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LETTER TO THE EDITOR

The third sum rule and the 'local mean-field theory' in a two-component quantum plasma

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Abstract. It is proved that the 'local mean-field theory' in a two-component quantum plasma never satisfies the perfect screening sum rule and the third sum rule simultaneously unless the 'local field corrections' depend on frequency.

The so called 'local mean-field theory' (LFT), as is well known, gives a useful framework for the treatment of correlation effects. Though this theory contains unknown quantities, namely, particle momentum distribution function and 'local field correction', the framework itself is never an approximation. In the following, the exact expression of the third sum rule for the spectral function of a charge-density response function in a two-component quantum plasma will be presented with emphasis on the existence of a singular term and it will be proved that no LFT with frequency-indepenent 'local field corrections' satisfies the perfect screening sum rule and the third sum rule simultaneously. This discussion is similar to that of Goodman and Sjölander (1973), Sjölander (1974) in a uniform electron liquid with positive background.

Let us consider a uniform, non-relativistic quantum plasma which is neutral as a whole and contained in a large box of unit volume with periodic boundary condition. Let average number density, mass, charge, and magnitude of spin of i species of particle be n_i, m_i, e_i and σ_i, respectively, where $i=1, 2$. When a fictitious external electric field with wavevector $\boldsymbol{q}$ and frequency ω coupling only with j species of particles is applied adiabatically, the linear response of the charge density of i species of particles is described by $D^{\mathrm{r}}_{ij}(\boldsymbol{q}, \omega)$ which is the Fourier transform of the retarded-response function defined as

$$D^{\mathrm{r}}_{ij}(\boldsymbol{q}, t-t') = -\mathrm{i}\theta(t-t')\langle[\rho_i(\boldsymbol{q}, t), \rho_j^{\dagger}(\boldsymbol{q}, t')]\rangle.$$

In the above expression, $\langle\ldots\rangle$ means the canonical ensemble average and $\rho_i(\boldsymbol{q}, t)$ is the Heisenberg representation of the $\boldsymbol{q}$th charge-density fluctuation operator of i component, $\rho_i(\boldsymbol{q})$.

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The third frequency moment $M_{3,ij}(q)$ of $v(q)D^{\mathrm{r}}_{ij}(\boldsymbol{q},\omega)$ can be calculated as usual from the Hamiltonian of the system and is

$$M_{3,ij}(q)=\delta_{ij}M^{(0)}_{3,i}(q)+\omega_i^2\omega_j^2\Big(1+\sum_{i'}[\delta_{ii'}-\delta_{ij}(n_{i'}e_{i'}/n_ie_i)](g_{i'j}(r=0)-1)/3$$

$$+\sum_{\boldsymbol{q}'(\neq 0)}(\boldsymbol{q}\cdot\boldsymbol{q}'/qq')^2[(1-\delta_{\boldsymbol{q}',\boldsymbol{q}})g_{ij}(\boldsymbol{q}'-\boldsymbol{q})-g_{ij}(\boldsymbol{q}')]\Big), \tag{1}$$

where $v(q)=(4\pi/q^2)(1-\delta_{q,0})$, $M^{(0)}_{3,i}(q)=8\pi e_i^2K_i q^2/m_i^2+\pi n_ie_i^2q^4/m_i^3$, $\omega_i^2=4\pi n_ie_i^2/m_i$, K_i is the average kinetic energy of i component and $g_{ij}(r)$ is the pair distribution function whose Fourier transform $g_{ij}(\boldsymbol{q})$ is defined by $g_{ij}(\boldsymbol{q})=(\langle\rho_i(\boldsymbol{q})\rho_j(\boldsymbol{q})\rangle-n_ie_i^2\delta_{ij})/(n_ie_in_je_j)$. Though in a classical theory $g_{ij}(r)$ for unlike charges, as is well known, has the short-range divergence, this may be eliminated by the quantum effects in the case of the system discussed here. Equation (1) gives the third sum rule for the spectral function of $v(q)D^{\mathrm{r}}_{ij}(\boldsymbol{q},\omega)$. Note the second term in the large parentheses on the right-hand side of equation (1). This term exists only in the multi-component system and does not vanish even in the long-wavelength limit. The existence of this singular term introduces a basic difficulty into LFT as described above.

According to LFT, $D^{\mathrm{r}}_{ij}(\boldsymbol{q},\omega)$ of the two-component plasma is expressed as (see Vashishta *et al* 1974):

$$D^{\mathrm{r}}_{ij}(\boldsymbol{q},\omega)=\{\delta_{ij}D^{(0)}_i-D^{(0)}_1D^{(0)}_2[\delta_{ij}(\psi_{11}+\psi_{22})-\psi_{ij}]\}/\Delta, \tag{2}$$

where

$$\Delta(q,\omega)=(1-\psi_{11}D^{(0)}_1)(1-\psi_{22}D^{(0)}_2)-D^{(0)}_1\psi_{12}\psi_{21}D^{(0)}_2,$$

$$\psi_{ij}(\boldsymbol{q},\omega)=v(q)(1-G_{ij}(\boldsymbol{q},\omega)),$$

and

$$D^{(0)}_i(\boldsymbol{q},\omega)=e_i^2\sum_{\boldsymbol{k},\sigma}\frac{n_i(\boldsymbol{k},\sigma)-n_i(\boldsymbol{k}+\boldsymbol{q},\sigma)}{\omega-\boldsymbol{kq}/m_i-q^2/2m_i+\mathrm{i}0^+}.$$

It can be proved on the basis of an equation of motion for a response function that equation (2) itself is never an approximation. Any approximations taken are for real momentum distribution function, $n_i(\boldsymbol{k},\sigma)$ and the so called 'local field correction', $G_{ij}(\boldsymbol{q},\omega)$. The condition that the third frequency moment of $v(q)D^{\mathrm{r}}_{ij}(\boldsymbol{q},\omega)$ obtained from the high frequency expansion of equation (2) is equal to equation (1) is given by

$$G_{ij}(\boldsymbol{q},\infty)=\sum_{i'}[\delta_{ii'}-\delta_{ij}(n_{i'}e_{i'}/n_ie_i)](1-g_{i'j}(r=0))/3$$

$$+\sum_{\boldsymbol{q}'(\neq 0)}(\boldsymbol{q}\cdot\boldsymbol{q}'/qq')^2[(1-\delta_{\boldsymbol{q}',\boldsymbol{q}})g_{ij}(\boldsymbol{q}'-\boldsymbol{q})-g_{ij}(\boldsymbol{q}')], \tag{3}$$

which gives the exact expression of the 'local field correction' in the high frequency limit. We note that the first and second terms of equation (3) correspond to the second and third terms in the large parentheses of equation (1), respectively; the first term of equation (3) exists only in the multi-component system and becomes dominant in the long-wavelength 'local field'.

Let us assume a theory in which 'local field corrections' do not depend on the frequency. Let us denote these by $G_{ij}(\boldsymbol{q})$. If this theory satisfies the third sum rule, then $G_{ij}(\boldsymbol{q})$ must be equal to equation (3). This, however, involves such an unphysical result as the dissatisfaction of the perfect screening sum rule as shown below. This sum rule states that $1/\epsilon(\boldsymbol{q}, 0)$ vanishes as $q \to 0$, where $\epsilon(\boldsymbol{q}, \omega)$ is the generalised dielectric function expressed as $1/\epsilon(\boldsymbol{q}, \omega) = 1 + v(q)\Sigma_{i,j}D^{\mathrm{r}}_{ij}(\boldsymbol{q}, \omega)$. Noticing that $G_{ij}(\boldsymbol{q})$ and $D_i^{(0)}(\boldsymbol{q}, 0)$ are of the order of q^0 as $q \to 0$, we see with the use of equation (2) that this sum rule is satisfied unless

$$\lim_{q\to 0}(G_{12}(\boldsymbol{q}) + G_{21}(\boldsymbol{q}) - G_{11}(\boldsymbol{q}) - G_{22}(\boldsymbol{q}) + G_{11}(\boldsymbol{q})G_{22}(\boldsymbol{q}) - G_{12}(\boldsymbol{q})G_{21}(\boldsymbol{q})) = 0.$$

The left-hand side of this condition is calculated from equation (3) and is equal to $(n_1e_1 + n_2e_2)^2(1 - g_{12}(r = 0))/(3n_1e_1n_2e_2)$. Therefore, in the two-component plasma where $n_1e_1 + n_2e_2 = 0$, the perfect screening sum rule is not satisfied.

As understood from the above discussion, this difficulty is due to the singular term in equation (1). This term is related to the non-conservation of the total charge-current. In fact, it is $v(q)\langle[[\boldsymbol{q}\boldsymbol{J}_i, H], \boldsymbol{q}\boldsymbol{J}_j]\rangle$, where $\boldsymbol{J}_i$ and H are the total charge-current of i component and the Hamiltonian, respectively. In such a system, the contribution of the *multiparticle* excitations to the long-wavelength response competes with that of plasmons as shown by Pines and Nozieres (1966). Therefore, the singular term may be connected with the response of the *multiparticle* excitations to the high frequency external field.

From the discussion in this Letter, we conclude as follows. In the two-component quantum plasma:

(i) the contribution of the *multiparticle* excitations to the low frequency response cannot be approximated to that to the high frequency response without the introduction of some unphysical result;

(ii) the frequency dependence of G_{ij} is essential for the description valid for both low and high frequency phenomena as far as the framework of LFT is defined by equation (2).

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