Plasmon modes and energy gap in electronic bilayers

S. Ranganathan
Department of Physics, Royal Military College of Canada, Kingston, Ontario, Canada K7K 7B4

R. E. Johnson
Department of Mathematics and Computer Science, Royal Military College of Canada, Kingston, Ontario, Canada K7K 7B4
(Received 29 July 2003; revised manuscript received 14 November 2003; published 19 February 2004)

Analysis of the dynamic structure factors of strongly coupled classical, symmetric electronic bilayers obtained from molecular dynamics simulation confirms the existence of two longitudinal collective modes. The in-phase mode resembles the optical mode seen in single-layer two-dimensional systems, while the out-of-phase mode shows an energy gap at wave numbers $q \rightarrow 0$ for interlayer separations d less than about 1.5 (in units of the Wigner-Seitz radius). These dispersion results corroborate recent molecular dynamics data obtained using a different algorithm and analysis, and for a lower value of the plasma parameter Γ. The energy gap is seen not to be very sensitive to the value of Γ. The analysis of our data has brought out an interesting feature: a bifurcation of the out-of-phase dispersion curve for a high value of $\Gamma(=80)$ for intermediate values of d. This feature is not seen for lower values of $\Gamma(=40)$ and has not been predicted by any theoretical model.

DOI: 10.1103/PhysRevB.69.085310 PACS number(s): 73.21.Ac, 73.22.Lp, 61.20.Ja

I. INTRODUCTION

Layered electronic systems have been the focus of recent research; interest is based on the fact that such systems can now be routinely fabricated in semiconductor devices and other physical tools. A good representative model of such a system that is amenable to theoretical and molecular dynamics (MD) analysis is a bilayer consisting of electrons in two parallel layers embedded in a neutralizing background and separated by distance d. The particles satisfy classical statistics, have the same density in the two layers and interact with the $1/r$ Coulomb potential. The single-component bilayer is equivalent to a two-component single-layer system with an interaction potential matrix $V_{11}(r)=V_{22}(r)=e^2/r$ and $V_{12}(r)=V_{21}(r)=e^2/\sqrt{r^2+d^2}$, where e is the electronic charge. This system is completely defined by two parameters: the interlayer separation d and the coupling constant $\Gamma=e^2/ak_BT$, where $a=(n\pi)^{-1/2}$ is the Wigner-Seitz radius and n is the surface density of particles. There have been theoretical investigations of both static and dynamic properties of such systems.[1–5] Recently, MD simulations[6–9,14] have provided much-needed results for comparison with those of the theoretical models. In this paper we focus on the collective modes of strongly coupled electronic bilayers; in particular, we obtain the dispersion relations for the in-phase and out-of-phase modes from the pertinent dynamic structure factors. We are then able to consider the question of the existence of an energy gap in the out-of-phase modes.

Before analyzing the MD data, it is useful to summarize the theories pertaining to collective excitations in bilayers. Two longitudinal modes have been identified: an in-phase mode in which the particles in the two layers oscillate in phase, and a mode with oscillations 180° out of phase. All theoretical models predict that the resulting dispersion relation for the in-phase mode is similar to that of a single-layer two-dimensional electron gas (2DEG), and that the frequency ω in terms of wave number q behaves as $\sqrt{q}$ for $q \rightarrow 0$, typical of an optical mode. However, the theories differ with regard to the small q behavior of the out-of-phase mode. The random-phase-approximation (RPA) predicts an acoustic mode ($\omega \sim q$ for $q \rightarrow 0$) for the long-wavelength behavior of this mode;[10] the RPA is applicable in the weak coupling regime ($\Gamma \ll 1$) where the particle correlations can be ignored. The effects of interlayer and intralayer correlations, essential for strongly coupled bilayers, have been taken into account using the Singwi-Tosi-Land-Sjolander (STLS) approximation[11] or the quasilocalized charge approximation (QLCA).[12] The two methods arrive at different predictions regarding the out-of-phase mode: the QLCA predicts a nonzero energy gap as $q \rightarrow 0$, while the STLS does not. It may be possible to reconcile these approaches by considering the effects of damping which may render the oscillator strength to be very small;[5] however, one needs to compare with experimental or MD results for a verification of the various theoretical predictions. Experimental results cannot readily be used for comparison because real systems do have quantum features, and the interaction potentials are more complicated than the ones assumed in theory. Recent experiments on dispersion of plasmon modes involve large interlayer separations where the energy gap is not evident.[13] Another tool for investigation of collective mode phenomena is computer simulation. The object of this paper is to present MD results for the dispersion relations of in-phase and out-of-phase longitudinal modes of a strongly coupled bilayer, and to use these results to study the energy gap. Although our simulation involves classical systems, it should describe the features of a quantum bilayer in a qualitative fashion. Very recently, MD results that indicate an energy gap in such systems have been published.[14] Our approach is different both in computational technique and in methodology. Our simulation uses a different algorithm and a higher value of the coupling constant, and our analysis is based on the more appropriate $S(q,\omega)$. Our results should produce a much-needed confirmation of their results and a further validation of theoretical approaches.

Our MD calculations are based on a generalized Ewald

 ©2004 The American Physical Society

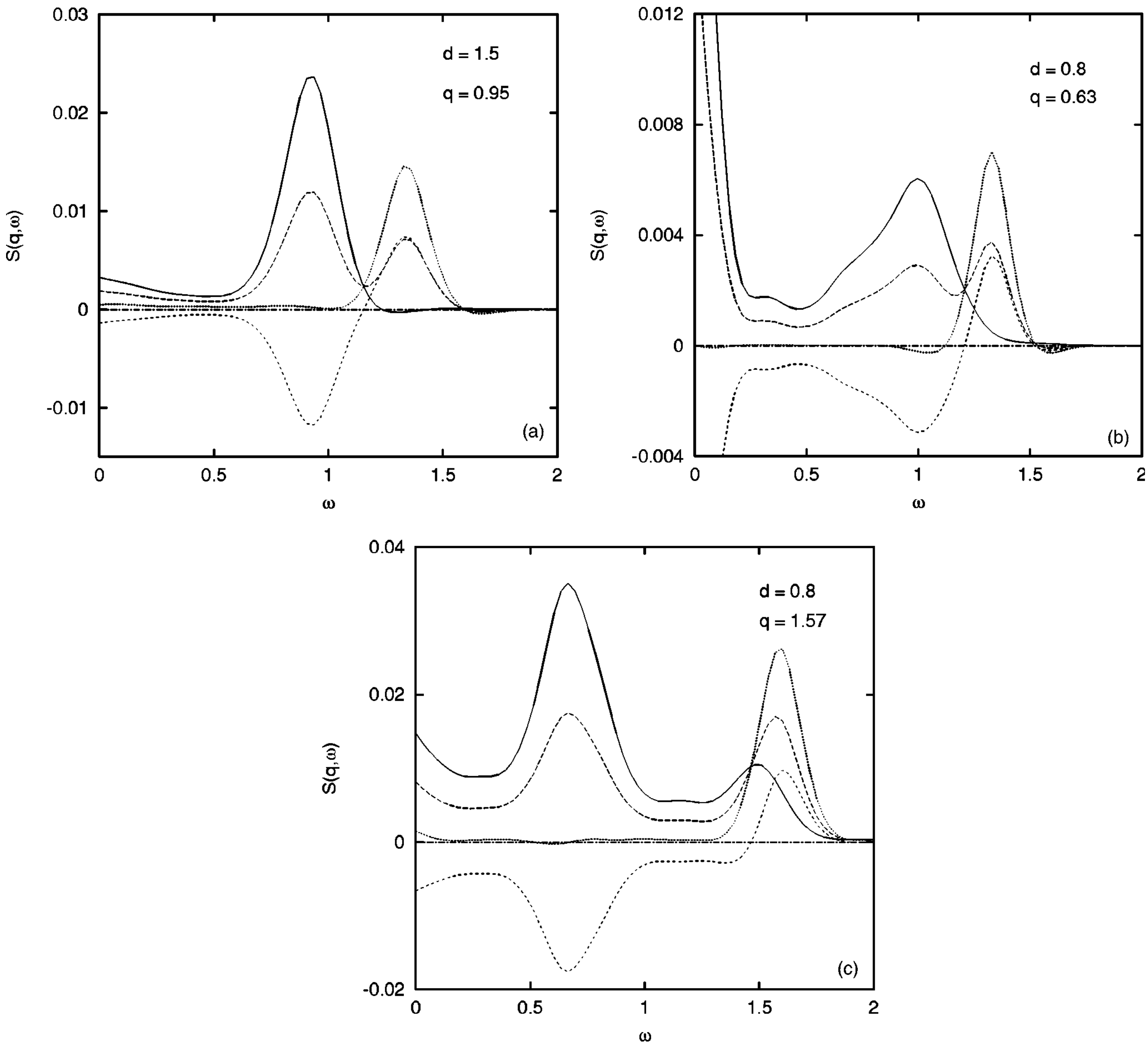

FIG. 1. Dynamical structure factors $S_{11}(q,\omega)$ (long dash), $S_{12}(q,\omega)$ (short dash), $S_+(q,\omega)$ (dot), and $S_-(q,\omega)$ (solid) for $\Gamma=80$: (a) $d=1.5$, $q=0.95$; (b) $d=0.8$, $q=0.63$; (c) $d=0.8$, $q=1.57$. Quantities plotted in these figures are all in dimensionless units as defined in the text. Also note that smooth curves through our data points are used.

sum dynamics algorithm which has been used to investigate static and dynamic properties of a classical, symmetric bilayer.[7–9] In particular, the dynamic structure factors $S_{11}(q,\omega)$ and $S_{12}(q,\omega)$ for $\Gamma=80$ and various values of d have been obtained.[9] The reader is referred to this paper for details regarding the simulation, the evaluation of the quantities of interest and the reliability checks considered. All quantities involved are in dimensionless units: distance in units of WS radius a, wave vector q in units of $1/a$, time in units of $\tau=\sqrt{ma^3/e^2}$, where m is the electron mass and ω is frequency in units of $1/\tau$. Our previous studies[7,8] have shown that a bilayer with $\Gamma=80$ (which is in a liquid phase for a single-layer 2DEG), undergoes dramatic changes in its structure, pair correlation functions, diffusion coefficient, and single particle properties as the interlayer separation changes. Therefore, we concentrate on $\Gamma=80$ to investigate the dispersion relations and the energy gap; it appears that this state may provide a better test for confirmation of theory than do smaller values of Γ.

Two longitudinal modes appear in these correlation functions and a separation of these modes can be accomplished by a linear combination: the in-phase modes then appear in $S_+(q,\omega)=S_{11}(q,\omega)+S_{12}(q,\omega)$, and the out-of-phase modes in $S_-(q,\omega)=S_{11}(q,\omega)-S_{12}(q,\omega)$. A collective mode, if any, appears as a peak at a nonzero frequency in these spectra. Since the number of particles in each layer was taken to be 512, the corresponding minimum value of q that can be investigated by our MD simulation is 0.157. Thus, an extrapolation of our results to $q\rightarrow 0$ is needed in order to investigate the energy gap.

We considered a number of discrete values of q between 0.157 and 2.56, (consistent with our MD), and selected d between 0.15 and 5.0. Previous MD results[14] have been presented in terms of longitudinal current correlation functions $L_+(q,\omega)=\omega^2 S_+(q,\omega)$ and $L_-(q,\omega)=\omega^2 S_-(q,\omega)$. It is known that if the collective peak in $S(q,\omega)$ is sharp, it will also appear as a sharp peak in $L(q,\omega)$ at essentially the same frequency. But if the peak is broad, it can appear somewhat distorted in $L(q,\omega)$ and its position may also be slightly different. For larger q, $L(q,\omega)$ may show a side peak where none exists in $S(q,\omega)$. In general, while it is safe to use $L(q,\omega)$ for small q, it is more prudent to analyze $S(q,\omega)$ for collective behavior. We observed one distinct peak in the S_+ and L_+ spectra for every d and q which we considered. This was not always true for S_-: in many cases, but not all, the central peak of $S_-(q,\omega)$ is very dominant and any collective peaks are considerably damped. By considering $L_-(q,\omega)$ one eliminates the central peak and augments the others. We have analyzed our results using $S_-(q,\omega)$ and wherever possible $L_-(q,\omega)$, and have checked that the correlation functions satisfy the zeroth and second moment sum rules.

II. RESULTS

To show how the behavior of $S_{11}(q,\omega)$ and $S_{12}(q,\omega)$ translates to that of $S_+(q,\omega)$ and $S_-(q,\omega)$, we have plotted these four functions together in Figs. 1(a)–1(c) for $\Gamma=80$ and representative values of d and q. In Fig. 1(a), for $d=1.5$ and $q=0.95$ we see that $S_{11}(q,\omega)$ and $S_{12}(q,\omega)$ are almost mirror images of each other except near the second peak, where they merge almost completely. Thus $S_+(q,\omega)$ and $S_-(q,\omega)$ each have one well defined collective peak, but at different values of ω. Such a pattern occurs quite often, though not in such a striking fashion, as illustrated in Fig. 1(b) for $d=0.8$ and $q=0.63$. Here also, $S_+(q,\omega)$ and $S_-(q,\omega)$ have well defined single peaks at different values of ω. However, in Fig. 1(c) with $d=0.8$ and q increased to 1.6, we see that, while $S_{11}(q,\omega)$ and $S_{12}(q,\omega)$ still are mirror images of each other for small ω, the heights of their second peaks are quite different. These features then yield just one collective peak for $S_+(q,\omega)$, but two distinct collective peaks for $S_-(q,\omega)$; the shorter peak at larger ω has its origin in the difference in height of the second peaks in $S_{11}(q,\omega)$ and $S_{12}(q,\omega)$. For $\Gamma=80$ such a pattern is seen for d between about 0.6 and 1.1 for certain values of q. This phenomenon produces a second branch of the dispersion relation for the out-of-phase plasmon mode and will be discussed in detail later in this paper. On the other hand, $S_+(q,\omega)$ always displays just a single peak for any d, and for q values that are small enough to yield a collective behavior. It should be emphasized that if the second peak heights in $S_{11}(q,\omega)$ and $S_{12}(q,\omega)$ are essentially the same, there will not be a second peak in $S_-(q,\omega)$.

While the out-of-phase modes are clearly discernible in the plots of $S_-(q,\omega)$ for larger values of d, the same is not true for smaller d. To clarify, we have plotted in Figs. 2(a) and 2(b) $S_{11}(q,\omega)$, $S_{12}(q,\omega)$, $S_-(q,\omega)$, and $L_-(q,\omega)$ for $d=0.15$ and 0.4. The value of q is 0.63. Note that the ω values in the figures have been restricted in the range 0.8 to 2.8 so as to focus just on the collective peak structure. The complete graphs for $S_{11}(q,\omega)$ and $S_{12}(q,\omega)$ for these states are shown in Ref. 9. It is seen that the out-of-phase peak does not show up very clearly in $S_-(q,\omega)$, though that peak does exist as can be seen distinctly in $L_-(q,\omega)$. Thus we use $L_-(q,\omega)$ plots for the dispersion relation curve when we know that such a mode must exist but is not seen unambiguously in $S_-(q,\omega)$ plots. It should be emphasised that the in-phase mode always shows up clearly in $S_+(q,\omega)$ for any d.

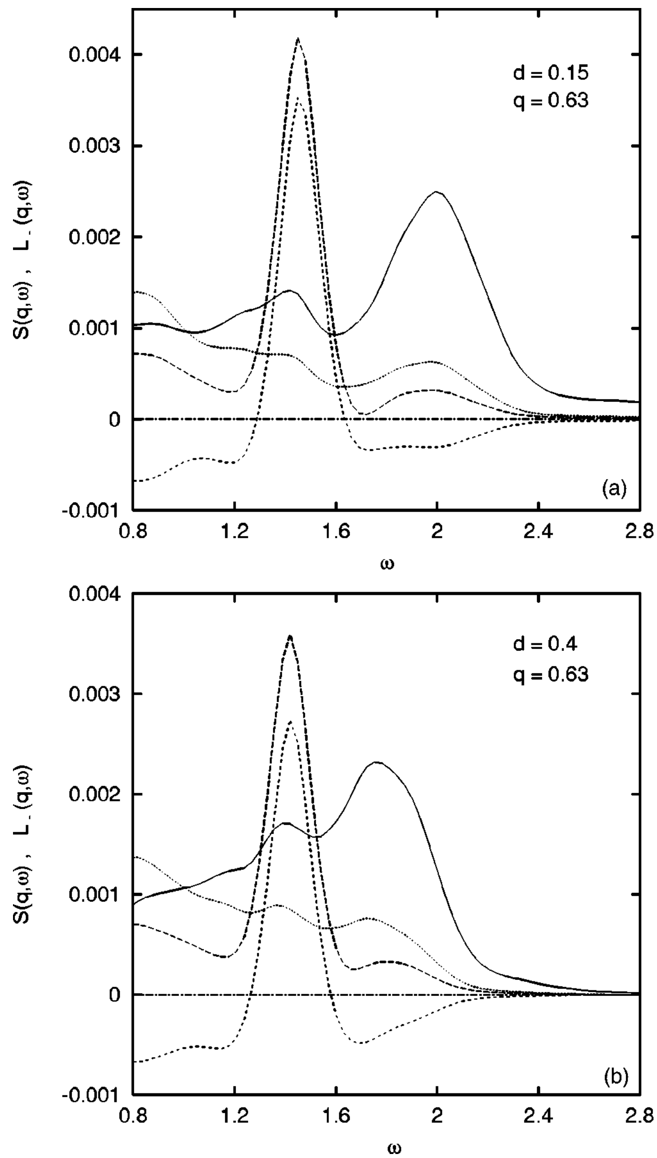

FIG. 2. $S_{11}(q,\omega)$ (long dash), $S_{12}(q,\omega)$ (short dash), $S_-(q,\omega)$ (dot), and $L_-(q,\omega)$ (solid) for $\Gamma=80$: (a) $d=0.15$, $q=0.63$; (b) $d=0.4$, $q=0.63$.

However, when Γ is reduced to 40 (corresponding to the state investigated by Donkó *et al.*[14]), the two peak structure in $S_{11}(q,\omega)$ is not seen. This is shown in Figs. 3(a) and 3(b) for the same values of d and q as in Figs. 1(b) and 1(c), respectively. This suggests that the bilayer must be strongly coupled ($\Gamma\cong 80$) to produce two out-of-phase plasmon modes.

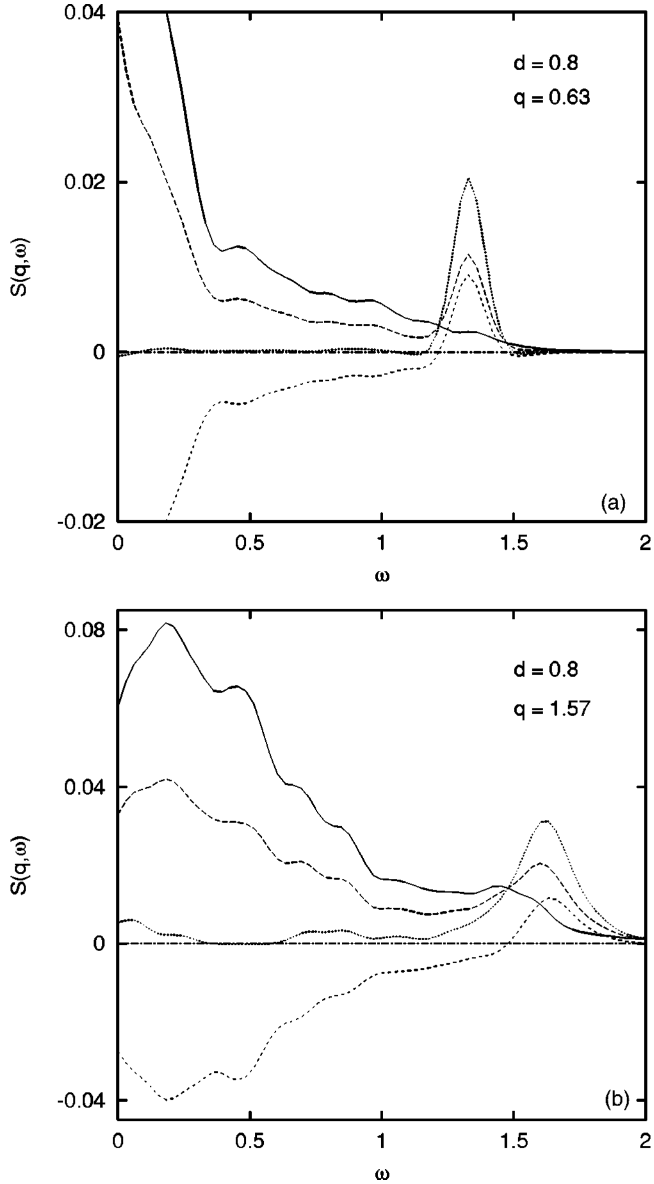

FIG. 3. $S_{11}(q,\omega)$ (long dash), $S_{12}(q,\omega)$ (short dash), $S_{+}(q,\omega)$ (dot), and $S_{-}(q,\omega)$ (solid) for $\Gamma=40$: (a) $d=0.8$, $q=0.63$; (b) $d=0.8$, $q=1.57$.

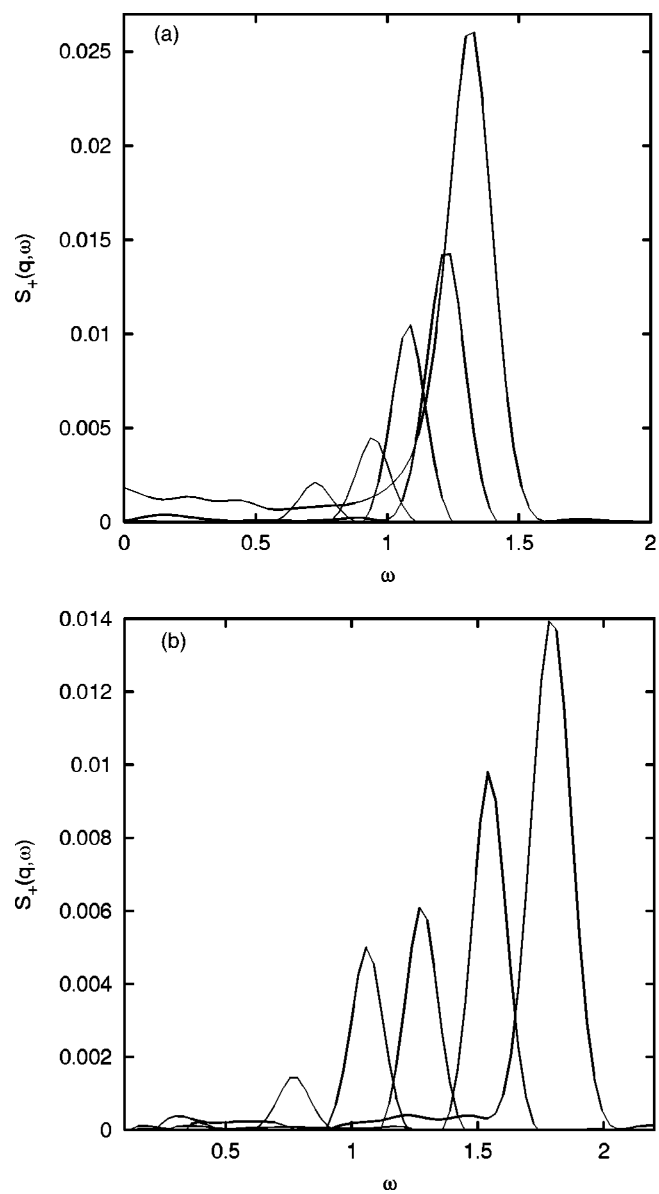

FIG. 4. $S_{+}(q,\omega)$ for $\Gamma=80$ and $q=0.16$, 0.31, 0.47, 0.79, 1.26 (left to right): (a) $d=2.0$; (b) $d=0.4$.

Figures 4(a) and 4(b) show the in-phase plasmon for $\Gamma=80$ with a rather large $d(=2.0)$ and a small $d(=0.4)$ for q between 0.16 and 1.26. In both plots the collective peak frequency is seen to decrease to 0 as q approaches 0; such a pattern is seen for all d. This optical mode is in agreement with theoretical predictions, although we have not analyzed its exact quantitative behavior.

However, as shown in Figs. 5(a), 5(b), and 5(c), $S_{-}(q,\omega)$ behaves quite differently as d is varied. For a large d, [such as 2.0 in Fig. 5(a)], there is only one collective peak frequency for the range of q displayed; it decreases to 0 as q approaches 0, qualitatively similar to that seen in Fig. 4(a) for $S_{+}(q,\omega)$. There is similar behavior for all d greater than about 1.5. For smaller d, the behavior of $S_{-}(q,\omega)$ is quite different: as q approaches 0 the collective peak frequency approaches a nonzero value called the ''energy gap.'' This is well illustrated in Fig. 5(b), where we have plotted $L_{-}(q,\omega)$ rather than $S_{-}(q,\omega)$ for $d=0.8$ for small values of q from 0.16 to 0.63. It is clear that as q approaches 0 the peak frequency is essentially a constant near $\omega=1$. Such an energy gap was observed in the out-of-phase plasmon mode for all d less than approximately 1.5.

Furthermore, for $\Gamma=80$ and d between 0.6 and 0.95, we discovered that $S_{-}(q,\omega)$ exhibits a two peak structure for certain values of q. This feature is illustrated in Fig. 5(c) for $d=0.8$ and $q=1.26$, 1.57, and 1.89, while its origin is explained by Fig. 1(c). Thus, for $d=0.8$ and q less than about 0.63, there is a single small side peak at $\omega\cong1$, but for $q>0.63$, there is a bifurcation in the dispersion relation plot. The branch normally seen in weakly coupled bilayers is that in which the peak frequency increases with q, but here we see another branch in which the peak frequency *decreases* with q. Our data show that the double peak structure in

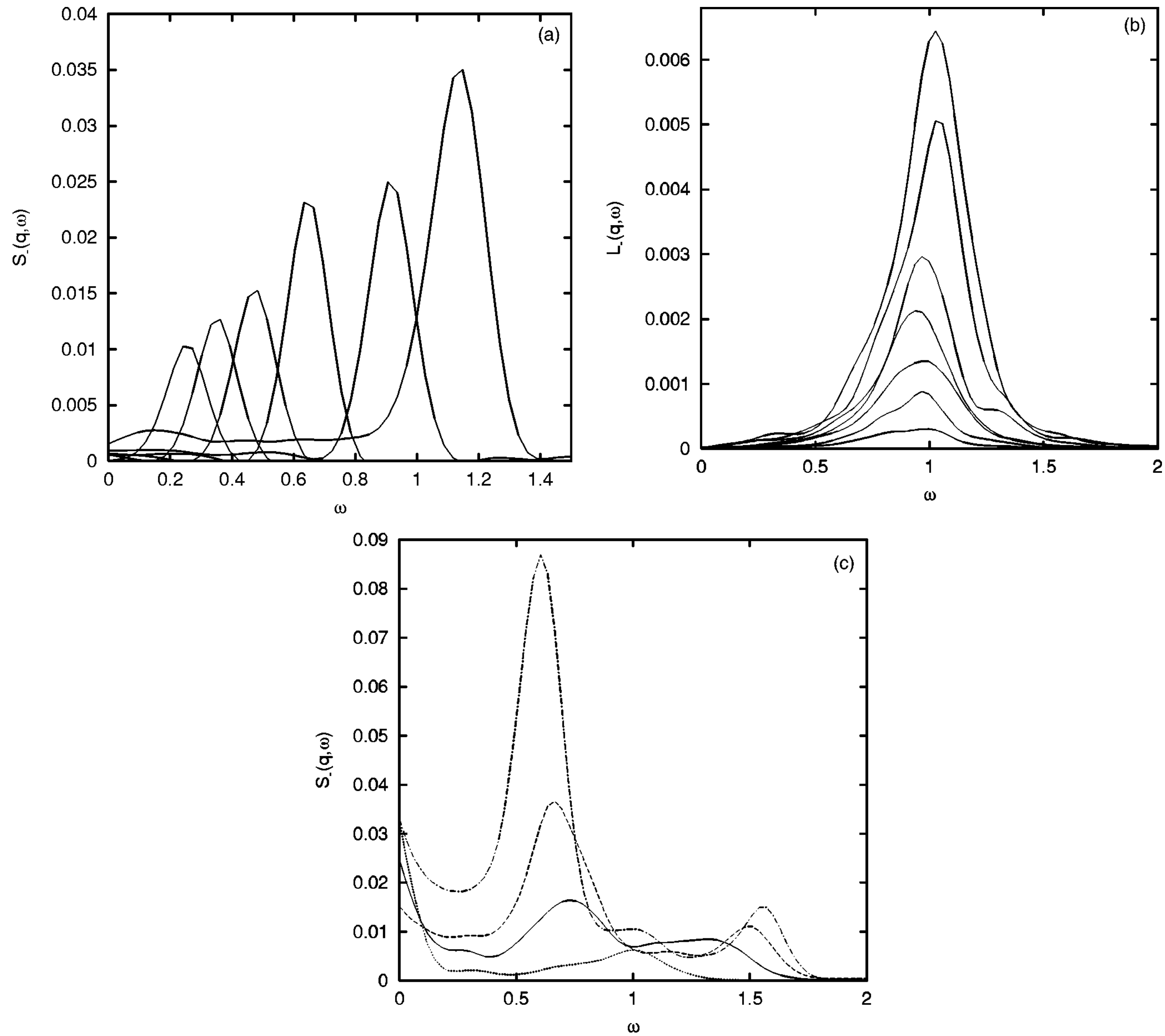

FIG. 5. (a). $S_{-}(q,\omega)$ for $\Gamma=80$, $d=2.0$ and $q=0.16$, 0.22, 0.31, 0.47, 0.79, 1.26 (left to right). (b) $L_{-}(q,\omega)$ for $\Gamma=80$, $d=0.8$ and $q=0.16$, 0.22, 0.31, 0.35, 0.47, 0.57, 0.63 (bottom to top). [Note that these peaks are not as clearly visible in $S_{-}(q,\omega)$.] (c) $S_{-}(q,\omega)$ for $\Gamma=80$, $d=0.8$ and $q=0.63$ (dotted), 1.26 (solid), 1.57 (dashed), 1.89 (dash-dot).

$S_{-}(q,\omega)$ occurs for $0.6<d<1.1$ at $\Gamma=80$. This behavior is not seen for $\Gamma=40$ as can be deduced from Figs. 3(a) and 3(b), and from earlier MD results.[14]

Our results indicate that there are two longitudinal (plasmon) modes in a strongly coupled bilayer, and that the out-of-phase mode has two branches for intermediate d. The dispersion relations for the two modes are displayed in Fig. 6(a). Recall that the minimum value of q that can be studied in our MD is 0.157. The in-phase mode dispersion $\omega_{+}(q)$ is shown for nine values of d from 0.15 (top, solid) to 5.0 (bottom, solid). The out-of-phase mode dispersion $\omega_{-}(q)$ is displayed for three values of d from 1.5 (bottom, dashed)to 5.0 (top, dashed). All of the in-phase dispersion relation plots approach 0 as for small $q\rightarrow 0$ and behave similar to $\sqrt{q}$ for small q. This is the expected behavior of the optical mode and is in agreement with theoretical predictions. The dispersion relation for the out-of-phase mode for $d>1.5$ seems to show a linear dependence on q for small q, typical of an acoustic mode. It should also be noted that for large d $(=5.0)$, the graphs of $\omega_{+}(q)$ and $\omega_{-}(q)$ essentially merge. Experimental results, albeit for a much lower value of Γ, show such a merging pattern.[5,13]

However, for $d<1.5$, the out-of-phase dispersion does not go to 0 as $q\rightarrow 0$. Figure 6(b) shows a plot of $\omega_{-}(q)$ for eight values of d from 0.15 (top) to 1.1 (bottom). Here we have chosen to plot only the upper portion of the dispersion curve; the bifurcation is discussed in the next paragraph. It is clear that the graphs approach a constant nonzero value for small q. This establishes that an energy gap exists for d less than about 1.5. As mentioned earlier, theoretical models based on STLS approximation[11] do not predict an energy gap, while those based on QLCA (Ref. 12) do. Our results thus validate

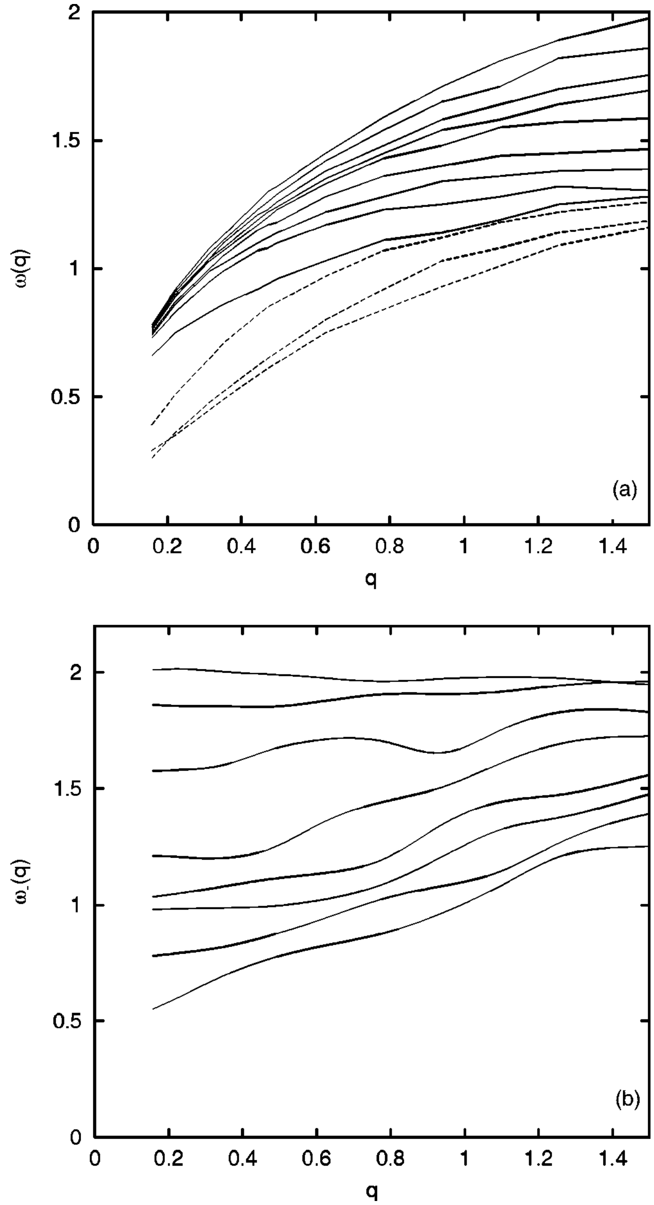

FIG. 6. (a) In-phase mode dispersion $\omega_+(q)$ (solid) for $\Gamma=80$ and $d=0.15$, 0.3, 0.6, 0.7, 0.8, 1.1, 1.5, 2.0, 5.0 (top to bottom); out-of-phase mode dispersion $\omega_-(q)$ (dashed) for $\Gamma=80$ and $d=1.5$, 2.0, 5.0 (bottom to top). (b) $\omega_-(q)$ for $d=0.15$, 0.3, 0.4, 0.6, 0.7, 0.8, 0.95, and 1.1 (top to bottom).

the latter theory as well as recently published MD results for $\Gamma=40$.[14]

Figure 7 shows the complete dispersion relation curves for the out-of-phase plasmon mode $\omega_-(q)$ for three values of d that show bifurcation. For these values of d and q sufficiently large, $S_-(q,\omega)$ shows a two peak structure, indicating the existence of two collective modes. The split occurs around $q=1.25$ for $d=0.95$ and around a much smaller $q=0.5$ for $d=0.6$. This behavior is not seen at $\Gamma=40$ (at least for q less than 2.5), suggesting that it occurs only in very strongly coupled bilayers. We are not aware of any theoretical model that has predicted this new phenomenon.

Finally, in Fig. 8 we have plotted the energy gap values

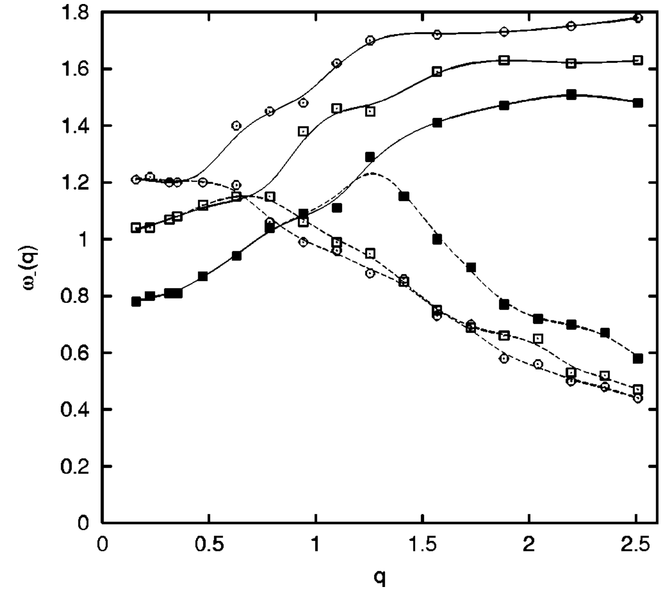

FIG. 7. Both branches of $\omega_-(q)$ for $\Gamma=80$ and $d=0.6$, 0.7, 0.95 (top to bottom as seen at the left edge). Our data points are shown.

$\omega_-(q\to 0)$ in units of 2D plasma frequency $\omega_0=\sqrt{2\pi n e^2/ma}(=\sqrt{2}/\tau)$, as a function of the interlayer separation d. Our results for $\Gamma=80$ were obtained using Fig. 5(b) with extrapolation, so are somewhat coarse. The data for $\Gamma=40$ were taken from Ref. 14. Together, they indicate that the energy gap is quite insensitive to the coupling parameter.

III. CONCLUSIONS

We have performed a detailed analysis of the two dynamic structure factors in an electronic bilayer system and identified how the side peaks develop and contribute to the

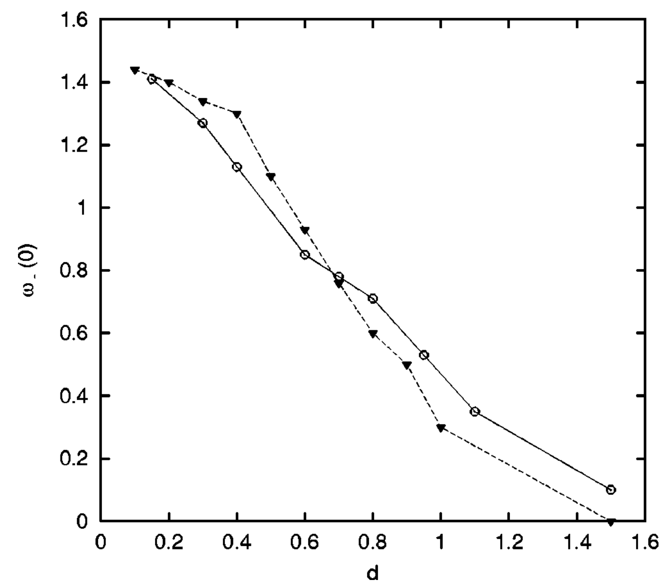

FIG. 8. Energy gap $\omega_-(q\to 0)$ as a function of d: $\Gamma=80$ (solid) and $\Gamma=40$ (dashed). The unit used for the ordinate here is $(\sqrt{2}/\tau)$ to agree with Ref. 14.

dispersion curves. Our dispersion results for $\Gamma=80$ are very similar to the recent MD results for $\Gamma=40$.[14] We have used a different algorithm and a different analysis, and our corroborating results serve as a validation of the two approaches. Thus, we conclude that (i) an energy gap exists, without question, in classical electronic bilayers for small interlayer separations, (ii) its value is not sensitive to the coupling parameter Γ, and (iii) it is in qualitative agreement with the predictions of the QLCA theory.[4] Experiments have been performed for weakly coupled quantum bilayer systems and they do not show an energy gap.[13] This is so because the interlayer separations in these experiments are quite large. It would be most interesting to perform such experiments for smaller d to see if the energy gap develops. An interesting feature discovered in our findings is the splitting of the out-of-phase dispersion relation for strongly coupled bilayers at intermediate interlayer separations. For $\Gamma=80$, the splitting occurs only for values of d from about 0.5 to 1.0, and the value of q where this occurs increases as d is decreased. This feature is not seen for lower values of the plasma parameter and has not been predicted by any theory, as far as we are aware.

ACKNOWLEDGMENTS

This research was supported in part by a grant from the Academic Research Program (ARP) of the Department of National Defence, Canada.

[1] V. I. Valtchinov, G. Kalman, and K. B. Blagoev, Phys. Rev. E **56**, 4351 (1997).

[2] C. Zhang, Phys. Rev. B **49**, 2939 (1994).

[3] L. Swierkowski, D. Neilson, and J. Szymanski, Aust. J. Phys. **46**, 423 (1992); L. Liu, L. Swierkowski, D. Neilson, and J. Szymanski, Phys. Rev. B **53**, 7923 (1996).

[4] G. J. Kalman, V. Valtchinov, and K. I. Golden, Phys. Rev. Lett. **82**, 3124 (1999).

[5] J. Ortner, Phys. Rev. B **59**, 9870 (1999).

[6] Z. Donkó and G. J. Kalman, Phys. Rev. E **63**, 061504 (2001).

[7] S. Ranganathan, R. E. Johnson, and K. N. Pathak, Phys. Rev. E **65**, 051203 (2002).

[8] S. Ranganathan and R. E. Johnson, Phys. Rev. E **67**, 041201 (2003).

[9] R. E. Johnson and S. Ranganathan, Phys. Rev. B **69**, 085309 (2004), the preceding paper.

[10] S. Das Sarma and A. Madhukar, Phys. Rev. B **23**, 805 (1981).

[11] K. S. Singwi, M. P. Tosi, R. H. Land, and A. Sjolander, Phys. Rev. **176**, 589 (1968).

[12] G. Kalman and K. I. Golden, Phys. Rev. A **41**, 5516 (1990); K. I. Golden and G. J. Kalman, Phys. Plasmas **7**, 14 (2000); K. I. Golden and G. Kalman, J. Phys. A **36**, 5865 (2003).

[13] T. B. Mitchell *et al.*, Science **282**, 1290 (1998); D. S. Kainth *et al.*, Phys. Rev. B **59**, 2095 (1999); D. S. Kainth *et al.*, J. Phys.: Condens. Matter **12**, 439 (2000).

[14] Z. Donkó, G. J. Kalman, P. Hartmann, K. I. Golden, and K. Kutasi, Phys. Rev. Lett. **90**, 226804 (2003).