

# Dynamic Excitation Modes of Couples Electron-Hole Quantum-Well Structure

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**Abstract :** We have theoretically investigated the role of many-body correlations in determining the dynamic excitation modes of coupled electron-hole quantum-well structure over a wide range of particle number density  $r_s$  and well spacing  $d$ . The intra-and interwell correlations are treated on the same footing within the self-consistent dynamic mean-field approximation. The excitation modes of the system are obtained from the calculation of the imaginary part of the frequency and wave vector dependent linear density response function  $\text{Im} \chi(q, \omega)$ . In addition to the usual single particle excitations, the coupled bilayer supports two collective excitation modes (plasmons), namely, the in-phase and out-of-phase modes. The in-phase mode is strongly affected by manybody correlations. As an interesting result, we find that  $\text{Im} \chi(q, \omega)$  exhibits, in the sufficiently close approach of two wells, a strong peak at small  $\omega$  at finite  $q$ . The appearance of this strong peak in  $\text{Im} \chi(q, \omega)$  indicates that it costs relatively very little energy to excite the system into a density-modulated state of wave vector  $q$ . This new peak in  $\text{Im} \chi(q, \omega)$  could possibly be used as an experimental probe to detect the existence of a density-modulated ground state in the coupled electron-hole quantum-well system.

**IndexTerms - Quantum well, number density, plasmons.**

## I. INTRODUCTION

In this paper<sup>[1]</sup>, we investigated the ground-state behaviour of the symmetric electron-hole (e-h) quantum-well structure by employing the dielectric formalism and treating correlations beyond the static local-field theories within the dynamical or quantum version of the Singwi, Tosi, Land, and Sjolander (qSTLS) approach<sup>[2]</sup>. As an important result, our study revealed that the liquid phase in the e-h bilayer could become unstable against phase transition in to a coupled Wigner crystal (WC) ground state at sufficiently low density in the close approach of two layers. Notably, the critical density for the phase transition was predicted to shift towards the higher-density side as compared to the corresponding value in the case of an isolated electron layer. Moreover, at densities higher than the critical density for crystallization, the qSTLS theory predicted transition to a charge-density-wave (CDW) ground state, thus implying a crossover from the CDW state to the WC state at a critical value of carrier density. The prediction of Wigner crystallization agreed qualitatively with the findings of the diffusion Monte Carlo calculations of De Palo et. al.<sup>[3]</sup>. In our calculations, the transition to the density modulated phase, i.e., the WC or CDW phase, appeared in the form of a divergence in the liquid state static density susceptibility at a finite wave vector value. Also, the intra-and interlayer pair-correlation functions exhibited pronounced in-phase oscillations typical of an ordered crystalline phase near the transition region. Earlier, Szymanski et. al. had obtained qualitatively similar results for the e-h ground state by using the so-called semi-STLS approach.

If the static properties, viz. the static pair correlation functions and the static density susceptibility, are so markedly affected near the transition region, it would be interesting and important to examine the behaviour of dynamic properties of the e-h bilayer at near system parameters associated with the phase transition of the system into a density-modulated phase. In particular, one could speculate to find the signs of the above structural phase transition in the dynamic excitation spectrum. This makes our motivation for the present work. In this paper, we intend to look into the behaviour of the dynamic excitation modes of the symmetric e-h quantum well structure - a quantity that is directly measurable, for instance, in the X-ray inelastic scattering experiments<sup>[4]</sup>. In Sec. 2, we present in brief the bilayer model and the theoretical formalism used. Results and discussion are given in Sec. 3. Conclusions are reported in Sec. 4.

## II. THEORETICAL FORMALISM AND FONTS

We consider a double-quantum-well structure with  $d$  as the center-to-center well separation. The carriers are electrons in one well and holes in the other. The motion of carriers is free along the  $xy$  plane and under the action of a double-well potential profile in the  $z$  direction. We assume that the wells are extremely narrow and the potential barriers along the  $z$  axis are high enough so that the particles occupy only the lowest-energy subband for the  $z$  motion and there is negligible overlap between the wave functions of the carriers in the two wells. The wells are assumed to be identical in each respect except for the charge of carriers. Also, the bilayer system is assumed to be embedded in a

uniform charge neutralizing background. On neglecting the effect of integrating over the finite extent of the particle wave function in the  $z$  direction, the Coulomb interaction potential among the carriers is obtained as

$$V_{ij}(q) = \alpha_{ij}(q)V(q)e^{-q|i-j|d} \tag{1}$$

where  $i = 1, 2$  is the layer index  $\alpha_{ij} = (-1)^{|i-j|}$  and  $V(q) = 2\pi e^2 / (q\epsilon_0)$ , is the intralayer interaction potential, with  $\epsilon_0$  being the background dielectric constant.

In the dielectric approach, the density-density linear response function  $\chi(q, \omega)$  plays the role of a central quantity in determining the many-body properties of the system. For the double layer system, the response function can be compactly expressed in the form of a  $2 \times 2$  matrix, and in the generalized mean-field approximation the elements of the inverse of the density response matrix are given by :

$$\chi_{ij}^{-1}(q, \omega) = \frac{\delta_{ij}}{\chi_i^0(q, \omega)} - V_{ij}(q)[1 - G_{ij}(q, \omega)] \tag{2}$$

where  $\chi_i^0(q, \omega)$  is the density response function of non-interacting carriers in layer (i.e., the Stern function<sup>[5]</sup>) and  $G_{ij}(q, \omega)$  is the dynamic local-field correction (LFC) factor accounting for the correlation effects among the carriers in the layers  $i$  and  $j$ . In the quantum version of the STLS approach<sup>[1]</sup>,  $G_{ij}(q, \omega)$  is given by

$$G_{ij}(q, \omega) = -\frac{1}{n} \int \frac{dq'}{4\pi^2} \frac{\chi_i^0(q, q'; \omega)V_{ij}(q')}{\chi_i^0(q, \omega)V_{ij}(q)} \times [S_{ij}(|q - q'|) - \delta_{ij}] \tag{3}$$

Here,  $\chi_i^0(q, q'; \omega)$  is the in-homogeneous density response function of non-interacting electrons and  $S_{ij}(q)$  is the static density structure factor. The fluctuation-dissipation theorem, which relates  $S_{ij}(q)$  with the imaginary part of the linear response function as

$$S_{ij}(q) = -\frac{\eta}{n\pi} \int_0^\infty d\omega \text{Im} \chi_{ij}(q, \omega) \tag{4}$$

closes the set of qSTLS equations for the density response function. Evidently, the response function calculation has to be carried out numerically in a self-consistent way.

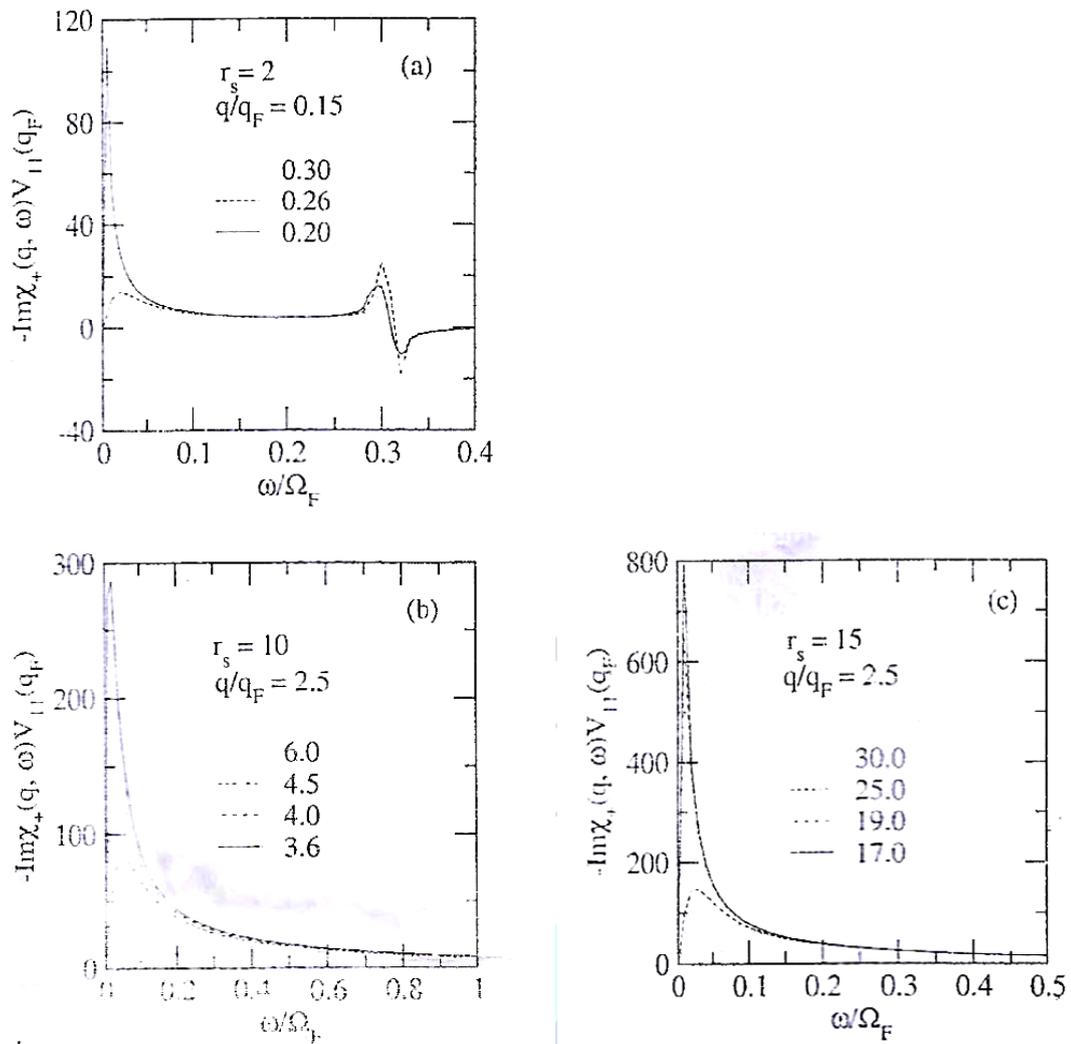
The dynamic excitation spectrum can be obtained from the imaginary part of the diagonalized density response function as<sup>[6]</sup>

$$\chi^\pm(q, \omega) = \frac{\chi_1^0(q, \omega)}{1 - \chi_1^0(q, \omega)[\varphi_{11}(q, \omega) \pm \varphi_{12}(q, \omega)]} \tag{5}$$

with  $\varphi_{11}(q, \omega) = V_n(q)[1 - G_n(q, \omega)]$  and  $\varphi_{12}(q, \omega) = V_{12}(q)[1 - G_{12}(q, \omega)]$ . The + and - signs correspond, respectively, to the in-phase and out-of-phase ( $\pi$ ) modes of the density modulations in the two layers.

### III. RESULTS AND DISCUSSION

It is straight forward to obtain the imaginary part of  $\chi^\pm(q, \omega)$  from Eq. (5). The only inputs required are the real and imaginary parts of the intra- and interlayer LEC factors and these can be determined numerically from Eq. (3) by using the self-consistent results of  $S_{ij}(q)$ ;  $S_{ij}(q)$  are, in turn, obtained numerically from the self-consistent solution of Eqs.(2)-4).

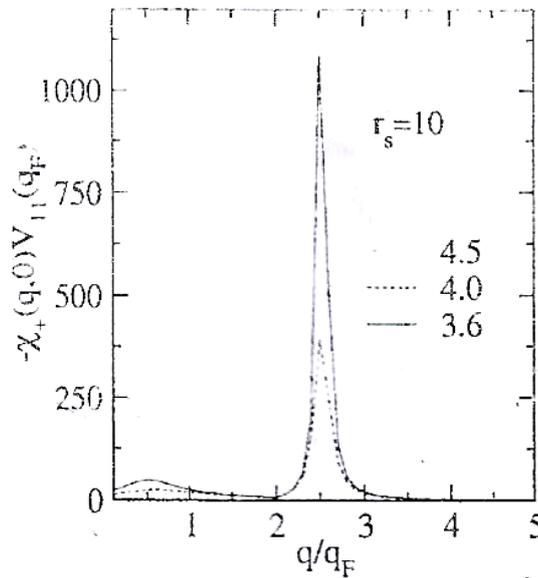


**Fig. 1 : (a)-(c)**  $Im \chi_{\pm}(q, \omega)$  vs.  $\omega/\Omega_F$  at different values of  $r_s$ ,  $q/q_F$  and  $d/a_0$ . Legends indicates the values of  $d/a_0$  and  $\Omega_F$  is the Fermi energy.

In this way, we calculate  $Im \chi_{\pm}(q, \omega)$  in the entire  $q - \omega$  plane over a wide range of density  $r_s$  and spacing  $d$ , but the results are reported here only for those values of system parameters at which the static density susceptibility  $\chi_{\pm}(q, 0)$  is given in I.  $r_s = 1/a_0(n\pi)^{1/2}$ , is the dimensionless density parameter, with  $n$  as the areal density of carriers and  $a_0$  the Bohr atomic radius.

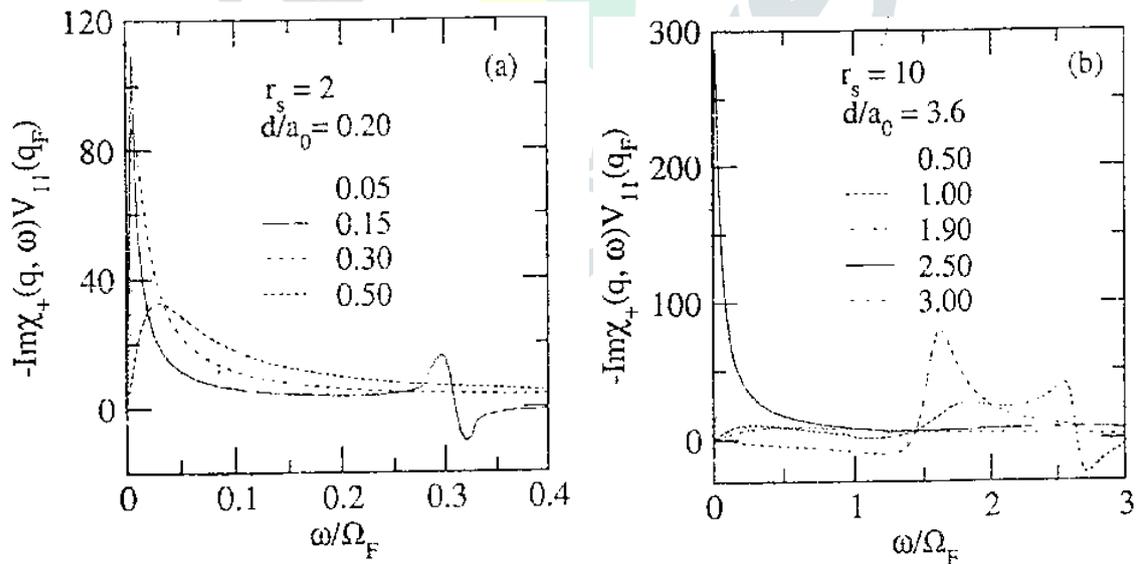
For the e-h bilayer, it is the in-phase mode, i.e.  $\chi_{+}(q, 0)$ , which can exhibit singular behaviour. Therefore, we plot in Fig. 1 (a-c) the results of  $Im \chi_{+}(q, \omega)$  as a function of frequency  $\omega$  by keeping the wave vector  $q$  fixed at a value equal to the one associated with the density-modulated phase at layer parameters lying in the transition region. We note that  $Im \chi_{+}(q, \omega)$  exhibits a sharp peak at small  $\omega$  at relatively smaller layer spacing, and decreasing the spacing makes the peak to grow higher in its strength and to move towards origin, i.e.  $\omega = 0$ . As the layer spacing approaches the critical  $d$  associated with the onset of density-modulated phase, the position of the low-frequency peak in  $Im \chi_{+}(q, \omega)$  seems to converge to  $\omega = 0$ . This in turn implies that it costs the system close to the transition point nearly zero or very little energy to excite it from the homogeneous liquid phase into an in-phase inhomogeneous density-modulated state having wave vector  $q_c$ .

For sake of completeness, we have also reproduced the behaviour of static density susceptibility  $\chi_{+}(q, 0)$  at  $r_s = 10$  and  $d/a_0 = 4.5, 4.0$  and  $3.6$  in Fig. 2. It is apparent that  $\chi_{+}(q, 0)$  exhibits a strong peak at  $q/q_F \approx 2.5$  and this peak seems to diverge for  $d/a_0 < 3.6$ ;  $q_F$  is 2D Fermi wave vector. This result, seen in conjunction with Fig. 1(b), strongly suggests that the presence of the phase transition to the density-modulated phase may show up in the dynamic excitation spectrum in the form of a new peak at vanishing frequency for  $q/q_F \approx 2.5$ .



**Fig. 2 :**  $\chi+(q,0)$  vs.  $q/q_F$  at different values of  $d/a_0$  for  $r_s = 10$ . Legends indicate the values of  $d/a_0$ .

We have also plotted in Fig. 2(a-b) the  $q$ -dependence of  $Im\chi+(q,\omega)$  by keeping  $d$  fixed at the critical spacing associated with the instability at  $r_s = 2$  and  $10$ . It is apparent that as  $q$  approaches, at a given  $r_s$ , the wave vector value of the density- modulated phase  $q_c$ , the peak in  $Im\chi+(q,\omega)$  grows to its maximum strength and its location approaches  $\omega = 0$ , and increasing  $q$  beyond  $q_c$  results in making this peak less strong and moving it towards higher-frequency side on the  $\omega$  axis. This once again supports our viewpoint that the liquid phase could become spontaneously unstable against transition into an inhomogeneous phase of density modulation wave vector  $q_c$  in the sufficiently close approach of the two layers. Apart from this, we notice the presence of a double-peak structure in  $Im\chi+(q,\omega)$  in the intermediate wave vector region - a feature also predicted to occur in an isolated electron layer<sup>[7]</sup>. Also, it may be noted that  $Im\chi+(q,\omega)$  assumes negative values at certain  $q - \omega$  points in violation with the fact that the dynamic structure factor is a positive definite quantity. This is one of the shortcomings of the qSTLS theory.



**Fig. 3 :** (a)-(b)  $Im\chi+(q,\omega)$  vs.  $\omega/\Omega_F$  at different values of  $r_s$ ,  $d/a_0$  and  $q/q_F$ . Legends indicate the values of  $q/q_F$  and  $\Omega_F$  is the Fermi energy..

**IV. CONCLUDING REMARKS**

In conclusion, we find that the instability of the liquid phase in the e-h bilayer may appear in the form of softening of the in-phase dynamic excitation mode. Although not reported here, we have found qualitatively similar behaviour of the dynamic excitation spectrum for the e-e bilayer; here, it is the out-of-phase mode that shows the softening behaviour. The observation of the soft mode in the form of a new peak appearing in the imaginary part of the in-phase

(out-of-phase) liquid-state density-density response function at small  $\omega$  and finite  $q$  could possibly be used as an experimental probe to detect the existence of a density-modulated ground state in the e-h (e-e) quantum well system.

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