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 wave function 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.

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Pairing is a central concept in many-body physics. It is based 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 which attractive interactions cause electrons to perfectly anticorrelate in momentum and spin, forming Cooper pairs. In second quantization, this is described by the BCS variational wave function

$$|\psi_{\mathrm{BCS}}\rangle = \prod_k (u_k + v_k A_k^\dagger)|0\rangle, \tag{1}$$

where $A_k^\dagger \equiv c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger$ 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.

Today, pairing and the creation of strongly correlated states of atoms is a key research topic. With the enhancement of atomic interactions due to Feshbach resonances, it has been possible both to produce Cooper pairs of fermionic atoms [1–3] 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 may induce collapse. Two work-arounds are based on optical lattices, either loaded with hard-core bosonic atoms [4] or, as in recent experiments [5], with metastable localized pairs supported by strong repulsive interactions.

In this Letter we propose a method to dynamically create long-range pairs of bosons which, instead of attractive interactions, uses entangled states as a resource. The method starts by loading an optical lattice of arbitrary geometry with entangled bosons that form an insulator. One possible family of initial states

$$|\psi\rangle \sim \prod_{i=1}^{L} A_{ii}^\dagger |0\rangle, \qquad A_{ij} = \begin{cases} c_{i\uparrow}c_{j\uparrow} \pm c_{i\downarrow}c_{j\downarrow} \\ c_{i\uparrow}c_{j\downarrow} + c_{j\uparrow}c_{i\downarrow} \end{cases}, \tag{2}$$

are on-site pairs created by loading a lattice with two atoms per site and tuning their interactions, as demonstrated in Ref. [6]. A larger family includes states created by exchange interactions between atoms hosted in the unit cells of an optical superlattice [7,8]

$$|\psi\rangle \sim \prod_{i=1}^{L/2} A_{2i-1,2i}^\dagger |0\rangle, \qquad A_{ij} = \begin{cases} c_{i\uparrow}c_{j\uparrow} \pm c_{i\downarrow}c_{j\downarrow} \\ c_{i\uparrow}c_{j\downarrow} \pm c_{j\uparrow}c_{i\downarrow} \end{cases}. \tag{3}$$

We propose to dynamically increase the mobility of the atoms, entering the superfluid regime. During this process, pairs will enlarge 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 [9], the evolution considered here is not adiabatic and the survival of entanglement is ensured by a symmetry of the interactions.

This Letter 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 (2) and (3) 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 quasiexact 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 [10]

$$H = -\sum_{\langle i,j\rangle,\sigma} J_\sigma c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i\sigma\sigma'} \frac{1}{2} U_{\sigma\sigma'} c_{i\sigma}^\dagger c_{i\sigma'}^\dagger c_{i\sigma'} c_{i\sigma}. \tag{4}$$

Atoms move on a d-dimensional lattice ($d = 1, 2, 3$) jumping between neighboring sites with tunneling amplitude J_σ, 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 on different lattice sites.

As mentioned in the introduction, we want to design a protocol that begins with an insulator of localized entangled states (2) and (3) and, by crossing the quantum phase transition, produces a gas of generalized Cooper pairs of bosons. In our proposal we restrict ourselves to symmetric interactions and hopping amplitudes $U \equiv U_{\uparrow\uparrow} = U_{\downarrow\downarrow} = U_{\uparrow\downarrow} \geq 0$; $J \equiv J_\uparrow = J_\downarrow \geq 0$. 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 (4), with time-dependent but symmetric interaction $U_{\sigma\sigma'} = U(t)$ and hopping $J_\sigma = J(t)$, the resulting state will have a paired structure at all times,

$$|\psi(t)\rangle = \sum_\pi c(t;\pi) A^\dagger_{\pi_1\pi_2}, \ldots, A^\dagger_{\pi_{2L-1}\pi_{2L}}|0\rangle, \qquad (5)$$

where $c(t;\pi)$ are complex coefficients and the sum over π denotes all possible permutations of the indices.

The proof of this result begins with the introduction of a set of operators $C_{ij} := \sum_\sigma c^\dagger_{i\sigma} c_{j\sigma}$ which form a simple Lie algebra $[C_{ij}, C_{kl}] = C_{il}\delta_{jk} - C_{kj}\delta_{il}$. The evolution preserves the commutation relations and maps the group onto itself. This is evident if we rewrite the Hamiltonian

$$H = -J\sum_{\langle i,j\rangle} C_{ij} + \frac{U}{2}\sum_i (C_{ii})^2. \qquad (6)$$

The evolution operator satisfies a Schrödinger equation $i\hbar \frac{d}{dt} V(t) = H(t)V(t)$, 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 focus on the evolution of state (3), given by $|\psi(t)\rangle = V(t)\prod_{i=1}^{L/2} A^\dagger_{2i-1,2i}|0\rangle$. We will use the commutation relations between the generators of the evolution and the pair operators $[A_{ij}, C_{kl}] = \delta_{ik}A_{lj} + \delta_{jk}A_{il}$, which are valid for any of the pairs in Eq. (3). 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 $C_{ij}|0\rangle = 0$ and recover Eq. (5). A similar proof applies to the on-site pairs (2).

A particular case is the abrupt jump into the noninteracting regime $U = 0$. Integrating this problem with initial conditions (2) and (3) the evolved state becomes

$$|\psi(t)\rangle = \prod_{x=1}^{N} \sum_{i,j} w(i-x, j-x, t) A^\dagger_{ij}|0\rangle. \qquad (7)$$

The wave packets 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 approaching a Bessel function for large times [11]. We remark that though the pair wave functions (5) and (7) include valence bond states, they are more general because particles may overlap or form triplets.

In a general case, computing the many-body pair wave function $c(t;\pi)$ is an open problem. Nevertheless we can prove that the final state does not become the ground state of the superfluid regime, no matter how slowly one changes the hopping and interaction. For the states in (3) this is evident from the lack of translational invariance. Let us thus focus on the state (2) generated by $A_{ii} = c_{i\uparrow}c_{i\downarrow}$, which has an equal number of spin-up and down particles $N_{\uparrow,\downarrow} = N/2$. The ground state of the same sector in the superfluid regime $U = 0$ is a number squeezed, two-component condensate [9] $|\psi_{NN}\rangle \propto \tilde{c}^{\dagger N/2}_{0\uparrow}\tilde{c}^{\dagger N/2}_{0\downarrow}|0\rangle$, with $\tilde{c}_{0\sigma} = \frac{1}{\sqrt{L}} \times \sum_{i=1}^{L} c_{i\sigma}$. We can also write this ground state as an integral over condensates with atoms polarized along different directions

$$|\psi_{NN}\rangle \propto \int d\theta e^{-iN\theta/2}(\tilde{c}^\dagger_{0\uparrow} + e^{i\theta}\tilde{c}^\dagger_{0\downarrow})^N|0\rangle. \qquad (8)$$

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

$$|\psi_{NN}\rangle \xrightarrow{MI} \sum_{\vec{n}, \sum n_k = N/2} \prod_k (c^\dagger_{k\uparrow})^{n_k}(c^\dagger_{k\downarrow})^{2-n_k}|0\rangle. \qquad (9)$$

Since this state is not generated by the $A_{ii} = c_{i\uparrow}c_{i\downarrow}$ operators, we conclude that this particular state (2), 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. Indeed, numerical simulations indicate that the evolved versions of (2) and (3) are no longer eigenstates of (4).

For the rest of this Letter we focus on two important states: the triplet pairs generated on the same site [6] and the singlet pairs generated on neighboring sites [7,8],

$$|\psi_T\rangle = \prod_{i=1}^{L} \frac{1}{2}(c^{\dagger 2}_{i\uparrow} + c^{\dagger 2}_{i\downarrow})|0\rangle, \qquad (10)$$

and

$$|\psi_S\rangle = \prod_{i=1}^{L/2} \frac{1}{\sqrt{2}}(c^\dagger_{2i-1\uparrow}c^\dagger_{2i\downarrow} - c^\dagger_{2i-1\downarrow}c^\dagger_{2i\uparrow})|0\rangle, \qquad (11)$$

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

$$\begin{aligned} G^T_{ij} &:= \langle c^\dagger_{i\uparrow}c^\dagger_{j\uparrow}c_{i\downarrow}c_{j\downarrow}\rangle - \langle c^\dagger_{i\uparrow}c_{i\downarrow}\rangle\langle c^\dagger_{j\uparrow}c_{j\downarrow}\rangle, \\ G^S_{ij} &:= \langle c^\dagger_{i\uparrow}c^\dagger_{j\downarrow}c_{j\uparrow}c_{i\downarrow}\rangle - \langle c^\dagger_{i\uparrow}c_{i\downarrow}\rangle\langle c^\dagger_{j\downarrow}c_{j\uparrow}\rangle, \end{aligned} \qquad (12)$$

combined in two different averages

$$G_{\Delta\geq 0} = \frac{1}{L-\Delta}\sum_{i=1}^{L-\Delta} G_{i,i+\Delta}, \qquad \bar{G} = \sum_{\Delta=0}^{L-1} G_\Delta \tag{13}$$

and what we call the pair size

$$R \equiv \frac{\sum_\Delta |\Delta| \times |G_\Delta|}{\sum_\Delta |G_\Delta|}. \tag{14}$$

A variant of the correlator G^T has been used as a pairing witness for fermions [12]. We expect these correlators to give information about the pair size and distribution also in the superfluid regime. This can be justified rigorously for an abrupt jump into the superfluid, in which the pair wave packets remain orthogonal and G_Δ and R characterize the spread of the wave functions $w(i, j, t)$. First, note that the single-particle expectation values such as $\langle c_{i\downarrow}^\dagger c_{i\uparrow}\rangle$ are exactly zero since $N_\uparrow$ and $N_\downarrow$ are even for the triplet state ψ_T and balanced for the singlet state ψ_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. (12) and (7) gives

$$\begin{aligned} G_{ij}^T &= \sum_x |w(i-x, j-x, t)|^2 4, \\ G_{ij}^S &= -\sum_x |w(j-x, i-x, t)|^2, \end{aligned} \tag{15}$$

where we have used the symmetry of the wave function, $w(i, j, t) = w(j, i, t)$. Particularized to the initial states, the triplet ψ_T gives $G_{ij}^T = \delta_{ij}$, $G_\Delta^T = \delta_{\Delta 0}$, $\bar{G}^T = 1$, and $R^T = 0$, as expected from on-site pairs. The singlet pairs described by ψ_S, on the other hand, yield a nonzero G_{ij}^S only if i and j are the indices of the two ends of a singlet pair. Thus $G_\Delta^S = -\frac{1}{2}\delta_{\Delta 1}$, $\bar{G}^S = -\frac{1}{2}$, and $R^S = 1$.

For a realistic study of the evolved paired states we have simulated the evolution of ψ_T and ψ_S under the Bose-Hubbard model as the hopping increases diabatically in time

$$J(t) = v(tU/\hbar)U, \tag{16}$$

with ramp speeds $v = 0.5$, 1, and 2 in dimensionless units. The simulations were performed using matrix product states (MPS) on one-dimensional lattices with up to 20 sites and open boundary conditions [13–15]. After several convergence checks, we chose $D = 30$ for the MPS matrix size and $dt = 5 \times 10^{-4}\hbar/U$ for the time steps. For these small lattices, we expect the simulations to appropriately describe even the superfluid regime, where the small energy gaps and the high occupation number per site make the MPS algorithm more difficult.

In Fig. 1 we plot the instantaneous values of the correlators and pair sizes along the ramp. Let us begin with the triplet pairs: initially the only relevant contribution is the

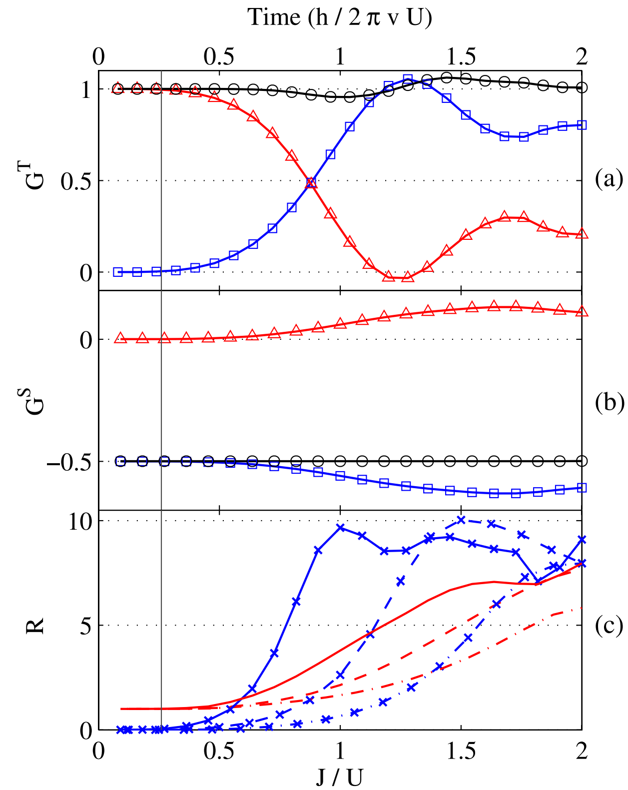

FIG. 1 (color online). We plot the (a) triplet and (b) singlet correlators for the evolution of ψ_T and ψ_S, respectively, at a ramp speed $v = 1$ [see Eq. (16)] and in a lattice of $L = 20$ sites. The circles, triangles, and squares denote $\bar{G}$, G_0, and their difference. (c) Pair size R for the singlet (line) and triplet (cross) states, for a ramp speed $v = 0.5$, 1, and 2 (solid curves, dashed curves, dash-dotted curves). The vertical line $J/U = 1/3.84$ marks the location of the phase transition.

short-range pair correlation G_0^T, then the pair size increases monotonically up to $R \sim L/2$, where it saturates. At this point, the pairs have become as large as the lattice permits, given that the density is uniform. The singlets have a slightly different dynamics. The antisymmetry of the spin wave function prevents two bosons of one pair to share the same site and thus $R = 1$ initially. This antisymmetry seems also to affect the overlap between pairs, as it is evidenced both in the slower growth $R(t)$ and in the smallness of G_0^S. Note that when the ramp is stopped (not shown here), the pair correlations persist but oscillate as the particles bounce off from each other and from the borders of the lattice.

Concerning the speed of the process, we have simulated ramps over a time scale 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 [16].

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. A numerical study of the scaling of this entropy up to $L = 20$ sites, together with analytical estimates using the wave function (7), shows that the entropy is far from the limit $O(N/2)$, which corresponds to perfectly splitting N distinguishable pairs among both lattice halves. We conjecture this is due to the pairs being composed of bosonic particles.

The pairing correlators $G^{T,S}$ can be decomposed into density-density correlations and measured using noise interferometry [17,18]. To prove this, let us introduce the Schwinger representation of angular momenta $S_x(i) = \frac{1}{\sqrt{2}}(c^\dagger_{i\uparrow}c_{i\downarrow} + c^\dagger_{i\downarrow}c_{i\uparrow})$, $S_y(i) = \frac{1}{\sqrt{2}}(c^\dagger_{i\uparrow}c_{i\downarrow} - c^\dagger_{i\downarrow}c_{i\uparrow})$, and $S_z(i) = \frac{1}{2}(c^\dagger_{i\uparrow}c_{i\uparrow} - c^\dagger_{i\downarrow}c_{i\downarrow}) = \frac{1}{2}(n_{i\uparrow} - n_{i\downarrow})$. For the states considered here, the correlation matrix is real (15). We can thus focus on its real part $\tilde{G}_{ij} = 2\,\mathrm{Re}(G_{ij})$, which is related to simple spin correlations

$$\tilde{G}^{T,S}_{ij} = \tfrac{1}{2}\langle S_x(i)S_x(j)\rangle \mp \tfrac{1}{2}\langle S_y(i)S_y(j)\rangle - \tfrac{1}{2}\langle S_x(i)\rangle\langle S_x(j)\rangle \pm \tfrac{1}{2}\langle S_y(i)\rangle\langle S_y(j)\rangle. \tag{17}$$

We introduce two global rotations in the hyperfine space of the atoms $U_{x,y} = \exp[\pm i\frac{\pi}{2}\sum_k S_{y,x}(k)]$, which take the S_x and S_y operators into the S_z, respectively. These rotations can be implemented experimentally without individual addressing and can be used to transform the spin correlators into density operators. For instance,

$$\langle S_x(i)S_x(j)\rangle = \tfrac{1}{4}\langle U^\dagger_x(n_{i\uparrow} - n_{i\downarrow})(n_{j\uparrow} - n_{j\downarrow})U_x\rangle \tag{18}$$

shows that the S_xS_x 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. [19]. 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 obviated 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 $t = 100\hbar/U$, which is longer than the evolution times suggested here.

In summary, in this Letter we have proposed a novel method to dynamically engineer Cooper-pair-like correlations between bosons. Our proposal represents a natural extension of current experiments with optical superlattices [7,8]. It begins with a Mott insulator of bosonic atoms loaded in an optical lattice and forming entangled pairs, that have been created using quantum gates [6–8]. This state is diabatically melted into the superfluid regime so that the system becomes a stable gas of long-range correlated pairs. Unlike other systems, pairing is created dynamically, using entanglement as a resource, and supported by symmetries instead of attractive interactions. The generated states and the numerical and analytical tools developed in this work form a powerful toolbox to study, both experimentally and theoretically, issues like entanglement distribution and decoherence of many-body states. Future work will involve the quest for other resource states and diabatic protocols that lead to stronger correlations or more exotic states [20].

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