Quantum Coulomb crystals in a two - component system

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Abstract: When electrons in a solid are excited to a higher energy band they leave behind a vacancy in the original band. Such holes behave like positively charged particles. We predict that holes can spontaneously order into a regular lattice in semiconductors with sufficiently flat valence bands. The critical hole to electron effective mass ratio required for this phase transition is found to be of the order of 80 in three dimensions and 30 in two dimensions. A unified phase diagram of Coulomb crystals in two-component systems is derived and verified by first-principle path-integral Monte Carlo simulations (submitted to [1]).

Two component Coulomb crystal

Crystallization appears to be a fundamental property common to all charged particle systems. The necessary condition for the existence of a crystal in one-component plasmas (OCP) is that the mean Coulomb interaction energy, strongly exceeds the mean kinetic energy. The vast majority of Coulomb matter in the Universe, however, exists in the form of neutral plasmas, containing (at least) two oppositely charged components (two-component plasma, TCP). Here we analyze the crystallization conditions in a TCP.

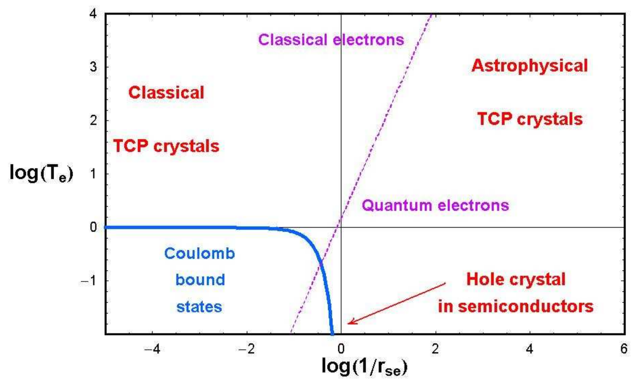


Fig. 1. Location of the two-component Wigner crystals in the density-temperature plane (qualitative picture). Astrophysical ion crystals in White Dwarf stars and neutron stars are embedded into an extremely dense quantum electron gas and span the parameter range $M = 10,000,\dots,100,000$, $Z = 6,\dots,23$ (carbon to iron) and $\Theta = 1,\dots,100$. Crystals in neutral or complex plasmas are surrounded by a dilute classical electron gas and M and Z may reach 10^{12} and 10^5 , respectively. The predicted hole crystals in semiconductors exist in the presence of quantum electrons, they have $Z = \Theta = 1$, and M has to exceed the critical value.

1 Analytical estimations

Condition for ion (hole) crystal in a TCP:

$$1)\Gamma \geq \Gamma^{cr}, r_{sh} \geq r_{sh}^{cr} \quad (1)$$

2) absence of electron-ion bound states

$$r_{se} = \bar{r}_e/a_B > r_s^{cr}$$

This is fulfilled if electrons can tunnel out of the atom (pressure ionization of atoms, Mott effect),

$$\frac{1}{r_{se}} \geq \frac{1}{r^{Mott}(T_e)}, \quad (2)$$

, $r^{Mott}(T_e) \simeq 1.2$ 10%

$$M \geq M^{cr}(T_e) = \frac{r_s^{cr}}{Z^{4/3} r^{Mott}(T_e)} - 1, \quad (3)$$

which exists in a finite electron density range between

$$n^{(1)}(T_e) = \frac{3}{4\pi}\left(\frac{1}{r^{Mott}(T_e)}\right)^3 \quad (4)$$

and

$$n^{(2)}(T_e) = n^{(1)}(T_e)\left(\frac{M+1}{M^{(cr)}(T_e)+1}\right)^3 \quad (5)$$

and below the temperature T^*, which is estimated by the crossing point of the classical and quantum asymptotics of an OCP crystal

$$T_e^\star = 2d\frac{Z^2\Theta(M+1)}{\Gamma^{cr} r_s^{cr}}. \quad (6)$$

where $E_B = \frac{Ze^2}{4\pi\varepsilon_o\varepsilon_r}\frac{1}{2a_B}$ and $a_B = \frac{\hbar^2}{m_r}\frac{4\pi\varepsilon_o\varepsilon_r}{Ze^2}$ [ε_r and [m_r] are the back-ground dielectric constant and the reduced mass, [$m_r = m_h^{-1}(1+M)$], yielding the requirement $Z^{4/3}(M+1)r_{se} > r_s^{cr}$.

Example : 3D (2D) e-h plasma with $\Theta = \tau = 1, \Gamma^{cr} = 83(31)$.

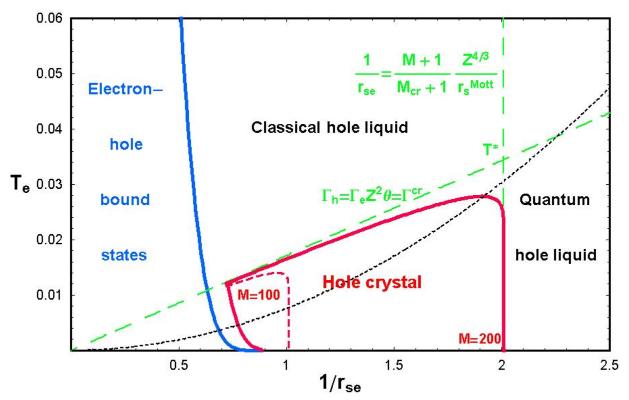
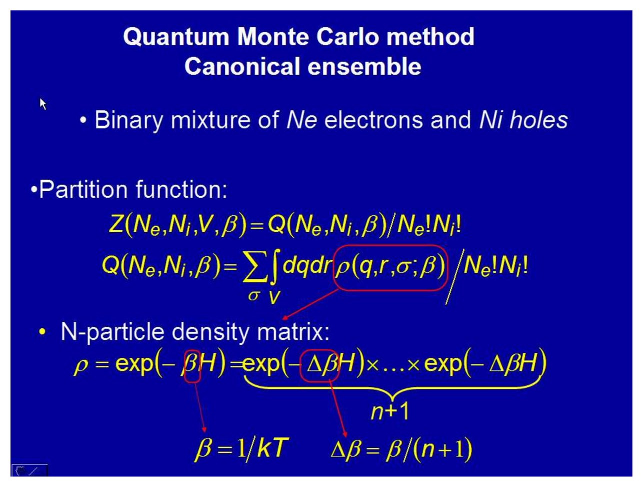
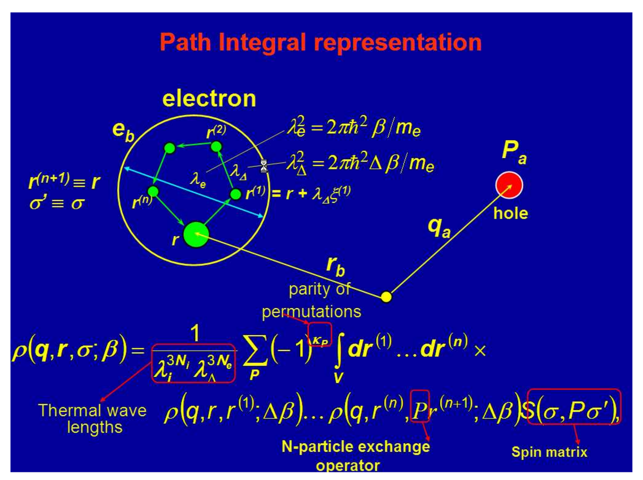


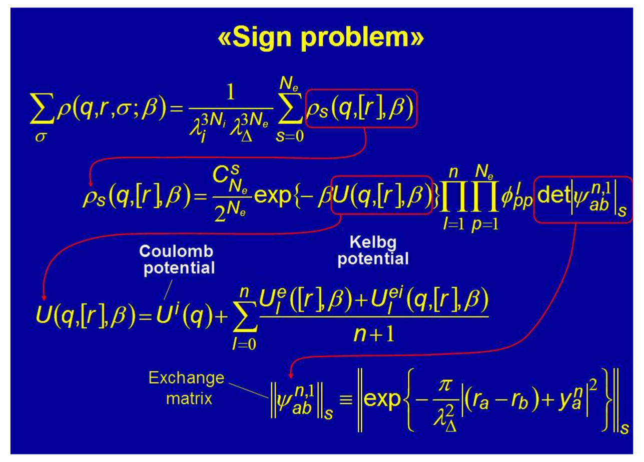
Fig. 2. Phase diagram of the two-component plasma in the vicinity of the hole crystal. The blue line indicates the boundary of the Coulomb bound state phase given by $r^{Mott}(T_e) \simeq 1.2$,and the dotted black line divides the holes into classical and quantum ones. The red line marks the boundary of the hole crystal for the case of $M = 200, Z = \Theta = 1$, , with the asymptotics (dashed green lines), $T_e = T_e^2$ and $n = n_e^2$, Eq. (7) where $K = (M+1)/(M^{cr}+1)$. The dashed red line corresponds to $M = 100$.

2 Model and simulation idea

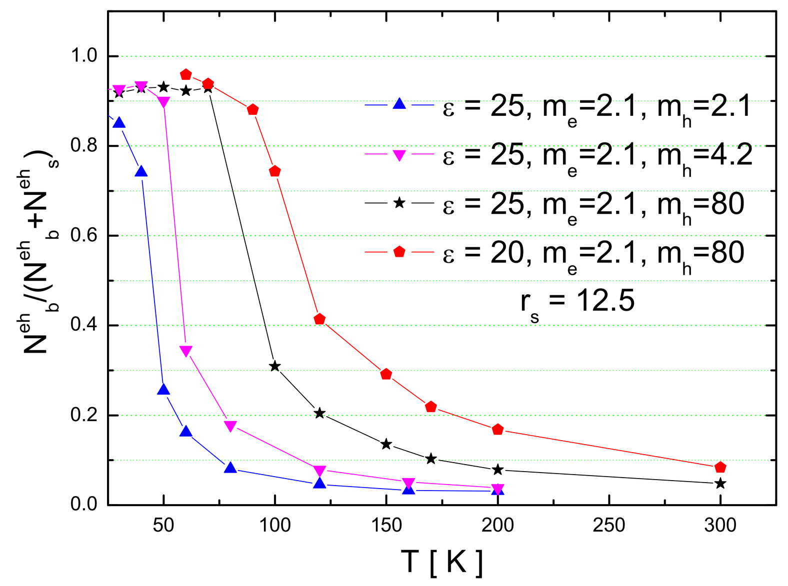
- Binary mixture of N_e quantum electrons and N_h quantum holes at temperature $T_e = T_h$.
- DPIMC simulations of electron-hole plasma [2, 3, 4]with Kelbg potential for Coulomb particles







3 Fraction of e-h bound states



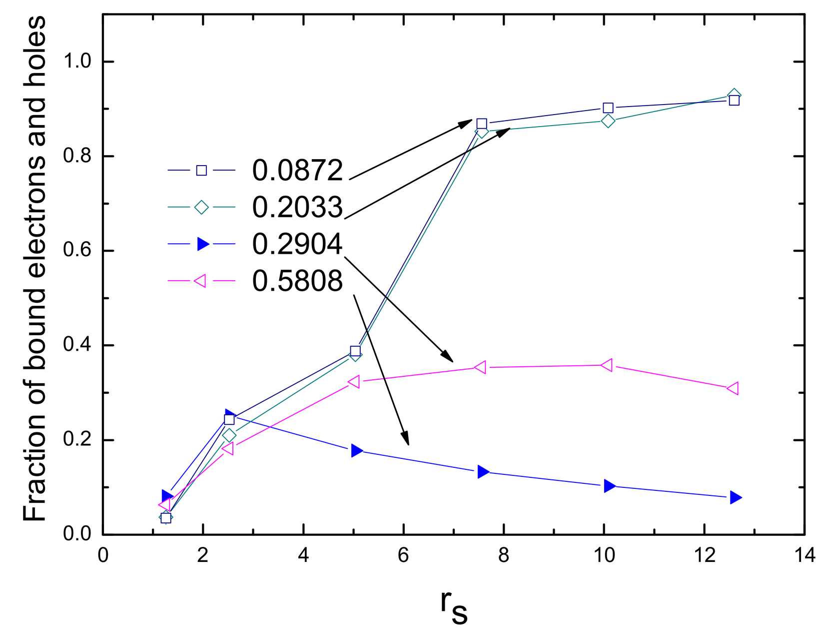
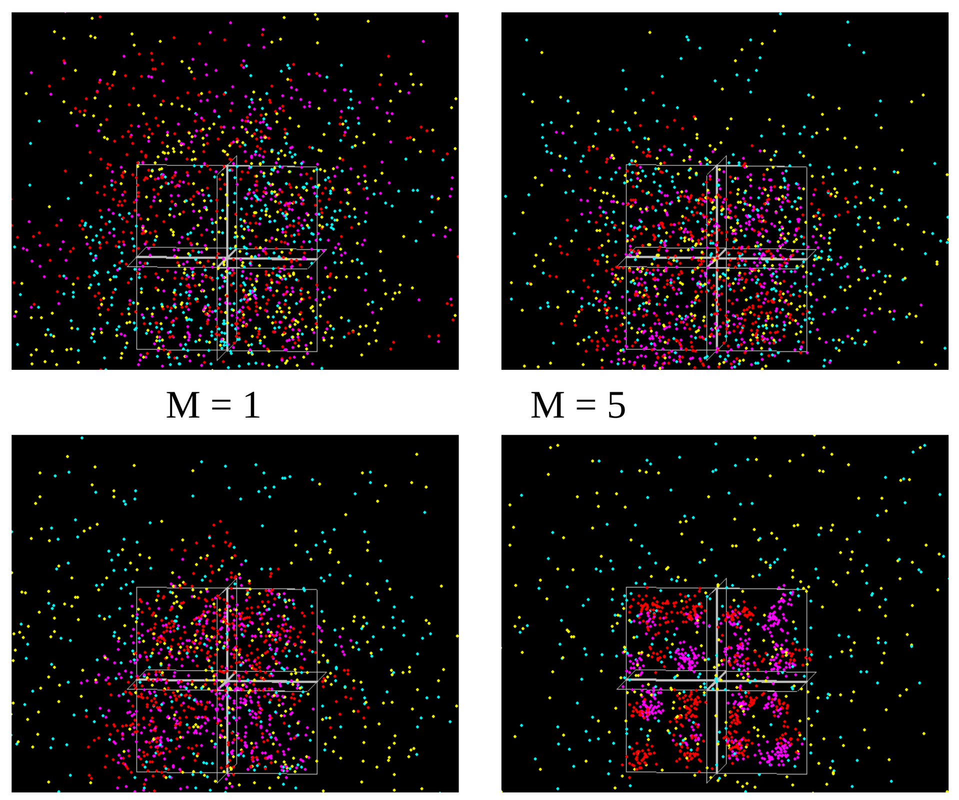


Fig. 3. Electron-hole bound state fraction (including excitons and bi-excitons) in a $3d$ semiconductor ($Z = \Theta = 1, M = 40$) versus density for characteristic temperatures given inside the figure.

4 Typical snapshots



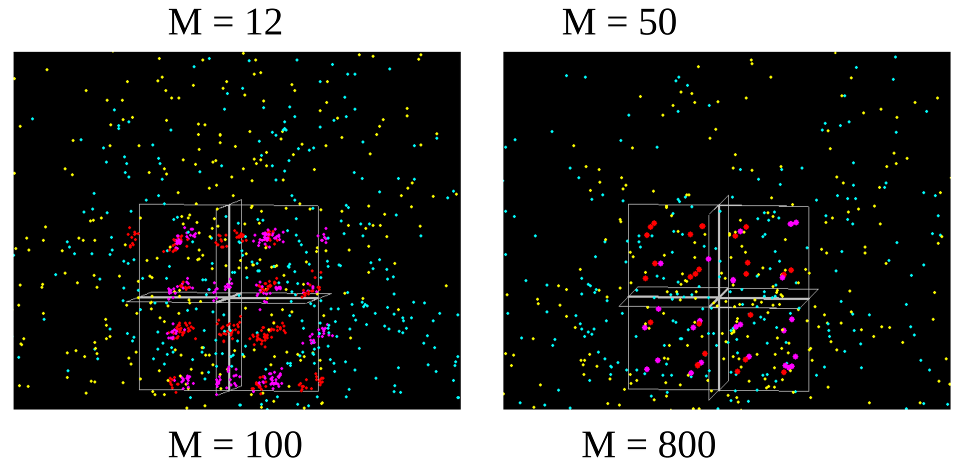


Fig. 4. Snapshots of an electron-hole system at $T = 0.096$ and $r_e = 0.63$ for different mass ratio. Blue (yellow) dots represent the fully delocalised electrons with spin up (down), clouds of red (pink) dots denote holes with spin up (down). Grey lines indicate the main simulation box in space which is periodically repeated in all directions.

5 Pair distribution functions and fluctuations

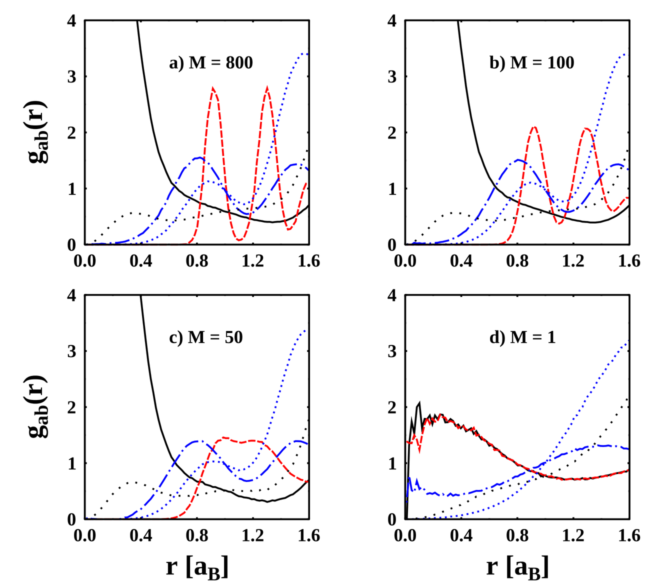


Fig. 5. Electron-electron (blue, dash-dots), hole-hole (black, full line) and electron-hole (red, dotted line) pair distribution functions for different mass ratios and $T = 0.096, r_s = 0.63$

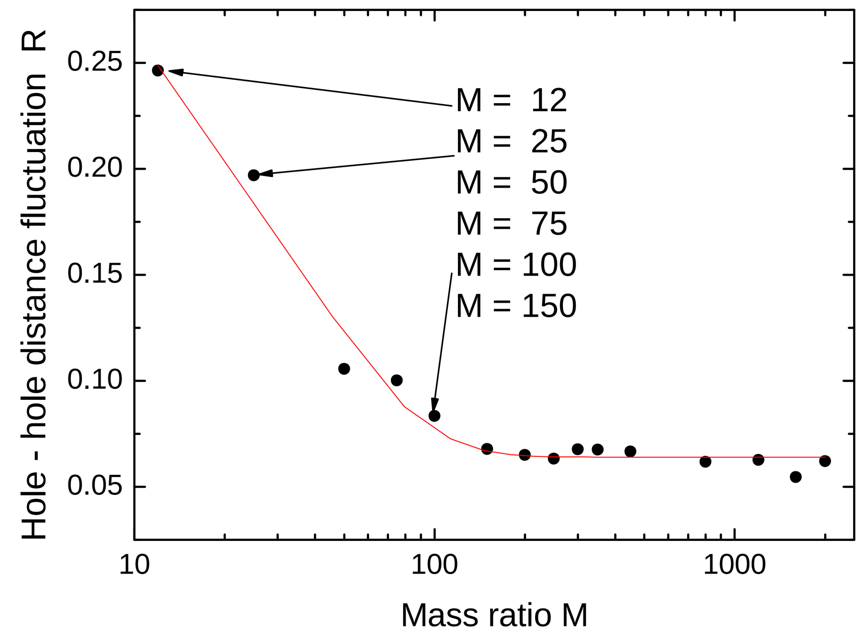
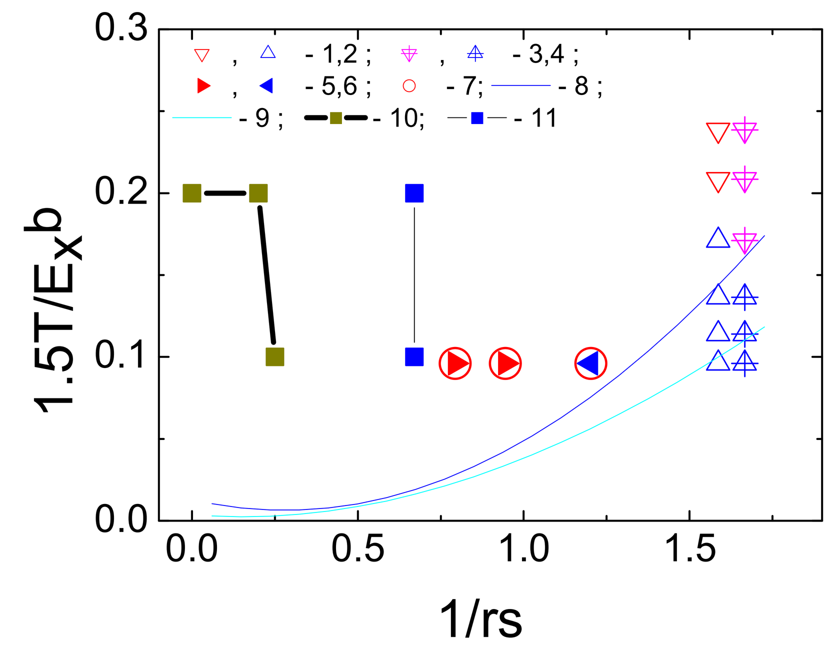


Fig. 6. Mean square relative hole-hole distance fluctuations (normalized to the mean inter-particle distance) as a function of mass ratio for $T_e = 0.096$ and $r_e = 0.63$.

6 DPIMC phase diagram

Notation of the the next Fig. 7 are the following: Points: 1 - liquid, 2 - crystal for $M = 800, m_e = 1, \varepsilon = 1$; 3 - liquid, 4 - crystal -4 for $M = 100, m_e = 1, \varepsilon = 1$; 5 - liquid, 6 - crystal for $M = 800, m_e = 1, \varepsilon = 1$; 7 - liquid for $M = 400, m_e = 2.1, \varepsilon = 25$. Lines: 8 - melting line crystal - liquid; 9 - melting line glass - liquid for $M = 100, m_e = 2.1, \varepsilon = 25$; 9 - e-h bound states fraction 50%, 10 - e-h bound states fraction 10%.



In [5] thermodynamic properties of the condensed excitonic phase of the intermediate valent system $TmSe_{0.45}Te_{0.55}$ have been measured between 1.5 K and 300 K and high pressure, as a first experiment of its kind. Fig. 1 shows the temperature-pressure diagram of the condensed excitonic phase. Transition between excitonic phase and semi-metallic phase has been predicted by Mott and Kohn [6, 7].

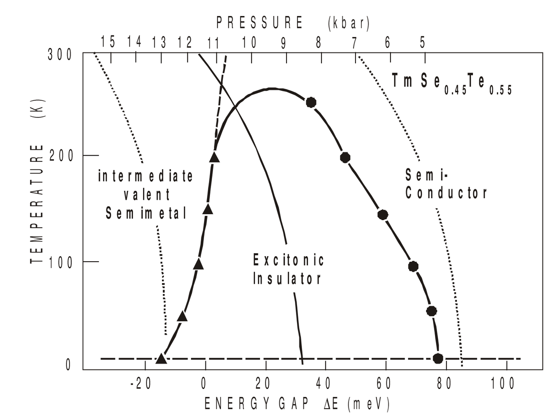


Fig. 8 Excitonic phase diagram of $TmSe_{0.45}Te_{0.55}$ taken from [5]. Experimental points designated by symbols. "Isobars" in the semi-conducting and semi-metallic phase are shown as dotted lines, whereas an "isobar" entering the excitonic phase is shown by a full line. In the lower abscissa the energy gap ΔE is plotted (negative values refer to the metallic state).

References

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