Supersolids in confined fermions on one-dimensional optical lattices

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Using quantum Monte Carlo simulations, we show that density-density and pairing correlation functions of the one-dimensional attractive fermionic Hubbard model in a harmonic confinement potential are characterized by the anomalous dimension $K_{\rho}$ of a corresponding periodic system, and hence display quantum critical behavior. The corresponding fluctuations render the SU(2) symmetry breaking by the confining potential irrelevant, leading to structure form factors for both correlation functions that scale with the same exponent upon increasing the system size, thus giving rise to a (quasi)supersolid.

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The recent experimental observation of nonclassical rotational inertia in solid $^4$He revived the interest in the possible coexistence of superfluidity and crystalline order, a phase named a supersolid (SS), proposed long ago in spite of arguments against it. Such arguments seem to be validated by quantum Monte Carlo (QMC) simulations and theoretical work showing that a defect-free crystal of $^4$He does not show off-diagonal long-range order (ODLRO). Further numerical simulations suggest that ODLRO may arise from domain walls or in a metastable state such that the existence of a pure supersolid phase in $^4$He is still under debate.

Alternative paths towards the realization of a SS were recently suggested for quantum gases on optical lattices, e.g., for bosons with dipolar interactions Bose-Fermi mixtures, Bose-Bose mixtures frustrated lattice geometries or extended interactions by loading the atoms in higher bands. Most of the proposals, however, are based on mean-field approximations that tend to be unstable with respect to phase separation, as shown by QMC simulations. Also the presence of a confining potential is in general neglected, discarding the coexistence of phases that may obscure the experimental determination of a SS.

Another system where a SS phase is well known to exist is the fermionic Hubbard model with an attractive contact interaction [the first two terms in Eq. (1) below]. In contrast to the mentioned bosonic systems, where vacancies or defects lead to a SS, here diagonal and ODLRO result from an SU(2) symmetry, relating density and pairing amplitudes at density $n = 1$. While the experimental realization of such a model is at least debatable in solid state systems, fermions with attractive contact interaction were recently achieved with quantum gases by means of Feshbach resonances, leading to pairing and superfluidity.

Even the observation of superfluidity with fermions in an optical lattice for a dense system ($n \sim 1$) was announced recently bringing very close the realization of an SU(2)-symmetric SS.

Still, the presence of a confining potential could inhibit the formation of the SS, since it explicitly breaks the above-mentioned SU(2) symmetry, as discussed in detail below. We show, however, based on QMC simulations of the one-dimensional (1D) attractive fermionic Hubbard model in a harmonic potential, (i) that density-density (DD) and pairing correlation functions are characterized by the anomalous dimension $K_{\rho}$ of the corresponding periodic model, and (ii) that in spite of the confinement, conditions can be reached where the structure form factors of both correlation functions diverge with the same power as the system tends toward the thermodynamic limit. Hence, a proper treatment of long-ranged quantum fluctuations shows that the SU(2) symmetry breaking becomes irrelevant, thus giving rise to a SS state.

In the following, we consider the Hamiltonian

$$H = -t \sum_{j,\sigma}(c_{j+1\sigma}^{\dagger}c_{j\sigma} + h.c.) - U \sum_{j} n_{j\uparrow}n_{j\downarrow} + V \sum_{j=0}^{N}(x_{j} - Na/2)^{2} n_{j},$$

where $c_{j\sigma}^{\dagger}$ and $c_{j\sigma}$ are creation and annihilation operators, respectively, for fermions on site $j$ (position $x_{j} = ja$), where $a$ is the lattice constant) with spin $\sigma = \uparrow, \downarrow$. The local density is $n_{j} = n_{j\uparrow} + n_{j\downarrow}$, where $n_{j\sigma} = c_{j\sigma}^{\dagger}c_{j\sigma}$. The contact interaction is attractive ($U > 0$) and the last term models the potential of the confining trap with $N$ (even) sites. The QMC simulations were performed using a projector algorithm ($\theta \simeq 30/\pi$) having parameter $\theta = 0.1/t$, the corresponding systematic error has no effect on the results. We use in general $\Delta \tau = 0.1/t$.

It is well known that a particle-hole transformation $d_{j\tau}^{\dagger} = (-1)^{j}c_{j\tau}^{\dagger}$, $d_{j\tau} = c_{j\tau}$, applied to the Hamiltonian leads to a repulsive Hubbard model in the presence of a spatially varying magnetic field $h_{j} = 2V(x_{j} - Na/2)^{2}$. If $\langle n_{j\uparrow}\rangle = \langle n_{j\downarrow}\rangle$, then $n_{j}^{2} \equiv \langle d_{j\uparrow}^{\dagger}d_{j\uparrow}\rangle + \langle d_{j\downarrow}^{\dagger}d_{j\downarrow}\rangle = 1$, i.e., the new system is half filled. If, furthermore, $h_{j} = 0$, i.e., for $V = 0$, a Mott insulator with dominating antiferromagnetic correlations results for the repulsive system.

In terms of the operators of Eq. (1), this implies that...
for $V = 0$ and $n = 1$ the DD correlation function $N_{j\ell} = \langle n_j n_{\ell} \rangle - \langle n_j \rangle \langle n_{\ell} \rangle$ and the pairing correlation function $P_{j\ell} = (\Delta_j \Delta_{\ell}^*)$, with $\Delta_j = c_j^\dagger c_{j+}$, obey

$$N_{j\ell} = 2(-1)^{|j-\ell|} P_{j\ell},$$

and will be the dominating correlation functions, with the same power-law decay. This identifies the state as a SS. However, the presence of a confining potential breaks this SU(2) symmetry, so that for $V \neq 0$ the SS is expected to be destroyed. In the following we show that, due to quantum critical fluctuations, even for $V \neq 0$ the SS is nevertheless recovered.

A first important question is whether, in the presence of a confining potential, which produces a spatial dependence of the density, the correlation functions will each exhibit a decay with a single power. In fact, this is no longer the case if one relies on the local density approximation (LDA)\textsuperscript{27}. However, we find that the LDA is not appropriate to describe the physics of the model in Eq.~(1). In Fig.\textsuperscript{1} we show the density profile for $N_f = 74$ fermions, $U/t = 4$, and a characteristic density $\tilde{\rho} = 1$. As shown before\textsuperscript{27} the characteristic density defined as $\tilde{\rho} = N_f a (V/t)^{1/2}$ relates systems with different sizes, number of particles, and confining harmonic potentials in the same way as the particle density does for periodic systems of different sizes. Figure\textsuperscript{1} shows that the presence of the confining potential produces density oscillations on a short distance scale ($\sim a$), which are absent in periodic systems. These oscillations preclude the use of the LDA as a sensible approximation, since it would require a slowly varying density.

We study next the DD and pairing correlations using QMC simulations. Since in the presence of quasi-long-range order a divergence is expected for a particular wave vector $k$ in a periodic system, we examine the eigenvalue equation for DD correlations,

$$\sum_{\ell} N_{j\ell} \phi_{\ell}^\mu = N^\mu \phi_{j}^\mu,$$

which reduces to a Fourier transformation for a periodic system, i.e., the eigenvectors $\phi_{\ell}^\mu$ are plane waves, each mode characterized by a particular $k$ vector. Interestingly, we find that even inside a harmonic trap most of the modes $\phi_{\ell}^\mu$ can still be assigned each to a characteristic wave vector. This can be seen by considering the moduli of the Fourier transform $[\sim \sum_{\ell} \phi_{\ell}^\mu \exp(ikx_{\ell})]$ of each $\phi_{\ell}^\mu$. As shown in Fig.\textsuperscript{2}(a), most of the modes $\mu$, with $N^\mu$ in ascending order, have a dominant component each of which can be related to a wave vector $k$ (actually, both $\pm k$ due to reflection symmetry). We checked that regions where a clear identification of a dominant $k$ vector is not possible at all correspond to the lowest eigenvalues that arise from the vanishing density at the edges of the fermionic cloud in Fig.\textsuperscript{1} Results of a similar analysis for the eigenvectors $\varphi_{\ell}^\mu$ of the pairing correlations $P_{j\ell}$,

$$\sum_{\ell} P_{j\ell} \varphi_{\ell}^\mu = P^\mu \varphi_{j}^\mu,$$

are shown in Fig.\textsuperscript{2}(b). We find that the highest eigenvalues of the pairing correlation function have the largest weight around $k = 0$, i.e., pairs are formed by fermions with opposite momenta. This unbiased result helps to understand why even in trapped systems, where translation invariance is broken and momentum is not a “good” quantum number, pairing correlations have been observed predominantly between atoms with opposite momenta.\textsuperscript{29}
to attain a SS. This is achieved in the periodic case for the slope of \( n = 0.71 \). The resulting density is \( n = 0.71 \). Inset: position of the \( 2k_F \) peak as a function of \( U \) in the harmonic trap for \( \tilde{\rho} = 1 \).

Since each mode \( \mu \) can be assigned rather clearly to a wave vector \( k \), we can map each eigenvalue \( N^\mu \) to \( N(k) \) as in a periodic system. Figure 3 shows the result of such an assignment (○), according to the salient features shown in Fig. 2(a). We superimposed in Fig. 3 the results for a periodic system (⊔), for which the density was fixed by identifying the wave vector corresponding to the maximum in \( N(k) \) of the confined system with \( 2k_F \) of the periodic system (black vertical line), where \( k_F \) is the Fermi momentum, establishing in this way a link between a trapped system with a characteristic density \( \tilde{\rho} \) and a periodic system of density \( n = 2k_Fa/\pi \). Such an identification is based on the observation that, in a 1D fermionic system with attractive interactions, \( 2k_F \) oscillations in the charge channel are dominating. The inset shows the position of the peak as a function of \( U \), which for the range \( 2 \leq U/t \leq 8 \) does not change appreciably. Hence, the identification is possible for a wide range of parameters and does not depend on any particular fine tuning.

While the identification of \( N(k) \) in the periodic and the confined systems deteriorates at wave vectors beyond \( 2k_F \) (with a number of points at zero or close to it due to the regions where the density vanishes), it is remarkably good close to \( k = 0 \). For a periodic system the DD correlation function obeys \( N(k) \rightarrow K_\rho |k|a/\pi \) for \( k \rightarrow 0 \).

Therefore, the anomalous dimension \( K_\rho \) that determines the power-law decay of the \( 2k_F \) oscillations that dominate at large distances can be directly obtained from the slope of \( N(k) \) for \( k \rightarrow 0 \). Figure 4 shows that the mapping proposed here leads to the identification of \( K_\rho \) also for the confined system. In fact, such an identification is possible in general, as shown in Fig. 4 where a comparison of the values of \( K_\rho \) obtained for a confined system with \( \tilde{\rho} = 1 \) and those obtained by Bethe ansatz for \( \langle n \rangle = 0.7 \) is shown.

We are now in a position to determine the conditions to attain a SS. This is achieved in the periodic case for \( n = 1 \), i.e., \( 2k_Fa = \pi \). We thus increase \( \tilde{\rho} \) until the maximum of \( N(k) \) in the confined system appears at \( k = \pi/a \). This is shown in Fig. 5 where the mapping described above was made for both the DD \( \langle N(k) \rangle \) and pairing \( \langle P(k) \rangle \) vs number of fermions \( N_f \) in a double-logarithmic scale.

FIG. 3: (Color online) \( N(k) \) for the confined (○) case with the same parameters as in Fig. 4. Superimposed are the results for a periodic system (⊔) with \( 2k_F \) given by the black vertical line. The resulting density is \( n = 0.71 \). Inset: position of the \( 2k_F \) peak as a function of \( U \) in the harmonic trap for \( \tilde{\rho} = 1 \).

FIG. 4: (Color online) Anomalous dimension \( K_\rho \) extracted from the slope of \( N(k) \) for the confined system (×) vs \( U \) for \( \tilde{\rho} = 1.0 \) and \( \langle n \rangle = 0.71 \). Superimposed are the results for a periodic system obtained from Bethe ansatz (○) for \( \langle n \rangle = 0.7 \) (Ref. 23).

FIG. 5: (Color online) (a) \( N(k) \) for the confined case for \( \tilde{\rho} = 2.34 \) (○); other parameters as in Fig. 4. Superimposed are the results for a periodic system (⊔) with density \( n = 1.0 \). (b) \( P(k) \) for the confined (○) and periodic systems (⊔) with the same parameters as in (a). Inset: largest eigenvalues for the DD \( \langle N(k = \pi) \rangle \) and pairing \( \langle P(k = 0) \rangle \) vs number of fermions \( N_f \) in a double-logarithmic scale.
fined system follow closely the behavior in the periodic system. As in the case of \( \rho = 1 \), the power-law behavior of the \( 2k_F \) oscillations in \( N(k) \) for the trapped system is determined by the same \( K_\rho \) as in the periodic case. Moreover, in the periodic case, due to the above mentioned SU(2) symmetry, the relationship Eq. (2) holds between the correlation functions. This means in a periodic system that \( P(k) = N(\pi/a - k)/2 \), a relation that is obeyed in Fig. 5 (C). Remarkably, and to a very good approximation, this symmetry is seen to be present also in the confined system (●). Hence, in spite of the explicit breaking of the SU(2) symmetry by the confining potential, this symmetry is recovered in the correlations, which display quasi-long-range order. This fact is reminiscent of the universality found for hard-core bosons confined on a 1D lattice, where the power-law decay of the one-particle density matrix remains unaffected by the presence of a confining potential. In fact, in the limit \( U/t \to \infty \) of Eq. (1), the resulting on-site pairs reduce to hard-core bosons. Here, we find that, due to the long-ranged fluctuations, once the appropriate characteristic density is found, the SU(2) symmetry is restored with high accuracy for the considered values of \( U \).

The inset of Fig. 5 shows the scaling behavior of the largest eigenvalues \( N(k = \pi) \) and \( P(k = 0) \) for the harmonically confined system as a function of the number of particles for \( \rho = 2.34 \) and \( U/t = 4 \). Both indeed diverge with the same power law, and, as discussed above, differ in magnitude within statistical errors by a factor of 2, as expected when the SU(2) symmetry is present. Hence, we show explicitly that quasi-long-range order is present in both the charge density and pairing channel with a unique exponent, giving rise to a SS state even in the trapped system.

In summary, on the basis of QMC simulations (i) we have shown that quasi-long-range order in a confined system of attractive fermions is characterized by the single exponent \( K_\rho \) of the related periodic system, and given a prescription to relate both systems; (ii) we have also shown that this identification leads to systems where diagonal and off-diagonal quasi-long-range order arise with the same exponent, such that they correspond to a supersolid in one dimension. These results clearly show that a SS state is attainable experimentally with fermionic quantum gases with two degenerate hyperfine states confined in one-dimensional tubes with an axial optical lattice, a configuration that was already realized with fermions with repulsive interactions.

**Note Added:** After this work was completed and submitted, we became aware of a related Letter by G. Xianlong et al.

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