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Third-frequency-moment sum rule for electronic multilayers

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The authors establish the third-frequency-moment sum rules for the density-density reponse matrix of electronic multilayer structures modeled as an array of N parallel two-dimensional (2D) electron-plasma monolayers. Layer densities and spacings between adjacent layers need not be equal. Contact is made with previously established sum rules for the isolated 2D electron liquid and type-1 infinite superlattices. The case of the equal-density bilayer is considered and its third frequency-moment-sum-rules for the in-phase and out-of-phase inverse dielectric functions are formulated.

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Satisfaction of the third-frequency-moment sum rule has been recognized [1] as an important test of the reliability of model dynamical theories of plasmas in a strongly correlated Coulomb liquid phase. To date, ω^3 sum rules for the external density-density response function $\hat{\chi}$ (which describes the response of the system to an external scalar potential perturbation) and its inverse dielectric function relative $1/\varepsilon=1+\hat{\chi}\phi$ have been derived and extensively analyzed for a variety of strongly coupled plasma configurations, most notably: (i) the three-dimensional (3D) one-component plasma (OCP) [1–4], (ii) the 2D electron liquid [1,5–7], (iii) binary ionic mixtures in a neutralizing uniform background [8,9], and (iv) type-1 semiconductor superlattices (comprised of an infinite number of equal-density 2D electron or hole layers with the same spacing d between adjacent layers) [10].

In this Brief Report, we establish from first principles ω^3 sum rules which apply not only to (iv) above, but more generally to electronic multilayer structures where the number of layers is *finite* and where areal densities and spacings between adjacent layers *need not be equal*. This is the main goal. The formulation of the in-phase and out-of-phase ω^3 sum rules for the special case of the equal-density electronic bilayer (consisting of two quasi-2D electron or hole liquids separated by a fixed distance d in a double quantum well) follows. The strong coupling limit of the latter, which is satisfied by the quasilocalized charge (QLC) theory of Ref. [11] and which is built into Ortner's interpolation formula [12] for the inverse dielectric function, is especially timely in view of the significance of interlayer interactions in the sum rule and the need to further resolve [12,13] conflicting theoretical predictions [11,14] concerning the role of interlayer interactions in the dispersion of the out-of-phase plasma mode: the ω^3 sum rule conserving QLC theory [11] predicts that strong interlayer correlations beyond the random-phase approximation (RPA) bring about a remarkable long-wavelength energy gap $[\omega^2(q=0)>0]$ in the out-of-phase acoustic plasma mode of electronic bilayers; by contrast, no such energy gap is predicted by the mean field theory approaches of Ref. [14] which either (i) focus on intralayer correlations and ignore interlayer correlations beyond the RPA (when it is physically not justifiable) or (ii) take account of the latter, but not in a way that structurally satisfies the third-frequency-moment sum rule.

The electronic multilayer model to be considered here consists of an array of N quasi-two-dimensional infinitely thin electron-plasma layers, each of large but bounded area V_{2D} and parallel to the xy plane; $n_A=N_A/V_{2D}$ is the mean areal density of the 2D electron liquid in layer $A(A=1,2,\ldots,N)$. The Coulomb interaction energy for the system is $\phi^{AB}(r)=e^2/[r^2+|z_A-z_B|^2]^{1/2}$ with Fourier transform $\phi^{AB}(q)=(2\pi e^2/q)\exp(-q|z_A-z_B|)$; r is the separation distance and q the wave number in the xy plane; z_A and z_B locate layers A and B along the z axis.

We begin by introducing the external density-density response matrix $\hat{\chi}(\mathbf{q},\omega)$ defined through the consitutive relation

$$\eta_A(\mathbf{q},\omega)=-e\sum_B \hat{\chi}^{AB}(\mathbf{q},\omega)\hat{\Phi}_B(\mathbf{q},\omega) \qquad (1)$$

linking the average particle density response in layer A to perturbing external scalar potentials $\hat{\Phi}_B(\mathbf{q},\omega)\equiv\hat{\Phi}(\mathbf{q},\omega,z_B)$; $B=1,2,\ldots.N$. The generalized relation [15]

$$[\varepsilon^{-1}(\mathbf{q},\omega)]^{AB}=\delta^{AB}+\sum_C \hat{\chi}^{AC}(\mathbf{q},\omega)\phi^{CB}(q), \qquad (2)$$

for the inverse dielectric matrix then follows from the relationship between the external and screened density-density response matrices [15]; Kronecker delta δ^{AB} is an element of the (NXN) identity matrix.

We wish to evaluate the $l=1,3$ frquency-moment matrix elements

$$\langle \omega^l \rangle^{AB}(\mathbf{q}) = \frac{1}{\pi}\int_{-\infty}^{\infty} d\omega\, \omega^l \,\mathrm{Im}\, \hat{\chi}^{AB}(\mathbf{q},\omega) \tag{3}$$

in the exact high-frequency expansion

$$\mathrm{Re}\, \hat{\chi}^{AB}(\mathbf{q},\omega\to\infty) = -(1/\omega^2)\langle\omega\rangle^{AB} - (1/\omega^4)\langle\omega^3\rangle^{AB}(\mathbf{q}) - \cdots. \tag{4}$$

The appropriate starting point for the calculation is the multilayer fluctuation-dissipation theorem

$$\mathrm{Im}\, \hat{\chi}^{AB}(\mathbf{q},\omega) = -\frac{1}{2\hbar V_{2D}}\int_{-\infty}^{\infty} dt\, e^{i\omega t}\langle[n_{\mathbf{q}}^{A}(t), n_{-\mathbf{q}}^{B}(0)]\rangle, \tag{5}$$

which is derived following the standard application of the statistical-mechanical-linear-response procedure of Kubo to electronic multilayers; $n_{\mathbf{q}}^A = \Sigma_i \exp(-i\mathbf{q}\cdot\mathbf{x}_i^A)$ is the Fourier transform of the local-density operator ($\mathbf{x}_i^A$ refers to particle i in layer A), and the angle brackets denote averaging over the equilibrium ensemble.

The $l=1$ f sum rule coefficient

$$\langle\omega\rangle^{AB} = \frac{1}{i\hbar V_{2D}}\langle[\dot{n}_{\mathbf{q}}^{A}, n_{-\mathbf{q}}^{B}]\rangle = -(n_A k^2/m)\,\delta^{AB} \tag{6}$$

readily results from substituting Eq. (5) into Eq. (3) and performing the routine commutator algebra for the Hamiltonian and local-density operators.

The more involved calculation of the $l=3$ sum rule coefficient

$$\langle\omega^3\rangle^{AB}(\mathbf{q}) = \frac{1}{i\hbar V_{2D}}\langle[\ddot{n}_{\mathbf{q}}^{A}, \dot{n}_{-\mathbf{q}}^{B}]\rangle \tag{7}$$

is carried out by repeated use of Heisenberg's equation followed by some lengthy commutator algebra. We obtain

$$\begin{aligned}\langle\omega^3\rangle^{AB}(\mathbf{q}) = &-(1/m)\sqrt{n_A n_B}\,q^2\{(\hbar q^2/2m)^2\delta^{AB} + 3(q^2/m) \\ &\times\langle E_{\mathrm{kin}}\rangle\delta^{AB} + \omega_{2D}^{A}(q)\,\omega_{2D}^{B}(q) \\ &\times e^{-q|z_A - z_B|} + D^{AB}(\mathbf{q})\},\end{aligned} \tag{8}$$

where $\langle E_{\mathrm{kin}}\rangle = (1/mN_A)\Sigma_i\langle(\mathbf{q}\cdot\mathbf{p}_i^A)^2\rangle/q^2$ is the expectation value of the 2D kinetic energy per particle for an interacting system, $\omega_{2D}^A(q) = [2\pi e^2 n_A q/m]^{1/2}$ is the 2D plasma frequency of layer A, and

$$\begin{aligned}D^{AB}(\mathbf{q}) &= \frac{1}{mV_{2D}}\sum_{\mathbf{q}'}[(\mathbf{q}\cdot\mathbf{q}')^2/q^2]\Big\{\phi^{AB}(q')S^{AB}(|\mathbf{q}-\mathbf{q}'|) \\ &\quad - \delta^{AB}\sum_C \sqrt{n_C/n_A}\,\phi^{AC}(q')S^{AC}(q')\Big\}\end{aligned} \tag{9}$$

is the contribution due to Coulomb correlations beyond the random-phase approximation (RPA); $S^{AB}(q') = [1/(N_A N_B)^{1/2}]\langle n_{\mathbf{q}'}^{A}, n_{-\mathbf{q}'}^{B}\rangle - (N_A N_B)^{1/2}\delta_{\mathbf{q}'}$ is the structure function. Equation (8) is the principal result of the present report. Its classical counterpart is readily obtained by observing that in the $\hbar\to 0$ limit the first right-hand-side term of Eq. (8) vanishes and $\langle E_{\mathrm{kin}}\rangle = k_B T$.

Going to the isolated 2D layer limit ($N=1$, $A=B=1$, $|z_A - z_B| = 0$), one readily recovers from Eq. (8) the correct 2D ω^3-sum rule coefficient reported in Refs. [1] and [6]. Going to the opposite limit ($N\to\infty$) and letting the mean areal densities and spacings between layers be equal, the ensuing periodicity of the resulting type-1 superlattice configuration allows one to invoke an additional Fourier transformation along the z axis, i.e., $\hat{\chi}(\mathbf{q},q_z,\omega) = \Sigma_A \hat{\chi}^{AB}(\mathbf{q},\omega)\exp[-iq_z(z_A - z_B)]$, and one readily recovers the superlattice ω^3 sum rule coefficient reported in Ref. [10].

An especially interesting structure is the equal-density ($n_1 = n_2 = n$) bilayer consisting of two identical 2D electron liquids separated by distance d; the interaction potentials are $\phi^{11}(r) = e^2/r$ and $\phi^{12}(r) = e^2/(r^2+d^2)^{1/2}$ with Fourier transform $\phi^{11}(q) = \phi_{2D}(q) = 2\pi e^2/q$ and $\phi^{12}(q) = \phi_{2D}(q)e^{-qd}$. For this particular case where the inverse dielectric matrix can be diagnolized, we proceed directly to the calculation of the frequency-moment-sum rules for the resulting in-phase (+) and out-of-phase (−) elements $\varepsilon_{\pm}^{-1}(\mathbf{q},\omega)$. From Eqs. (2), (6), (8), and

$$\varepsilon_{\pm}^{-1}(\mathbf{q},\omega) = [\varepsilon^{-1}(\mathbf{q},\omega)]^{11} \pm [\varepsilon^{-1}(\mathbf{q},\omega)]^{12}, \tag{10}$$

one readily obtains

$$\int_{-\infty}^{\infty} d\omega\,\omega\,\mathrm{Im}\,\varepsilon_{\pm}^{-1}(\mathbf{q},\omega) = -\pi\omega_{2D}^2(q)(1\pm e^{-qd}), \tag{11}$$

$$\begin{aligned}\int_{-\infty}^{\infty} d\omega\,\omega^3\,\mathrm{Im}\,\varepsilon_{\pm}^{-1}(\mathbf{q},\omega) &= -\pi\omega_{2D}^2(q)(1\pm e^{-qd})\{(\hbar q^2/2m)^2 \\ &\quad + 3(q^2/m)\langle E_{\mathrm{kin}}\rangle + \omega_{2D}^2(q)(1\pm e^{-qd}) \\ &\quad + D^{11}(\mathbf{q}) \pm D^{12}(\mathbf{q})\},\end{aligned} \tag{12}$$

where $\omega_{2D}(q) = [2\pi e^2 nq/m]^{1/2}$ and $D^{11}(q)$ and $D^{12}(q)$ are expressed in terms of equilibrium pair correlation functions $g^{AB}(q) = (1/n)[S^{AB}(q) - \delta^{AB}]^{11}$:

$$\begin{aligned}D^{11}(\mathbf{q}) = \omega_{2D}^2(q)(1/V_{2D})\sum_{\mathbf{q}'}\frac{(\mathbf{q}\cdot\mathbf{q}')^2}{q^3 q'}[g^{11}(|\mathbf{q}-\mathbf{q}'|) \\ - g^{11}(q') - g^{12}(q')e^{-q'd}],\end{aligned} \tag{13}$$

$$D^{12}(\mathbf{q}) = \omega_{2D}^2(q)(1/V_{2D})\sum_{\mathbf{q}'}\frac{(\mathbf{q}\cdot\mathbf{q}')^2}{q^3 q'} \times g^{12}(|\mathbf{q}-\mathbf{q}'|)e^{-q'd}. \tag{14}$$

In conclusion, we have established the general third-frequency-moment sum rules for type-1 electronic multilayers consisting of a finite number of parallel 2D electron-plasma monolayers; layer densities and spacings between adjacent layers need not be equal. Finally, we observe that only the interlayer correlations survive in the $q=0$ limit of Eq. (9):

$$D^{AA}(0) = -(e^2/2m)\sum_{C\neq A}\sqrt{n_C/n_A}\times\int_0^\infty dq\, q^2 S^{AC}(q) e^{-q|z_A-z_C|}, \tag{15}$$

$$D^{AB}(0) = (e^2/2m)\int_0^\infty dq\, q^2 S^{AB}(q) e^{-q|z_A-z_B|} \quad (A\neq B). \tag{16}$$

The correspondence between Eqs. (15) and (16) and the $q=0$ energy gap that emerges in the QLC description of plasma mode dispersion in equal-density bilayers [11] and superlattices [16] suggests the existence of the gap in the QLC description of all type-1 multilayer structures exhibiting strong interlayer Coulomb interactions.

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