Supersolid state in a fermionic optical lattice system

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Abstract. We study ultracold fermionic atoms loaded in an optical lattice with a confining potential. By combining dynamical mean-field approximation with a two-site impurity solver, we demonstrate that a supersolid state, where an $s$-wave superfluid coexists with a density-wave state of checkerboard pattern, is stabilized by attractive onsite interactions on a square lattice. The stability of the supersolid state in the thermodynamic limit is also addressed.

Ultracold fermionic atoms in an optical lattice have attracted considerable interest since the successful observation of the Fermi surface. More recently, further interesting phenomena have been observed such as superfluid and Mott insulating states, which stimulates further theoretical investigations on fermionic optical lattice systems. One of the interesting questions is how an $s$-wave superfluid (SSF) state coexists or competes with a density wave (DW) state. This provides an important issue in condensed matter physics since it is related to the possibility of the supersolid state. It is known that in homogeneous systems on bipartite lattices, except for one dimension, the DW and SSF ground states are degenerate at half filling, which means that the supersolid state is realizable in principle. However, the degenerate ground state is unstable against hole doping, where the supersolid state immediately changes to a genuine SSF state. On the other hand, the optical lattice system has a chance to realize the supersolid state due to the existence of an additional confining potential. In fact, the possibility of the supersolid state, where the DW and SSF states coexist, has been suggested in a small cluster on square lattice. However, it is not clear how stable the supersolid state is in the thermodynamic limit, which may be important for experimental observations. Motivated by this, we study ultracold fermionic atoms in the optical lattice to discuss how the supersolid state is stabilized when the system size is increased.

Let us consider a fermionic optical lattice system described by the following attractive Hubbard Hamiltonian,

$$H = -t \sum_{\langle i,j \rangle} c_{i\sigma}^\dagger c_{j\sigma} - U \sum_i n_{i\uparrow} n_{i\downarrow} + \sum_i \left[ V_0 r_i^2 - \mu \right] n_{i\sigma},$$

where $c_{i\sigma} (c_{i\sigma}^\dagger)$ annihilates (creates) a fermion at the $i$th site with spin $\sigma$ and $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$. $t$ is the nearest-neighbor hopping, $U$ the attractive interaction, and $\mu$ the chemical potential. $r_i$ is the distance measured from the center of the system and $V_0$ the curvature of the harmonic potential. Here, the length characteristic of the harmonic potential is defined as $d = (V_0/t)^{1/2}$.

The ground-state properties of the Hubbard model on inhomogeneous lattices have theoretically been studied by means of various methods such as Bogoljubov-de Gennes
equations [22], Gutzwiller approximations [23, 24], and variational Monte Carlo simulations [25]. However, these methods may be difficult to describe the coexisting phase like a supersolid in the strong coupling regime. The density matrix renormalization group method [20, 18] and quantum Monte Carlo method [26, 17] are efficient for one-dimensional systems, but may be difficult to apply to higher-dimensional systems with large clusters. We here use dynamical mean-field approximation (DMFA) [27], which incorporates local particle correlations precisely. This method also has an advantage in treating the SSF and DW states on an equal footing in the strong coupling regime, which allows us to discuss the supersolid state in the optical lattice [19].

In the framework of DMFA, the lattice Green’s function is described in terms of the site-diagonal self-energy $\hat{\Sigma}_i (i\omega_n)$ as

$$\hat{G}^{-1}_{\text{lat}} (i\omega_n)_{ij} = \delta_{ij} \left[ i\omega_n \hat{\sigma}_0 + \left( \mu - V_0 i\pi T \right) \hat{\sigma}_z - \hat{\Sigma}_i (i\omega_n) \right] - t \delta_{(ij)} \hat{\sigma}_z, \tag{2}$$

where $\hat{\sigma}_z$ is the $z$ component of the Pauli matrix, $\hat{\sigma}_0$ the identity matrix, $\mu$ the chemical potential, $\omega_n = (2n + 1)\pi T$ the Matsubara frequency, and $T$ the temperature. A DMFA self-consistent loop is iterated under the condition that the site-diagonal component of the lattice Green function is equal to the local Green function obtained from the effective impurity model,

$$\hat{G}_{\text{lat}}^{-1} (i\omega_n)_{ii} = \hat{G}_{\text{imp}}^{-1} (i\omega_n)_{ii} + \hat{\Sigma}_i (i\omega_n). \tag{3}$$

When DMFA is applied to our inhomogeneous system, one has to solve the effective impurity models $L$ times by iteration, where $L$ is the system size. Therefore, a proper impurity solver is necessary to discuss the system-size dependence of the ground state. To this end, we use a two-site approximation [28, 29], where the effective bath is replaced by only one site in the method. In spite of this simplicity, this method has an advantage in taking into account both low- and high-energy properties reasonably well within restricted numerical resources [19, 29, 30, 31]. Furthermore, we can make use of the symmetry of the square lattice in the framework of DMFA, which is guaranteed by the fact that the point symmetry characteristic of the square lattice is not broken even in the supersolid state [19]. For example, when the system with 5801 sites ($r < 38.0$) is treated, one can deal with only 595 inequivalent sites. These enable us to treat the optical lattice with large clusters to discuss the stability of the supersolid state in the thermodynamic limit.

**Figure 1.** (Color Online) Density profile $\langle n_{i\sigma} \rangle$ when $U/t = 5$, $d = 20.0$ and $N \sim 2850$.

**Figure 2.** (Color Online) Pair potential $\Delta_i$ when $U/t = 5$, $d = 20.0$ and $N \sim 2850$.

We perform DMFA to calculate the local density $\langle n_{i\sigma} \rangle = 2T \sum_{n=0} \text{Re} [G_{ii}(i\omega_n)] + 1/2$ and the pair potential $\Delta_i = 2T \sum_{n=0} \text{Re} [F_{ii}(i\omega_n)]$, where $G_{ii}(i\omega_n)[F_{ii}(i\omega_n)]$ is the normal (anomalous)
part of the local Green’s function at \( i \)th site. In Figs. 1 and 2, we show the results for the optical lattice system with \( U/t = 5 \), \( d = 20 \) and \( N \sim 2850 \) at the temperature \( T = 0.05 \), where 
\[ N = \sum_{i\sigma} \langle n_{i\sigma} \rangle. \]
We find that ultracold fermions are confined in the region \( r < 34 \). It is also found that the checkerboard pattern appears in the density profile in the doughnut-like region \( (12 < r < 28) \), which implies the existence of the DW state with the two-sublattice structure. On the other hand, the pair potential appears in the whole region with \( \langle n_i \rangle \neq 0 \), where the SSF state is realized in the region, as shown in Fig. 2. These results lead to the conclusion that the supersolid state is indeed stabilized in the doughnut region, where the DW state coexists with the SSF state. This is consistent with our previous result with \( d = 6.5 \) [19] and suggests that the supersolid state is stable even in larger cluster systems.

To clarify how the supersolid state is affected by the system size, we perform DMFA for several clusters with different \( d \), and fixed \( U/t \) and \( \mu/t \). The obtained profiles of the local density and the pair potential are shown in Figs. 3 and 4. Since we have dealt with finite systems, all data are discrete in \( r \). Nevertheless, it is found that the obtained results are well scaled by \( d \) although some fluctuations appear due to finite-size effects in a small \( d \) case. Since the effective particle density \( \tilde{n} = N/\pi d^2 \) is almost constant in the above cases, we can say that the supersolid state discussed here is stable in the thermodynamic limit \( (N \to \infty, d \to \infty) \) and \( \tilde{n} \sim 2.3 \). Note that this result does not necessarily imply that the supersolid state is realized in the homogeneous system with arbitrary fillings, where the supersolid state might be realizable only at half filling [9, 10, 11, 12, 13, 14]. Therefore, a confining potential is essential to stabilize the supersolid state in the optical lattice system. The ground state properties in the optical lattice system with different effective particle densities \( \tilde{n} \) and the Coulomb interactions \( U/t \) will be reported elsewhere.

In summary, we have investigated the fermionic attractive Hubbard model in the optical lattice with harmonic confinement. By combining DMFA with a two-site approximation, we have found that the supersolid state, in which the SSF state coexists with the DW state, is indeed stabilized. It has been also clarified that a confining potential plays a key role in stabilizing the supersolid state in large clusters. There are a lot of interesting problems to be explored in this context. An imbalanced fermionic system with \( N_\uparrow \neq N_\downarrow \) may be especially interesting, since the so-called Fulde-Ferrell-Larkin-Ovchinnikov superfluid state with a spatially modulated order parameter may compete with the DW state, giving rise to a novel supersolid state.
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