Collective excitations of strongly coupled bilayer charged Bose liquids in the third-frequency-moment sum rule

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We calculate the collective excitation modes of strongly coupled bilayer charged Bose systems. We employ the dielectric matrix formulation to study the correlation effects within the random-phase approximation (RPA), the self consistent field approximation Singwi, Tosi, Land, and Sjölander (STLS), and the quasilocalized charge approximation (QLCA), which satisfies the third-frequency-moment ($\langle\omega^3\rangle$) sum rule. We find that the QLCA predicts a long-wavelength correlation-induced energy gap in the out-of-phase plasmon mode, similar to the situation in electronic bilayer systems. The energy gap and the plasmon density of states are studied as a function of interlayer separation and coupling parameter r_s. The results should be helpful for experimental investigations.

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I. INTRODUCTION

The layered two-dimensional (2D) electron systems have attracted a great deal of theoretical and experimental interests in the last two decades. The motivation for studying these systems is provided by a number of observed static and dynamic phenomena entirely due to interlayer Coulomb interactions such as the quantum Hall effect and insulating Wigner crystal and interlayer Coulomb drag effects.[1] A system of charged bosons is an important construct to study similar phenomena and to discern the differences brought by quantum statistics. Recently, an important impetus to study charged bosons in various dimensions has been the recognition of the layered charged Bose (CB) systems as a possible model for high-temperature superconductors.[2–4]

The intralayer and interlayer many-body correlations play a central role in determining several properties, such as correlation energy and pair-correlation function, of layered systems. Charged particles in one layer act as a polarizing background for the particles in the other one, then the strength of correlations is remarkably increased in the presence of many layers. The quantitative degree of these relative correlations has been determined by quantum Monte Carlo simulations in bilayer electron and hole systems.[5]

The long-wavelength ($q\to 0$) behavior of collective excitations, or plasmons, in weak and strong-interaction regimes is one of the issues under investigation in bilayer systems. When the interlayer distance is large enough, i.e., an uncoupled bilayer system, each layer has a 2D plasma mode with a long-wavelength dispersion $\omega(\boldsymbol{q})\sim\sqrt{q}$. However, when they are near each other, the interlayer Coulomb interaction becomes more effective, and the system displays two different longitudinal modes: in-phase mode $[\omega_+(\boldsymbol{q})]$ in which two layers oscillate in unison and out-of-phase mode $[\omega_-(\boldsymbol{q})]$, where the oscillation phase of the layers differs by π. These modes are, respectively, termed optical and acoustic plasmons, and have already been observed in the inelastic-light-scattering experiments.[6]

The dispersion of collective modes $\omega_\pm(\boldsymbol{q})$ in a bilayer CB system and in particular their long-wavelength ($q\to 0$) behavior is the subject of the present paper. The interaction strength between the charged bosons in a layer is characterized by the dimensionless parameter r_s. For $r_s \ll 1$, the system is a weakly coupled liquid well described by the random-phase approximation (RPA). Both intralayer and interlayer interactions get stronger and the system essentially becomes strongly correlated with increasing r_s. The correlation effects beyond RPA are usually included via a low-frequency, or static, local-field (LF) factor in the widely used self-consistent field (SCF) approximation of Singwi, Tosi, Land, and Sjölander[7] (STLS). Tanatar and Das[8] included the interaction effects at the RPA level to study the plasmon dispersion of double layer CB system with nonidentical particle densities and masses. They found plasmon dispersions similar to those of a bilayer electron gas. Moudgil *et al.*[4] studied the ground state of a bilayer CB system by treating the intralayer correlation effects within the STLS, but interlayer correlations within the RPA. They concluded that the system will be unstable against a phase transition into an inhomogeneous charge-density wave ground state below a critical spacing between the layers.

In the study of dielectric properties of quantum liquids, the frequency-moment sum rules provide some exact conditions for the dielectric function $\varepsilon(\boldsymbol{q},\omega)$ of quantum liquids to obey. Evidently, satisfaction of these sum rules is an important criterion for an acceptable dynamic approximation. The third-frequency moment ($\langle\omega^3\rangle$) is the lowest-order moment that exhibits the correlation effects. It constrains the asymptotic form of the LF factor in the long-wavelength limit. It was shown by Iwamoto[9] that the collective excitations give major contributions to this sum rule. Therefore, for a complete description of the collective modes in quantum liquids one must resort to an approach which satisfies the $\langle\omega^3\rangle$ sum rule. The $\varepsilon(\boldsymbol{q},\omega)$ obtained within the quasilocalized charge approximation (QLCA) of Golden and Kalman[10] satisfies the $\langle\omega^3\rangle$ sum rule in strongly correlated quantum liquids. The QLCA was proposed in order to explain the plasmon dispersions in the high-temperature classical Coulomb fluids. Its main feature is that at strong coupling, the charges are trapped in local potential fluctuations.[11,12]

As far as the long-wavelength behavior of $\omega_+(\boldsymbol{q})$ mode is concerned, both STLS and QLCA yield the optical-modelike behavior $\omega_+(q\to 0)\sim\sqrt{q}$. Nevertheless, they predict quite different feature for the $\omega_-(\boldsymbol{q})$ mode. The QLCA expression for the LF factor has a finite value as $q\to 0$, this fact leads to an energy gap $[\omega(\boldsymbol{q})>0$ for $q=0]$, while the STLS expression vanishes as $q\to 0$; therefore, it yields a gapless $\omega_-(\boldsymbol{q})$ mode. Kalman and Golden[13] discussed the reason of this discrepancy in detail and concluded that the QLCA is the correct model for bilayer systems due to two main reasons. The first reason is that $\varepsilon(\boldsymbol{q},\omega)$ expression obtained in the QLCA satisfies the $\langle\omega^3\rangle$ sum rule, while STLS expression does not. The second reason is the fact that the bilayer systems can be mapped onto a single two-component 2D layer, and the upward frequency shift of the plasmon mode in two-component ionic mixtures is known for a long time. Indeed, this feature has been predicted by computer experiments.[14–16] It is known that although the STLS approximation describes one-component systems quite well, it fails in describing two-component systems.[17] Ortner[18] argued that the neglecting of damping processes overestimates the correlation effects and concluded that a correct account of damping processes leads to absence of an energy gap in a bilayer system, confirming prediction of the STLS approach.

The aim of this paper is to analyze the collective excitations in a strongly coupled bilayer CB system using the well-established $\langle\omega^3\rangle$ sum rule. For this task we resort to the QLCA. The results are compared with those computed within the RPA and STLS schemes. Thus, the appearance of a gap in $\omega_-(q)$ in a system other than the electron gas is established.

II. MODEL AND THEORY

We consider two identical infinite layers with equal density n of spinless charged bosons separated by a distance d, which is comparable to the average interparticle spacing (Wigner-Seitz radius) $r_0=1/\sqrt{n\pi}$ in a single layer. For the charge neutrality, it is assumed that each layer is embedded in a rigid uniform neutralizing background of opposite charge. The finite-thickness effects, disorder effects, and interlayer quantum tunneling are ignored. Then, we have a strictly 2D symmetric bilayer system with constant particle density in each layer. We further assume that the system is in the condensate phase at absolute zero temperature $(T=0)$.

Each layer is characterized by the dimensionless coupling parameter $r_s=r_0/a_B^\star$, where $a_B^\star=\hbar^2\varepsilon_0/(e^2m^\star)$ is the effective Bohr radius in terms of the background dielectric constant ε_0 and effective boson mass $m^\star$. Therefore, one needs only two parameters to define a symmetric bilayer CB fluid: interlayer separation distance d and coupling parameter r_s. The intralayer and interlayer Coulomb interaction potentials, $\phi_{11}(\boldsymbol{r})$ and $\phi_{12}(\boldsymbol{r})$, respectively, between the charged particles with in-layer $\boldsymbol{r}$ and interlayer separations d are

$$\phi_{11}(\boldsymbol{r})=\phi_{22}(\boldsymbol{r})=\phi_{2D}(\boldsymbol{r})=e^2/(\varepsilon_0 r),$$

$$\phi_{12}(\boldsymbol{r})=\phi_{21}(\boldsymbol{r})=e^2/(\varepsilon_0\sqrt{r^2+d^2}),$$

$$\phi_{11}(\boldsymbol{q})=\phi_{2D}(\boldsymbol{q})=2\pi e^2/(\varepsilon_0 q),$$

$$\phi_{12}(\boldsymbol{q})=\phi_{2D}(\boldsymbol{q})e^{-qd}. \tag{1}$$

The $\varepsilon(\boldsymbol{q},\omega)$ of a quantum liquid describes its density response to an external potential $\phi(\boldsymbol{q})$ coupled to the density fluctuations in the system. Within the linear-response theory, it is related to the density-density response function $\chi(\boldsymbol{q},\omega)$ as

$$[\varepsilon(\boldsymbol{q},\omega)]^{-1}=1+\phi(\boldsymbol{q})\chi(\boldsymbol{q},\omega). \tag{2}$$

In the SCF approximations treating the correlation effects beyond the RPA, the system responds to an external potential through the noninteracting response function $\chi_0(\boldsymbol{q},\omega)$ modified by a static LF factor $G(\boldsymbol{q})$, which embodies the short-range exchange-correlation effects between the particles. As a result, in SCF approximations $\chi(\boldsymbol{q},\omega)$ of a single-layer system is given by

$$\chi(\boldsymbol{q},\omega)=\frac{\chi_0(\boldsymbol{q},\omega)}{1-\phi(\boldsymbol{q})[1-G(\boldsymbol{q})]\chi_0(\boldsymbol{q},\omega)}. \tag{3}$$

At $T=0$, $\chi_0(\boldsymbol{q},\omega)$ of a CB liquid reads

$$\chi_0(\boldsymbol{q},\omega)=\frac{2nE_q}{(\omega+i\eta)^2-E_q^2}, \tag{4}$$

where $E_q=\hbar^2q^2/(2m^\star)$ is the free-particle energy and η is a positive infinitesimal quantity.

As noted in Sec. I, a one-component bilayer system is equivalent to a two-component single-layer system, which is described by a dielectric matrix. This matrix can easily be diagonalized for symmetric bilayers by separating the in-phase (+) and out-of-phase (−) modes in terms of $\phi_\pm(\boldsymbol{q})=\phi_{11}(\boldsymbol{q})\pm\phi_{12}(\boldsymbol{q})$,

$$\varepsilon_\pm(\boldsymbol{q},\omega)=1-\frac{\phi_\pm(\boldsymbol{q})\chi_0(\boldsymbol{q},\omega)}{1+\phi_{2D}(\boldsymbol{q})\chi_0(\boldsymbol{q},\omega)[G_{11}(\boldsymbol{q})\pm G_{12}(\boldsymbol{q})]}. \tag{5}$$

Lu and Golden[12] derived the $\langle\omega^3\rangle$ sum rule for a symmetric bilayer system as

$$\frac{1}{\pi}\int_{-\infty}^{\infty}d\omega\omega^3\ \mathrm{Im}[\varepsilon_\pm(\boldsymbol{q},\omega)]^{-1}$$
$$=-\omega_p^2(q)[1\pm e^{-qd}]\left\{\omega_p^2(q)[1\pm e^{-qd}]+3\frac{q^2}{m^\star}\langle E_{\mathrm{kin}}\rangle+\left(\frac{\hbar q^2}{2m^\star}\right)^2-\omega_p^2(q)[G_{11}(\boldsymbol{q})\pm G_{12}(\boldsymbol{q})]\right\}, \tag{6}$$

where $\omega_p(q)=[\phi_{2D}(q)nq^2/m^\star]^{1/2}$ is the 2D plasmon frequency.

The intralayer and interlayer local-field factors, $G_{11}(\boldsymbol{q})$ and $G_{12}(\boldsymbol{q})$, respectively, are given in the QLCA by

$$G_{11}(\boldsymbol{q})=-\frac{1}{N}\sum_{\boldsymbol{k}}\frac{(\boldsymbol{q}\cdot\boldsymbol{k})^2}{q^4}\frac{\phi_{11}(k)}{\phi_{2D}(q)}[S_{11}(\boldsymbol{q}-\boldsymbol{k})-S_{11}(\boldsymbol{k})]+\frac{1}{N}\sum_{\boldsymbol{k}}\frac{(\boldsymbol{q}\cdot\boldsymbol{k})^2}{q^4}\frac{\phi_{12}(k)}{\phi_{2D}(q)}S_{12}(\boldsymbol{k}),$$

$$G_{12}(\boldsymbol{q}) = -\frac{1}{N}\sum_{\boldsymbol{k}} \frac{(\boldsymbol{q}\cdot\boldsymbol{k})^2}{q^4} \frac{\phi_{12}(k)}{\phi_{2D}(q)} S_{12}(\boldsymbol{q}-\boldsymbol{k}). \tag{7}$$

On the other hand, in the STLS approach they read

$$G_{11}(\boldsymbol{q}) = -\frac{1}{N}\sum_{\boldsymbol{k}} \frac{\boldsymbol{q}\cdot\boldsymbol{k}}{q^2} \frac{\phi_{11}(k)}{\phi_{2D}(q)} [S_{11}(\boldsymbol{q}-\boldsymbol{k})-1],$$

$$G_{12}(\boldsymbol{q}) = -\frac{1}{N}\sum_{\boldsymbol{k}} \frac{\boldsymbol{q}\cdot\boldsymbol{k}}{q^2} \frac{\phi_{12}(k)}{\phi_{12}(q)} S_{12}(\boldsymbol{q}-\boldsymbol{k}). \tag{8}$$

The RPA expressions are restored by setting $G_{AB}(\boldsymbol{q})=0$ in Eq. (5).

The static structure factors $S_{AB}(\boldsymbol{q})$ appearing in Eqs. (7) and (8) define the instantaneous density fluctuations due to the intralayer and interlayer correlations. They are related to $\chi_{AB}(\boldsymbol{q},\omega)$ through the fluctuation-dissipation theorem,

$$S_{AB}(\boldsymbol{q}) = -\frac{\hbar}{\pi n}\int_0^\infty d\omega \chi_{AB}(\boldsymbol{q},i\omega). \tag{9}$$

The collective eigenmodes of a quantum liquid are determined by the zeros of the dielectric function, i.e., $\varepsilon(\boldsymbol{q},\omega_p)=0$. Therefore, from Eq. (5) we obtain the modes of a bilayer CB liquid as

$$\omega_\pm^2(\boldsymbol{q}) = \frac{q_n^4}{r_s^4} - \frac{8q_n}{r_s^3}[G_{11}(\boldsymbol{q}) \pm G_{12}(\boldsymbol{q}) \mp e^{-qd} - 1], \tag{10}$$

where $q_n \equiv qr_0$ and $\mathrm{Ry}^\star = 1/(2m^\star a_B^\star)$ is the effective Rydberg. Note that these dispersion relations are exact and analytical expressions (valid for all values of q) and go beyond the RPA. This follows from the simple form of $\chi_0(\boldsymbol{q},\omega)$ for the CB systems [Eq. (4)].

The plasmon density of states (DOS) is obtained similarly to other density-of-states computations in condensed-matter physics: $\rho(\omega)=\Sigma_{\boldsymbol{q}}\delta[\omega-\omega_\pm(\boldsymbol{q})]$. In our case it reduces to

$$\frac{\rho[\omega_\pm(\boldsymbol{q})]}{N} = \frac{\boldsymbol{q}_n^\star(\omega)}{2\left|\frac{d\omega_\pm(\boldsymbol{q}_n)}{d\boldsymbol{q}_n}\right|_{\boldsymbol{q}_n^\star}}. \tag{11}$$

Here N is the number of bosons in each layer and $\boldsymbol{q}_n^\star$ is the root of the equation $\omega_\pm(\boldsymbol{q})=\omega$.

III. RESULTS AND DISCUSSION

We start presenting our results first by comparing the static LF factors computed within the QLCA and STLS schemes. Evidently, this task requires the knowledge of the static structure factors $S_{AB}(\boldsymbol{q})$. In our computations in the QLCA we used the $S(\boldsymbol{q})$ data of De Palo *et al.*[19] obtained via the reptation quantum Monte Carlo (RQMC) method for systems of 56 charged bosons. Gold[20] calculated the LF factors of a single-layer 2D CB condensate and presented analytic expressions for its density dependence within a sum-rule version of the STLS approximation. The STLS LF factor data we use in our calculations are obtained from these analytic expressions. On the other hand, we confined our calculations to approximate $S_{12}(\boldsymbol{q})$ within the RPA via Eq. (9). This is largely because the interlayer LF factor is not available from QMC simulations. Such an approximation was employed by Moudgil *et al.*[4] and should be valid as $d/r_0 > 1$.

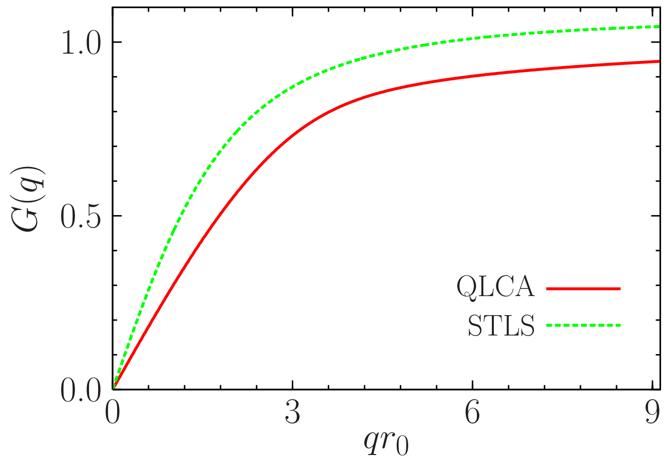

FIG. 1. (Color online) Static LF factor of a single-layer CB liquid versus normalized wave number qr_0 for density $r_s=10$.

Figure 1 displays the static LF factor of a single-layer CB system; both curves have similar features. The most distinguishing difference is observed in the large wave-number limit: the STLS $G(\boldsymbol{q})$ becomes larger than unity.

The intralayer and interlayer LF factors calculated within the QLCA [Eq. (7)] are plotted in Fig. 2 at different r_s and normalized interlayer separation $\bar{d}=d/r_0$ values. At a given r_s, $G_{11}(\boldsymbol{q})$ increases whereas $G_{12}(\boldsymbol{q})$ decreases very fast with increasing interlayer distance. We see that when $\bar{d}=2$ the bilayer system effectively becomes a single layer one at all densities studied. At large q, Eqs. (7) and (8) become

$$G_{11}(q\to\infty) = 1 - g_{11}(\boldsymbol{r}=0) + O(1/q),$$

$$G_{12}(q\to\infty) = 1 - g_{12}(\boldsymbol{r}=0)\exp(-qd), \tag{12}$$

in which $g_{AB}(\boldsymbol{r}=0)$ are intralayer and interlayer pair-correlation functions at contact. They may be obtained from the static structure functions $S_{AB}(\boldsymbol{q})$: $g_{AB}(\boldsymbol{r})=1+(1/N)\Sigma_{\boldsymbol{q}}[S_{AB}(\boldsymbol{q})-\delta_{AB}]\exp(-i\boldsymbol{q}\cdot\boldsymbol{r})$. In the single-layer limit, or $d\to\infty$, Eq. (12) yields the Kimball identity,[21]

$$\lim_{x\to\infty}[1-G_{11}(\boldsymbol{q})] = g_{11}(\boldsymbol{r}=0). \tag{13}$$

In the long-wavelength limit we only have interlayer correlations. This is clearly seen in Fig. 2. Our findings are qualitatively similar to those obtained in electronic bilayer systems.[22]

As discussed in Sec. II, energy spectrum of the collective excitations in a strongly coupled bilayer system is of interest. One may compute the plasmon dispersion by Eq. (10). We plot our results as a function of r_s in Fig. 3. It is clearly seen that the $\langle\omega^3\rangle$ sum rule leads to a finite correlation-induced

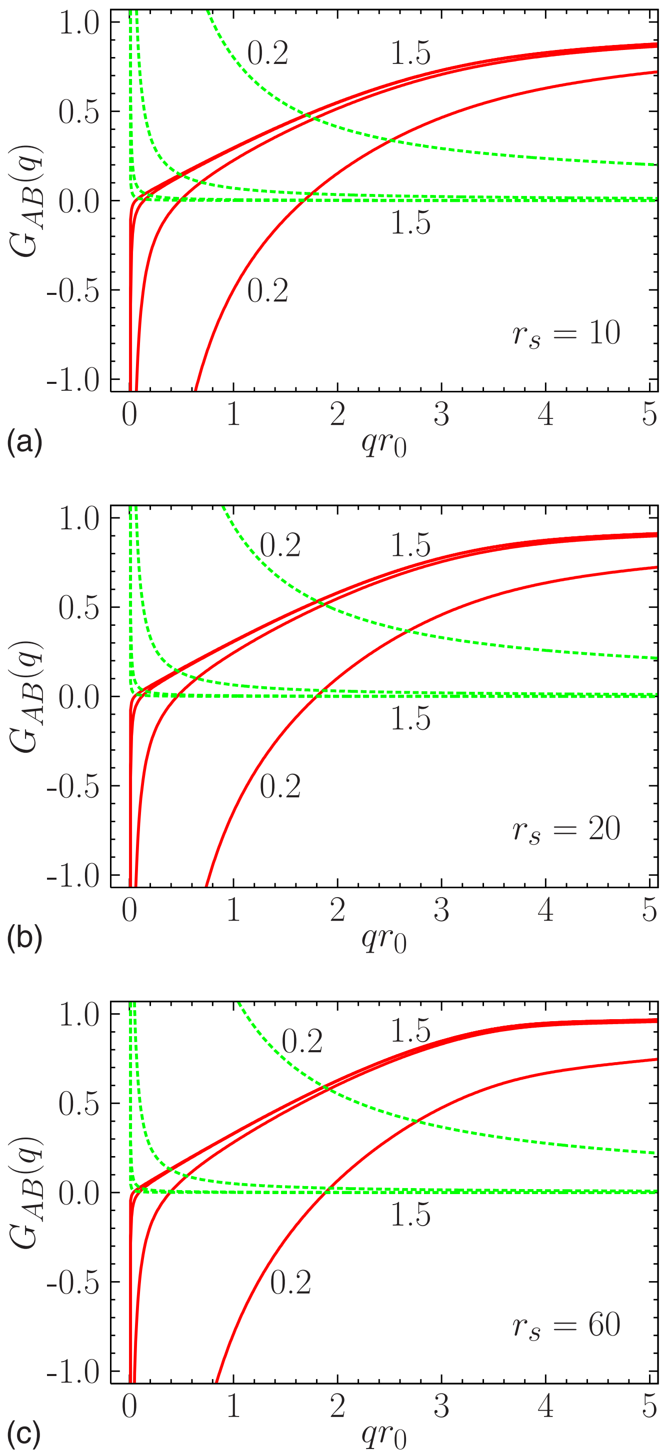

FIG. 2. (Color online) Intralayer (11, solid curves) and interlayer (12, dashed curves) LF factors for a symmetric bilayer CB fluid at r_s=10, 20, and 60 for dimensionless interlayer separation distances $\bar{d}$=0.2, 0.5, 1, and 1.5. In each plot, the highest-lying $G_{11}(\boldsymbol{q})$ curve corresponds to $\bar{d}$=1.5; the lowest-lying $G_{12}(\boldsymbol{q})$ curve corresponds to $\bar{d}$=1.5.

energy gap in the out-of-phase mode; i.e., $\omega_-(q\to 0)\neq 0$.

The long-wavelength limit of the plasmon dispersions are obtained by noting that $G_{11}(q\to 0)=-G(r_s,d)/q$ and $G_{12}(q\to 0)=G(r_s,d)/q$ as in the case of bilayer electron systems,[23]

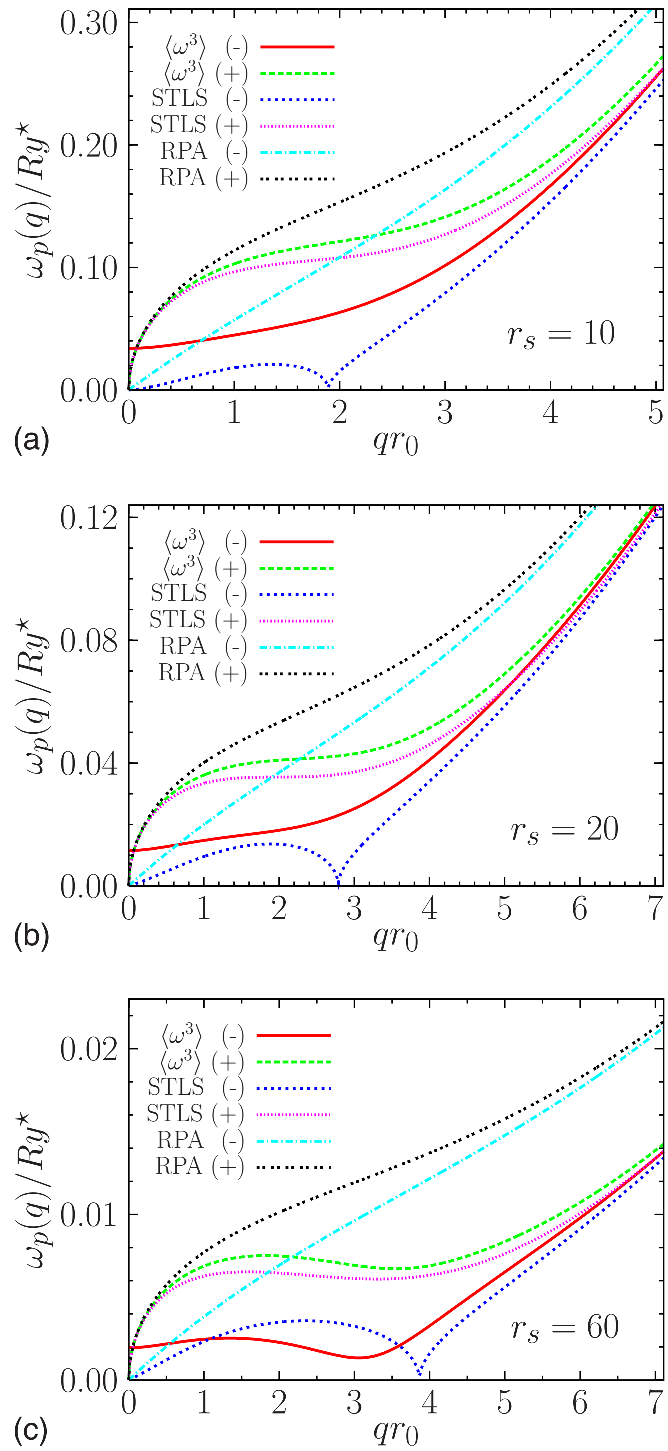

FIG. 3. (Color online) In-phase (+) and out-of-phase (−) plasmon dispersions of a symmetric bilayer CB system with r_s=10, 20, and 60. The interlayer distance is fixed at $\bar{d}$=0.5.

$$\omega_\pm^2(\boldsymbol{q}) = \frac{16 r_0}{r_s^3}\begin{cases} q \\ G(r_s,d) \end{cases}, \tag{14}$$

where the upper and lower expressions refer to the in-phase and out-of-phase modes, respectively. We observe that $\omega_-(\boldsymbol{q})$ exhibits a gap at q=0 due to the specific form the QLCA LF

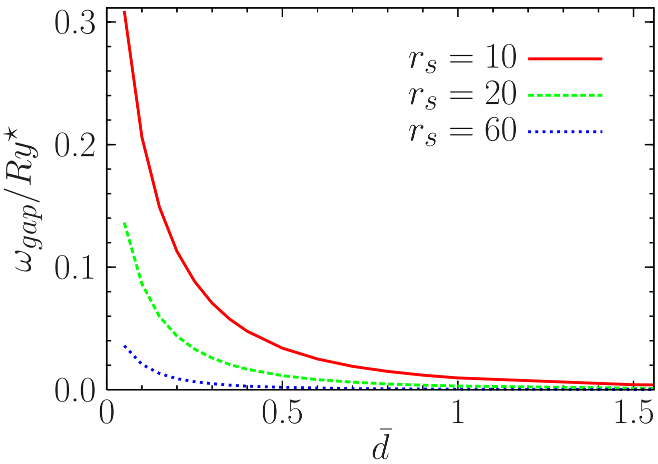

FIG. 4. (Color online) Energy gap $\omega_-(q\to 0)$ as a function of interlayer separation $\bar{d}$ for r_s=10, 20, and 60.

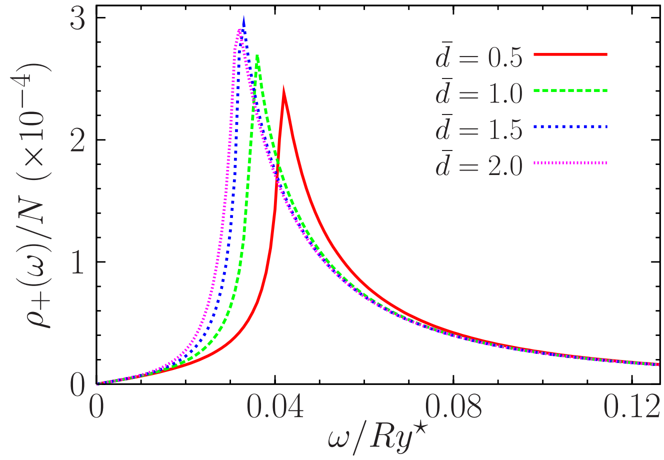

FIG. 6. (Color online) Plasmon DOS for in-phase modes in a bilayer CB liquid at coupling constant r_s=20 computed within the QLCA for various layer separations.

factors have in the long-wavelength limit. However, the RPA and STLS approaches yield no such energy gap in the out-of-phase mode.

The correlation-induced energy gap is displayed in Fig. 4 as a function of interlayer separation distance $\bar{d}$ for various densities. We find that for a given density, the energy gap decreases sharply with increasing $\bar{d}$. Indeed, it almost vanishes around $\bar{d}$=2 for r_s=10 and 20 and around $\bar{d}$=1 for r_s =60, where the system becomes very strongly correlated.

The plasmon DOS is of both theoretical and experimental importance. It is a useful quantity for analyzing the photoelectron spectra in layered materials particularly high-temperature superconductors.[24,25]

In the present case of a bilayer CB fluid, the plasmon modes in various theoretical approaches discussed above are expected to yield different results for the plasmon DOS. Figure 5 shows that the plasmon DOS for in-phase modes calculated from Eq. (11) exhibits a peak structure and this peak is enhanced by the inclusion of LF factor. In Fig. 6 we notice that the peak shifts toward low energies within the QLCA as the interlayer separation is increased. Furthermore, the peak height increases and the peak gets broader as we go to single-layer limit.

One can clearly see the influence of the correlation-induced energy gap on the plasmon DOS for the out-of-phase mode at coupling parameter r_s=20 in Fig. 7. Here the peak is also proportional to the interlayer separation as in the in-phase modes. We surmise that similar qualitative behavior should be expected of electron bilayers. The plasmon DOS clearly displays the correlation-induced energy gap in the out-of-phase mode. The peak in Fig. 7 is also proportional to the interlayer separation as in the in-phase modes. Thus, an indirect way to test the predictions of various theoretical models would be to conceive experiments measuring the plasmon DOS in bilayer systems.

In summary, we have considered the collective excitation modes of a bilayer charged Bose system. The ground-state correlations at low density were described by a number of

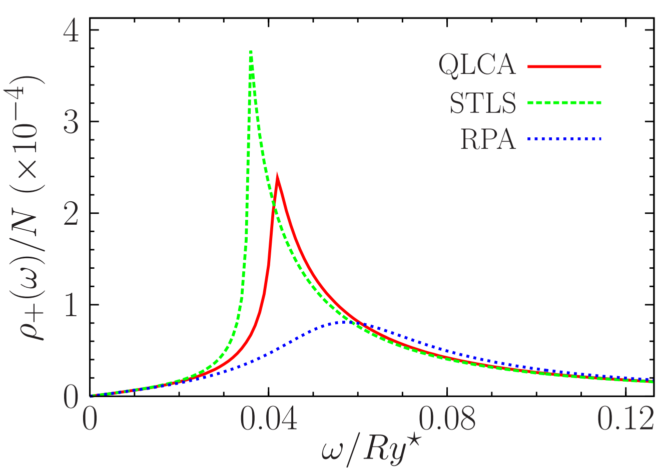

FIG. 5. (Color online) Plasmon DOS for in-phase modes of a bilayer CB liquid with respect to normalized plasmon energy computed in different approaches at r_s=20 and $\bar{d}$=0.5.

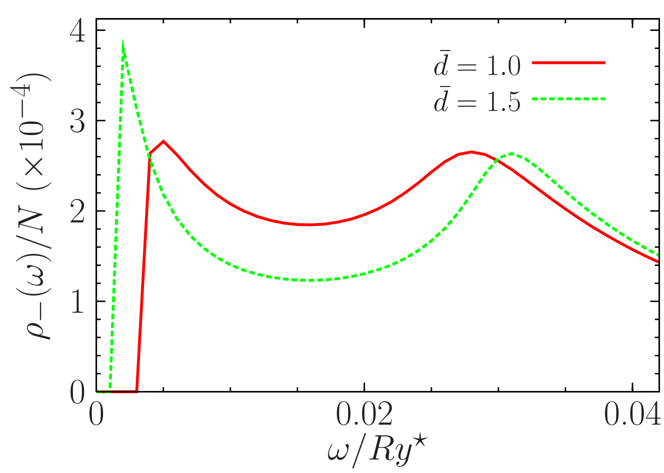

FIG. 7. (Color online) Plasmon DOS for out-of-phase modes in a bilayer CB liquid with r_s=20 computed within the QLCA in the single-layer limit.

theoretical approaches. Within the third-frequency-moment sum rule we have found that the out-of-phase mode $\omega_{-}(\boldsymbol{q})$ exhibits a gap at long wavelengths similarly to the situation in bilayer electron systems and classical layered charged-particle systems. We have calculated the plasmon DOS in various approximations which may be helpful to confirm the existence of such gapped modes in experimental situations.

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