Study of Finite Width Effects on Wigner Crystallization in Symmetric Electron-Hole Bilayer

Tarun Kumar Dey[1] and Brahma Nand Jha[2]

[1]Post Graduate Department of Physics, L. S. College, Muzaffarpur-842001
[2]Department of Physics, M.S.S.G College, Areraj, B.R.A Bihar University, Muzaffarpur – 842001.

Abstract : We examine the role played by the finite width of the layers in determining the critical density for the onset of Wigner crystallization in a symmetric electron-hole bilayer system. Such a phase transition can appear, for instance, in the liquid-state static density susceptibility in the form of a divergence at a wave vector representing the period of density prevailing in the crystal phase. In this perspective, we have theoretically calculated the static density susceptibility over a wide range of the carrier density r_s and the interlayer spacing *d*, by incorporating the effect of finite width of the two layers. The correlations among carriers (both the intra- and interlayre) are treated beyond the static mean-field theories by using the dynamical self-consistent mean-field approximation of Hasegawa and Shimizu. Our study reveals, parallel to the one where finite width effects are ignored, that the electron-hole liquid may become unstable with respect to the Wigner crystal phase above a critical r_s value (say r_s^c) for *d* lower than a critical spacing, while the charge-density-wave state might be the stable phase for $r_s < r_s^c$, r_s^c turns out to be lower as compared to the corresponding value for an isolated layer, and thus implying that the electron-hole correlations act to stabilize the Wigner crystal phase over the homogeneous liquid phase. On comparison of our results with similar studies without finite width effects, we find that the inclusion of these effects have tendency to augment the critical r_s for Winger crystallization.

IndexTerms - Crystallization, electron-hole-bilayer system, phase transition.

I. INTRODUCTION

During the last decade, the systems composed of two or more layers of electrons have attracted a great deal of interest both at the theoretical and experimental fronts. Such electron systems can be fabricated with a very good precision, for instance, at the interface of a semiconductor heterostructure, and this unit can be repeated periodically in the transverse direction to have a system of two or more layers. Many interesting and unusual phenomenon have been discovered in these systems due entirely to the presence of additional layers of carriers. Prominent among these are the observations of the new quantum hall states and the insulating Wigner crystal (WC) phase in the electron bilayer system. The existence of the WC state has also been predicted by the recent theoretical[1,2] and computer simulation[3] studies. Very recently[2,4], the coupled electron-hole (e-h) bilayer system, where electrons are substituted by holes in one of the layers, has got considerable attention mainly due to this system being more strongly correlated than its electron counterpart at the same number density of carriers. Here, in addition to the formation of the WC state, the possibility of the excitonic paring[4] is also predicted at sufficiently small spacing.

However, in all of the theoretical as well as simulation studies made so far, each layer in the bilayer system is assumed to have practically zero width, whereas the situation is quite different in real physical conditions; in particular, the experimentally grown electron (or hole) layers have finite width due to finite amount of extension in the carrier wave function along the transverse direction. The consideration of the finite width of the layer should modify the strength of interaction among carriers, and consequently, the overall behaviour of the system. To investigate the ground state of the coupled e-h bilayer by including the finite width of the two layers makes the main objective of the present work. In particular, we wish to examine its effect on the existence of the liquid-Wigner-crystal phase transition. In Sec.2, we outline the theoretical procedure used. Results and discussion are given in Sec.3, followed by conclusion in Sec. 4.

II. THEORETICAL FORMALISM

As in the previous theoretical studies[1,3], we proceed by calculating the liquid-state density susceptibility of the system. The phase transition into a density-modulated phase, if any, may appear in the form of a divergence in the susceptibility at a wave vector representing the period of density modulation existing in the crystal phase. Within the generalized mean-field approximation, the dynamic density response function for the double layer system can be compactly expressed in the form of a 2 × 2 matrix, with the elements of the inverse of the response matrix given by

$$\chi_{ij}^{-1}(q,\omega) = \frac{\delta_{ij}}{\chi_i^0(q,\omega)} - V_{ij}(q)\left[1 - G_{ij}(q,\omega)\right] \quad \text{..... (1)}$$

where $\chi_i^0(q,\omega)$ is the density response function of non-interacting *i*, *Vij(q)* is the Coulomb interaction potential, and $G_{ij}(q,\omega)$ is the dynamic local-field correction (LFC) accounting for the correlation effects among the carriers in the layers *i* and *j*.

$V_{ij}(q)=\alpha_{ij}V(q)F_{ij}(q)$, where $\alpha_{ij}=+1$ for $i=j$ and -1 otherwise, $V(q)=2\pi e^2/(q\varepsilon)$ (ε being the dielectric constant of the background material) and $F_{ij}(q)$ is the form factor given by

$$Fij(q)=\int dz\int dz' e^{-q|z-z'|}\left|\zeta_i(z)\right|2\left|\zeta_J(z')\right|2 \quad \text{..... (2)}$$

with $\zeta_i(z)$ being the solution of the Schrodinger equation

$$\left[-\frac{\eta^2}{2m_i^*}\frac{d^2}{dz^2}+V(z)\right]\zeta_i(z)=E_z\zeta_i(z) \quad \text{..... (3)}$$

for the motion along *z*-direction. m_i^* is the effective mass of carriers in the *i*th layer. *V(z)* is the net potential experienced by carriers in the *z*-direction. It contains, in addition to the Hartree term, the effect of exchange-correlations and this makes the calculation of $\zeta_i(z)$ an extremely complex problem. We use here the model of Fang and Howard[5], where the in-layer form factor is given by

$$F_{ij}(q)=\left(1+\frac{q}{b}\right)^{-3}\left(1+\frac{9}{8}\frac{q}{b}+\frac{3}{8}\left(\frac{q}{b}\right)^2\right) \quad \text{..... (4)}$$

Here, $b=\left(33\pi m_i^* e2n/\left(2\varepsilon\hbar^2\right)^{1/3}\right)$ with a being the in-layer density of carriers. For the inter-layer interaction, the effect of layer-width is expected to be small and therefore, we ignore it and take $F_{ij}(q)=\exp(-qd)$, with *d* being the centre - to - center layer spacing. Evidently, setting $F_{ij}(q)=1$, corresponds to ignoring the width of the layer.

In the dynamical mean-field approximation[6] of Hasegawa and Shimizu, $G_{ij}(q,\omega)$ is given as

$$G_{ij}(q,\omega)=-\frac{1}{n}\int\frac{dq'}{4\pi^2}\frac{\chi_i^0(q,q';\omega)V_{ij}(q')}{\chi_i^0(q,\omega)V_{ij}(q)}\times\left[S_{ij}(|q-q'|)-\delta_{ij}\right] \quad \text{..... (5)}$$

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 structure factor. The fluctuation-dissipation theorem, which relates $S_{ij}(q)$ with the imaginary part of the linear response function as

$$S_{ij}(q)=-\frac{\eta}{n\pi}\int_0^\infty d\omega lm\,\chi_{ij}(q,\omega) \quad \text{..... (6)}$$

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

The static density susceptibility can be obtained by diagonalizing the density response matrix (1) as

$$\chi\pm(q,0)=\frac{2}{\chi_e^{-1}(q,0)+\chi_h^{-1}(q,0)\pm\Delta} \quad \text{..... (7)}$$

with

$$\Delta=-\sqrt{\left(\chi_e^{-1}(q,0)-\chi_h^{-1}(q,0)^2\right)+4V_{eh}^2(q)\left(1-G_{eh}(q,0)\right)^2}$$

and

$$\chi\pm(q,0)=\frac{\chi_1^0(q,0)}{1-V_{ij}(q)\left(1-G_{ij}(q,0)\right),\chi_1^0(q,0)} \quad \text{..... (8)}$$

The + and - signs correspond, respectively, to the in-phase and out-of-phase (π) modes of the density modulations in the two layers.

III. Results and Discussion

We now look for the poles of Eq. (7). However, this can only be achieved numerically since the LFC's in our approach (Eq. (5)) can only be determined numerically from the self-consistent solution of Eqs. (1), (5) and (6). But, it is evident from Eq. (7) that it is $\chi+(q,0)$ that can have divergence in the e-h layer system. It is appropriate to point out here that in all our numerical calculations we have taken the effective mass of holes to be equal to that of elections.

We infer from our numerical calculations that $\chi+(q,0)$ exhibits quite generally a peak-like behaviour in the region of sufficiently close approach of two layers. The overall character of this behaviour is seen to depend upon the carrier density r_s and the interlayer spacing *d*. $r_s=1/a_0^*(n\pi)^{1/2}$ is the usual (in-layer) density parameter with a_0^* the effective Bohr atomic radius. For smaller r_s values, $\chi+(q,0)$ contains a single peak at $q/q_F>0.5$; q_F is the Fermi wave vector.

However, with increase in r_s there starts developing a second peak in $\chi+(q,0)$ in the region $q/q_F > 2$ (Fig. 1(a)) with its strength growing monotonically with increasing r_s. Results of $\chi+(q,0)$ are given in Fig. 1(a-c) at some selected values of r_s and *d*. It can be noticed that the peak-height becomes stronger with decreasing *d*. But, we encounter at each r_s a critical spacing d_c below which is becomes almost impossible to obtain a self-consitent solution of Eqs. (1), (5) and (6) and, hence the $\chi+(q,0)$; for instance $d_c/a_0^* \approx 4.6$ at $r_s = 10$. Although we are not able to calculate $\chi+(q,0)$ for $d < d_c$, $\chi+(q,0)$ appears to diverge in this *d*-region. Our results show that the small-*q* peak dominates for $r_s = 16$ and the large-*q* peak dominates thereafter. The small-*q* peak indicates instability of the liquid towards a charge-density-wave (CDW) ground state, while the large-*q* peak, whose position lies close to the reciprocal lattice vector of a triangular lattice, could indicate instability against a coupled WC ground state.

At this point, it is interesting to know the behaviour of other properties of the system near the instability region. In view of this, we have plotted, for instance in Fig. (2) the intra- and interlayer pair-correlation functions at $r_s = 20$ and $d/a_0^* = 25$ and 19. These functions exhibit pronounced in-phase oscillations near the instability region, which are typical of an ordered phase. This behaviour of correlation functions supports further our claim of interpreting the (seemingly) diverging behaviour of $\chi+(q,0)$ at $q/q_F \approx 2.4$ as a signature of the liquid-Winger crystal phase transition.

To calculate the role of the finite width of the layers, we now compare our results with the corresponding studies where these effects are ignored.

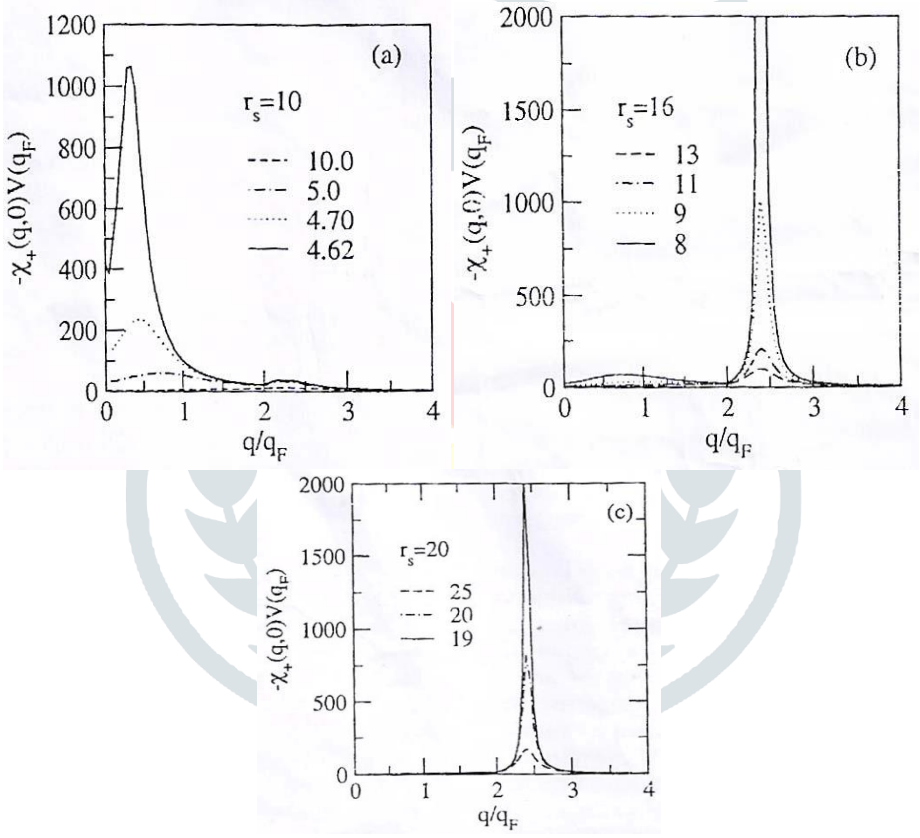

Fig. 1 (a-c) $\chi+(q,0)$ vs. q/q_F at different r_s and d/a_0^* ; the legends indicate the values of d/a_0^*.

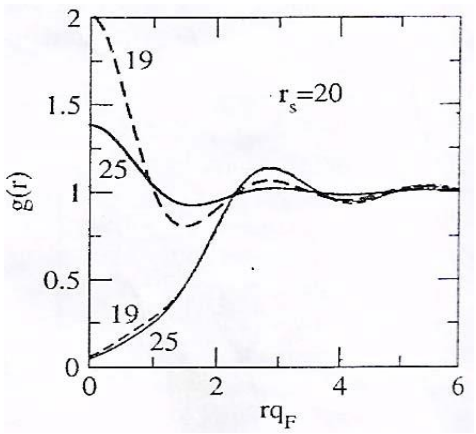

Fig. 2 : Pair-correlation function $g(r)$ vs. rq_F at $r_s = 20$ for $d/a_0^* = 25$ (solid curves) and 19 (dashed curves); thin and thick curves represent, respectively, $g_{11}(r)$ and $g_{12}(r)$.

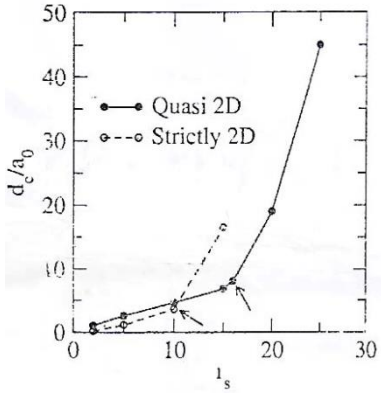

Fig. 3 : Points of instability d_c / a_0^* vs. r_s, with (quasi 2D) and without (strictly 2D) finite width. The arrow indicate the crossover point.

The comparison is compactly summarized in Fig. (3) where we have displayed the points of instability, as a function of r_s, with and without the finite width of the layers. It can be noticed that the inclusion of the finite width results in an increase in critical r_s i.e., a decrease in carrier density, for the liquid-Wigner crystal transition. Apart from this shift in the critical density, the e-h bilayer exhibits, at the qualitative level, a behaviour similar to that without considering the finite width. For instance, we have comapred in Fig. (4) the behaviour of pair-correlation function at $r_s = 10$ and $d / a_0^* = 10$, with and without the finite width.

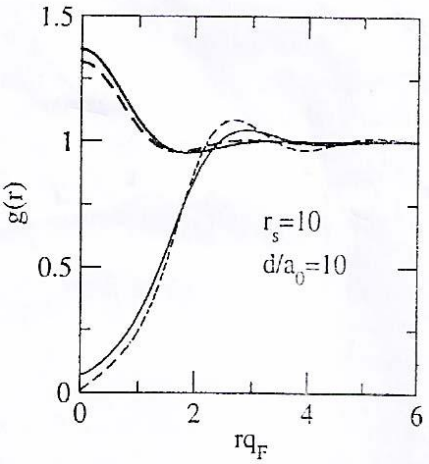

Fig. 4 : Pair-correlation function $g(r)$ vs. rq_F at $r_s = 10$ for $d / a_0^* = 10$; solid and dashed curves are with and without finite width, respectively.

IV. CONCLUSIONS

In conclusion, we find that the inclusion of the finite width of layers in the e-h bilayer shifts the critical density for Wigner crystallization towards higher r_s by a noticeable factor of about 1.6. Thus, our study demonstates in a clear way the importance of finite width effects and in particular. It underlines that these effects should be considered before we compare any theoretical or the simulation predictions with the experimental observations.

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