Emergence of Mixed Quintet Superfluidity in the Chain of Partially Polarized Spin-3/2 Ultracold Atoms

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The system of ultracold atoms with hyperfine spin $F = 3/2$ might be unstable against the formation of quintet pairs if the interaction is attractive in the quintet channel. We have investigated the behavior of correlation functions in a model including only $s$-wave interactions at quarter filling by large-scale density-matrix renormalization-group simulations. We show that the correlations of quintet pairs become quasi-long-ranged, when the system is partially polarized, leading to the emergence of various mixed superfluid phases in which BCS-like pairs carrying different magnetic moment coexist.

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Introduction: Recently ultracold atomic and molecular systems have been in the focus of theoretical and experimental studies not only in atomic and molecular physics but also in condensed matter physics. Atomic systems with hyperfine spin degrees of freedom higher than 1/2 can show completely new behavior for both bosonic and fermionic systems. For repulsive interaction Mott insulating phases, (chiral) spin liquid states, resonating plaquette order, spin-quadrupole and even higher multipole order or a generalized Peierls-like distortion can occur. For attractive interactions bound trionic and quartet states have been predicted for one- and three-dimensional systems as well.

In addition to the usual singlet BCS pairs, nonsinglet pairs may also occur if the appropriate component of the interaction is attractive. A general description of different high-spin pair states was given by Ho and Yip. High spin fermions may form spin-2 (quintet) pairs, which are of particular interest owing to their exotic properties. Moreover ultracold atomic systems of $F = 3/2$ fermions are excellent candidates for studying the consequences of high symmetries, since they possess SO(5) rather than SO(3).

For a long time magnetic ordering and superconductivity were thought to be incompatible. In fact highly symmetric states, since they possess SO(5) rather than SO(3).

In this paper, we study the possible formation of local quintet pairs and their stability in a one-dimensional chain of fermionic atoms with hyperfine spin $F = 3/2$, when the interaction is attractive in the quintet channel. We consider a quarter-filled system, that is the number of particles is equal to the number of sites.

We show that if spin states with different spin components are unequally populated, quintet pairs can become stable. Note that in a one-dimensional model, where no true long-range order may exist, a superfluid state is claimed to be stabilized, when the corresponding correlation function shows algebraic—instead of exponential—

decay. The superfluid phases will be characterized by the spin quantum number of the pairing operators appearing in the correlation function. As will be seen, the type of stable quintet pairs depends on the coupling constants (scattering lengths) and the spin-imbalance. It is worth noting that our model contains only $s$-wave interaction indicating that quintet pairing phases can be stabilized via $s$-wave Feshbach resonance. This can help in the possible experimental realization of Cooper-like pairs with high multiplicity by avoiding the difficulties due to inelastic loss in $p$-wave scatterings.

Formulation of the problem: The scattering processes between particles with hyperfine spin $F$ can be classified into independent spin channels characterized by the total spin $S$ of the scattered atoms. Accordingly, the interaction part of the Hamiltonian is $V = \sum_{S=0}^{2F} g_S \mathcal{P}_S$, where $\mathcal{P}_S$ projects onto the total spin $S$ subspace and $g_S$ is the coupling constant in the corresponding channel. The projectors are expressed via the pairing operators as $\mathcal{P}_S = \sum_{m,i} P_{S,m,i}^{\dagger} P_{S,m,i}$, which are defined through the Clebsch-Gordan coefficients and the creation operator of fermions, $c_{\alpha,i}^{\dagger}$ at site $i$, with spin component $\alpha = \pm 3/2, \pm 1/2$, as $P_{S,m,i}^{\dagger} = \sum_{m,3} \langle \frac{3}{2} \frac{3}{2} \alpha \beta | S, m \rangle c_{\alpha,i}^{\dagger} c_{\beta,i}^{\dagger}$, where $m$ is the $z$ component of the total spin of the two scattering particles.

Starting from a fermionic spin-3/2 Hubbard-like model with on-site interaction, the only contributing terms are antisymmetric under the exchange of the spin of the two colliding atoms, therefore, only the $S = 0$ and $S = 2$
terms may appear. Thus the Hamiltonian of the system reads as
\[
\mathcal{H} = -t \sum_{i,\alpha} (c_{\alpha,i}^\dagger c_{\alpha,i+1} + \text{H.c.}) + g_0 P_0 + g_2 P_2,
\]
where \( t \) measures the hopping amplitude between neighboring sites. In optical lattices \( t \approx 2\omega R^3 e^{-2k^2/\pi} \), with \( \zeta = (V_0/\omega R)^{1/4} \), where \( V_0 \) is the potential depth, and \( \omega R = \hbar^2 k^2/2m_{\text{atom}} \) is the recoil energy for atoms of mass \( m_{\text{atom}} \) in a lattice with lattice constant \( a \). The coupling \( g_S \) measured in units of the transverse confinement energy is related to \( V_0 \) and the \( s \)-wave scattering length in the total spin \( S \) scattering channel, \( a_S \), as \( g_S \approx \pi^2 a_S/(2a) \). For attractive couplings \( (g_0 < 0, g_2 < 0) \) the above Hamiltonian suggests that singlet and quintet pairs are competing. Although the SU(4) line \( (g_0 = g_2) \) is expected to be the most relevant experimentally, the region with repulsive interaction in the singlet channel \( (g_0 > 0) \) and attractive interaction in the \( S = 2 \) channel turns out to be more favorable for quintet pairing. Therefore, besides the SU(4) line, we will consider the case \( g_0 > 0, g_2 < 0 \), where quintet pairing competes with density waves, as seen if the interaction term \( \Delta \) is rewritten in terms of the density, \( n_i = \sum_\alpha n_{\alpha,i} = \sum_\alpha c_{\alpha,i}^\dagger c_{\alpha,i} \), and the \( P_2 \) quintet projector as \( U/2 \sum_i n_i^2 + V P_2 \), with couplings \( U = 2g_0, V = g_2 - g_0 \). In a system with more than two components, not only pairs, but trions, too, may be formed. We did not consider such a possibility. Although three-body losses \(^{17} \) may be important in this system, large three-body losses may suppress threefold occupation of sites and may stabilize pairs as has been shown in Ref. \(^{18} \).

Analytic calculation in the weak-coupling limit \(^{19} \) shows that the leading instability for \( g_0 > 0, g_2 < 0 \) is the formation of site- or bond-centered spin singlet quartets, which are formed from an equal number of atoms with \( \alpha = \pm 1/2, \pm 3/2 \). In order to search for possible conditions that might stabilize the quintet Cooper pairs in one dimension we have studied numerically the phase diagram of model \(^{11} \) for \( g_2 \leq 0 \) at quarter filling.

**Numerical procedure:** Density-matrix renormalization-group (DMRG) simulations have been performed with open boundary condition up to \( L = 64 \) sites, keeping 500–2000 block states and using up to 8 sweeps. Properties of various phases have been determined by analyzing the spatial variation of correlation functions of different pairs, \( \chi_{Sm}(i) = \langle P_{Sm,1}^i P_{Sm,1+1}^i \rangle \), with \( m = 0 \) for \( S = 0 \), and \( m = 0, \pm 1, \pm 2 \) for \( S = 2 \), of quartets, \( \chi_Q(i) = \langle Q(i) Q_{1+i} \rangle \) with \( Q(i) = c_{3/2,1}^i c_{1,2}^i c_{-3/2,1}^i c_{1,2}^i \), as well as density and spin-density correlation functions, \( \chi_\alpha(i) = \langle n_{1/2} n_{1+i} \rangle - \langle n_{1/2} \rangle \langle n_{1+i} \rangle \), \( \chi_\delta(i) = \langle n_{3/2} n_{1+i} \rangle - \langle n_{3/2} \rangle \langle n_{1+i} \rangle \), where \( n_{1/2} = \sum_\alpha n_{\alpha,1/2} \). In the rest of the paper—for better visibility—only the quintet pairing correlation functions \( \chi_{2m} \) are shown in the figures for the five \( m \) values.

**Numerical results:** The analysis of these functions confirmed the absence of quintet Cooper pairs when all spin components are equally populated, since \( \chi_{2m} \) decays exponentially for all \( m \) [see Figs. \(^{11} \)\(a\), \(^{3} \)\(a\), and \(^{4} \)\(a\)]. We have found, in agreement with Ref. \(^{6} \) that \( \chi_Q \) and \( \chi_n \) decay algebraically in the regime where a phase composed of site-centered quartets was predicted by weak-coupling analysis.

The spin-singlet quartets could, however, be broken and quintet pairs could be stabilized, if a population imbalance occurs in the number of fermions with different spin components. Spin imbalance can for example be generated by switching on a weak magnetic field \( (B) \) which couples linearly to the magnetization \( \tilde{m} = \frac{1}{4} \sum_i \langle \tilde{n}_i \rangle \) (measured in units of Bohr magneton). The stability of quintet pairs is indicated by the slow decay of the correlation function of quintet pairs. Even for reasonably small spin imbalance, \( \chi_Q \) decays faster or vanishes, while the correlation of singlet Cooper pairs \( \langle \chi_{0,0} \rangle \) behaves in the same way as \( \chi_{2,0} \). Therefore, in what follows we present the correlation functions \( \chi_{2m} \) for increasing spin imbalance from \( \tilde{m} = 0 \) up to the maximum value \( \tilde{m} = 3/2 \).

**SU(4) symmetric model:** First we present results for the SU(4) symmetric model where we have found three different superfluid phases as the polarization is increased. Although it is difficult to determine the phase boundaries explicitly the correlation functions behave differently for small \( (\tilde{m} \text{ around } 1/3) \), intermediate \( (\tilde{m} \text{ somewhat below } 1) \), and for large \( (\tilde{m} > 1) \) values of \( \tilde{m} \), as can be inferred from Fig. \(^{11} \). For \( \tilde{m} = 1/3 \), the correlation functions for quintet pairs with \( m = \pm 2 \) show the slowest decay (Fig. \(^{11} \)\(b\)). We denote this phase by \( SF_{5}(2, -2) \), where the subscript 5 indicates the quintet nature of the superfluid (SF) phase and the numbers in brackets gives the \( m \) index of the dominant \( \chi_{2m} \) correlation functions. In this regime, the correlation function of the quartets decays only slightly faster than that of

FIG. 1. (Color online) The quintet correlation functions \( \chi_{2m} \) as a function of the distance \( i \) for \( \tilde{m} = 0 \) (all \( \chi_{2m} \) are equal), \( 1/3, 2/3 \) and \( 1 \) calculated at \( g_0 = g_2 = -1 \).
the dominant quintets. Note, that the occurrence of this state is highly nontrivial, since naively one can expect the dominance of pairs formed of fermions with the majority spin components $\alpha = 3/2$ and $1/2$, while pairs formed of fermions with $\alpha = -1/2$ and $-3/2$ would be suppressed.

A different behavior is found at $\tilde{m} = 1$ (Fig. 1(d)), where the correlation function of quintet pairs with $m = 2$, 1, and 0 ($\chi_{2,2}$, $\chi_{2,1}$ and $\chi_{2,0}$) shows algebraic decay. The correlation functions $\chi_{2,-1}$ and $\chi_{2,-2}$, and also $\chi_{Q}$ vanish within our numerical accuracy, since the number of fermions with $\alpha = -1/2$ and $-3/2$ is much less than that with $\alpha = 3/2$. Similar reason is behind the smaller weight of the $\chi_{2,1}$ and $\chi_{2,0}$ quintet pairs, but they decay algebraically with the same exponent as $\chi_{2,2}$. The corresponding phase is denoted by $SF_5(2,1,0)$.

The magnetization value $\tilde{m} = 2/3$ (see Fig. 1(c)) belongs to a region where the system possesses a transitional behavior between $SF_5(2, -2)$ and $SF_5(2, 1, 0)$. Here it is difficult to decide whether some of the correlation functions decay algebraically or exponentially. Nevertheless, it is clear that the dominant superfluid instability in this region is again characterized by different coexisting quintet pairs.

Slightly above $\tilde{m} = 1$, an effective two-component system with the usual FFLO state develops, where only $\chi_{2,2}$ is finite and all other $\chi_{2m}$ are zero. This phase is denoted by $SF_5(2)$ and will be discussed in more detail below.

The $g_0 > 0$, $g_2 < 0$ quadrant: The calculation for the SU(4) symmetric model shows that various exotic mixed superfluid phases can exist in which BCS-like pairs carrying different magnetic moments coexist. The differing behavior of the correlation functions is related to the number of atoms needed to form the pairs. Therefore, it is interesting to see how the number of atoms with $\alpha = -3/2, -1/2$, and $1/2$ decreases while more and more atoms have $\alpha = 3/2$ as the total polarization of the system is increases. These numbers depend on the interaction between the particles. For the sake of convenience, in what follows, we will consider the quadrant $g_0 > 0$, $g_2 < 0$, because the decay of correlation functions is easiest to analyze there. We have found two types of dependence of $\langle n_{\alpha,i} \rangle$ on $\tilde{m}$ as displayed in Fig. 2. The regions, where one or the other behavior is realized, correspond roughly to the regions separated by the line $g_0 = -3g_2$, where the ground state at $\tilde{m} = 0$ is a site-centered or bond-centered phase. The difference is also apparent in the different behavior of the site energy, $\epsilon_{\tilde{m}}$, as a function of $\tilde{m}$ (see the inset in Fig. 2(a)).

In the whole quadrant $g_0 > 0$, $g_2 < 0$ the model becomes independent of $g_0$ for $\tilde{m} \geq 1$ due to the absence of fermions with $\alpha = -3/2$ and $-1/2$. The only surviving quintet correlation function, $\chi_{22}$, shows an algebraic decay as shown in Fig. 3(c) and (d) in agreement with the results of Batrouni et al. [14], since in the $\tilde{m} \geq 1$ regime our model can be mapped exactly to their two-component model. This phase, in our notation $SF_5(2)$, is equivalent to the well-known FFLO state.

In contrast to this, for $\tilde{m} < 1$ the population imbalance of fermions with different spin components shows markedly different character in the two regions of the coupling space. For $g_0 < -3g_2$ (Fig. 2(a)) all spin components have finite weight for $\tilde{m} < 1$. As a consequence, the density of spin quintet pairs decreases, but $\chi_{22}$ remains the slowest decaying correlation function at least
when $\tilde{m} \geq 1/2$ (see Fig. 3(b)). In addition, also $\chi_{2-2}$ decays algebraically, although, with smaller weight and somewhat larger exponent. This mixed phase is the same SF$_5(2, -2)$ phase which was found along the SU(4) line for moderate magnetizations. Although, it is difficult to distinguish between an exponential or algebraic decay of the correlation functions below $\tilde{m} \approx 1/2$, quintet pairing is still the dominant instability even slightly below $\tilde{m} = 1/2$. Even though all the four spin components have finite weight, the other correlation functions $\chi_{2m}$ with $m = 0$, and $\pm 1$ decay exponentially (Fig. 3(b)) for $\tilde{m} < 1$.

A different behavior is found for $g_0 > -3g_2$ (Fig. 2(b)). As the polarization decreases from $\tilde{m} = 1$ to a value slightly above $3/4$, the density of atoms with $\alpha = -3/2$ remains zero, half of the atoms have $\alpha = 3/2$, while the density of atoms with $\alpha = \pm 1/2$ varies linearly with $\tilde{m}$. $\chi_{2-2}$ and $\chi_{2-1}$ are equal to zero in this range and $\chi_{20}$ decays exponentially (Fig. 4(d)). On the other hand, the slowest decaying correlation functions, $\chi_{21}$ and $\chi_{22}$, show algebraic decay with identical exponent, therefore we call this phase SF$_5(2, 1)$. As $\langle n_{-1/2} \rangle$ is increasing, the density of $m = 1$ pairs also increases and the number of $m = 2$ pairs decreases. At $\tilde{m} = 3/4$ we have found that the $m = 1$ and $m = 2$ quintet pairings remain the dominant instability, however, as $\tilde{m}$ is decreasing, the correlations $\chi_{2-1}$ and $\chi_{2-2}$ start to increase (see Fig. 4(c)). For even weaker polarization again the SF$_5(2, -2)$ state is stabilized (Fig. 4(b)), suppressing the naively expected pairs formed by the majority components of the fermions.

**Conclusions:** In this work, we have investigated possible quintet-pair formation in the system of $F = 3/2$ cold atoms in one-dimensional optical traps at quarter filling via large-scale, high precision DMRG simulations of various correlation functions. We have found that sufficiently strong spin-imbalance can stabilize different exotic quintet superfluid states, where pairs with different magnetic moments coexist. We have found that for large magnetizations the dominant superfluid instability is determined by the most populated fermion components. For moderate magnetization, however, a different behavior was found: in the SF$_5(2, -2)$ phase the correlation function of pairs with the largest spin projections, $m = \pm 2$, show the slowest decay, which probably indicates the emergence of an effective antiferromagnetic exchange between the pairs suppressing the quasi-long range order of all other quintet pairs.

Quantum degeneracy of spin-3/2 fermionic atoms could probably be realized experimentally since several atoms, e.g., $^{132}$Cs, $^{9}$Be, $^{135}$Ba, $^{137}$Ba or $^{201}$Hg (see Ref. 1) and 9 have $F = 3/2$ as lowest hyperfine manifold. Higher spin fermion mixtures have already been realized very recently$^{21}$ and these higher spin systems might also show similar instability against quintet superfluidity as found in this paper for spin-3/2 fermions. The interaction between alkaline earth atoms or between atoms having similar orbital structure, i.e., a closed outer orbit, have SU(N) symmetry with very good accuracy. The interaction between a series of spinor bosonic isotopes of alkali atoms also turned out to be nearly SU(N) symmetric$^{22}$.

It is expected that the superfluid state found along the SU(4) line ($g_0 = g_2$) is relatively easy to realize. Nevertheless, the rapid development of experimental techniques with ultracold atoms raises the hope that quantum degeneracy of multicomponent fermionic atoms with non SU(N) symmetric ground state will also be achieved in the near future.

There are several possibilities to probe these many-body correlation effects and to detect the coexisting quintet pairs with different magnetic moments. The pair gap can be studied by radio-frequency spectroscopy or momentum-resolved Bragg-spectroscopy, although these measurements have the disadvantage that the pair gap is the same for quintet pairs with different $m$, since the s-wave scattering length in the quintet channel does not depend on $m$. Magnetic moment of the pairs can be measured independently from the pair gap, e.g., via a Stern-Gerlach-like experiment by applying inhomogeneous external magnetic field.

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