pressure difference. Hence, to analyze this difference in more detail it is sufficient to consider a system of charged particles in a magnetic field without taking into account the Coulomb interactions. In other words, already in a magnetized free-particle system the effect would arise. As a further simplification we shall assume the system to be non-degenerate. Since the boundaries play an essential role we have to include these carefully. Let us consider therefore a system of charged particles in a slab-like geometry, with the x-coordinates of the particles confined to a finite region. The magnetic field is taken in the direction of the positive z-axis. We shall calculate the pressure tensor of the system by using perturbation theory with respect to the magnetic interactions. A similar method has been used before to study the surface currents in magnetized plasmas [8],[9]. Using the Landau gauge we write the Hamiltonian for a single particle as $H = H_0 + H_1$, with $H_0 = (1/2m)p^2 + V(x)$ and $H_1 = -\omega_c x p^y + \frac{1}{2} m\omega_c^2 x^2$. Here $V(x)$ is the infinitely steep potential which confines the system to the slab. Furthermore, $\omega_c = eB/mc$ is the cyclotron frequency. Up to second order in the field strength one finds for the one-particle partition function Z:

$$Z = \mathrm{tr}\,\left(e^{-\beta H}\right) = Z_0(1 - \frac{1}{24}\beta^2\hbar^2\omega_c^2) \quad , \tag{21}$$

with Z_0 the one-particle partition function for the field-free system confined to the slab. The thermodynamic pressure up to second order is thus independent of the field:

$$p_{\mathrm{therm}} = \frac{n}{\beta} \quad . \tag{22}$$

The components of the volume-averaged mechanical pressure tensor can likewise be evaluated with the help of perturbation theory. For the zz-component of the pressure tensor one immediately gets for any field strength:

$$V^{-1}\int^V d\mathbf{r}\,\langle T^{zz}(\mathbf{r})\rangle = p_B = \frac{n}{\beta} \quad , \tag{23}$$

so that (19) is recovered.

On the other hand, the yy-component of the pressure tensor

$$V^{-1}\int^V d\mathbf{r}\,\langle T^{yy}(\mathbf{r})\rangle = p_B - \tfrac{3}{2}\delta p_B = \frac{n}{mZ}\mathrm{tr}\,[e^{-\beta H}(p^y - m\omega_c x)^2] \quad , \tag{24}$$

does depend on the field strength. Employing perturbation theory up to second order one gets

$$\mathrm{tr}\,[e^{-\beta H}(p^y - m\omega_c x)^2] = \frac{m}{\beta}Z_0(1 + \frac{1}{24}\beta^2\hbar^2\omega_c^2) \quad . \tag{25}$$

Combining this result with (21) we obtain

$$p_B - \tfrac{3}{2}\delta p_B = \frac{n}{\beta}(1 + \frac{1}{12}\beta^2\hbar^2\omega_c^2) \quad , \tag{26}$$

and hence

$$\delta p_B = -\frac{1}{18}n\beta\hbar^2\omega_c^2 \quad . \tag{27}$$

Finally, the average magnetization in first order of the field strength follows by differentiation of Z:

$$V^{-1}\int^V d\mathbf{r}\ \langle M(\mathbf{r})\rangle = -\frac{1}{12}n\beta\hbar^2\frac{\omega_c^2}{B} \quad , \tag{28}$$

so that (20) is confirmed as well. The volume-averaged mechanical pressure tensor is indeed found to be anisotropic.

More insight in the behaviour of the pressure tensor of this model system is obtained by evaluating the profiles of the components of the mechanical pressure tensor near the boundary of the slab. In second-order perturbation theory one arrives at the following results

$$\langle T^{ii}(\mathbf{r})\rangle = \frac{n}{\beta}F^i(\xi) + \frac{1}{12}n\beta\hbar^2\omega_c^2 G^i(\xi) \quad . \tag{29}$$

Here ξ stands for the reduced coordinate $(2m/\beta\hbar^2)^{1/2}x$. The functions F^i have the simple form:

$$F^x(\xi) = 1 \quad , \quad F^y(\xi) = F^z(\xi) = 1 - e^{-\xi^2} \quad . \tag{30}$$

For vanishing field the tangential components of the mechanical pressure tensor vanish at the wall; only the component perpendicular to the wall retains its bulk value. In second order of the field strength the profiles change. The functions $G^i(\xi)$ are combinations of exponential functions and error functions:

$$\begin{aligned} G^x(\xi) &= 1 - (1+\xi^2)e^{-\xi^2} + \sqrt{\pi}\xi^3\,\mathrm{erfc}(\xi) \quad , \\ G^y(\xi) &= 1 - (1 - 4\xi^2 - \tfrac{3}{2}\xi^4)e^{-\xi^2} - 6\sqrt{\pi}\xi^3(1 + \tfrac{1}{4}\xi^2)\,\mathrm{erfc}(\xi) \quad , \\ G^z(\xi) &= \tfrac{1}{2}\xi^4 e^{-\xi^2} - \tfrac{1}{2}\sqrt{\pi}\xi^5\,\mathrm{erfc}(\xi) \quad . \end{aligned} \tag{31}$$

They have been plotted in Figure 1. As the figure shows, the second-order terms of all components of the pressure tensor vanish at the wall. Away from the wall the various cartesian components have a different behaviour, however: whereas the second-order component in the direction of the field vanishes in the bulk as well, the second-order components in the directions transverse to the field acquire a finite value in the bulk. It now becomes clear why the mechanical and thermodynamic pressures can differ. The thermodynamic pressure measures the change of the free energy when the position of the boundary changes. Hence, it is determined by the pressure tensor at the wall. On the other hand, the mechanical pressure averaged over the sample is determined by the bulk value. The bulk and wall values of the pressure can be different, if a steep change of the pressure tensor near the wall occurs. This can happen, if the divergence of the pressure tensor is compensated by a force which takes large values near the wall. This is indeed the case for a magnetized charged particle system, since the electric current density and hence the Lorentz force density is concentrated in a thin layer near the wall.

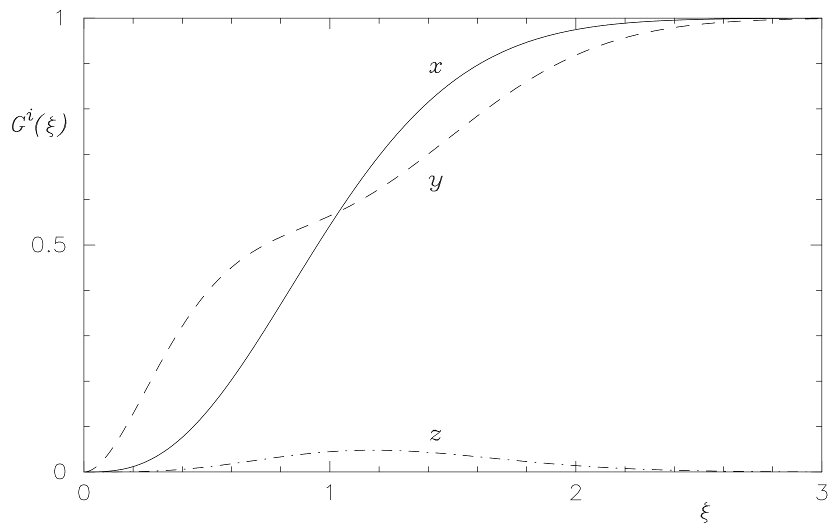

Fig. 1. The profile functions for the x, y and z components of the field-dependent part of the pressure tensor near the wall.

The above expressions have been obtained on assuming that the free-particle system is non-degenerate. For a completely degenerate system one can derive similar results. The general relation (20) between the anisotropic part of the mechanical pressure tensor and the total magnetization is corroborated in that case as well.

5. Compressibility relation

For a classical one-component plasma the structure factor in fourth-order of the wavenumber is determined by the isothermal compressibility. In quantum theory one expects that the charge fluctuation expression $\mathcal{K}V^{-1}\langle Q(\mathbf{k})Q(-\mathbf{k})\rangle_T$ with $\mathcal{K}$ denoting the Kubo transform, and T truncation (i.e. subtraction of the product of averages), is likewise given by the compressibility in fourth-order of k. General statements to that effect can be found in the literature [10]. However, in particular for magnetized plasmas, where mechanical and thermodynamic pressures are different, no proof of the so-called compressibility rule appears to be available. Even if the compressibility rule is taken for granted for magnetized plasmas as well, it is not clear which pressure is meant in the definition of the compressibility. Of course, a formal proof of the rule would be helpful in deciding this question.

To evaluate the fourth-order terms of the charge fluctuation expression we start from an identity that can be derived [11] from the continuity equation and the equation of motion:

$$\mathcal{K}\frac{1}{V}\langle Q(\mathbf{k})Q(-\mathbf{k})\rangle_T^{(4)} = -\frac{e}{m\omega_p^2\cos\theta}\mathcal{K}\frac{1}{V}\langle \hat{\mathbf{k}}\cdot\mathsf{T}(\mathbf{k})\cdot\hat{\mathbf{B}}\; Q(-\mathbf{k})\rangle_T^{(2)} \quad . \tag{32}$$

Here a superscript (n) indicates the order with respect to the wavenumber. Furthermore, ω_p is the plasma frequency, $\hat{\mathbf{k}}$ a unit vector in the direction of the wavevector, and

$\cos\theta = \hat{\mathbf{k}}\cdot\hat{\mathbf{B}}$. The right-hand side of (32) can be reduced to even lower-order quantities by using once more the continuity equation and the equation of motion, since one has for local operators Ω [11]:

$$
\begin{aligned}
&\mathcal{K}\frac{1}{V}\langle\Omega(\mathbf{k})Q(-\mathbf{k})\rangle_T^{(2)} = \\
&= \frac{1}{\hbar\beta\omega_p^2\cos\theta}\frac{1}{V}\langle[\Omega(\mathbf{k})\,,\,\mathbf{J}(-\mathbf{k})\cdot\hat{\mathbf{B}}]\rangle^{(1)} - \frac{e}{m\omega_p^2\cos\theta}\mathcal{K}\frac{1}{V}\langle\Omega(\mathbf{k})\hat{\mathbf{k}}\cdot\mathsf{T}(-\mathbf{k})\cdot\hat{\mathbf{B}}\rangle_T^{(0)}\,. \quad (33)
\end{aligned}
$$

The commutator at the right-hand side can be evaluated easily for any operator $\Omega(\mathbf{k})$ of the type of the kinetic or the potential pressure, i.e. for sums of one-particle local operators depending on $\boldsymbol{\pi}_\alpha$ and for sums of purely configurational two-particle operators. One finds for such operators

$$
\begin{aligned}
&\frac{1}{V}\langle[\Omega(\mathbf{k})\,,\,\mathbf{J}(-\mathbf{k})\cdot\hat{\mathbf{B}}]\rangle^{(1)} = \\
&= \frac{\hbar e\cos\theta}{m}\frac{1}{V}\langle\Omega(\mathbf{k}=0)\rangle - \frac{ie}{m}\frac{1}{V}\left\langle\left[\sum_\alpha \boldsymbol{\pi}_\alpha\cdot\hat{\mathbf{B}}\,\mathbf{r}_\alpha\cdot\hat{\mathbf{k}},\Omega(\mathbf{k}=0)\right]\right\rangle \quad . \qquad (34)
\end{aligned}
$$

The right-hand side of (33), with (34), is related to the variation of the average of $\Omega(\mathbf{k}=0)$ at varying volume. To prove this we proceed as in section 3 and write for a change of the boundary determined by $\delta\boldsymbol{\epsilon}$:

$$
\begin{aligned}
\delta\left[\frac{1}{V}\langle\Omega(\mathbf{k}=0)\rangle\right] &= -\delta(\log Z)\frac{1}{V}\langle\Omega(\mathbf{k}=0)\rangle \\
&\quad -\frac{\beta}{ZV}\sum_n \delta E_n\, e^{-\beta E_n}\ <\psi_n|\Omega(\mathbf{k}=0)|\psi_n> \\
&\quad -\frac{\delta V}{V^2}\,\langle\Omega(\mathbf{k}=0)\rangle + \frac{1}{ZV}\sum_n e^{-\beta E_n}\,\delta <\psi_n|\Omega(\mathbf{k}=0)|\psi_n> \quad . \qquad (35)
\end{aligned}
$$

The variations of Z and δE_n have been derived already in section 3. In the last term the variation of the eigenstates in the matrix element follows from the Schrödinger equation at constant $\bar{\mathbf{r}}_\alpha$:

$$
<\psi_m|\delta\psi_n> = \frac{1}{E_n - E_m}\ <\psi_m|\delta H|\psi_n> \quad , \qquad (36)
$$

for $n \neq m$, if we assume the spectrum to be non-degenerate. Inserting these variations in (35) one recognizes the Kubo transform of the fluctuation formula for δH and Ω. In fact, we get

$$
\delta\left[\frac{1}{V}\langle\Omega(\mathbf{k}=0)\rangle\right] = -\beta\,\mathcal{K}\frac{1}{V}\langle\Omega(\mathbf{k}=0)\;\delta H\rangle_T - \frac{\delta V}{V^2}\,\langle\Omega(\mathbf{k}=0)\rangle + \frac{1}{V}\langle\delta\Omega(\mathbf{k}=0)\rangle\,. \quad (37)
$$

The last term at the right-hand side is the average value of the variation of $\Omega(\mathbf{k}=0)$ at constant $\bar{\mathbf{r}}_\alpha$. It can easily be found for the operators of the type specified below (33). For instance, for a sum of one-particle operators of the form

$$
\Omega(\mathbf{r}) = \tfrac{1}{2}\sum_\alpha\{f(\boldsymbol{\pi}_\alpha),\delta(\mathbf{r}-\mathbf{r}_\alpha)\} \quad , \qquad (38)
$$

with $f(x)$ a polynomial of x, one finds

$$\delta\Omega(\mathbf{k}=0) = \sum_\alpha \delta\boldsymbol{\pi}_\alpha \cdot \frac{\partial}{\partial\boldsymbol{\pi}_\alpha} f(\boldsymbol{\pi}) \quad , \tag{39}$$

with

$$\delta\boldsymbol{\pi}_\alpha = -\delta\tilde{\boldsymbol{\epsilon}} \cdot \boldsymbol{\pi}_\alpha + \frac{e}{2c}[(\delta\boldsymbol{\epsilon}\cdot\mathbf{B})\wedge\mathbf{r}_\alpha - (\mathrm{tr}\,\delta\boldsymbol{\epsilon})(\mathbf{B}\wedge\mathbf{r}_\alpha)] \quad . \tag{40}$$

The left-hand side of (37) can depend on the deformation tensor only through its trace. Hence, we may choose $\delta\boldsymbol{\epsilon}$ in a way that best suits our purposes. Let us take $\delta\boldsymbol{\epsilon} = \hat{\mathbf{B}}\hat{\mathbf{k}}\delta\varepsilon$, with a scalar $\delta\varepsilon$. Then one has $\delta V = V\delta\varepsilon\cos\theta$. Furthermore, δH gets the form $-\delta\varepsilon\,\hat{\mathbf{k}}\cdot\mathsf{T}(\mathbf{k}=0)\cdot\hat{\mathbf{B}}$, as follows from (14) and (15). Finally, (39) becomes quite simple, since the terms between square brackets in (40) cancel. The final result for an operator of the form (38) is

$$\begin{aligned}\delta\left[\frac{1}{V}\langle\Omega(\mathbf{k}=0)\rangle\right] &= \beta\,\mathcal{K}\frac{1}{V}\langle\Omega(\mathbf{k}=0)\,\hat{\mathbf{k}}\cdot\mathsf{T}(\mathbf{k}=0)\cdot\hat{\mathbf{B}}\rangle_T\,\delta\varepsilon - \cos\theta\,\frac{1}{V}\langle\Omega(\mathbf{k})\rangle\,\delta\varepsilon \\ &\quad + \frac{i}{\hbar}\,\frac{1}{V}\left\langle\left[\sum_\alpha \boldsymbol{\pi}_\alpha\cdot\hat{\mathbf{B}}\,\mathbf{r}_\alpha\cdot\hat{\mathbf{k}},\Omega(\mathbf{k}=0)\right]\right\rangle\delta\varepsilon \quad .\end{aligned} \tag{41}$$

The same result is found for operators that are sums of purely configurational two-particle operators, like the potential pressure tensor.

Upon comparing (33)-(34) to (41) one arrives at a relation for $\delta\,[V^{-1}\langle\Omega(\mathbf{k}=0)\rangle]$, which can be rewritten as

$$V\frac{\partial}{\partial V}\left[\frac{1}{V}\langle\Omega(\mathbf{k}=0)\rangle\right] = -\beta q_v\,\mathcal{K}\frac{1}{V}\langle\Omega(\mathbf{k})\,Q(-\mathbf{k})\rangle_T^{(2)} \quad . \tag{42}$$

Combination with (32) gives

$$\mathcal{K}\,\frac{1}{V}\langle Q(\mathbf{k})Q(-\mathbf{k})\rangle_T^{(4)} = -\frac{1}{\beta m\omega_p^2\cos\theta}\,\frac{\partial}{\partial n}\left[\frac{1}{V}\langle\hat{\mathbf{k}}\cdot\mathsf{T}(\mathbf{k}=0)\cdot\hat{\mathbf{B}}\rangle\right] \quad . \tag{43}$$

Employing (18) we may write the right-hand side as $-(1/\beta m\omega_p^2)\partial p_B/\partial n$. Thus we have found

$$\mathcal{K}\,\frac{1}{V}\langle Q(\mathbf{k})Q(-\mathbf{k})\rangle_T^{(4)} = -\frac{1}{\beta m n\omega_p^2\kappa_T} \quad , \tag{44}$$

where the isothermal compressibility has been defined as $\kappa_T^{-1} = n(\partial p_B/\partial n)$ at constant T and B.

The relation (44) is the compressibility rule we have been after. It contains the derivative of the component of the mechanical pressure in the direction of the field. The latter is equal to the thermodynamic pressure, as we have seen in section 3. Hence, the right-hand side of (44) can be written in terms of a second derivative of the free energy per particle, as is the case for the unmagnetized plasma.

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