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Structures of quantum 2D electron–hole plasmas

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Abstract
We investigate structures of 2D quantum electron–hole (e–h) plasmas by the direct path integral Monte Carlo method (PIMC) in a wide range of temperature, density and hole-to-electron mass ratio. Our simulation includes a region of appearance and decay of the bound states (excitons and biexcitons), the Mott transition from the neutral e–h plasma to metallic-like clusters, formation from clusters of the hexatic-like liquid and formation of the crystal-like lattice.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

Strongly correlated two-dimensional quantum Coulomb systems are the subject of intensive discussions [1, 2]. In particular, it is known that the competition between electrostatic and kinetic energies in an electron gas may be the reason for an unusual phase diagram of a 2D system of electrons. The liquid state of such a system is stable when the kinetic energy dominates while the electrostatically favored 'Wigner' triangular crystal is stable in the opposite case [3]. If there is a strong competition between these two kinds of energies, different situations are possible. The question under discussion is the existence of the intermediate anisotropic liquid phase (hexatic) under melting of crystal into isotropic liquid. Moreover, the physical mechanism of melting can be influenced by the interaction with substrate and defects. Currently, all mentioned phenomena can be extensively investigated by a consistent first-principle numerical simulation, and in this brief paper we present the most interesting results of our numerical experiments by the direct PIMC method.

2. Path integral Monte Carlo approach

Let us consider a two-component neutral e–h plasma. In particular, the properties of such plasma at different hole-to-electron mass ratios are very useful for the understanding of phase diagrams of semiconductors [4]. Thermodynamics of e–h plasma are defined by the partition function Z, which for the case of N_e electrons and N_h holes ($N_e = N_h$) is given by $Z(N_e, N_h, V, \beta) = Q(N_e, N_h, \beta)/N_e!N_h!$, with $Q(N_e, N_h, \beta) = \sum_\sigma \int_V \mathrm{d}r\, \mathrm{d}q\, \rho(q, r, \sigma; \beta)$, where $\beta = 1/k_B T$, $\sigma = (\sigma_e, \sigma_h)$, r, σ_e denote the space and spin electron coordinates, while q, σ_h denote the space and spin hole coordinates. The exact density matrix $\rho(q, r, \sigma, \beta)$ of a quantum system for low temperature and high density is in general not known but can be constructed using a path integral representation [5, 6]. Thus we take into account interaction, exchange (through permutation operators) and spin effects for both electrons and holes. The maximum statistical and systematic errors in our simulations are not more than 5%.

3. Simulation results

We are interested in strong Coulomb correlation effects such as bound states (excitons, bi-excitons, many particle clusters), their transformation and eventual breakup at increasing density (Mott effect). Beyond the Mott density, we expect the possibility of the hole crystallization if the hole mass is sufficiently large [7]. Below, the density of the two-component plasma is characterized by the Brueckner parameter r_s defined as the ratio of the mean distance between particles $d = [1/\pi(n_e + n_h)]^{1/2}$ and the 3D exciton Bohr radius a_B, where n_e and n_h are the electron and hole 2D densities. The dimensionless temperature will be presented as a ratio of the temperature and the 3D electron–hole binding energy (Rydberg), which includes the reduced effective mass and dielectric constant.

We analyze some spacial distribution functions and related spin-resolved typical 'snapshots' of the e–h state in the simulation box for different particle densities, temperatures and hole-to-electron mass ratios M. Due to the limited size of the paper all results are illustrated at $M = 800$ which is higher than the critical value for crystallization ($M \approx 60$, see [7] for details). At this value of mass ratio we obtain the most remarkable physical effects. According to the path integral representation of the density matrix, each electron and hole is represented by several tens of points ('beads'). The spatial distribution of the beads of each quantum particle is proportional to its spatial probability distribution. Figure 1 shows that the typical size of the cloud of beads for electrons is several times larger than the one for the heavy holes. At low temperature and low ($r_s = 6$) and middle ($r_s = 2$) densities practically all holes are closely covered by electron beads. From a physical point of view this means that electrons and holes form bound states, i.e. excitons, bi-excitons and many particle clusters. The existence of the bound states is also supported by the behavior of the pair distribution functions, exhibiting pronounced maxima at the distances of about half and a bit more of the Bohr radius (see g_{eh} in figure 1). We note that raising the temperature at a fixed density leads to a temperature-induced ionization of the bound states. As a result we found a substantial number of free electrons and holes.

From figure 2 it follows that the growth of density results in the increase of the number of particles in clusters. The structural analysis of large many-particle clusters shows the hexagonal ordering of heavy holes inside liquid-like clusters (upper right panel). In this panel there are only two clusters: one is in the center of the Monte Carlo cell, while the second one is divided into four parts (in each corner) due to the periodic boundary conditions of the Monte Carlo cell. Here besides the inner normal hexagonal structure the holes due to the strong Coulomb repulsion form the filament-like structures of the clouds of beads at the bounds of

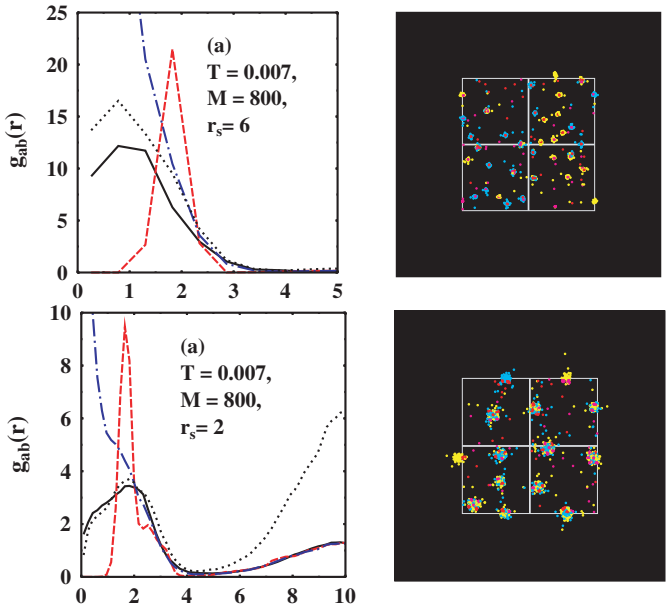

Figure 1. Pair distribution functions (left column) and snapshots of the Monte Carlo cell (right column). Left column: g_{ee} (black solid line), g_{hh} (red dashed line), g_{eh} (blue dot-dashed line) at temperature $T/Ry = 0.007$, the hole-to-electron mass ratio $M = 800$ and densities related to the Brueckner parameter $r_s = 6$ and $r_s = 2$. Right column: red and magenta clouds—holes, yellow and cyan clouds—electrons with the opposite spin directions.

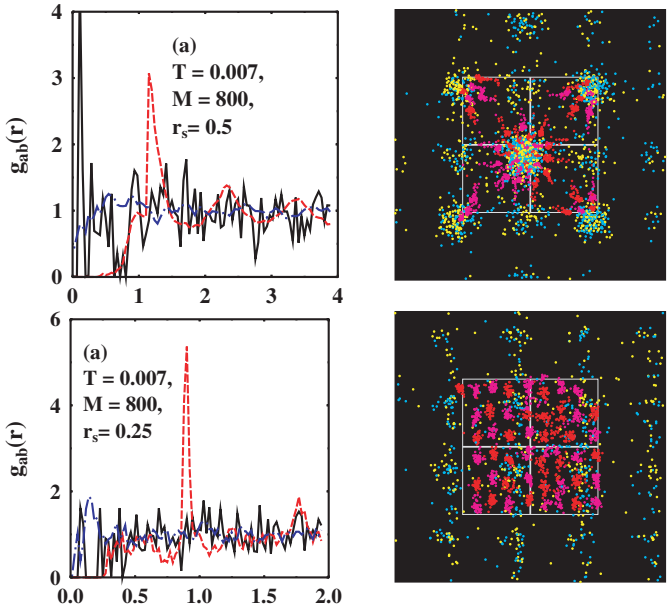

Figure 2. Pair distribution functions (left column) and snapshots of the Monte Carlo cell (right column) at temperature $T/Ry = 0.007$, the hole-to-electron mass ratio $M = 800$ and densities related to the Brueckner parameter $r_s = 0.5$ and $r_s = 0.25$. Notations are the same as in figure 1.

clusters. The filament-like structures are fully 2D topological effect as in 3D case the holes in analogous many-particle clusters have normal liquid-like ordering [6, 8].

If the particle density is high enough ($r_s = 0.25$), the electron wavelength becomes larger than the mean inter-particle distance d and even larger than the size of the Monte Carlo cell which is seen by the large extension of the clouds of electron beads. For $r_s \leqslant 0.5$ clusters become unstable because two electrons bounded to neighboring holes start to overlap allowing for electron tunneling from one cluster to the other (Mott effect). Since the hole wavelength is significantly smaller than the electron wavelength, it may still be smaller than d and the structure of the hole beads resembles a liquid-like or a crystal-like state. If the hole mass exceeds a critical value, the holes may even form a crystal-like structure [7] (lower right panel in figure 2). Here the holes form a crystal-like structure, while the electron density demonstrates the Bloch oscillations. At this very high density the type of the hole 'crystal' is influenced by the boundary conditions of the Monte Carlo cell (finite-size effect). The detailed analysis of the type of the crystal-like structure is possible for a much more bigger number of particles in the Monte Carlo cell.

4. Conclusion

In this paper we have presented a computer simulation analysis of strong Coulomb correlations in dense two-dimensional two-component quantum plasmas at low temperatures. In particular, the formation and dissociation of bound states, such as excitons, bi-excitons and many particle clusters, is analyzed and the density–temperature regions of their occurrence are identified. We have shown that, above the Mott point, two-component plasmas with large mass anisotropy show interesting Coulomb correlation phenomena: with increasing density holes can undergo a phase transition to a Coulomb hexatic-like liquid and to a Wigner crystal which is embedded into a degenerate electron gas. The crystal-like formation in a two-component plasma is possible for large enough hole-to-electron mass ratios [7].

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