Variational Monte Carlo calculation of two-dimensional Wigner crystal under lattice commensurability

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Wigner crystallization, which breaks the translational symmetry due to the long-range Coulomb interactions, is a fundamental problem in strongly correlated electron systems. By the diffusive quantum Monte Carlo method (DQMC), the critical electron density for crystallization is obtained as $r_s = r_0/a_B^* \simeq 150$ for a three-dimensional electron gas ($r_0 = (\pi n_e)^{-1/2}$, a_B^*: the effective Bohr radius) [1]. The critical value of r_s is lowered down to $r_s \simeq 31$ for a two-dimensional electron gas [2, 3]. In addition to the Coulomb interaction, the lattice commensurability reduces the critical Coulomb interaction for crystallization [4].

In this work, we studied the Wigner crystallization in spinless Fermion systems on a square lattice at finite fillings by highly accurate simulation based on the many-variable variational Monte Carlo (mVMC) method [5]. By performing the calculations up to the order of 10^3 sites, we determine the transition points for $n = 2, 4, 8, 12, 16$ and draw the phase diagram as functions of r_s and $1/n$ as shown in Fig. 1.

In contrast to the previous works by path-integral renormalization group (PIRG) [4], we found that the transition points at finite fillings becomes significantly small. Nevertheless, the transition points seem to continuously connect to its continuum limits, which is consistent with the previous works. We also examined the nature of the associated metal-insulator transition by calculation the momentum distribution and the charge gap [6].

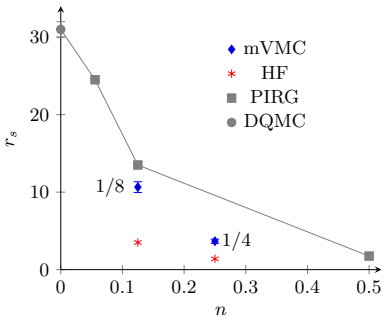

Figure 1: Phase diagram in the plane of the electron-density and r_s. We also show the result of the Hartree-Fock (HF) approximation.

References

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