Quantum Monte Carlo Simulations of Quantum Crystals and Supersolids

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Strong correlation regime and quantum phase transition*s* into crystal phase controlled by the density are studied for a set 2D quantum systems and clusters - dipole Bose atom*s,* dipole exciton*s* and Rydberg atoms by *Q*uantum Monte Carlo simulations.
Essential peculiarities in excitation spectra, in structure and condensate depletion with density will be discussed. We have studied also the possible existence of a supersolid phase of a two-dimensional dipolar crystal using quantum Monte Carlo methods at zero temperature. Our results show that the commensurate solid is not a supersolid in the thermodynamic limit. The presence of nonequilibrium vacancies or interstitials turn the solid into a supersolid phase even when a tiny fraction of them are present. The residual interaction between vacancies is repulsive making a *quasi-equilibrium* dipolar supersolid possible. The ground state of the system is not the supersolid with defects but ideal crystal. But there is large energy barrier between these two states. So supersolid with defects is metastable state.

A mesoscopic system of dipolar bosons trapped by a harmonic potential is considered.
The system has a number of physical realizations including dipole excitons, atoms with large dipolar moment, polar molecules, Rydberg atoms in inhomogenious electric field.
In dimensionless units the system is described by two control parameters, the number of particles and the strength of the interparticle interaction. We have shown that when the interparticle interaction is strong enough a mesoscopic crystal cluster is formed. As the strength of interactions is decreased a multi-stage melting takes place. Off-diagonal order in the system is tested using natural orbitals analysis. We have found that the system might be Bose condensed even in the case of strong interparticle interactions. There is a set of parameters for which a spatially ordered structure is formed while simultaneously the fraction of Bose condensed particles is non zero. This might be considered as a realization of a mesoscopic supersolid.

Crystallization of Rydberg gas and mesoscopic clusters of Rydberg atoms due to van der Waals repelling (instead of van der Waals attraction of atoms in ground state) is discussed.
Supersolid formation in the system of Rydberg crystal embedded in BEC of nonexcited atoms is analyzed. Two-stage melting of Rydberg clusters is discussed.

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