TWO-BODY CORRELATIONS AND
THE UNDERLYING PHASE TRANSITIONS IN BILAYERS

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Abstract

The pair correlation functions for a bilayer system of classical electrons has been calculated through a two-component HNC formalism. The results show changes in the structure of the correlation functions as the interlayer distance is increased from zero to about twice the Wigner-Seitz radius. These changes are indicative of structural phase transitions which are expected to take place in the crystallized phase and whose short range orders the liquid phases emulate.

Ms. No PACS numbers: 73.20.Dx, 73.40.Gk.

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I. INTRODUCTION

Electronic bilayer systems (2D electron liquids in a neutralizing background, separated by a distance \( d \), each having density \( n = 1/\pi a^2 \), \( a \) being the Wigner-Seitz radius) have attracted a great deal of attention, both in condensed matter physics \([1–3]\) and in relation to the Penning trapped ion experiments \([4,5]\). It has been realized \([3,6]\) that correlations play a more important role in such systems than in the 2D layer or in 3D bulk systems.

Although attempts have been made to estimate the interlayer correlation functions \([3,6,7]\) no reliable calculation on them has so far been available. In this paper we report on the results of HNC calculations of the correlation functions of a classical bilayer for a wide range of \( \Gamma = e^2/akT \) and \( d/a \) values. While in most experimental situations strong magnetic fields are present, and in the semiconductor bilayers the electronic liquid is degenerate, the classical model is expected to be quite reliable in the high \( \Gamma \) or high \( r_s \) domain where the electrons are quasi-localized.

II. CALCULATION

The calculation is based on mapping the bilayer into a 2D two-component single layer with an interaction matrix \([8]\)

\[
\begin{align*}
\phi_{11}(r) &= \phi_{22}(r) = \frac{e^2}{r} \\
\phi_{12}(r) &= \frac{e^2}{\sqrt{r^2 + d^2}}.
\end{align*}
\]

(1) (2)

The mapping makes it possible to apply the two-component HNC formalism, which is well known \([8]\). The resulting system of equations is

\[
\begin{align*}
g_{ij}(r) &= h_{ij}(r) + 1 \\
h_{ij}(r) &= \exp(H_{ij} - \phi_{ij}(r)) - 1 \\
H_{ij}(r) &= h_{ij}(r) - c_{ij}(r) \\
h_{12}(k) &= \frac{c_{12}(k)}{B(k)}
\end{align*}
\]

(3) (4) (5) (6)
\[ h_{11}(k) = \frac{c_{11}(k) + A_{12}(k)h_{12}(k)}{1 - A_{11}(k)} \]  \hspace{1cm} (7)

\[ A_{ij}(k) = nc_{ij}(k) \]  \hspace{1cm} (8)

\[ B(k) = [1 - A_{11}(k)]^2 - [A_{12}(k)]^2. \]  \hspace{1cm} (9)

The system of equations is solved by using Lado’s method \cite{4} with the following parameters: maximal radial distance \( R \approx 29 \), \( \alpha \approx 2.8 \), \( N = 500 \). Using as convergence monitor the maximum difference between the input array elements and the corresponding elements after one HNC iteration, it was found that the difference for the intralayer correlation function always exceeds the difference for the interlayer function. Therefore, only the former was monitored, and the iterative solution was obtained for a maximum difference less than \( \varepsilon = 5 \times 10^{-5} \).

### III. RESULTS

Our results for \( g_{11}(r) \) and \( g_{12}(r) \) are summarized in Figs. 1, 2 and 3, 4, 5. For low \( \Gamma \) values the most interesting effect is the generation of a partially filled correlation hole in layer 2 above a particle in layer 1. The correlation hole empties both with increasing \( \Gamma \) and decreasing \( d \) (see Figs. 1, 2 and 7).

Qualitatively new effects appear for high \( \Gamma \) values, where the quasilocalization of the particles becomes important. It has been proposed \cite{2, 5} that in the crystalline phase (for a monolayer \( \Gamma_{\text{crit}} = 137 \); for a bilayer the \( \Gamma_{\text{crit}}(d) \) has not been established, but probably is of the same order of magnitude; see comment below) a number of structural phase transitions take place as \( d/a \) changed. Here in the liquid phase one sees a rather dramatic manifestation of the change of short-layer order which reflects the underlying structural phase transitions, as \( d/a \) is varied from 0 to 2.

At \( d = 0 \) (when the two layers collapse into one single 2D layer) the two correlation functions \( g_{11}(r) \) and \( g_{12}(r) \) are identical, since the two ”species” are now one and the same and the correlation function is that of a 2D liquid with double density \((2n)\). In the underlying
crystalline phase "species 1" and "species 2" particles are randomly distributed on the vertices of a triangular lattice with lattice constant $a_\Delta = 1.35a$. As $d/a$ is increased $g_{11}(r)$ and $g_{12}(r)$ remain similar, but develop different amplitudes, $g_{11}(r) < g_{12}(r)$. This reflects the change of the first and second coordination numbers $q_{11}^{(1)}$, $q_{12}^{(1)}$ and $q_{11}^{(2)}$, $q_{12}^{(2)}$ (estimated here from the peak values of $rg_{11}(r)$ and $rg_{12}(r)$) and a tendency of the two species to occupy alternating rows of the triangular lattice which leads to a centered rectangular lattice (Fig. 9). This transition seems to be completed around $d/a = 0.2$ where the position of the first peak of $g_{11}(r)$ and that of $g_{12}(r)$ begin to separate (Fig. 3), marking the gradual transformation of the rectangular structure into a centered square lattice (Fig. 9). At $d/a = 0.65$ the first and the second peaks of $g_{11}(r)$ ($R_{11}^{(1)}$ and $R_{11}^{(2)}$) merge (Figs. 4 and 6) which we can interpret as the formation of the latter structure. During these processes the $q_{12}^{(1)}/q_{11}^{(1)}$ ratio changes from 1 (at $d = 0$) to its maximum 1.66 (at $d/a = 0.4$) (Fig. 7), qualitatively corroborating the above picture. The abrupt formation of a distant second shell at $d/a = 0.65$ is indicative of an underlying (equilateral) square or rhombic structure. Indeed, for $d/a > 0.65$ the transformation into a centered rhombic lattice (Fig. 9) can be seen by the shrinking of $R_{12}^{(1)}$ (Fig. 6). By $d/a = 1.5$ the rhombic structure transforms into a centered triangular lattice (Fig. 9) where the particles of the second layer sit over the holes created in the first layer. This is indicated by the reversal of the decrease of $R_{12}^{(1)}$ (as particle 2 shifts from the center of the rhombus into the center of the triangle, and the settling of $R_{11}^{(1)}$, $R_{11}^{(2)}$ and $R_{12}^{(1)}$ near their expected values $a_\Delta$, $\sqrt{3}a_\Delta$ and $\sqrt{3}/3a_\Delta$, with $a_\Delta = 1.90a$, respectively. Although the staggered triangular is the final equilibrium structure for $d/a > 1.5$, further increase of $d$ weakens the correlations between the layers to the point that by $d/a = 3$ the interlayer correlations practically vanish (Fig. 8).

The $d/a$ values of the structural phase transitions predicted from the comparison of the respective Madelung energies [24] show reasonable agreement with our results. However, it should be emphasized, that in the considered $\Gamma$-range system is liquid and the various lattice sites are not actual positions of the electrons, but rather positions of local energy minima, and indicative of the positions of the successive high probability "shells" in the liquid phase.
Finally, one may wonder whether the bilayer system crystalizes at a lower $\Gamma_{\text{crit}}$ value than a single 2D layer, as conjectured by Ref. 3. Although no definitive answer can be given on the basis of the calculations performed here, an inspection of Figs. 1 and 2 shows that there is certainly no tendency for the short-range order to set on a lower $\Gamma$-values than in the case of a 2D layer.

(This work has been partially supported by NSF Grant PHY–9115714.)
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Fig. 1 Intralayer correlation function for different Γ values at $d/a = 1$.

Fig. 2 Interlayer correlation function for different Γ values at $d/a = 1$.

Fig. 3 Intralayer and interlayer correlation functions.

Fig. 4 Intralayer and interlayer correlation functions.

Fig. 5 Intralayer and interlayer correlation functions.

Fig. 6 Positions of the first and second peaks of the intralayer and interlayer correlation functions as indicators of the nearest neighbour positions.

Fig. 7 Normalized values of the first and second peak amplitudes of the interlayer and intralayer correlation functions as indicators of the first and second coordination numbers, $q_{11}^{(i)}$ and $q_{12}^{(i)}$.

Fig. 8 The value of the interlayer correlation function at $r = 0$ for different Γ values, indicating the degree of correlation between the layers.

Fig. 9 The four principal lattice structures.
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