Bose-Einstein Condensation of Particle-Hole Pairs in Ultracold Fermionic Atoms Trapped within Optical Lattices

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We investigate the Bose-Einstein condensation (BEC, superfluidity) of particle-hole pairs in ultracold Fermionic atoms with repulsive interactions and arbitrary polarization, which are trapped within optical lattices. In the strongly repulsive limit, the dynamics of particle-hole pairs can be described by a hard-core Bose-Hubbard model. The insulator - superfluid and charge-density-wave(CDW) - superfluid phase transitions can be induced by decreasing and increasing the potential depths with controlling the trapping laser intensity, respectively. The parameter and polarization dependence of the critical temperatures for the ordered states (BEC and/or CDW) is discussed simultaneously.

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In recent years, the demonstration of Bose-Einstein condensation of particle-particle pairs in homogeneous or confined two-component (spin-1/2) ultracold fermionic atoms has triggered great theoretical and experimental interest. The BCS-BEC crossover in ultracold Fermi atomic gases near a Feshbach resonance has been predicted by using the resonance superfluidity theory [1], and been observed in experiments [2]. For the fermionic atoms trapped within optical lattices, the s-wave or d-wave particle-particle pairs can undergo a phase transition to a superfluid state when the inter-component interaction is attractive or repulsive [3].

With the mechanism of the superfluidity of atom-atom pairs in ultracold Fermi atomic gases being explored more and more deeply, the question arises whether the atom-hole pairs in ultracold Fermi atomic gases can undergo a BEC phase transition similar to electron-hole pairs [4]. Firstly, due to the essentially non-equilibrium nature of the system of particle-hole pairs, which usually does not appear in the system of particle-particle pairs, the particle-hole system becomes an ideal system for exploring the non-equilibrium quantum mechanics at the frontier of many-body physics. Additionally, since all condensed particle-hole pairs can emit photons in tandem, the quantum coherence in such a condensate will reveal novel optical effects and nonlinear optical dynamics, which can not be shown by the condensate of particle-particle pairs. This provides possible applications in ultrafast digital logical elements and quantum computation. Furthermore, the controllable interaction strength and kinetic energy (or hopping strength) in the atomic systems open up the very exciting potential to investigate macroscopic quantum coherence and superfluidity under some extreme conditions that never exist in traditional electronic systems.

In this letter, we show that the atom-hole pairs in arbitrarily polarized spin-1/2 ultracold Fermi atoms with repulsive interaction, which are trapped within optical lattices, can undergo a superfluid phase transition similar to the ultracold bosonic atoms confined in optical lattices [5]. In the strongly repulsive limit, the dynamics of atom-hole pairs can be described by a hard-core Bose-Hubbard model. Then, the phase transition is analyzed with the derived Bose-Hubbard model. At the same time, the critical temperature for the ordered states (charge-density-wave and/or Bose-Einstein condensation) is discussed within the mean-field theory.

Consider an ensemble of arbitrarily polarized ultracold fermionic atoms occupying two different hyperfine states |S⟩ and |P⟩, which are trapped within the optical lattices. For simplicity, we assume the optical lattice potentials as $V^s_p(x) = \sum_{j=1}^{d} V^s_p \cos^2(kx_j)$. The wave vector $k$ is determined by the laser wave-lengths, $d$ (=1, 2 or 3) is the dimension of the optical lattices, and $V^s_p$ are proportional to the laser intensity. For sufficient low temperature, all atoms will be localized into the lowest Bloch band, and the system can be described by an asymmetric Fermi-Hubbard Hamiltonian:

$$H = -\sum_{\langle i,j \rangle} \left( t_{s} f_{si}^{\dagger} f_{sj}^{\phantom{\dagger}} + t_{p} f_{pi}^{\dagger} f_{pj}^{\phantom{\dagger}} \right) + \sum_{i} (\epsilon_s n_{si} + \epsilon_p n_{pi}) + U \sum_{i} n_{si} n_{pi}. \quad (1)$$

Here $f_{\sigma i}^{\dagger}$ ($f_{\sigma i}$) are fermionic creation (annihilation) operators for localized atoms in state |$\sigma$⟩ on site $i$, $n_{\sigma i} = f_{\sigma i}^{\dagger} f_{\sigma i}$. The symbol $\langle i,j \rangle$ represents summing over the nearest-neighbors and $\epsilon_s$ ($\epsilon_p$) is the single-atom energy of the atoms in state |S⟩ (|P⟩). The state-dependent tunneling (hopping) $t_{s}$($t_{p}$) between nearest neighbors can be induced by varying the potential depth $V^s_0$($V^p_0$) with controlling the laser intensity $\beta$. Usually, the tunneling strengths increase with the decrease of potential depths. Below the unitary limit, the on-site interaction $U$ is proportional to the s-wave scattering length between atoms occupying different hyperfine states. The s-wave scattering between atoms occupying the same hyperfine state is absent due to the Pauli blocking.
The average number of atoms per site (filling number) $n$ and the polarization $\gamma$ of the considered system are defined as

$$n = \sum_i (n_{si} + n_{pi})/N_L, \quad (2)$$

$$\gamma = \sum_i (n_{si} - n_{pi})/\sum_i (n_{si} + n_{pi}). \quad (3)$$

The symbol $N_L$ is the total number of lattice sites. In the following, we focus our interests on the half-filled case ($n = 1$), i.e., one atom per site.

The ground state energy per atom depends upon both the polarization and the energy difference ($\Delta \epsilon = \epsilon_p - \epsilon_s$) between two occupied states. With the definition of polarization, the ground states can be divided into five different regimes: non-polarized (NP) ground states with $\gamma = 0$, partially polarized in state $|S\rangle$ (PPS) with $0 < \gamma < 1$, partially polarized in state $|P\rangle$ (PPP) with $-1 < \gamma < 0$, fully polarized in state $|S\rangle$ (FPS) with $\gamma = 1$ and fully polarized in state $|P\rangle$ (FPP) with $\gamma = -1$.

For the one-dimensional lattices ($d = 1$) with state-independent hopping ($t_s = t_p = t$), these regimes can be exactly obtained with the Bethe-ansatz [8]. The $\Delta \epsilon$ has two critical values

$$\Delta \epsilon_1^c = \begin{cases} \left| \frac{U}{2} - 2t + 4t \int_0^\infty \frac{J_1(u)du}{u^{1+\exp([U/2])}} \right| & \text{for } U < 0, \\ 0 & \text{for } U > 0, \end{cases} \quad (4)$$

and

$$\Delta \epsilon_2^c = \begin{cases} 2t + \left| \frac{U}{2} \right| & \text{for } U < 0, \\ \sqrt{\frac{U^2}{4} + 4t^2} - \frac{U}{2} & \text{for } U > 0, \end{cases} \quad (5)$$

corresponding to the boundaries between different regimes. Here, $J_1(u)$ is the first kind Bessel function with first order. The non-polarized, partially polarized and fully polarized regimes satisfy $|\Delta \epsilon| \leq \Delta \epsilon^c$, $\Delta \epsilon_1^c < |\Delta \epsilon| < \Delta \epsilon_2^c$ and $|\Delta \epsilon| \geq \Delta \epsilon_2^c$ respectively (see Fig. 1).

In the strongly repulsive limit ($0 < t_{s,p} \ll U$), the Fermi-Hubbard model is equivalent to an anisotropic spin-1/2 Heisenberg model [8]. For the case of infinitely repulsive limit ($U/t_{s,p} \rightarrow +\infty$), the ground states (lowest energy states) have only one atom for each site, and their charge degrees of freedom are frozen. Under the strongly repulsive condition, $U/t_{s,p} \gg 1$, one can introduce the bosonic operators

$$b_j^+ \leftrightarrow f_{j1}^+ f_{pj}^-, \quad b_j \leftrightarrow f_{pj}^+ f_{j1}^-, \quad n_j = b_j^+ b_j \leftrightarrow \frac{1}{2} + \frac{1}{2} (n_{sj} - n_{pj}), \quad (6)$$

for the atom-hole pairs on site $j$. The operator $b_j^+$ ($b_j$) creates (annihilates) a pair of S-atom (atom in $|S\rangle$) and P-hole (hole in $|P\rangle$) on site $j$. These operators with different lattice indices are commutative. However, to exclude the multiple occupation at each lattice which comes from Pauli blocking, the operators with same lattice indices have a property like Fermi particles. In other words, the interaction between bosons on the same lattice is infinitely repulsive. Using the perturbation theory developed by Takahashi [8] ($b$ and $b^+$ correspond to $\sigma^-$ and $\sigma^+$), up to third order terms of the perturbation parameters (hopping strengths), we obtain the atom-hole pairs obey the hard-core Bose-Hubbard Hamiltonian

$$H_B = -\mu \sum_i n_i + J \sum_{\langle i,j \rangle} b_i^+ b_j + V \sum_{\langle i,j \rangle} n_i n_j. \quad (7)$$

Denoting $t_p = \alpha t_s = \alpha t$, we obtain the hopping strength $J = 4t_p t_s / U = 4\alpha^2 t^2 / U$, the nearest neighbor interaction strength $V = 2(t_s^2 + t_p^2) / U = 2(1 + \alpha^2) t^2 / U$ and the chemical potential $\mu = \Delta \epsilon + ZV / 2 = \Delta \epsilon + Z(1 + \alpha^2) / 2$. For the cubic lattices, the total number of the nearest neighbors $Z$ equals 2$d$. The above hard-core Bose-Hubbard model can be mapped onto an anisotropic spin-1/2 XXZ Heisenberg model with $J_{xy} = J$, $J_z = V$ and an effective magnetic field $B_z = \Delta \epsilon / \hbar$. The antiferromagnetic-Z order, XY-order and fully magnetized states in XXZ model correspond to the CDW phase, superfluid phase and fully polarized insulator phase of the atom-hole pairs, respectively [8,10]. The superfluidity means the Bose condensation of atom-hole pairs in their momentum spaces.

At zero temperature, the ground states for the atom-hole pairs have three different phases: (i) charge-density-wave phase similar to a solid phase with zero polarization ($\gamma = 0$) corresponds to the half-filled case of the hard-core Bose-Hubbard model ($\langle b^+ b \rangle = 1/2$), (ii) Bose-Einstein condensation phase with non-zero superfluid order parameter ($\langle b \rangle$), and (iii) insulator phase with the largest polarization ($\langle \gamma \rangle = 1$) corresponds to the empty ($\langle b^+ b \rangle = 0$) or the fully-filled ($\langle b^+ b \rangle = 1$) case of the hard-core Bose-Hubbard model. The difference between superfluid and insulator phases indicates that it need a non-fully polarized atomic gases to support the atom-hole BEC. From the equivalence between the
For fixed values of hopping ratio $\alpha$ of arbitrary dimensionality with hopping ratio $t$, transitions occur at a first order phase transition. The points on this separatrix means the coexistence of both phases, they represents the supersolid phase. These conditions also show the CDW - superfluid and insulator - superfluid transitions occur at $|\Delta\epsilon|/U = (Z/2)(t/U)^2(1/\alpha)^2$ and $|\Delta\epsilon|/U = Z(t/U)^2(1/\alpha)^2$, respectively.

In FIG. 2, we show the phase diagram for lattices of arbitrary dimensionality with hopping ratio $\alpha = 2$. For fixed values of hopping ratio $\alpha$, energy difference $\Delta\epsilon$ and on-site repulsive interaction strength $U$, increasing (decreasing) the hopping strength $t$ will induce an insulator-superfluid (solid-superfluid) transition. This means that Bose condensation of the atom-hole pairs exists for medium hopping strengths. For larger (smaller) hopping strength, the ground states fall into the phase of CDW (fully polarized insulator). In the case of state-independent hopping, $\alpha = 1$, the CDW region becomes a line localized at $\Delta\epsilon = 0$. This is consistent with the results of the antiferromagnetic phase in Refs. [3].

At finite temperatures, due to the thermal fluctuations, the ordered phases will be destroyed when the temperature is above some critical temperatures. Within the framework of the mean-field theory [12], a continuous phase transition between the CDW and the normal liquid (NL) takes place at the critical temperature

$$T_{CDW}^c = \frac{Z}{k_B} \cdot \frac{2\alpha^2}{U} \cdot (1 - \gamma^2).$$

and a similar phase transition between the superfluid and the normal liquid occurs at

$$T_{SF}^c = \frac{Z}{k_B} \cdot \frac{2\alpha^2}{U} \cdot \frac{\gamma}{\arctanh(\gamma)}.$$  

Here, $k_B$ is the Boltzmann constant. The bicritical polarizations $\gamma = \pm \gamma_{BC}(\alpha)(\gamma_{BC} > 0)$ are given by $T_{SF}^c = T_{CDW}^c$ and $|\gamma| \neq 1$. Below the critical temperatures, there are two coexistence regions of CDW and superfluid, which correspond to the supersolid regions. The boundaries between the superfluid and supersolid and between CDW and supersolid can be obtained by using the Landau expansion [13]. At zero temperature, the critical polarization corresponding to the superfluid-supersolid transition is given as $\gamma_{SFC}^c = [(1 - \alpha)/(1 + \alpha)]$. For the case of state-independent hopping ($\alpha = 1$), the critical polarization $\gamma_{SFC}^c = 0$, it means that the CDW/solid and supersolid regions shrink to a line localized at $\gamma = 0$. This indicates that the atom-hole BEC in non-polarized atoms with state-independent hopping has the highest critical temperature for the superfluid phase.

The finite temperature phase transitions rely on the hopping ratio $\alpha$ and the polarization $\gamma$. For state-independent hopping ($\alpha = 1$), CDW - NL and superfluid - NL transitions occur in non-polarized ($|\gamma| = 0$) and polarized case ($|\gamma| \neq 0$), respectively. For state-dependent hopping ($\alpha \neq 1$), the transition routes become more complex. The CDW - NL, supersolid - CDW - NL, superfluid - supersolid - CDW - NL, and superfluid - NL phase transitions take place when $\gamma = 0$, $0 < |\gamma| \leq \gamma_{SFC}^c$, $\gamma_{SFC}^c < |\gamma| < \gamma_{BC}$, and $|\gamma| \geq \gamma_{BC}$, respectively.

The critical temperatures are determined by both the parameters and the polarization. The parameter dependence is similar to the one of Refs. [3], $T^c \propto t^2/U$. Thus, to increase the critical temperatures, one has to decrease the potential strengths $V_{0,1}^{s,p}$ to increase the hopping strengths. The polarization dependence of the critical temperatures and the finite temperature phase diagram are shown in FIG. 3 for the state-dependent hopping case with $\alpha = 2$.

The previous consideration includes only the terms up to the third order of the perturbation parameter. Including up to the fifth order terms, the Hamiltonian (7) reads as

$$H_B = -\mu \sum_i n_i + J_1 \sum_{\langle i,j \rangle} b_i^\dagger b_j + J_2 \sum_{\langle \langle i,k \rangle \rangle} b_i^\dagger b_k + V_1 \sum_{\langle i,j \rangle} n_i n_j + V_2 \sum_{\langle \langle i,k \rangle \rangle} n_i n_k.$$  

Here, $\langle \langle i,k \rangle \rangle$ represents summing over the next-nearest-neighbors. The parameters are determined by $\mu = \Delta\epsilon + Z(V_1 + V_2)/2$, $J_1 = 4t_{p}^4(1 - 2t_{s}^4+t_{s}^2)/U$, $V_1 = 4t_{p}^4(t_{s}^2+t_{p}^2 - t_{s}^4-t_{s}^2-t_{p}^4)/U^2$, $J_2 = 4t_{p}^4(1+t_{s}^2)/U^2$, and $V_2 = 4t_{p}^4(3t_{s}^4+3t_{p}^4-4t_{s}^2+t_{p}^4)/(2t_{s}^2)^2$. The corresponding critical temperatures
are formulated as

\[ T_{CDW}^C = \frac{Z}{2k_B} \cdot (V_1 - V_2) \cdot (1 - \gamma^2), \tag{11} \]

\[ T_{SF} = \frac{Z}{2k_B} \cdot (J_1 + J_2) \cdot \frac{\gamma}{\text{arctanh}(\gamma)}. \tag{12} \]

Because \( J_2 \ll J_1 \approx J \) and \( V_2 \ll V_1 \approx V \), the above equations indicate that the critical temperatures are only shifted a little bit by the high-order terms.

In summary, we have demonstrated the existence of Bose-Einstein condensation of atom-hole pairs in arbitrarily polarized ultracold fermionic atoms confined in optical lattices with half filling. In the strongly repulsive limit, the atom-hole pairs obey a hard-core Bose-Hubbard Hamiltonian. For a polarized insulator phase, the particle-hole pairs undergo an insulator - superfluid transition when the hopping between nearest neighbors is increased. For a charge-density-wave (CDW) phase, the pairs undergo a CDW - superfluid transition when the hopping is decreased. The mean-field results indicate that the finite temperature phase transition depends upon not only the system parameters but also the polarization.

To realize the considered model, one can prepare an ultracold two-component atomic Fermi gases with arbitrary polarization \[ \text{[2]} \], then load them into an optical lattice with one atom per site. The optical lattices can be produced with a series of standing-wave lasers. Similar to the experimental realization of Tonks gas \[ \text{[3]} \] (however the physical details are only loosely related), the strongly repulsive limit \( U/t_{s,p} \gg 1 \) can be reached by increasing the s-wave scattering length with Feshbach resonances \[ \text{[17]} \] (but still below the unitary limit \[ \text{[16]} \]) and/or by decreasing the hopping strengths \( t_{s,p} \) with controlling the laser intensity. The applied magnetic field will also induce an energy difference between two occupied levels due to the Zeeman effects. To observe the superfluidity of the atom-hole pairs, one can use Bragg scattering approach to detect the elementary excitations spectrum of cold atoms by monitoring the scattered atoms versus the frequency difference between two lasers \[ \text{[17]} \], which form the light grating. In the superfluid phase, it will appear a distinguished peak corresponding to the collective Bogoliubov quasi-particle excitations. In a condensed system of interacting atom-hole pairs within an applied electromagnetic field, the stimulated two-photon emission (second order harmonics emission) process can also give a credible evidence for the atom-hole BEC \[ \text{[18]} \]. In this process, the number of the condensed atom-hole pairs decreases with the emission of the second order harmonics of the applied light.

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