Dynamical creation of bosonic Cooper-like pairs

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We propose a scheme to create a metastable state of paired bosonic atoms in an optical lattice. The most salient features of this state are that the wavefunction of each pair is a Bell state and that the pair size spans half the lattice, similar to fermionic Cooper pairs. This mesoscopic state can be created with a dynamical process that involves crossing a quantum phase transition and which is supported by the symmetries of the physical system. We characterize the final state by means of a measurable two-particle correlator that detects both the presence of the pairs and their size.

Pairing is a central concept in many-body physics. It consists on the existence of quantum or classical correlations between pairs of components of a many-body system. The most relevant example of pairing is BCS superconductivity. In a superconductor, an attractive interaction causes electrons to organize into Cooper pairs, bosonic quantum objects where electrons are perfectly anticorrelated in momentum and in spin. In the language of second quantization this is described by the BCS variational wavefunction

$$|\psi_{\text{BCS}}\rangle = \prod_k \left( u_k + v_k A_k \right) |0\rangle,$$  \hfill (1)

where $A_k \equiv c_{k\uparrow}^\dagger c_{k\downarrow}^\dagger$ is an operator that creates one such Cooper pair. Remarkably, the fact that pairing occurs in momentum space means that the constituents of the pairs are delocalized and share some long-range correlation.

Nowadays, pairing is also a key research topic in the field of ultracold atoms. While atomic interactions are short range, they can be enhanced using Feschbach resonances. These resonances allow both to create Cooper pairs of fermionic atoms \cite{1,2,3} and to observe the crossover from these large, delocalized objects to a condensate of bound molecular states. Realizing similar experiments with bosons is difficult, because attractive interactions can induce collapse. In the paper by Paredes \cite{4} it is suggested to load an optical lattice with hard-core bosonic atoms in two internal states that attract each other so as to induce BCS-like pairing. A different approach, followed in Ref. \cite{5}, is to load an optical lattice with pairs of atoms in the regime of strong repulsive interactions. Such metastable on-site pairs are robust and survive about 700 ms in the lattice.

In this Letter we propose a method to create long-range paired states of bosonic atoms using entangled states as a resource. The method uses an optical lattice of arbitrary geometry which is loaded with entangled bosons in an insulator state. We will consider both on-site pairs

$$|\psi\rangle \sim \prod_{i=1}^L A_{ij}^L |0\rangle, \quad A_{ij} = \left\{ \begin{array}{ll} c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger \pm c_{i\downarrow} c_{j\uparrow} & \text{if } i < j, \\ c_{i\uparrow} c_{j\downarrow} \pm c_{i\downarrow}^\dagger c_{j\uparrow}^\dagger & \text{if } i = j, \\ c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger c_{i\downarrow} c_{j\uparrow} & \text{if } i > j. \end{array} \right. \hfill (2)$$

such as the ones demonstrated in Ref. \cite{6} and a larger family of singlet and triplet states

$$|\psi\rangle \sim \prod_{i=1}^{L/2} A_{j-i,2i}^L |0\rangle, \quad A_{ij} = \left\{ \begin{array}{ll} c_{i\uparrow} c_{j\downarrow} \pm c_{i\downarrow} c_{j\uparrow} & \text{if } i < j, \\ c_{i\uparrow} c_{j\downarrow} \pm c_{i\downarrow} c_{j\uparrow} & \text{if } i = j, \\ c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger c_{i\downarrow} c_{j\uparrow} & \text{if } i > j. \end{array} \right. \hfill (3)$$

some of which have been created using optical superlattices \cite{7,8}. We propose to dynamically increase the mobility of the atoms, entering the superfluid regime. During this process, the pairs will grow in size until they form a stable gas of long-range Cooper-like pairs that span about half the lattice size. Contrary to works on the creation of squeezed states \cite{9}, the evolution considered here is not adiabatic and the survival of entanglement is ensured by a symmetry of the interactions.

This paper is organized as follows. First, we present the Hamiltonian for bosonic atoms which are trapped in a deep optical lattice, have two degenerate internal states and spin independent interactions. Next, we prove that by lowering the optical lattice and moving into the superfluid regime, the Mott-Bell entangled states \cite{10,11,12,13} evolve into a superfluid of pairs. We then introduce two correlators that detect the singlet and triplet pairs and their approximate size. These correlators are used to interpret quasi-exact numerical simulations of the evolution of two paired states as they enter the superfluid regime. Finally, we suggest two procedures to measure these correlators and elaborate on other experimental considerations.

We will study an optical lattice that contains bosonic atoms in two different hyperfine states ($\sigma = \uparrow, \downarrow$). In the limit of strong confinement, the dynamics of the atoms is described by a Bose-Hubbard model

$$H = - \sum_{(i,j),\sigma} J_\sigma c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i,\sigma\sigma'} \frac{1}{2} U_{\sigma\sigma'} c_{i\sigma}^\dagger c_{i\sigma'}^\dagger c_{i\sigma'} c_{i\sigma}, \hfill (4)$$

Atoms move on a $d$-dimensional lattice ($d = 1, 2, 3$) jumping between neighboring sites with tunneling amplitude $J_\sigma$, and interacting on-site with strength $U_{\sigma\sigma'}$. The Bose-Hubbard model has two limiting regimes. If the interactions are weak, $U \ll J$, atoms can move freely through the lattice and form a superfluid. If interactions are
strong and repulsive, \( U \gg J \), the ground state is a Mott insulator with particles pinned to different lattice sites.

As mentioned in the introduction, we want to design a protocol that begins with a localized entangled state \( |2 \rangle \) and \( |3 \rangle \), and, by increasing the mobility of atoms, enlarge these pairs until the final state describes a gas of generalized Cooper pairs of bosons. In our proposal we restrict ourselves to symmetric interaction and hopping amplitudes

\[
U \equiv U_{11} = U_{1} = U_{11} \geq 0; \quad J \equiv J_{1} = J_{1} \geq 0. \tag{5}
\]

This symmetry makes the system robust so that, even though bosons do not stay in their ground state, they remain a coherent aggregate of pairs, unaffected by collisional dephasing. We will formulate this more precisely.

Let us take an initial state of the form given by either Eq. (2) or (3). If we evolve this state under the Hamiltonian \( \hat{H} \), with time-dependent but symmetric interaction \( U_{\sigma} = U(t) \) and hopping \( J_{\sigma} = J(t) \), the resulting state will have a paired structure at all times

\[
|\psi(t)\rangle = \sum_{k} c(t,k) A_{k1,k2}^{\dagger} \ldots A_{k_{2L-1},k_{2L}}^{\dagger} |0\rangle,
\]

where \( c(t,k) \) are complex coefficients to be determined.

The proof of this result begins with the introduction of a set of operators \( C_{ij} \) which form a simple Lie algebra \( [C_{ij},C_{kl}] = C_{ik}\delta_{jl} - C_{jl}\delta_{ik} \). The evolution preserves the commutation relations and maps the group onto itself. This is evident if we rewrite the Hamiltonian

\[
H = -J \sum_{(i,j)} C_{ij} + \frac{U}{2} \sum_{i}(C_{ii})^{2}. \tag{7}
\]

The evolution operator satisfies a Schrödinger equation \( \hat{H} \frac{d}{dt} V(t) = H(t)V(t) \), with initial condition \( V(0) = \mathbb{I} \). Since the Hamiltonian only contains \( C_{ij} \) operators we conclude that \( V(t) \) is an analytic function of these generators. Let us now focus on the evolution of state \( |3\rangle \), given by \( |\psi(t)\rangle = V(t) \prod_{i=1}^{L/2} A_{2i-1,2i}^{\dagger}|0\rangle \). We will use the commutation relations between the generators of the evolution and the pair operators \( [A_{ij},C_{kl}] = \delta_{ik}A_{jl} + \delta_{jk}A_{il} \), which are valid for any of the pairs in Eq. (8).

Formally, it is possible to expand the unitary operator \( V(t) \) in terms of the correlators \( C_{ij} \) and commute all these operators to the right of the \( A \)'s, where we use \( C_{ij}|0\rangle = 0 \). After doing this one is left with Eq. (8).

A similar proof applies for the on-site pairs \( |2\rangle \) and for any initial state which already has a paired structure \( |0\rangle \).

The previous result includes a very simple case, which is the abrupt jump into the non-interacting regime, \( U = 0 \). This problem is integrable and for the initial conditions \( |2\rangle \) and \( |3\rangle \) the evolved state can be written as

\[
|\psi(t)\rangle = \frac{N}{n=1} \sum_{i,j} w(i-j,n-j,n,t) A_{ij}^{\dagger}|0\rangle. \tag{8}
\]

The wavepackets \( w(i,j,t) \) form an orthogonal set of states, initially localized \( w(i,j,0) \propto \delta_{ij} \) or \( w(i,j,0) \propto \delta_{ij+1} \) and for large times close to a Bessel function \( J_{\nu} \).

We remark that the pair wavefunctions \( |2\rangle \) and \( |3\rangle \) can include valence bond states, however represent a generalization both in the fact that pairs can overlap or be triplets.

In a general case, computing the many-body pair wavefunction, \( c(t,k) \), is an open problem. Nevertheless we can prove that the final state does not remain in the ground state in the superfluid regime, no matter how slowly one changes the hopping and interaction. For the states in \( |0\rangle \) this is evident from the lack of translational invariance.

Let us thus focus on the state \( |2\rangle \) generated by \( A_{ii} = c_{i1}c_{i1} \), which has an equal number of spin-up and down particles \( N_{11} = N/2 \). The ground state of the same sector in the superfluid regime, \( U = 0 \), is a number squeezed, two-component condensate

\[
|\psi_{NN}\rangle \propto c_{01}^{N/2}c_{0j}^{N/2}|0\rangle, \tag{9}
\]

with \( c_{0\sigma} = \frac{1}{\sqrt{L}} \sum_{i=1}^{L} c_{i\sigma} \). Note that we can also write this ground state as an integral over condensates with atoms polarized along different directions

\[
|\psi_{NN}\rangle \propto \int d\theta e^{-iN\theta/2}(c_{01}^{\dagger} + e^{i\theta}c_{01}^{\dagger})^{N}|0\rangle, \tag{10}
\]

When this state is evolved backwards in time, into the \( J = 0 \) regime, each condensate transforms into an insulator with different polarization yielding

\[
|\psi_{NN}\rangle \xrightarrow{\text{MI}} \sum_{n} \prod_{k} (c_{k1}^{\dagger})^{n_{k}} (c_{k1}^{\dagger})^{2-n_{k}}|0\rangle. \tag{11}
\]

Since this state is not generated by the \( A_{ii} = c_{i1}c_{i1} \) operators, we conclude that this particular state \( |2\rangle \), when evolved into the superfluid, leaves the ground state. Furthermore, since different pairs in Eq. (2) are related by global rotations, this statement applies to all of them.

For the rest of this Letter we focus on two important states: the triplet pairs generated on the same site \( |6\rangle \) and the singlet pairs generated on neighboring sites \( |4\rangle \), respectively. Our goal is to study the evolution of these states as the mobility of the atoms is increased, suggesting experimental methods to detect and characterize the pair structure. The main tools in our analysis are the following two-particle connected correlators

\[
G_{ij}^{T} := \langle c_{i1}^{\dagger}c_{j1}^{\dagger}c_{i1}c_{j1} \rangle - \langle c_{i1}^{\dagger}c_{i1} \rangle \langle c_{j1}^{\dagger}c_{j1} \rangle, \quad G_{ij}^{S} := \langle c_{i1}^{\dagger}c_{j1}^{\dagger}c_{j1}c_{i1} \rangle - \langle c_{i1}^{\dagger}c_{i1} \rangle \langle c_{j1}^{\dagger}c_{j1} \rangle, \tag{14}
\]}
combined in two different averages

\[ G_{\Delta \geq 0} = \frac{1}{L - \Delta} \sum_{i=1}^{L - \Delta} G_{i, i+\Delta}, \quad \tilde{G} = \sum_{\Delta=0}^{L-1} G_{\Delta} \]  

(15)

and what we call the pair size

\[ R = \frac{\sum_{\Delta} |\Delta| \times |G_{\Delta}|}{\sum_{\Delta} |G_{\Delta}|} . \]  

(16)

A variant of the correlator \( G^T \) has been used as a pairing witness of fermions \[11\]. We expect these correlators to give information about the pair size and distribution also in the superfluid regime. This can be justified rigorously in the case of an abrupt jump into the superfluid, where the pair wavepackets remain orthogonal and where \( G_{\Delta} \) and \( R \) characterize the spread of the wavefunctions \( w(i,j,t) \). First, note that the single-particle expectation values such as \( \langle c_i^\dagger \psi \rangle \) are exactly zero since \( N_i^T \) and \( N_i \) are even for the triplet state \( \psi_T \) and balanced for the singlet state \( \psi_S \). Second, the two-particle correlators only have nonzero contributions where the destruction and creation operators cancelled and subsequently created the same pair. Combining Eqs. (14) and (8) gives

\[ G^T_{ij} = \sum_n |w(i - n, j - n, t)|^2 \delta_{ij}, \quad G^T_{0} = \delta_{\Delta 0}, \quad G^T = \delta_{\Delta 1}, \quad R^T = 0 , \]  

(17)

\[ G^S_{ij} = - \sum_n |w(j - n, i - n, t)|^2 , \]  

(18)

where we have used the symmetry of the wavefunction, \( w(i,j,t) = w(j,i,t) \). Particularized to the initial states, the triplet \( \psi_T \) gives \( G^T_{ij} = \delta_{ij}, \ G^T_{0} = \delta_{\Delta 0}, \ G^T = \delta_{\Delta 1}, \ G^T = 1 \), and \( R^T = 0 \), as expected from on-site pairs. The singlet pairs described by \( \psi_S \), on the other hand, yield \( G^S_{ij} = -\frac{1}{2} (\delta_{ij+1} + \delta_{ij-1}) \), \( G^S_{1} = -\frac{1}{2} \delta_{\Delta 1}, \ G^S_{S} = -\frac{1}{2} \), and initially span two sites \( R^S = 1 \).

For a realistic study of the evolved paired states we have simulated the evolution of \( \psi_T \) and \( \psi_S \) under the Bose-Hubbard model as the hopping increases nonadiabatically in time

\[ J(t) = v \times (tU/h) \times U, \]  

(18)

with ramp speeds \( v = 0.5, 1 \) and \( 2 \) in adimensional units. The simulations were performed using Matrix Product States (MPS) on one-dimensional lattices with up to 20 sites and open boundary conditions \[12, 13\]. Given the small size of these lattices, we expect these simulations to appropriately describe even the superfluid regime, where the size of the energy gaps and the high occupation number per site make the MPS simulation more difficult.

For each of these simulations we have computed all correlators and pair sizes, values which are plotted in Fig. 4. Let us begin with the triplet pairs: initially the only relevant contribution is the short-range pair correlation \( G^T_{0} \); then the pair size increases monotonously from \( R = 0 \) up to \( R \sim L/2 \), where it saturates. At this point, the pairs have become as large as the lattice permits, given that we have uniform density and open boundary conditions. The singlets have a slightly different dynamics. The antisymmetry of the spin wavefunction prevents two bosons of one pair to share the same site and thus \( R = 1 \) initially. However, this antisymmetry seems also to affect the overlap between pairs, as it is evidenced both in the slower growth \( \tilde{R}(t) \) and in the smallness of \( G^S_{0} \).

Concerning the speed of the process, we have simulated ramps over a timescale which is comparable or even shorter than the typical interaction time, \( 1/U \), so that the process is definitely not adiabatic. Nevertheless, the pairs seem to have enough time to spread over these small lattices. Note also that the spreading of atoms begins right after the value \( J/U \simeq 1/3.84 \) where the one-dimensional Insulator-Superfluid phase transition takes place \[14\].

The system of delocalized Cooper-like pairs can also be regarded as a mean of distributing entanglement in the optical lattice. Following this line of thought we have used the von Neumann entropy to measure the entanglement between two halves of the optical lattice. Apart from a logarithmic contribution induced by the delocal-
ization of particles, which is also present in a single-component condensate, there is an additional contribution caused by the spreading of pairs across the lattice. However, this contribution does not reach a magnitude $O(N/2)$ which corresponds to perfectly splitting $N$ pairs between both lattice halves. We conjecture this is due to the pairs being composed of distinguishable particles.

The pairing correlators $G^{T,S}$ can be decomposed into density-density correlations and measured via the noise interferometry technique developed in Ref. [16] and applied in Ref. [10]. To prove this, let us introduce the Schwinger representation of angular momenta

$$S_x(i) := \frac{1}{\sqrt{2}}(c_{i\uparrow}^† c_{i\downarrow} + c_{i\downarrow}^† c_{i\uparrow})$$

$$S_y(i) := \frac{1}{\sqrt{2}}(c_{i\uparrow}^† c_{i\downarrow} - c_{i\downarrow}^† c_{i\uparrow})$$

$$S_z(i) := \frac{1}{2}(c_{i\uparrow}^† c_{i\downarrow} - c_{i\downarrow}^† c_{i\uparrow}) = \frac{1}{2}(n_{i\uparrow} - n_{i\downarrow}).$$

We will focus on the real part of the correlation matrices, defined as $\tilde{G}_{ij} = 2\text{Re}(G_{ij})$. For the family of states considered here this matrix is the same as the original one [See Eq. (17)] and it is related to simple spin correlations

$$\tilde{G}^{T,S}_{ij} = \frac{1}{2} (S_x(i) S_x(j)) \mp \frac{1}{2} (S_y(i) S_y(j)), \quad (20)$$

$$- \frac{1}{2} (S_x(i) S_y(j)) \pm \frac{1}{2} (S_y(i) S_y(j)).$$

We now introduce two global rotations in the hyperfine space of the atoms $U_{x,y} = \exp [\pm i \frac{\pi}{2} \sum_k S_y c(k)]$. The operators $U_x$ and $U_y$ take the $S_x$ and $S_y$ operators into the $S_z$, respectively. These rotations can be implemented experimentally without individual addressing. Using these unitaries we can relate the previous spin correlations to simple density operators. For instance

$$\langle S_x(i) S_x(j) \rangle = \frac{1}{4} \langle U_x^† (n_{i\uparrow} - n_{i\downarrow})(n_{j\uparrow} - n_{j\downarrow}) U_x \rangle,$$  

shows that the $S_x S_y$ arises from all possible density correlations after applying a $\pi/2$ pulse on the atoms.

Another possibility is to apply the ideas put forward in Ref. [10]. These methods rely on the interaction between coherent light and the trapped atoms to map quantum fluctuations of the atomic spin onto the light that crosses the lattice. Using this technique it should be possible to measure both the single-particle and the two-particle expectation values that constitute $G^{T,S}$.

Experimental imperfections are expected not to affect the nature of the final state. The influence of stray magnetic and electric fields can be cancelled by working with the singlet pairs, which are insensitive to global rotations of the internal states and have large coherence times. More important could be the influence of any asymmetry in the interaction constants. However, assuming this asymmetry to be of the order of 1%, the effect can only be noticeable after a time $t = 100h/U$, which is longer than the evolution times suggested here.

Summing up, in this Letter we have proposed a method to create a generalization of long-range Cooper pairs using bosonic atoms in an optical lattice. We suggest to prepare a Mott insulator of Bell pairs and dynamically melt this state into the superfluid regime. A spin independent interaction guarantees that pairing is preserved and that the system becomes a gas of long-range correlated pairs, which spread over approximately half the lattice size. This mechanism works even if the process is not adiabatic or the initial state does not have translational invariance. Most important, our proposal represents a natural extension of current experiments with optical superlattices [7, 8].

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