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Pressure and compressibility in a quantum one-component plasma

P John and L G Suttorp

Instituut voor Theoretische Fysica, Universiteit van Amsterdam, Valckenierstraat 65, 1018 XE Amsterdam, The Netherlands

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Abstract. With the help of scaling methods, a general relation is established between the thermodynamic pressure and the mechanical pressure tensor of an equilibrium one-component plasma in a magnetic field. The mechanical pressure tensor is shown to be anisotropic. A general proof of the compressibility sum rule for a magnetized quantum plasma is presented. Finally, fourth-order wavenumber inequalities for the static charge correlation function are derived.

1. Introduction

The pressure of a fluid system in equilibrium can be defined in several alternative ways. One way is via the microscopic pressure tensor, of which the divergence appears in the equation of motion for the momentum density. Performing the ensemble average, we arrive at the so-called mechanical pressure tensor.

A different standard way to define the equilibrium pressure is by taking the volume derivative of the free energy, which follows from the canonical partition function. In this way, one gets the thermodynamic pressure, which is a scalar quantity for fluid systems.

The normal way to establish a relation between the two pressures is via the virial theorem. For classical systems, the pressures turn out to be equivalent. For quantum systems, the proof of the equivalence is not so simple. There was much debate in the fifties concerning the details of the proof of the quantum-mechanical virial theorem for fluids of neutral particles with short-range interactions; however, this was eventually settled [1, 2]. For the electron gas, with long-range Coulomb interactions, the presence of the uniform background has to be taken into account [3].

When a magnetic field is present in an electron gas, the virial theorem loses its validity; this was demonstrated for the two-dimensional case in [4]. Furthermore, the mechanical pressure tensor may become anisotropic in the presence of a magnetic field, as was shown for a free electron gas in a magnetic field [5, 6].

In this paper, we will derive a general relation between the mechanical pressure tensor and the thermodynamic pressure for an equilibrium one-component quantum plasma in a magnetic field. This relation will be established with the use of scaling methods in section 3. It is valid for all densities and temperatures for which the plasma is in a fluid phase. As a result, the mechanical pressure tensor is found to be anisotropic for the interacting plasma in a magnetic field. The anisotropy will be shown to be caused by the Landau diamagnetic effect so that it is a pure quantum effect.

The existence of inequivalent pressures implies the existence of different compressibilities. In section 4, it will be demonstrated which compressibility enters the compressibility

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sum rule for the charge fluctuations. This is achieved by combining the scaling methods of section 3 and the microscopic equations of motion. For a vanishing magnetic field, the mechanical and the thermodynamic compressibilities coincide. The compressibility rule then has the same form as for a classical plasma, as was argued previously in [7]. A review of the compressibility rule for classical plasmas can be found in [8].

The compressibility rule gives information on the long-wavelength limit of the charge response function, which is an integral of the charge correlation function over imaginary times. Using inequalities derived in [9–11], one may also obtain information on the equal time or static charge correlation function in the form of upper and lower bounds. For the unmagnetized plasma, these bounds will be established in section 5.

The system we will be investigating is a quantum-mechanical plasma in a classical external magnetic field. The field is taken to be time-independent and homogeneous. The system is assumed to be in full equilibrium so that all its properties are independent of time. As a model, we will consider the one-component plasma (OCP). It consists of N interacting particles of charge e and mass m that move in a neutralizing inert background. The spin of the particles will be neglected. The background, which is assumed to be free of impurities, has a charge density $-q_V = -en = -eN/V$ where V is the volume of the system. We suppose the system to be in the fluid phase. Our treatment will take full account of the effects of quantum statistics. The results will be valid for arbitrary values of the magnetic-field strength and for any temperature and density in the fluid range.

2. Equations of motion

In this section, the equations that will be the starting point for the rest of the paper will be reviewed. The Hamiltonian of the magnetized OCP reads

$$H = \frac{1}{2m}\sum_{\alpha}\left[\boldsymbol{p}_\alpha - \frac{e}{c}\boldsymbol{A}(\boldsymbol{r}_\alpha)\right]^2 + \tfrac{1}{2}{\sum_{\alpha,\beta}}' \frac{e^2}{4\pi|\boldsymbol{r}_\alpha - \boldsymbol{r}_\beta|}$$

$$- n\sum_{\alpha}\int_V \mathrm{d}^3r\,\frac{e^2}{4\pi|\boldsymbol{r}-\boldsymbol{r}_\alpha|} + \tfrac{1}{2}n^2\int_V \mathrm{d}^3r\int_V \mathrm{d}^3r'\,\frac{e^2}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}. \tag{1}$$

Here, $\boldsymbol{p}_\alpha$ and $\boldsymbol{r}_\alpha$ are the momenta and positions of the particles and n is the number density. The vector potential $\boldsymbol{A}$ describes the magnetic field $\boldsymbol{B}$ in an arbitrary gauge. The prime at the summation indicates that the $(\alpha = \beta)$-term is excluded.

The charge density and the current density are defined by

$$Q(\boldsymbol{r}) = e\sum_{\alpha}\delta(\boldsymbol{r}-\boldsymbol{r}_\alpha) - q_V \tag{2}$$

$$\boldsymbol{J}(\boldsymbol{r}) = \frac{e}{2m}\sum_{\alpha}\{\boldsymbol{\pi}_\alpha, \delta(\boldsymbol{r}-\boldsymbol{r}_\alpha)\} \tag{3}$$

where we have introduced the mechanical momentum $\boldsymbol{\pi}_\alpha = \boldsymbol{p}_\alpha - (e/c)\boldsymbol{A}(\boldsymbol{r}_\alpha)$. The curly brackets denote the anti-commutator. The charge density and the current density are connected by the following equation of motion, which is just the continuity equation

$$\frac{\mathrm{i}}{\hbar}[H, Q(\boldsymbol{r})] = -\nabla\cdot\boldsymbol{J}(\boldsymbol{r}). \tag{4}$$

The equation of motion for the current density reads

$$\frac{\mathrm{i}}{\hbar}[H, J(r)] = -\frac{e}{m}\nabla \cdot \mathbf{T}(r) + \frac{e}{m}F(r) + \frac{e}{mc}J(r) \wedge B. \tag{5}$$

The quantities $\mathbf{T}$ and F appearing on the right-hand side are defined as follows. First, we have $\mathbf{T} := \mathbf{T}_{\text{kin}} + \mathbf{T}_{\text{pot}}$, where $\mathbf{T}_{\text{kin}}$ is the kinetic pressure tensor

$$T^{ij}_{\text{kin}}(r) = \frac{1}{2m}\sum_{\alpha}[\pi^i_\alpha \pi^j_\alpha \delta(r - r_\alpha) + \delta(r - r_\alpha)\pi^j_\alpha \pi^i_\alpha]. \tag{6}$$

The divergence of the potential pressure tensor can be written as

$$\nabla \cdot \mathbf{T}_{\text{pot}}(r) = \int_V \mathrm{d}^3r' \, \nabla_r \frac{e^2}{4\pi|r - r'|} D(r, r') \tag{7}$$

in which we introduce the abbreviation

$$D(r, r') = \sum_{\alpha,\beta}{}' \delta(r - r_\alpha)\delta(r' - r_\beta) - n\sum_\alpha \delta(r - r_\alpha) - n\sum_\beta \delta(r' - r_\beta) + n^2. \tag{8}$$

Lastly, F appearing in (5) is the force density

$$F(r) = -n\int_V \mathrm{d}^3r' \, \nabla_r \frac{e}{4\pi|r - r'|} Q(r'). \tag{9}$$

The implicit definition of the potential part of the pressure tensor can be turned into an explicit definition. The function $D(r, r')$ occurring in (7) is symmetric under an interchange of its arguments. In fact, to bring about this feature we had to split off the force density. Owing to the symmetry, we can write [12]

$$\begin{aligned}\mathbf{T}_{\text{pot}}(r) = -\tfrac{1}{2}\int_0^1 \mathrm{d}\lambda \int \mathrm{d}^3x \, \left(x\nabla_x \frac{e^2}{4\pi x}\right)\theta_V\left(r - \tfrac{1}{2}\lambda x\right)\theta_V\left(r + \left(1 - \tfrac{1}{2}\lambda\right)x\right) \\ \times D\left(r - \tfrac{1}{2}\lambda x, r + \left(1 - \tfrac{1}{2}\lambda\right)x\right)\end{aligned} \tag{10}$$

where θ_V is the characteristic function of the volume V, which is equal to 1 for arguments inside V and equals 0 elsewhere. We assume that the region V is convex, so that the potential pressure tensor vanishes outside V. If we integrate the potential part of the pressure tensor over the volume, the λ-integral drops out:

$$\int_V \mathrm{d}^3r \, \mathbf{T}_{\text{pot}}(r) = -\tfrac{1}{2}\int_V \mathrm{d}^3r \int \mathrm{d}^3x \left(x\nabla_x \frac{e^2}{4\pi x}\right)\theta_V(r)\theta_V(r + x)D(r, r + x). \tag{11}$$

Note that both the potential part and the kinetic part of the pressure tensor are symmetric.

3. Mechanical and thermodynamic pressure

In this section, we will establish a general relation between the mechanical pressure tensor and the thermodynamic pressure. The mechanical pressure tensor is the ensemble average of the microscopic pressure tensor that has been defined in the previous section in (6) and (10). The thermodynamic pressure is defined via a volume derivative of the free energy in the usual way.

To find a general relation between the two pressures, one has to write the thermodynamic pressure as the ensemble average of a microscopic quantity, like the mechanical pressure. A convenient way to achieve this is by carrying out the differentiation of the free energy through a scaling method. For neutral-particle systems with short-range interactions, this is the standard way to derive the virial theorem. A general discussion of the virial theorem in all its varieties may be found, for example, in [13]. Once the virial theorem is established, the equivalence of the mechanical pressure tensor and the thermodynamic pressure follows immediately. Along these lines, the equivalence of the two pressures for neutral-particle systems has indeed been proved [1, 2]. For systems of charged particles, however, the general argument to prove the equivalence of the two pressures cannot be taken over as such, at least not if a magnetic field is present. Nevertheless, the same scaling method can be used in this case to derive a more general relation between the two pressures, as we will hereafter show.

Let us consider a variation of the volume as follows. The boundary is scaled from $\boldsymbol{r}_{\mathrm{W}}$ to $\boldsymbol{r}_{\mathrm{W}} + \delta\boldsymbol{\epsilon}\cdot\boldsymbol{r}_{\mathrm{W}}$, where $\delta\boldsymbol{\epsilon}$ is a deformation tensor. As a result, the volume varies as $\delta V = V\,\mathrm{tr}\,\delta\boldsymbol{\epsilon}$. Furthermore, the free energy changes by an amount

$$\delta f = \frac{1}{NZ}\sum_n \delta E_n \mathrm{e}^{-\beta E_n} \tag{12}$$

where δE_n is the shift of the energy eigenvalue E_n. To determine this shift, one has to solve the Schrödinger equation for the Hamiltonian (1) with the deformed boundary conditions. Therefore, we also introduce new position variables $\boldsymbol{r}'_\alpha$ in the Schrödinger equation, such that all $\boldsymbol{r}'_\alpha$ lie inside the 'old' volume V. So

$$\boldsymbol{r}_\alpha \to \boldsymbol{r}'_\alpha = \boldsymbol{r}_\alpha - \delta\boldsymbol{\epsilon}\cdot\boldsymbol{r}_\alpha. \tag{13}$$

When we consider the energy eigenfunctions as functions of the new positions $\boldsymbol{r}'_\alpha$, we can write the change in the energy eigenvalues as

$$\delta E_n = \langle\psi_n|\delta H|\psi_n\rangle. \tag{14}$$

Here, δH is the variation of the Hamiltonian at fixed values of the position variables $\boldsymbol{r}'_\alpha$.

Under the deformation (13), the momentum scales as

$$\boldsymbol{p}_\alpha \to \boldsymbol{p}'_\alpha = \boldsymbol{p}_\alpha + \delta\tilde{\boldsymbol{\epsilon}}\cdot\boldsymbol{p}_\alpha. \tag{15}$$

If we insert the vector potential

$$\boldsymbol{A}(\boldsymbol{r}_\alpha) = \tfrac{1}{2}\boldsymbol{B}\wedge\boldsymbol{r}_\alpha + \nabla_\alpha\chi(\boldsymbol{r}_\alpha) \tag{16}$$

with an arbitrary gauge function χ, we can write the variation of the mechanical momentum according to (13) and (15) as

$$\delta\boldsymbol{\pi}_\alpha = -\delta\tilde{\boldsymbol{\epsilon}}\cdot\boldsymbol{\pi}_\alpha + \frac{e}{2c}[(\delta\boldsymbol{\epsilon}\cdot\boldsymbol{B})\wedge\boldsymbol{r}_\alpha - (\mathrm{tr}\,\delta\boldsymbol{\epsilon})\boldsymbol{B}\wedge\boldsymbol{r}_\alpha] - \frac{e}{c}\nabla_\alpha[\boldsymbol{r}_\alpha\cdot\delta\tilde{\boldsymbol{\epsilon}}\cdot\nabla_\alpha\chi(\boldsymbol{r}_\alpha)]. \tag{17}$$

The variation of the kinetic part of the Hamiltonian can then be calculated to be

$$\delta H_{\rm kin} = -\delta\epsilon : \int_V \mathrm{d}^3 r\, \mathsf{T}_{\rm kin}(\boldsymbol{r}) - (\mathrm{tr}\,\delta\epsilon)\boldsymbol{B}\cdot\int_V \mathrm{d}^3 r\, \boldsymbol{M}(\boldsymbol{r}) + \boldsymbol{B}\cdot\delta\tilde{\epsilon}\cdot\int_V \mathrm{d}^3 r\, \boldsymbol{M}(\boldsymbol{r}) - \frac{\mathrm{i}e}{\hbar c}\sum_\alpha [H, \boldsymbol{r}_\alpha\cdot\delta\tilde{\epsilon}\cdot\nabla_\alpha\chi(\boldsymbol{r}_\alpha)] \tag{18}$$

where we recognize the kinetic pressure tensor and where we have introduced the microscopic magnetization density $\boldsymbol{M}$

$$\boldsymbol{M}(\boldsymbol{r}) = \frac{e}{4mc}\sum_\alpha \{\boldsymbol{r}_\alpha \wedge \boldsymbol{\pi}_\alpha, \delta(\boldsymbol{r}-\boldsymbol{r}_\alpha)\}. \tag{19}$$

Along similar lines, one can easily show that the variation of the potential part of the Hamiltonian yields

$$\delta H_{\rm pot} = -\delta\epsilon : \int_V \mathrm{d}^3 r\, \mathsf{T}_{\rm pot}(\boldsymbol{r}). \tag{20}$$

Substituting (18) and (20) in the expression for the variation of the free energy (12) with (14), we find that the gauge-dependent term in (18) drops out, so that we get

$$\delta f = -v\delta\epsilon : (\bar{\mathsf{P}} - \boldsymbol{B}\bar{\mathsf{M}} + \boldsymbol{B}\cdot\bar{\mathsf{M}}\mathsf{U}) \tag{21}$$

where U is the unit tensor and $v = V/N$ is the volume per particle. Furthermore, we have introduced the volume-averaged mechanical pressure tensor $\bar{\mathsf{P}}$

$$\bar{\mathsf{P}} := V^{-1}\int \mathrm{d}^3 r\, \langle \mathsf{T}(\boldsymbol{r})\rangle \equiv V^{-1}\langle \mathsf{T}(\boldsymbol{k}=0)\rangle$$

and the volume-averaged macroscopic magnetization density $\bar{\mathsf{M}}$

$$\bar{\mathsf{M}} := V^{-1}\int \mathrm{d}^3 r\, \langle \boldsymbol{M}(\boldsymbol{r})\rangle \equiv V^{-1}\langle \boldsymbol{M}(\boldsymbol{k}=0)\rangle.$$

Clearly, the volume-averaged mechanical pressure tensor is equal to the uniform bulk value of the mechanical pressure tensor $\langle \mathsf{T}(\boldsymbol{r})\rangle$, where $\boldsymbol{r}$ is an arbitrary position in the bulk, since surface effects in the pressure will only be manifest in a thin layer near the boundary. On the other hand, the volume-averaged magnetization density is certainly not equal to the bulk value of the macroscopic magnetization density $\langle \boldsymbol{M}(\boldsymbol{r})\rangle$. In fact, the latter vanishes. All contributions to the total macroscopic magnetization and, hence, to its volume average originate from a thin layer near the boundary, where considerable macroscopic electric currents circulate. These currents give rise to the Landau diamagnetic effect in the system.

For fluid systems, the free energy per particle should be dependent on the volume of the system only and not on its shape. So, the variation of the free energy should only depend on the trace of the deformation tensor $\delta\epsilon$. Since one has $\delta v = v\,\mathrm{tr}\,\delta\epsilon$, we have found

$$\bar{\mathsf{P}} - \boldsymbol{B}\bar{\mathsf{M}} + \boldsymbol{B}\cdot\bar{\mathsf{M}}\mathsf{U} = p\mathsf{U}. \tag{22}$$

As a consequence, we can write the bulk mechanical pressure tensor as the sum of an isotropic part and an anisotropic part

$$\bar{\mathsf{P}} = p_{\rm B}\mathsf{U} - \tfrac{3}{2}\delta p_{\rm B}(\mathsf{U} - \hat{\boldsymbol{B}}\hat{\boldsymbol{B}}) \tag{23}$$

where $\hat{B}$ is a unit vector in the direction of the field and where the scalar coefficients are

$$p_{\mathrm{B}} = p \tag{24}$$

$$\delta p_{\mathrm{B}} = \tfrac{2}{3} B \cdot \bar{\mathbf{M}} \,. \tag{25}$$

We have proved that the (volume-averaged or bulk) mechanical pressure tensor is indeed anisotropic. It consists of an isotropic part that is trivially related to the thermodynamic pressure and an anisotropic part that is determined by the (volume-averaged) macroscopic magnetization density. For a diamagnetic response δp_{B} is negative. This means that the pressure in a direction transverse to the magnetic field is larger than that in a direction parallel to the field.

The relation between the mechanical and the thermodynamic pressure that has been obtained above is completely general. It is valid both for the interacting and the free electron gas in a magnetic field. For the latter rather special case, the anisotropy in the mechanical pressure and its relation to the magnetization has been found before via an explicit calculation [5, 6]. It should be noted that for classical systems in equilibrium, the pressure is always isotropic due to the Bohr–van Leeuwen theorem. Hence, the anisotropy for an equilibrium plasma found here is a pure quantum effect. Of course, for magnetized plasmas out of equilibrium, one often encounters an anisotropic pressure tensor, even in the classical case. Examples of such systems are well known from Vlasov theory. However, the anisotropy in that case has an altogether different cause. It can be due, for instance, to the occurrence of different temperatures for the velocity distribution functions in the directions parallel and orthogonal to the magnetic field, as may be the case if collisions are rare.

4. Compressibility relation

In this section, we shall prove a relation between the derivative of the ensemble average of an operator with respect to the density and the (Kubo-transformed) correlation function of the same operator and the charge. This relation enables us to find exact sum rules for the correlation functions, which can serve as touchstones to assess approximations used in obtaining frequency-dependent correlation functions. Furthermore, they are essential in deriving the long-wavelength collective modes of the system via the Mori–Zwanzig projection method [14].

The relation we are after will be established via the scaling arguments used in the previous section. With the help of this relation, we will be able to find the fourth-order term in the wavenumber expansion of the Kubo-transformed charge autocorrelation function $\mathcal{K}V^{-1}\langle Q(\boldsymbol{k})Q(-\boldsymbol{k})\rangle_{\mathrm{T}}$, with $\mathcal{K}$ denoting the Kubo transform and T denoting truncation. It has been argued that this fourth-order term has the same form as the fourth-order term in the structure factor of the classical OCP, at least for the unmagnetized plasma [7].

We start with an identity for an arbitrary local operator Ω:

$$\mathcal{K}\frac{1}{V}\langle\Omega(\boldsymbol{k})Q(-\boldsymbol{k})\rangle_{\mathrm{T}}^{(2)} = \frac{1}{\hbar\beta\omega_{\mathrm{p}}^{2}\cos\vartheta}\frac{1}{V}\langle[\Omega(\boldsymbol{k}), \boldsymbol{J}(-\boldsymbol{k})\cdot\hat{\boldsymbol{B}}]\rangle^{(1)}$$
$$\qquad - \frac{e}{m\omega_{\mathrm{p}}^{2}\cos\vartheta}\mathcal{K}\frac{1}{V}\langle\Omega(\boldsymbol{k})\hat{\boldsymbol{k}}\cdot\mathbf{T}(-\boldsymbol{k})\cdot\hat{\boldsymbol{B}}\rangle_{\mathrm{T}}^{(0)}. \tag{26}$$

The bracketed superscripts (n) mean that we consider the coefficient of the nth term in the wavenumber expansion. Furthermore, ω_{p} is the plasma frequency and ϑ the angle between the wavevector and the magnetic field. Identity (26) can be derived [15] from the Fourier-transformed counterparts of the equations of motion (4) and (5). Multiplying these equations with an operator Ω and taking the Kubo-transformed equilibrium average, one may employ an identity valid for all operators A and B

$$\mathcal{K}\frac{1}{V}\langle[H, A(\boldsymbol{k})]B(-\boldsymbol{k})\rangle_T = \beta^{-1}\frac{1}{V}\langle[B(-\boldsymbol{k}), A(\boldsymbol{k})]\rangle. \tag{27}$$

Upon solving the resulting equations for $\mathcal{K}\frac{1}{V}\langle\Omega(\boldsymbol{k})Q(-\boldsymbol{k})\rangle_{\mathrm{T}}^{(2)}$ in successive order of the wavenumber, we end up with (26).

The commutator on the right-hand side of (26) can be evaluated explicitly for operators of the type

$$\Omega_{\mathrm{kin}}(\boldsymbol{r}) = \tfrac{1}{2}\sum_{\alpha}\{f(\boldsymbol{\pi}_\alpha), \delta(\boldsymbol{r}-\boldsymbol{r}_\alpha)\} \tag{28}$$

and

$$\Omega_{\mathrm{pot}}(\boldsymbol{r}) = \int_0^1 \mathrm{d}\lambda \int \mathrm{d}^3x\, f(\boldsymbol{x})\theta_V(\boldsymbol{r}-\tfrac{1}{2}\lambda\boldsymbol{x})\theta_V(\boldsymbol{r}+(1-\tfrac{1}{2}\lambda)\boldsymbol{x})D(\boldsymbol{r}-\tfrac{1}{2}\lambda\boldsymbol{x}, \boldsymbol{r}+(1-\tfrac{1}{2}\lambda)\boldsymbol{x}). \tag{29}$$

These are one-particle operators depending on the (mechanical) momentum and two-particle configurational operators with background terms and a λ-integration, respectively. In the former, one has to properly symmetrize the π factors and the delta function. Both the charge density and the current density are of the form Ω_{kin}, while the microscopic pressure tensor is the sum of operators Ω_{kin} and Ω_{pot}.

For the calculation of the commutator of Ω_{kin} with $\boldsymbol{J}$, we use the identity

$$[\boldsymbol{\pi}_\alpha \cdot \hat{\boldsymbol{B}}, f(\boldsymbol{\pi}_\alpha)] = 0 \tag{30}$$

which follows from $[\pi_\alpha^i, \pi_\alpha^j] = (\mathrm{i}e\hbar/c)\epsilon^{ijk}B^k$. Then, one finds

$$\begin{aligned}\frac{1}{V}\langle[\Omega_{\mathrm{kin}}(\boldsymbol{k}), \boldsymbol{J}(-\boldsymbol{k})\cdot\hat{\boldsymbol{B}}]\rangle &= \frac{e\hbar}{m}k\cos\vartheta\frac{1}{V}\langle\Omega_{\mathrm{kin}}(\boldsymbol{k}=0)\rangle\\ &\quad - \frac{e}{4mV}\left\langle\sum_\alpha \hbar\boldsymbol{k}\cdot\hat{\boldsymbol{B}}\left[\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}_\alpha}, \left[\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}_\alpha}, f(\boldsymbol{\pi}_\alpha)\right]\right]\right\rangle\\ &\quad - \frac{e}{4mV}\left\langle\sum_\alpha\left\{\boldsymbol{\pi}_\alpha\cdot\hat{\boldsymbol{B}}, \left\{\left[\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}_\alpha}, f(\boldsymbol{\pi}_\alpha)\right], \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}_\alpha}\right\}\right\}\right\rangle.\end{aligned} \tag{31}$$

In leading (first) order in k, the second term on the right-hand side vanishes and we find for operators $\Omega(\boldsymbol{k}) = \Omega_{\mathrm{kin}}(\boldsymbol{k})$

$$\frac{1}{V}\langle[\Omega(\boldsymbol{k}), \boldsymbol{J}(-\boldsymbol{k})\cdot\hat{\boldsymbol{B}}]\rangle^{(1)} = \frac{e\hbar}{m}\cos\vartheta\frac{1}{V}\langle\Omega(\boldsymbol{k}=0)\rangle - \frac{\mathrm{i}e}{m}\frac{1}{V}\left\langle\left[\sum_\alpha \boldsymbol{\pi}_\alpha\cdot\hat{\boldsymbol{B}}\boldsymbol{r}_\alpha\cdot\hat{\boldsymbol{k}}, \Omega(\boldsymbol{k}=0)\right]\right\rangle. \tag{32}$$

In particular, if we take $\Omega_{\rm kin}(\boldsymbol{k})$ to be the kinetic part of the pressure tensor, we get

$$\frac{1}{V}\langle[\mathsf{T}_{\rm kin}(\boldsymbol{k}),\, \boldsymbol{J}(-\boldsymbol{k})\cdot\hat{\boldsymbol{B}}]\rangle^{(1)} = \frac{e\hbar}{m}\frac{1}{V}\left[\langle\mathsf{T}_{\rm kin}(\boldsymbol{k}=0)\rangle\hat{\boldsymbol{k}}\cdot\hat{\boldsymbol{B}} + \hat{\boldsymbol{k}}\hat{\boldsymbol{B}}\cdot\langle\mathsf{T}_{\rm kin}(\boldsymbol{k}=0)\rangle + \hat{\boldsymbol{B}}\cdot\langle\mathsf{T}_{\rm kin}(\boldsymbol{k}=0)\rangle\hat{\boldsymbol{k}}\right]. \tag{33}$$

In the first instance, the evaluation of the commutator of $\Omega_{\rm pot}$ with the current density leads to

$$\begin{aligned}\frac{1}{V}\langle[\Omega_{\rm pot}(\boldsymbol{k}),\, \boldsymbol{J}(-\boldsymbol{k})\cdot\hat{\boldsymbol{B}}]\rangle &= \frac{e\hbar}{m}\int_0^1 {\rm d}\lambda \int {\rm d}^3r \int {\rm d}^3x \left\{\left[(1-\tfrac{1}{2}\lambda){\rm e}^{-{\rm i}(\lambda/2)\boldsymbol{k}\cdot\boldsymbol{x}} + \tfrac{1}{2}\lambda{\rm e}^{{\rm i}(1-(\lambda/2))\boldsymbol{k}\cdot\boldsymbol{x}}\right]\boldsymbol{k}\cdot\hat{\boldsymbol{B}}f(\boldsymbol{x})\right.\\ &\quad\left. - {\rm i}\left[{\rm e}^{-{\rm i}(\lambda/2)\boldsymbol{k}\cdot\boldsymbol{x}} - {\rm e}^{{\rm i}(1-(\lambda/2))\boldsymbol{k}\cdot\boldsymbol{x}}\right]\hat{\boldsymbol{B}}\cdot\nabla_{\boldsymbol{x}}f(\boldsymbol{x})\right\}\\ &\quad\times\theta_V(\boldsymbol{r}-\tfrac{1}{2}\lambda\boldsymbol{x})\theta_V(\boldsymbol{r}+(1-\tfrac{1}{2}\lambda)\boldsymbol{x})\frac{1}{V}\langle D(\boldsymbol{r}-\tfrac{1}{2}\lambda\boldsymbol{x},\boldsymbol{r}+(1-\tfrac{1}{2}\lambda)\boldsymbol{x})\rangle. \end{aligned} \tag{34}$$

In zeroth order in k, the commutator vanishes as expected. In first order the commutator reads

$$\begin{aligned}\frac{1}{V}\langle[\Omega_{\rm pot}(\boldsymbol{k}),\, \boldsymbol{J}(-\boldsymbol{k})\cdot\hat{\boldsymbol{B}}]\rangle^{(1)} &= \frac{e\hbar}{m}\cos\vartheta\frac{1}{V}\langle\Omega_{\rm pot}(\boldsymbol{k}=0)\rangle - \frac{e\hbar}{m}\int_0^1 {\rm d}\lambda\int {\rm d}^3r\int {\rm d}^3x\,\hat{\boldsymbol{k}}\cdot\boldsymbol{x}[\hat{\boldsymbol{B}}\cdot\nabla_{\boldsymbol{x}}f(\boldsymbol{x})]\\ &\quad\times\theta_V(\boldsymbol{r}-\tfrac{1}{2}\lambda\boldsymbol{x})\theta_V(\boldsymbol{r}+(1-\tfrac{1}{2}\lambda)\boldsymbol{x})\frac{1}{V}\langle D(\boldsymbol{r}-\tfrac{1}{2}\lambda\boldsymbol{x},\boldsymbol{r}+(1-\tfrac{1}{2}\lambda)\boldsymbol{x})\rangle. \end{aligned} \tag{35}$$

We can write the last term as the average of the commutator of $\Omega_{\rm pot}(\boldsymbol{k}=0)$ with $\sum_\alpha \boldsymbol{\pi}_\alpha\cdot\hat{\boldsymbol{B}}\boldsymbol{r}_\alpha\cdot\hat{\boldsymbol{k}}$, as one can verify by explicit calculation. So one ends up with expression (32) again, which, hence, is valid for both types of operators.

Let us now consider the variation of the average of an operator $\Omega_{\rm kin}$ or $\Omega_{\rm pot}$ for a changing volume. After rescaling the particle positions and momenta, as in the previous section, the Hamiltonian H is replaced by $H+\delta H$. Since $\langle\Omega\rangle = {\rm tr}(\rho\Omega)$, with the density operator ρ defined as $\rho = \exp(-\beta H)/\,{\rm tr}[\exp(-\beta H)]$, we see that the rescaling amounts to replacing H by $H+\delta H$ and Ω by $\Omega+\delta\Omega$. Using a well known Kubo formula to rewrite the 'new' density operator, we find

$$\delta\left[\frac{1}{V}\langle\Omega(\boldsymbol{k}=0)\rangle\right] = -\beta\mathcal{K}\frac{1}{V}\langle\Omega(\boldsymbol{k}=0)\delta H\rangle_{\rm T} - \frac{\delta V}{V^2}\langle\Omega(\boldsymbol{k}=0)\rangle + \frac{1}{V}\langle\delta\Omega(\boldsymbol{k}=0)\rangle \tag{36}$$

where the second term on the right-hand side arises from varying the factor V^{-1}.

Evaluation of the variation of the operator $\Omega(\boldsymbol{k}=0)$ gives, for momentum-dependent operators,

$$\delta\Omega_{\rm kin}(\boldsymbol{k}=0) = \sum_\alpha \delta\boldsymbol{\pi}_\alpha\cdot\frac{\partial}{\partial\boldsymbol{\pi}_\alpha}f(\boldsymbol{\pi}_\alpha) \tag{37}$$

where the terms in the derivative should be ordered in such a way that each factor π_α in turn is replaced by $\delta\pi_\alpha$. The variation $\delta\pi_\alpha$ of the mechanical momentum is given in (17). The average of the variation of operators $\Omega_{\rm kin}$, as given in (37), can be written as a commutator:

$$\frac{1}{V}\langle\delta\Omega_{\rm kin}(k=0)\rangle = \frac{\mathrm{i}}{\hbar}\frac{1}{V}\left\langle\left[\sum_\alpha r_\alpha\cdot\delta\tilde{\epsilon}\cdot p_\alpha, \Omega_{\rm kin}(k=0)\right]\right\rangle. \tag{38}$$

If we substitute (38) and (18)–(20) in (36), we see that the gauge-dependent part χ drops out. One gets for $\Omega = \Omega_{\rm kin}$

$$\begin{aligned}\delta\left[\frac{1}{V}\langle\Omega(k=0)\rangle\right] &= \beta K\frac{1}{V}\langle\Omega(k=0)\\ &\quad\times[\delta\epsilon : \mathsf{T}(k=0) - B\cdot\delta\tilde{\epsilon}\cdot M(k=0) + (\operatorname{tr}\delta\epsilon)B\cdot M(k=0)]\rangle_{\rm T}\\ &\quad-\frac{\delta V}{V^2}\langle\Omega(k=0)\rangle + \frac{\mathrm{i}}{\hbar}\frac{1}{V}\left\langle\left[\sum_\alpha r_\alpha\cdot\delta\tilde{\epsilon}\cdot\left(\pi_\alpha + \frac{e}{2c}B\wedge r_\alpha\right), \Omega(k=0)\right]\right\rangle.\end{aligned} \tag{39}$$

The variation of configurational operators $\Omega_{\rm pot}$ can be found directly by rescaling both r_α, x and r in the way given in (13). It reads

$$\begin{aligned}\frac{1}{V}\langle\delta\Omega_{\rm pot}(k=0)\rangle &= \int_0^1 \mathrm{d}\lambda\int\mathrm{d}^3r\int\mathrm{d}^3x\,[x\cdot\delta\tilde{\epsilon}\cdot\nabla_x f(x)]\theta_V(r-\tfrac{1}{2}\lambda x)\theta_V(r+(1-\tfrac{1}{2}\lambda)x)\\ &\quad\times\frac{1}{V}\langle D(r-\tfrac{1}{2}\lambda x, r+(1-\tfrac{1}{2}\lambda)x)\rangle.\end{aligned} \tag{40}$$

Just as in the calculation of the commutator of the current density with $\Omega_{\rm pot}$, we can rewrite this last equation as a commutator:

$$\frac{1}{V}\langle\delta\Omega_{\rm pot}(k=0)\rangle = \frac{\mathrm{i}}{\hbar}\frac{1}{V}\left\langle\left[\sum_\alpha r_\alpha\cdot\delta\tilde{\epsilon}\cdot\pi_\alpha, \Omega_{\rm pot}(k=0)\right]\right\rangle. \tag{41}$$

Substituting (41) and (18)–(20) in (36), we see that the gauge-dependent part χ drops out again. We can write the commutator in the last equation in the same way as the commutator appearing in the last term of (39), since the extra term depends only on the position. Therefore, it commutes with $\Omega_{\rm pot}$ and we find that expression (39) is valid for both types of operators.

The variation of the volume-averaged equilibrium value of a local operator Ω, as given by (39), can only depend on the change of the density (or the volume) and not on the change in shape of the system. Hence, the right-hand side should depend on the deformation tensor through its trace only. Therefore, we may choose $\delta\epsilon$ in a convenient way. Let us take $\delta\epsilon = \hat{B}\hat{k}\delta\epsilon$ with a scalar $\delta\epsilon$. With this choice, the field-dependent terms drop out in (39). The final result is then

$$\begin{aligned}\delta\left[\frac{1}{V}\langle\Omega(k=0)\rangle\right] &= \beta K\frac{1}{V}\langle\Omega(k=0)\hat{k}\cdot\mathsf{T}(k=0)\cdot\hat{B}\rangle_{\rm T}\delta\epsilon - \cos\vartheta\frac{1}{V}\langle\Omega(k=0)\rangle\delta\epsilon\\ &\quad+\frac{\mathrm{i}}{\hbar}\frac{1}{V}\left\langle\left[\sum_\alpha\pi_\alpha\cdot\hat{B}r_\alpha\cdot\hat{k}, \Omega(k=0)\right]\right\rangle\delta\epsilon\end{aligned} \tag{42}$$

valid for both types of operators.

Using (26), (32) and (42), we arrive at an expression for the variation of an operator which can be rewritten as

$$\frac{\partial}{\partial n}\left[\frac{1}{V}\langle\Omega(\boldsymbol{k}=0)\rangle\right]=\beta e\mathcal{K}\frac{1}{V}\langle\Omega(\boldsymbol{k})Q(-\boldsymbol{k})\rangle_{\mathrm{T}}^{(2)}. \tag{43}$$

This is a general expression for the derivative of the ensemble average of a volume-averaged operator with respect to the density. On the right-hand side, the Kubo-transformed correlation function for the operator and the second-order wavenumber charge density appear. For a classical one-component plasma, a similar relation was derived on the basis of identities for configurational correlation functions [16]. The scaling method described above can be applied to the classical case as well.

Relation (43) may be called the generalized Stillinger–Lovett relation. In fact, as an example of the use of (43), one may substitute $\Omega(\boldsymbol{k})=Q(\boldsymbol{k})+eN\delta_{\boldsymbol{k},0}$. In that case, the derivative on the left-hand side gives a trivial result. As a consequence, one recovers the well known Stillinger–Lovett relation for the second-order term in the wavenumber expansion of the Kubo-transformed charge autocorrelation function

$$\mathcal{K}\frac{1}{V}\langle Q(\boldsymbol{k})Q(-\boldsymbol{k})\rangle_{\mathrm{T}}^{(2)}=\beta^{-1}. \tag{44}$$

The general relation found above can also be used to obtain a result for the fourth-order wavenumber charge autocorrelation function. In fact, employing the identity

$$\mathcal{K}\frac{1}{V}\langle Q(\boldsymbol{k})Q(-\boldsymbol{k})\rangle_{\mathrm{T}}^{(4)}=-\frac{e}{m\omega_{\mathrm{p}}^{2}\cos\vartheta}\mathcal{K}\frac{1}{V}\langle\hat{\boldsymbol{k}}\cdot\mathsf{T}(\boldsymbol{k})\cdot\hat{\boldsymbol{B}}Q(-\boldsymbol{k})\rangle_{\mathrm{T}}^{(2)} \tag{45}$$

which can be derived [15] from the equations of motion in a similar way as (26), we can write the fourth-order term of the charge autocorrelation function as

$$\mathcal{K}\frac{1}{V}\langle Q(\boldsymbol{k})Q(-\boldsymbol{k})\rangle_{\mathrm{T}}^{(4))}=-\frac{1}{\beta m\omega_{\mathrm{p}}^{2}\cos\vartheta}\frac{\partial}{\partial n}\left[\frac{1}{V}\langle\hat{\boldsymbol{k}}\cdot\mathsf{T}(\boldsymbol{k}=0)\cdot\hat{\boldsymbol{B}}\rangle\right]. \tag{46}$$

With the use of (23), we may transform the right-hand side to $-(1/\beta m\omega_{\mathrm{p}}^{2})\partial p_{\mathrm{B}}/\partial n$. So we have found

$$\mathcal{K}\frac{1}{V}\langle Q(\boldsymbol{k})Q(-\boldsymbol{k})\rangle_{\mathrm{T}}^{(4)}=-\frac{1}{\beta n m\omega_{\mathrm{p}}^{2}\kappa_{T}} \tag{47}$$

where the isothermal compressibility is defined as $\kappa_{T}^{-1}=n(\partial p_{\mathrm{B}}/\partial n)$ at constant B and β. The last equation is the compressibility sum rule we wanted to derive. It contains the derivative of the component of the volume-averaged mechanical pressure tensor in the direction of the field. The latter is equal to the thermodynamic pressure, as we have seen in (24). Hence, the fourth-order term in the wavenumber expansion of the Kubo-transformed charge autocorrelation function has indeed the same form as the fourth-order term in the structure factor of the classical one-component plasma. It should be stressed that the relation (47) is valid for an equilibrium magnetized quantum plasma at arbitrary density and temperature, at least if the plasma is in a fluid phase.

As a further example of the use of (43), one may take for $\Omega(\boldsymbol{k})$ the Fourier-transformed energy density $E(\boldsymbol{k})$. One finds

$$\mathcal{K}\frac{1}{V}\langle E(\boldsymbol{k})Q(-\boldsymbol{k})\rangle_{\mathrm{T}}^{(2)} = \beta^{-1}\left(\frac{\partial e_V}{\partial q_V}\right)_{B,\beta} \tag{48}$$

where $e_V = V^{-1}\langle E(\boldsymbol{k}=0)\rangle$ is the energy density.

Both (47) and (48) are useful for the derivation of the long-wavelength collective modes. In fact, the amplitudes of these modes are linear combinations of $Q(\boldsymbol{k})$, $\boldsymbol{J}(\boldsymbol{k})$ and $E(\boldsymbol{k})$. In deriving the modes by means of the projection-operator technique, one needs the inner products of these quantities that are defined as Kubo-transformed correlation functions [14].

5. Inequalities for the static charge correlation function

In the previous section, we derived an expression for the fourth-order term in the Kubo-transformed charge correlation function. With the use of this expression, we will show how information on the static charge correlation function, that is at imaginary time $\tau = 0$, can be obtained as well.

We will derive our result by using general inequalities derived in [9–11]. In these papers, the authors derived upper [9] and lower bounds [10, 11] for the static correlation function of general operators in terms of the static response function and moments of the spectral function. This is achieved as follows. One starts with the observation that the moments, the static correlation function and the static response function can all be written as an integral containing the spectral function and some other function. Knowing this, one can find constraints on the static correlation function in terms of suitable linear combinations of the moments and the static response function. In the mathematical literature, this is known as the generalized moment problem for Chebyshev–Markov systems.

Written in a form suitable for our purposes, the inequalities for the static charge autocorrelation function read

$$\mathcal{K}\frac{1}{V}\langle Q(\boldsymbol{k})Q(-\boldsymbol{k})\rangle_{\mathrm{T}} + \frac{1}{\beta\lambda^2}[\tfrac{1}{2}\lambda\coth(\tfrac{1}{2}\lambda) - 1]S_1 \leqslant \frac{1}{V}\langle[Q(\boldsymbol{k})]_{\tau=0}Q(-\boldsymbol{k})\rangle_{\mathrm{T}}$$
$$\leqslant \tfrac{1}{2}\mu\coth(\tfrac{1}{2}\mu)\mathcal{K}\frac{1}{V}\langle Q(\boldsymbol{k})Q(-\boldsymbol{k})\rangle_{\mathrm{T}} \tag{49}$$

where

$$S_n = \beta^{n+1}(-1)^n\frac{1}{V}\langle[[H,[H,\ldots,[H,Q(\boldsymbol{k})]\ldots],Q(-\boldsymbol{k})]\rangle \qquad n = 1, 3, 5, \ldots \tag{50}$$

$$\lambda = \sqrt{S_3/S_1} \tag{51}$$

$$\mu = \sqrt{S_1/[\beta\mathcal{K}V^{-1}\langle Q(\boldsymbol{k})Q(-\boldsymbol{k})\rangle_{\mathrm{T}}]}. \tag{52}$$

In (50), an n-fold repeated commutator with the Hamiltonian appears.

We want to use the inequalities for small values of the wavenumber. Hence, we need the small-wavenumber expansions of the various quantities in the upper and the lower bounds. From the results of the previous section, we know

$$\mathcal{K}\frac{1}{V}\langle Q(\boldsymbol{k})Q(-\boldsymbol{k})\rangle_{\mathrm{T}} = \beta^{-1}k^2 - \frac{k^4}{nk_{\mathrm{D}}^2\kappa_T} + \cdots \tag{53}$$

where k_D is the Debye wavevector, $k_D^2 = ne^2\beta$. This expansion has the same form, independent of the magnetic field. The moment S_1 can be evaluated in closed form:

$$S_1 = \beta^2\hbar^2\omega_p^2k^2 \qquad \forall\, k. \tag{54}$$

It is likewise independent of the magnetic field. The next moment S_3, however, does depend on the magnetic field. If the magnetic field vanishes, it has the expansion

$$S_3 = \beta^4\hbar^4\left[\omega_p^4k^2 + \frac{2\omega_p^2}{nm}k^4\left(e_V^{\mathrm{kin}} + \frac{2}{15}e_V^{\mathrm{pot}}\right) + \cdots\right] \tag{55}$$

where e_V^{kin} and e_V^{pot} are the kinetic- and the potential-energy density, respectively. For non-vanishing magnetic field, the leading-order terms already have a different form:

$$S_3 = \beta^4\hbar^4\omega_p^2[\omega_p^2 + \omega_c^2\sin^2\vartheta]k^2 + \cdots \tag{56}$$

where ω_c is the cyclotron frequency.

If we substitute the expressions (53)–(55) for the unmagnetized case in (49) and compare the terms in order k^2, we find that in this order the inequalities become an equality because the upper and lower bounds merge

$$\frac{1}{V}\langle Q(\boldsymbol{k})Q(-\boldsymbol{k})\rangle_{\mathrm{T}}^{(2)} = \tfrac{1}{2}\hbar\omega_p\coth\left(\frac{\beta\hbar\omega_p}{2}\right). \tag{57}$$

This confirms what is known already [7]. On the other hand, substituting (56) instead of (55), one finds that for the magnetized OCP, the bounds do not merge in second order of k. One is left with a rather uninteresting inequality. In fact, the static charge autocorrelation function in second order is known already [15].

The fact that the upper and lower bounds in second order coincide for the unmagnetized OCP implies that a non-trivial inequality for the fourth-order static correlation function can be obtained. One finds

$$-\frac{1}{nk_D^2\kappa_T} + \frac{2}{\beta nm\omega_p^2}\left(e_V^{\mathrm{kin}} + \frac{2}{15}e_V^{\mathrm{pot}}\right)\mathcal{F}(\beta\hbar\omega_p) \leqslant \frac{1}{V}\langle[Q(\boldsymbol{k})]_{\tau=0}Q(-\boldsymbol{k})\rangle_{\mathrm{T}}^{(4)}$$
$$\leqslant -\frac{1}{nk_D^2\kappa_T} + \frac{1}{nk_D^2\kappa_T}\mathcal{F}(\beta\hbar\omega_p). \tag{58}$$

Here, we have introduced the function $\mathcal{F}(x) = 1 - \mathcal{G}(x) + \frac{1}{2}x\mathcal{G}'(x)$, with $\mathcal{G}(x) = \frac{x}{2}\coth(\frac{x}{2})$. Note that $\mathcal{F}$ is negative definite. Since the function $\mathcal{F}(x)$ is of order x^4 for small x, we find up to order $\hbar^3$

$$\frac{1}{V}\langle[Q(\boldsymbol{k})]_{\tau=0}Q(-\boldsymbol{k})\rangle_{\mathrm{T}}^{(4)} = -\frac{1}{nk_D^2\kappa_T} \tag{59}$$

which is equal to the result for the classical OCP.

In higher orders of $\hbar$, the inequalities (58) give bounds for the static charge correlation function. In order for these bounds to be consistent, another inequality, which involves the kinetic-energy density, the potential-energy density and the compressibility, has to be satisfied, namely

$$\frac{2}{nm\omega_{\mathrm{p}}^2}\left(e_V^{\mathrm{kin}}+\frac{2}{15}e_V^{\mathrm{pot}}\right)\geqslant\frac{\beta}{nk_{\mathrm{D}}^2\kappa_{\mathrm{T}}}. \tag{60}$$

The validity of this inequality can be established by noting that $\mathcal{K}(1/V)\langle Q(\boldsymbol{k})Q(-\boldsymbol{k})\rangle_{\mathrm{T}}$, S_1 and S_3 are moments of a positive spectral function. The Schwarz inequality gives

$$\beta\mathcal{K}\frac{1}{V}\langle Q(\boldsymbol{k})Q(-\boldsymbol{k})\rangle_{\mathrm{T}}S_3\geqslant[S_1]^2 \tag{61}$$

which leads to (60).

The static charge correlation function for a quantum OCP in equilibrium is known in an approximate form only, on the basis of more or less drastic assumptions. The inequalities (58) for the Fourier-transformed static charge correlation function in fourth order of the wavenumber are rigorous bounds, which are useful as conditions that must necessarily be fulfilled by any approximate expression for the static correlation function in order to be internally consistent. As such, the inequalities can serve as a tool in assessing the validity of a phenomenological or fundamental approach that leads to such an approximate version of the static correlation function.

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