Metastable superfluidity of repulsive fermionic atoms in optical lattices

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In the fermionic Hubbard model, doubly occupied states have an exponentially large lifetime for strong repulsive interactions $U$. We show that this property can be used to prepare a metastable $s$-wave superfluid state for fermionic atoms in optical latices described by a large-$U$ Hubbard model. When an initial band-insulating state is expanded, the doubly occupied sites Bose condense. A mapping to the ferromagnetic Heisenberg model in an external field allows for a reliable solution of the problem. Nearest-neighbor repulsion and pair hopping are important in stabilizing superfluidity.

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Trapped cold atoms open the possibility to realize new quantum states of matter and to control them with an unprecedented precision. An especially exciting perspective is the possibility to study interacting quantum systems out of equilibrium. The high tunability in combination with the slow dynamics of cold atoms allows to investigate time-dependent processes, for example the quench from a superfluid to a Mott insulating state [1].

Thermal equilibrium is usually dominated by low-energy states of the system, while out of equilibrium also high-energy states can become important. In the continuum, high-energy states typically decay rapidly in the presence of interactions: High energy implies that the available phase space for inelastic scattering is large. In contrast, for lattice systems where the kinetic energy of a single particle cannot exceed its bandwidth $D$, a state with high energy, $E \gg D$ (e.g. a doubly occupied site in a strongly repulsive Hubbard model), cannot easily decay. This is a consequence of energy conservation: To dissipate the huge energy $E$, a complex many-particle scattering process is needed, with at least $n \gtrsim E/D$ participating particles. For local two-particle interactions such processes are expected to be exponentially suppressed for large $n$ (see below). This effect has been directly observed in measurements of the lifetime of doubly occupied lattices sites for bosonic $^{87}$Rb atoms in an optical lattice [2]: Starting from a dense cloud of atoms with many doubly occupied sites, the strength of the trapping potential was reduced in one direction, allowing the cloud to expand. Subsequently, many long-lived double occupancies were detected, with a lifetime exceeding their inverse tunneling rate by more than two orders of magnitude.

The large lifetime of doubly occupied lattice sites implies that one can easily create new metastable states of matter. Indeed, numerical simulations by Kollath et al. [3] show that metastable states form in the one-dimensional bosonic Hubbard model for strong repulsion.

An obvious question is whether the doubly occupied sites will Bose condense. For a bosonic Hubbard model, this question was investigated by Petrosyan et al. [4], but the authors found that instead the system will phase-separate: Due to nearest-neighbor attractive interactions, doubly occupied sites will stick together instead of forming a low-density superfluid. In this paper we will prove that for fermions, in contrast, a Bose condensate of spin singlets with $s$-wave symmetry will form. Interestingly, the many-particle wavefunction of the relevant homogeneous metastable superfluid state can be constructed in a controlled way. It has been known for a long time [5, 6] that a hidden SU(2) symmetry of the charge sector (called $SU_C(2)$ in the following) of the Hubbard model can be employed to build wavefunctions with off-diagonal long-range order (states with so-called “$\eta$ pairing”[5]). We shall show that these states can easily be realized just by expanding an atomic cloud in an optical lattice slowly compared to typical collision times but rapidly compared to the exponentially large lifetime of the doubly occupied states.

The condensation of doubly occupied sites can be detected by measuring the momentum distribution of fermion pairs [7]. The repulsively bound doubly occupied sites of the repulsive Hubbard model hop from site to site via virtual low-energy states. Therefore the sign of their effective hopping amplitude is reversed compared to bound pairs in the attractive Hubbard model. This implies that the condensation occurs at momentum $(\pi, \pi, \pi)$ [5, 6] rather than zero, allowing for an unambiguous detection of this state, see Fig. 1.

FIG. 1: Schematic plot of the momentum distribution of fermion pairs [7]. For attractive interactions, the Cooper pairs condense at momentum 0 (and corresponding reciprocal lattice vectors). In contrast, the metastable superconductivity of the repulsive Hubbard model arises at momentum $(\pm \pi, \pm \pi, \pm \pi)$. 
Setup. We consider the fermionic Hubbard model
\[
\mathcal{H} = -J \sum_{\langle ij \rangle, \sigma} c_i^\dagger c_j + U \sum_i n_i^\dagger n_i + V \sum_i r^2_i n_i
\] (1)
on a cubic lattice with a harmonic trapping potential of strength $V_i$. Here $J$ is the tunneling rate between neighboring sites of the optical lattice, $U > 12J = D$ is a strong repulsive interaction, and $n_i = c_i^\dagger c_i$, $n_i = n_i^\dagger + n_i$. The lattice distance $a$ is set to unity. 

As argued above, the total number of doubly occupied sites, $N_d = \sum_i n_i$, has an extremely long lifetime, due to the difficulty in loosing the large energy $U$. This can formally be seen using a well-known unitary transformation [8, 9], $\mathcal{H} \rightarrow \tilde{\mathcal{H}} = e^{iS} \mathcal{H} e^{-iS}$, $N_d \rightarrow \tilde{N}_d = e^{iS} N_d e^{-iS}$, called Schrieffer-Wolff transformation. For a given arbitrary order $n$, one can explicitly construct [9] a unitary operator $e^{iS}$, such that the commutator $[\tilde{N}_d, \tilde{\mathcal{H}}]$ vanishes exactly up to terms of order $1/U^n$. This proves that, in the limit of large $U$, the lifetime $\tau_d$ of doubly occupied sites grows faster than any power of $U$. The underlying physical reason, the energy bottleneck, has been described in the introduction. We therefore expect that, for $V_i = 0$, $\tau_d$ is exponentially large in $U/D$.

We consider an initial situation where the atoms are densely packed, with two atoms per site in the center of the trap (i.e. a band insulator state), and investigate the evolution of the system upon reducing the strength $V_i$ (i.e. curvature) of the trapping potential [10]. The initial system is in thermal equilibrium, and we assume vanishing entropy for simplicity (all of the following arguments remain valid as long as the entropy per particle remains small compared to unity). The radius of the atomic cloud is $r_d \sim N^{1/3}_d$. To avoid a decay of the doubly occupied states by a conversion of interaction energy into potential energy, the slope of the trapping potential at the edge of the cloud has to be small compared to $U$, $2V_i r_d \ll U$. Taking into account the Mott-insulating shell forming around the band-insulating core [11, 12, 14], one obtains from this condition the ratio of the numbers of singly and doubly occupied sites, $N_1/N_d \gg 1/N_d^{1/3}$. Nevertheless, the ratio $N_1/N_d$ can be made sufficiently small, such that singly occupied states can be neglected. Note that this is not required to obtain Bose condensation of double occupancies, but simplifies the theoretical analysis considerably.

Effective model. Neglecting singly occupied sites, the effective Hamiltonian after the Schrieffer-Wolff transformation [8, 9] reads [15] (up to constant contributions)
\[
\tilde{\mathcal{H}} = \frac{J^2}{U} \sum_{\langle ij \rangle} c_i^\dagger c_i^\dagger c_j c_j^\dagger + n_i^\dagger n_i (1 - n_{ji}) (1 - n_{ij}) \\
+ 2V_i \sum_i r^2_i n_i n_{i^\dagger} n_{i^\dagger}.
\] (2)
The first term describes the hopping of doubly occupied sites, the second an effective interaction. In the presence of singly occupied sites, the leading correction to (2) arises [9] from $J \sum_{\langle ij \rangle, \sigma} n_i^\dagger c_i^\sigma c_j n_{ji, -\sigma}$, which describes an exchange of a doubly and a singly occupied site. This term can be neglected when the local density of single occupancies is smaller than $J/U$. While this is not the case at the border of the atomic cloud in its initial configuration, it turns out to be valid in the scaling limit discussed below, as single occupancies are efficiently diluted when the trapping potential gets weaker.

It is useful to rewrite (2) in two different ways. First, one can identify the doubly occupied states with a boson $d_i^\dagger = c_i^\dagger c_i^\dagger$, such that (up to a constant)
\[
\tilde{\mathcal{H}} = \frac{J^2}{U} \sum_{\langle ij \rangle} d_i^\dagger d_j + \sum_{ij} V_{ij} n_i d_j n_{ij} + 2V_i \sum_i r^2_i n_i d_i
\] (3)with $n_i d_i = d_i^\dagger d_i$. Here $V_{ij} = \infty$ implements a hard-core constraint, and $V_{ij} = -J^2/U$ describes an attraction for nearest neighbors $i$ and $j$. Second, one can map the hard-core bosons to spins [4]. Starting from (2), this can be done by performing a particle-hole transformation for the down-spins only, $c_i^\dagger \rightarrow c_i^\dagger$, $c_i \rightarrow (1 - c_i)^\dagger$. This maps an empty site to a spin down and a doubly occupied site to a spin up. A finite magnetization in the $xy$ plane describes Bose condensation of pairs of fermions, see below. Identifying $S_i = \frac{1}{2} \sum_{\alpha \beta} c_i^\dagger \sigma_{\alpha \beta} c_i$ after this transformation, one obtains a ferromagnetic Heisenberg model in a magnetic field:
\[
\tilde{\mathcal{H}} = \frac{J^2}{U} \sum_{\langle ij \rangle} S_i \cdot S_j + 2V_i \sum_i r^2_i S_i^z.
\] (4)
The SU(2) symmetry of the first term in (4) is a direct consequence of the SU(2) symmetry of the charge sector of the underlying Hubbard model [5, 6]: For $V_i = 0$ and a chemical potential $\mu = U/2$, $\mathcal{H}$ (1) commutes with all three components of the particle-hole transformed operators $\sum_i S_i$ defined above - in the original variables, these are $(\eta + \eta^\dagger)/2$, $(\eta - \eta^\dagger)/(2i)$, and $\sum_i (n_i - 1)/2$ with $\eta = \sum_i (-1)^i c_i^\dagger c_i$.

For $V_i = 0$, the exact ground state of (4) for fixed particle density $n_{d}$ is a ferromagnetic state,
\[
|\Psi\rangle = e^{-i\omega \sum_i S_i^z} |\uparrow \uparrow \uparrow \ldots\rangle = e^{-i\frac{\omega}{2} \sum_i (-1)^i (c_i^\dagger c_i^\dagger + h.c.)}|0\rangle
\] (5)where $\cos \theta = 1 - 2n_d$ fixes the magnetization $S_z = n_d - \frac{1}{2}$ in $z$ direction. The rotational symmetry around the $z$ axis is spontaneously broken, which implies off-diagonal long-range order, $\langle c_i^\dagger c_{j}^\dagger \rangle = \langle d_i^\dagger \rangle = (\frac{1}{2})^i \sin \theta$, with momentum ($\pi, \pi, \pi$). The superfluid fraction, defined as $|\langle d_i^\dagger \rangle^2 / n_{d}\rangle$, is given exactly by $(1 - n_d)$ [16].

The initial thermally equilibrated state, described above, is not superfluid. A state with a finite expectation value of $(c_i^\dagger c_i^\dagger)$ can, however, easily be generated by reducing the trapping potential $V_i$ adiabatically, i.e., much
slower than the typical time scales of order $U/J^2$ arising from the dynamics of the effective Hamiltonian (2). If the whole experiment is furthermore performed on a time scale short compared to the (exponentially large) life time $\tau_0$ of doubly occupied sites, the system remains in the ground state of the effective Hamiltonian (2) [or, equivalently, (4)] with the number of doubly occupied sites (the total magnetization) kept fixed. To calculate how a finite superfluid fraction arises when $V_t$ is lowered for fixed $N_d$, we employ a mean-field approximation. We approximate the ground-state wavefunction of (4) by $|\Psi\rangle = \Pi_i |\tilde{n}_i\rangle$, where $|\tilde{n}_i\rangle$ describes a spin $i$ polarized in the $+\hat{n}_i$ direction. Here $\tilde{n}_i = \hat{n}(\mathbf{r}_i)$ is (in the limit of large $N$ and small $V_t$) a unit vector smoothly varying as a function of $\mathbf{r}$, which minimizes

$$E = \int d^3r \left[ \frac{J^2}{4U} \left( \nabla \cdot \hat{n}(\mathbf{r}) \right)^2 + V_t \mathbf{r} \cdot \hat{n}(\mathbf{r}) + 1 \right]$$

with the constraint $\int d^3r [\hat{n}(\mathbf{r}) + 1] = 2N_d$. The employed continuum limit becomes formally exact for a large number of atoms (typical optical-lattice experiments use $10^4$ to $10^5$ atoms). In this “scaling” limit it is convenient to measure distances in units of $N_d^{1/3}$, and all physical properties only depend on the dimensionless quantity $\alpha_t = V_t N_d^{4/3} U/J^2$. The initial state then corresponds to $\alpha_t = \infty$.

Results. When the confining potential $V_t$ gets weaker, the cloud of atom pairs expands (Fig. 2a), and simultaneously a condensate of fermionic pairs first emerges at the boundary of the band-insulating state, i.e. at the domain wall separating the spin-up and spin-down phases (Fig. 3a). When $\alpha_t$ becomes of order 1 and smaller, the maximum of $|\langle c_i^\dagger c_j^\dagger \rangle|$ moves to the center of the trap, and for $\alpha_t \rightarrow 0$ the condensate fraction shown in Fig. 3b approaches unity. The minimization of (6) then becomes equivalent to solving the Schrödinger equation of non-interacting bosons in a trap using $\hat{n} \approx |\Psi(\mathbf{r}), 0, -1 + \langle \Psi(\mathbf{r})^2/2)\rangle$.

Is the system a true superfluid? A superfluid is very different from a ferromagnet, as the excitation spectrum of the former is linear in momentum while it is quadratic in the latter. As the bosonic Hamiltonian (2) is equivalent to a ferromagnetic model, we conclude that, for $V_t = 0$, the doubly occupied states do not form a superfluid with a finite phase stiffness, but only a Bose-Einstein condensate as for non-interacting bosons: At low energy and density, the scattering length of the bosons vanishes, as the hard-core repulsion is exactly balanced by the short-range attraction. Furthermore, the SU(2) symmetry of the Hubbard model implies that the energy difference per volume of a phase-separated state (where doubly occupied sites stick together, i.e. where $\mathbf{S}$ points only up or down) and a superfluid state vanishes in the thermodynamic limit of the uniform system.

SU(2) symmetry breaking will therefore either stabilize the superfluid state or lead to phase separation. Let us list possible corrections to the Hubbard model (1) which break the SU(2) charge symmetry (at $V_t = 0$), but preserve the SU(2) spin symmetry. As the chemical potential is fixed by the particle number, the most
important contributions are two-site terms. The possible two-site terms are longer-range tunneling, assisted tunneling, pair tunneling, density-density and spin-spin interactions. For an optical lattice, where the lattice potential in $x$, $y$, and $z$ directions is independent, $V(x) = \sum_i V_i(x_i)$, the leading longer-range tunneling term is to the second-neighbor site in $x$, $y$ and $z$ direction. Its strength can be estimated as $J' \sim J^2/\Delta$ where $\Delta$ measures the gap to the next Bloch band of the lattice. Assisted next-neighbor tunneling of the form $-J\hat{c}_i^{\uparrow}\hat{c}_{i+1}^{\downarrow}(n_i-\alpha+n_i+\alpha-1)$ arises from the interaction correction to the local Wannier wavefunction of a fermion and is hence given by $\hat{J} \sim JU/\Delta$. Finally, both the next-neighbor density-density interaction, $U'(n_i-1)(n_j-1)$, and a next-neighbor pair-hopping term $J_p\hat{c}_i^{\uparrow}\hat{c}_i^{\downarrow}\hat{c}_j^{\uparrow}\hat{c}_j^{\downarrow}$ are given by matrix elements of Wannier states on adjacent sites, $U' \approx J_p/4 \sim U(J/\Delta)^2$. A next-neighbor spin-spin interaction is of similar size, but unimportant for the dynamics of doubly occupied and empty sites. One may also consider three-site terms, but those are easily seen to be subleading.

After the Schrieffer-Wolff transformation, the leading correction to the dynamics of double occupancies for $J < U \ll \Delta$ arises from the $U'$ repulsion term and the pair hopping $J_p$, as the tunneling terms only enter in second order via an intermediate singly occupied state. In fact, the contributions of $\hat{J}$ cancel, and the effect of $J'$ is $J'U/4 \sim J^4/(\Delta^2U)$, such that the effects of $U'$ and $J_p$ are larger by a factor of $(U/J)^2 \gg 1$. Hence, in the bosonic language we are left with

$$\Delta \mathcal{H} = \sum_{(ij)} 4U'(n_{d,i} - \frac{1}{2})(n_{d,j} - \frac{1}{2}) + J_p d_i^{\dagger}d_j$$

and both terms stabilize superfluidity. Translating into spins and using the same variational Ansatz as above, one obtains the leading correction to (6) in $d = 3$: $\Delta E = (6U' + 3J_p/2)\int d^3r \hat{n}_s^2$ where we used $\hat{n}_s^2 = 1$. It is convenient to parameterize the strength of the additional interactions by the dimensionless parameter

$$\gamma = (6U' + 3J_p/2)UN_d^{2/3}/J^2.$$  

For a typical experimental setup $\gamma \sim (U/\Delta)^2 N_d^{2/3}$ will be quite large, $10 \lesssim \gamma \lesssim 1000$. As shown in Figs. 2b and 3b, a large $\gamma$ leads to the expected expansion of the cloud and therefore to an enhancement of the superfluid fraction.

From our variational wavefunction, one can calculate the momentum distribution of the fermion pairs, $\langle d_k^\dagger d_k \rangle$. While the non-condensed fraction gives only a smooth background signal, the condensate gives rise to sharp peaks centered at $(\pm \pi, \pm \pi, \pm \pi)$, see Fig. 1 and Fig. 3c.

**Conclusion.** We have shown that, within the strongly repulsive Hubbard model, one can realize a metastable $s$-wave superfluid by expanding a band-insulating ground state. One experimental problem may be the preparation of the initial state, as in present optical-lattice experiments [13, 14] the entropy is not small, implying a sizeable fraction of singly occupied sites [14] even for large $V_t$. Fortunately, the condition for the onset of Bose condensation is not very strict. For non-interacting bosons, the entropy per particle has to be smaller than $3.6kb_B$.

The corresponding entropy per fermion of $1.8k_B$ can be reached by cooling non-interacting fermions down to $0.22 T_F$; considerably lower temperatures are nowadays obtained routinely [14]. It is, however, presently not clear how this entropy is distributed between singly and doubly occupied sites. Furthermore, it may not be simple to keep quasi-adiabatic conditions when the cloud is expanded [13, 14], as extrinsic heating processes limit the total time in which experiments are performed. While a quantitative estimate of these corrections is difficult, we are optimistic that, with present-day technology and suitably chosen experimental conditions, an exotic finite-momentum $s$-wave condensate can be realized and detected for strongly repulsive fermions in optical lattices.

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