Extended two-site Bose–Hubbard model with pair tunneling: spontaneous symmetry breaking,

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Extended two-site Bose–Hubbard model with pair tunneling: spontaneous symmetry breaking, effective ground state and fragmentation

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Abstract

The extended Bose–Hubbard model for a double-well potential with pair tunneling is studied through both exact diagonalization and mean field theory (MFT). When pair tunneling is strong enough, the ground state wavefunction predicted by the MFT is complex and doubly degenerate while the quantum ground state wavefunction is always real and unique. The time reversal symmetry is spontaneously broken when the system transfers from the quantum ground state into one of the mean field ground states upon a small perturbation. As the gap between the lowest two levels decreases exponentially with particle number, the required perturbation inducing the spontaneous symmetry breaking (SSB) is infinitesimal for particle number of typical cold atom systems. The quantum ground state is further analyzed with the Penrose–Onsager criterion, and is found to be a fragmented condensate. The state also develops the pair correlation and has non-vanishing *pair order parameter* instead of the conventional single particle order parameter. When this model is generalized to optical lattice, a pair superfluid can be generated. The mean field ground state can be regarded as effective ground state in this simple model. The detailed computation for this model enables us to offer an in-depth discussion of the relation between SSB and effective ground state, giving a glimpse on how nonlinearity arises in the SSB of a quantum system.

Keywords: extended Bose–Hubbard model, effective ground state, pair tunneling

(Some figures may appear in colour only in the online journal)

1. Introduction

The Bose–Hubbard model for a double-well potential has been extensively studied since the experimental realization of Bose–Einstein condensate. Rich physics has been explored with this simple model, including the Josephson effect [1, 2] and self-trapping phenomenon for the attractive interaction [3, 4]. Furthermore, this model is a prototype of the Bose–Hubbard model in periodic potentials, and can offer clues to phenomenon like superfluid to Mott insulator transition that occurs in the thermodynamic limit [5]. Due to its simplicity, one can carry out detailed and systematic studies of this two-site Bose–Hubbard model and obtain insights into many intriguing phenomena.

Here we study the Bose–Hubbard model for a double-well potential with pair tunneling, and show how the strong pair tunneling can change the underlying physics. (i) When the pair tunneling effect is strong enough, the mean field

ground state becomes doubly degenerate and each breaks the time reversal symmetry. In contrast, the wavefunction of the quantum ground state is always real and unique. Actually, the quantum wave wavefunction has large and equal overlap with both mean field wavefucntions. This is an analog of the NOON state in the phase space [6]. (ii) The model shows a general feature of a class of spontaneous symmetry breaking (SSB): the quantum ground state is unique while the effective (or mean field) ground state is degenerate. The onset of degeneracy in the effective ground state is accompanied by the appearance of quasi-degeneracy in the lowest quantum energy levels, where the energy gap decreases exponentially with particle number. The quantum ground state is unstable against small perturbations which mix up these quasi-degenerate levels. In experiments we always observe the effective ground state instead of the quantum one. Once one symmetry breaking state is chosen, the system needs an infinitely long time to restore the symmetry in the thermodynamic limit. (iii) The quantum ground state of this model is a fragmented condensate, corresponding to the superposition of two coherent simple condensates. It can be characterized by a *pair order parameter* instead of the single particle parameter. The extended Bose–Hubbard model can be generalized to optical lattice; in this case a pair superfluid [7, 8] can be generated by a certain perturbation.

In many condensed matter systems the quantum ground state cannot be observed in experiments. What is observed is the effective ground state whose energy is almost identical to its quantum counterpart while whose wave function has a finite difference from its quantum counterpart [9, 10]. The mean field ground states discussed here are the effective ground states. This simple Hubbard model allows us to offer a detailed comparison between the quantum ground state and the effective ground state, and discuss SSB in the perspective of effective ground state. We observe that there are two types of SSB: (i) the quantum ground state is degenerate; (ii) the quantum ground state is unique while the effective ground state is degenerate. The second type can be further divided into two subgroups according to the origin of the degeneracy. This may offer a fresh perspective into a question asked by Wen on a website, 'what is spontaneous symmetry breaking in QUANTUM systems?' [11].

2. Ground state of the model

The extended Bose–Hubbard model for a double-well potential can be described by the following Hamiltonian [12–14],

$$
\hat{H} = -t\left(\hat{a}^\dagger \hat{b} + \hat{a}\hat{b}^\dagger\right) + U_3(\hat{n}_a + \hat{n}_b - 1)\left(\hat{a}^\dagger \hat{b} + \hat{a}\hat{b}^\dagger\right)
$$
$$
+ \frac{U_0}{2}\left[\hat{n}_a(\hat{n}_a - 1) + \hat{n}_b(\hat{n}_b - 1)\right]
$$
$$
+ (U_1 + U_2)\hat{n}_a\hat{n}_b + \frac{U_2}{2}\left(\hat{a}^\dagger\hat{a}^\dagger\hat{b}\hat{b} + \hat{a}\hat{a}\hat{b}^\dagger\hat{b}^\dagger\right), \tag{1}
$$

with $\hat{a}^\dagger(\hat{a})$ and $\hat{b}^\dagger(\hat{b})$ being the creation (annihilation)

operators in well a (b). t is the usual single particle tunneling, U_0 is the usual onsite interaction, and U_1, U_2, U_3 describe the off-site interaction. Specifically, U_1 and U_2 are the inter-well particle interaction, and U_3 is the density-dependent tunneling. All these terms show up naturally provided that one expands the field operator in terms of the Wannier basis and preserves all the terms. In the standard Bose–Hubbard model, the terms involving U_1, U_2, U_3 are all neglected, as they are small compared with the hopping energy and the onsite interaction. Here the inter-well particle interaction (the last term in equation (1)) serves as an effective pair tunneling, which is the focus of this work. For ultracold dilute gases with short range interaction, the contact interaction captures the essential physics, so we assume $V(\mathbf{r}_1 - \mathbf{r}_2) = \frac{4\pi\hbar^2 a_s}{m}\delta(\mathbf{r}_1 - \mathbf{r}_2)$, a_s being the s-wave scattering length, and thus $U_1 = U_2$.

Below the transition temperature and for large particle number, the quantum model can be approximated by the mean field theory (MFT). By replacing the creation and annihilation operators with complex numbers, one obtains the MFT Hamiltonian,

$$
H = -J\left(a^*b + ab^*\right) + w_1 |a|^2|b|^2 + w_2\left(a^{*2}b^2 + a^2b^{*2}\right), \tag{2}
$$

where $J = t - (N - 1)U_3$, $w_1 = (2U_1 - U_0)N$, $w_2 = NU_1/2$. The ground state of this mean field Hamiltonian has been studied in [15]. It is convenient to introduce a pair of canonically conjugate variables, $\theta = \theta_b - \theta_a$ and $s = |b|^2 - |a|^2$, with $a = |a|\,e^{i\theta_a}$, $b = |b|\,e^{i\theta_b}$. We focus on the repulsive interaction case and tune the ratio between pair tunneling and single particle tunneling, $\lambda = w_2/J$. In the weak pair tunneling regime, $0 < \lambda < \frac{1}{2}$, the ground state is the fixed point $(s, \theta) = (0, 0)$, which has equal population and zero relative phase between the two wells. In the strong pair tunneling regime, $\lambda > \frac{1}{2}$, the ground state becomes two-fold degenerate with $(s, \theta) = \left(0, \pm\arccos\left(\frac{1}{2\lambda}\right)\right)$, which has zero population imbalance but nonzero relative phase between the two wells. The transition between these two scenarios occurs at the critical value $\lambda_c = 1/2$. In the discussion above, we assume that one can artificially tune λ, and postpone the discussion of the experimental realization of such tuning to section 5.

Our interest is in the connection between the quantum and mean field ground states. The quantum ground state can be obtained by diagonalizing the quantum Hamiltonian equation (1). In contrast to the mean field results, the quantum ground state is always real and non-degenerate no matter how strong the pair tunneling is. To elucidate and understand this subtle discrepancy, it is helpful to observe that the mean field ground state is actually the coherent state $(a\hat{a}^\dagger + b\hat{b}^\dagger)^N|0\rangle$ in the second quantized language. This allows us to calculate the inner product $f(s, \theta)$ between the quantum ground state and the classical one. In usual cases without pair tunneling effect or weak pair tunneling regime, the inner product $f(s, \theta)$ is a function with its single peak located at $(s, \theta) = (0, 0)$ and its width related to the quantum fluctuations caused by interaction. In the strong pair tunneling regime, the classical ground state becomes two degenerate fixed points $(0, \pm\Theta(\lambda))$, and
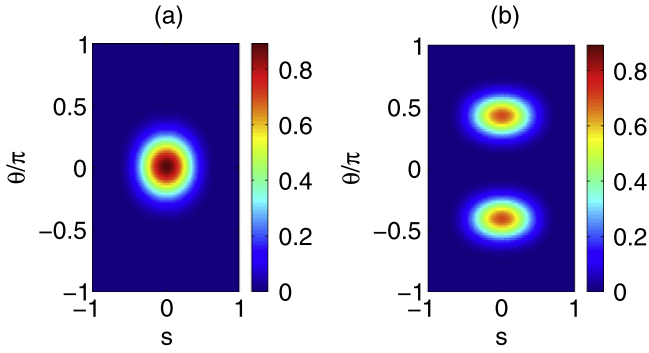
Figure 1. The inner product of the quantum ground state and the mean field ground state $|f(s, \theta)|$. (a) Weak pair tunneling regime: $U_1/U_0 = 0.02$ and $\lambda = 0.2 < \frac{1}{2}$. The mean field ground state is non-degenerate and $|f(s, \theta)|$ has only one peak. (b) Strong pair tunneling regime: $U_1/U_0 = 0.2$ and $\lambda = 2 > \frac{1}{2}$. The mean field ground state is two-fold degenerate and $|f(s, \theta)|$ has two peaks.

consequently $f(s, \theta)$ has two peaks located at those two fixed points. This is illustrated in figure 1, where $|f(s, \theta)|$ is plotted for a specific set of parameters, $N = 40$, $U_0/J = 0.5$, $U_1/U_0 = 0.02$ ($\lambda = 0.2$), and 0.2 ($\lambda = 2$).

Actually this state is the phase space analog of the self-trapping effect in a double-well potential for attractive particle interaction [3, 4, 16, 17]. The self-trapping effect occurs when the attraction between particles is strong enough, and then MFT predicts that all the particles will spontaneously occupy only one well, breaking the symmetry of the double-well potential explicitly. The quantum ground state is known as the NOON state, an equal superposition of particles occupying both wells, which in fact restores the symmetry. Here in our model MFT also gives two degenerate states breaking the symmetry of the potential, and the quantum ground state can be called the NOON state in the phase space.

3. Effective ground state and SSB

Our numerical solution of the quantum model shows when the mean field ground state becomes degenerate, the quantum energy levels exhibit the feature of quasi-degeneracy, where the energy gap between the lowest two states decreases exponentially with particle number (see figure 2). The quasi-degeneracy indicates that the quantum ground state is unstable; very small perturbation will mix up the quasi-degenerate states. For a typical cold atomic system with particle number up to $10^5 \sim 10^6$, an infinitesimal perturbation will drive the system into one of the degenerate *effective ground states*.

The effective ground state is associated with the experimental observability of a ground state. As there is always all kinds of noise in experiments, what is observed experimentally may not be the true ground state of the system, but the effective one. A well-known example is the gas to solid phase transition in free space [9, 10]. Since the center of mass momentum of the particles commutes with the whole
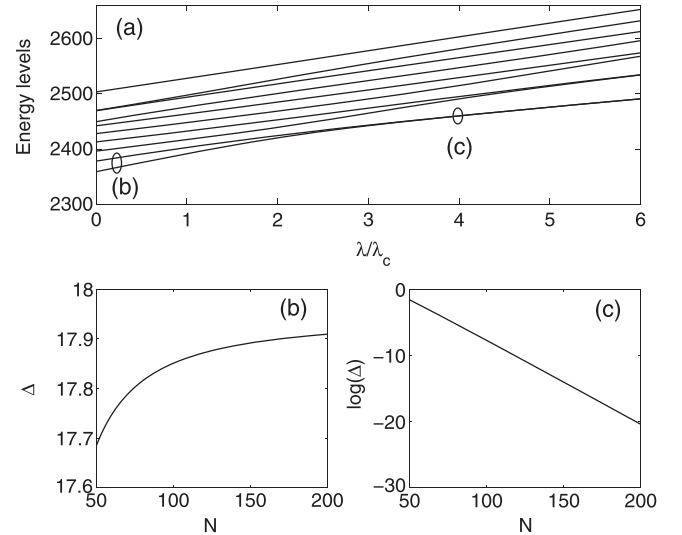

Figure 2. (a) The lowest 10 energy levels, rescaled with respect to J, as a function of pair tunneling strength, rescaled with respect to the critical strength λ_c. The energy spectrum shows quasi-degeneracy for strong pair tunneling. Particle number $N = 50$. (b) The energy gap Δ between the lowest two states as a function of particle number N at weak pair tunneling strength $\lambda/\lambda_c = 0.2$ (marked by an open circle near the left-lower corner in (a)). Δ increases with N before saturation. (c) $\log(\Delta)$ as a function of particle number N at strong pair tunneling strength $\lambda/\lambda_c = 4$ (marked by the other open circle in (a)). Δ decreases exponentially with N when the pair tunneling is strong.

Hamiltonian, the absolute ground state should be the eigenstate of center of mass momentum, namely, particles should be distributed homogeneously in the whole space. However, in the real world we always observe a localized solid. This is because the exact ground state is unstable against infinitesimal perturbation in the thermodynamic limit, and it will spontaneously decay into a symmetry-breaking effective ground state. The quantum time crystal [18] proposed by Wilczek is also such an effective ground state, whose existence needs the breaking of both translational and time reversal symmetries.

Suppose that we prepare one effective ground state. Since it is not the true ground state of the system, it will evolve under the quantum Hamiltonian. This process also determines the lifetime of the effective ground state observed in experiments. For this model, we find that the effective ground state evolves almost periodically with the period T as illustrated in figure 3. As the energy gap Δ between the first excited state and the ground state decreases with particle number N as $\Delta \sim \exp(-N)$, we have $T \sim 2\pi/\Delta \sim \exp(N)$. So for large particle number, the evolution period is remarkably long, then the system will always stay in the effective ground state during the course of experiments.

It should be emphasized that, in the discussion above, we always assume the particle number to be large enough for the conclusion to be valid. For systems of small particle number, e.g., $\lesssim 20$, the ground state observed in experiments may indeed be the quantum state, not the mean-field one. That is to say, there should be a crossover from the quantum
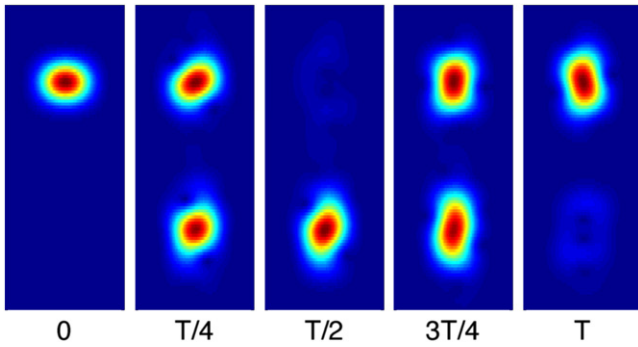
Figure 3. Evolution of one of the two effective ground states under the quantum Hamiltonian in the strong pair tunneling regime. $N = 50$ and $\lambda/\lambda_c = 20$. The color bar, axis ticks and labels are the same as figure 1.
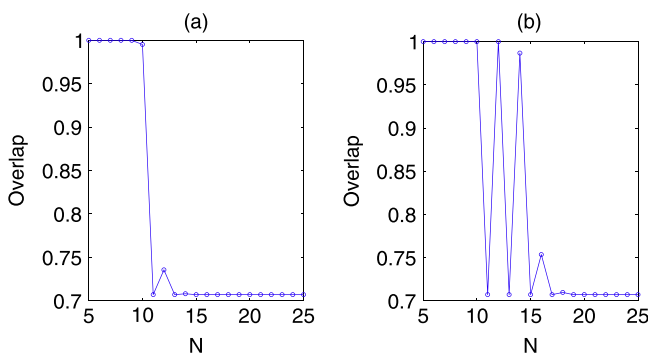

Figure 4. Evolution of the quantumness of the experimentally observed states with particle number in the strong pair tunneling regime for two strengths of perturbations: (a) $\delta/J = 10^{-4}$, (b) $\delta/J = 10^{-7}$. Here we choose $U_0/J = 0.5$, and $U_1/U_0 = 0.4$. The quantumness of a state is defined as its overlap with the exact quantum state without perturbations. When the particle number is very small, the energy gap is large compared to the external perturbation, so the perturbation does not change the state too much. In this case the quantumness is almost 1. When the particle number gets larger, the energy gap becomes smaller compared to perturbation, so the perturbation mixes up the quantum states and the resulted one is classical. For a classical state, its quantumness is not zero but around 0.7 by this definition.

ground state to the effective ground state as the particle number increases. The particle number in the crossover region depends crucially on the form and strength of external perturbations. As a specific example, we simulate the experiment by adding a small perturbation to the single particle tunneling term, that is, changing J to $J + \delta\sigma_y$. δ is many orders of magnitude smaller than J and σ_y is the Pauli matrix. Such a perturbation can originate from the single particle hopping of charged particles under external magnetic field or neutral particles under some artificial gauge field. We characterize the quantumness of the observed state in experiments by the overlap between the quantum ground state under the perturbation and the one without perturbation. If the overlap is one, the observed state is fully quantum. The simulation results are shown in figure 4 for a set of parameters of typical values. Under both strengths of perturbations, the observed states gradually evolve from the

quantum state to the classical one with the increase of particle number. Besides, the weaker the perturbation is, the larger particle number we need to observe the effective ground state in experiments. Note that the quantumness of the observed state exhibits some oscillations in the crossover region for weak perturbation. This is due to the oscillation of the lowest energy gap with the oddness and evenness of particle number. For small particle number, the energy gap is much smaller for odd particle number as there is an additional symmetry or quasi-degeneracy with respect to the distribution of particle number in the two wells.

We have already stated many times that for these boson systems, the mean-field ground state is just the effective ground state. The above calculations, in particular the results in figure 4, show convincingly that this is indeed the case for this simple Bose–Hubbard model. However, it is not well understood why the mean-field ground state is the effective ground state for boson systems. There are many indications, for example, the mean-field Gross–Pitaevskii equation has been able to explain many Bose–Einstein condensate experiments.

From this simple model, we see clearly that the two fundamental concepts, SSB and effective ground state, are closely related. We take this opportunity to discuss their relation. In the perspective of effective ground state, there are two different types of SSB. In the first type, the quantum ground state is degenerate; therefore, the effective ground state is also degenerate. At low temperatures, the system falls into one of the quantum degenerate states, breaking the symmetry. The well-known ferromagnetic ground state falls into this category.

In the second type of SSB, the quantum ground state is unique while the effective ground state is degenerate. In these systems, the degeneracy of the effective ground states arises from the quasi-degeneracy of the quantum energy levels: tiny perturbation can mix up these quasi-degenerate quantum states and generate these degenerate effective ground states, which are observed in experiments. Interestingly, this category can be further divided into two subgroups as the quasi-degeneracy has two different origins: (i) the quasi-degeneracy of the quantum energy levels is caused by the large volume size of the system. The gas–solid transition mentioned above [9, 10] and the Bose–Einstein condensation of ideal gas [19] are typical examples of this case. The degree of degeneracy in this subgroup is usually infinite. (ii) The quasi-degeneracy of the quantum energy levels is due to the interaction in the system. For systems in this subgroup, the energy gap usually decreases exponentially with particle number. Our model belongs to this subgroup along with many other systems reported elsewhere [20–24].

SSB is a familiar and well-studied concept in condensed matter physics. However, it is still not fully understood. Wen recently asked, 'what is spontaneous symmetry breaking in QUANTUM systems?' on a website [11]. This question highlights a dilemma that we all face: on the one hand, SSB can only happen for nonlinear systems; on the other hand, quantum systems are always linear. The connection between SSB and effective ground state that we have shown here may
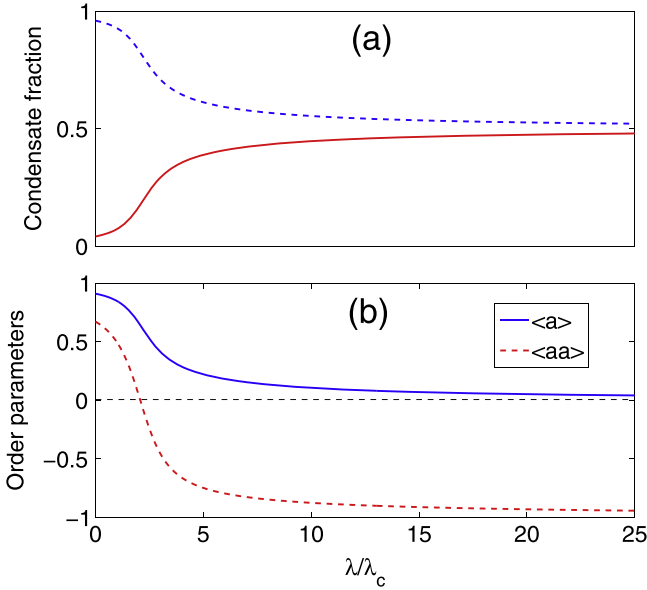
Figure 5. (a) Two fragmented condensate fractions of the quantum ground state as a function of pair tunneling strength. $N = 50$. (b) Order parameter $\langle \hat{a} \rangle$ (blue solid line) and pair order parameter $\langle \hat{a}\hat{a} \rangle$ (red dashed line) as a function of pair tunneling strength for the quantum ground state. They are rescaled with respect to $\sqrt{N/2}$ and $N/2$, respectively. $N = 50$.

provide a fresh perspective into this issue: nonlinearity needed for SSB is rooted in the degeneracy (or quasi-degeneracy) of quantum energy levels.

4. Fragmentation and pair order parameter

As our system is an interacting boson system, we use the Penrose–Onsager criterion [25] to further analyze its quantum ground state. The condensate fraction is given by n_i/N, where N is the total particle number and n_i are the eigenvalues of the reduced single particle density matrix. In lattice models, $\rho_1(i, j) = \langle \hat{a}_i^\dagger \hat{a}_j \rangle$. Here for the double-well potential, we have

$$\rho_1 = \begin{bmatrix} \langle \hat{a}^\dagger \hat{a} \rangle & \langle \hat{a}^\dagger \hat{b} \rangle \\ \langle \hat{b}^\dagger \hat{a} \rangle & \langle \hat{b}^\dagger \hat{b} \rangle \end{bmatrix}. \qquad (3)$$

As shown in figure 5(a), for strong pair tunneling, both of the condensate fractions are nonzero for large N. So, the system is in fact a fragmented condensate. This is consistent with the result in [13, 14] within the parameters that overlap. Those authors found that the fragmented condensate is stable against various perturbations. Here we have shown that the fragmented condensate is unstable under perturbations that break time reversal symmetry.

The fragmentation of the quantum ground state corresponds to the degeneracy of mean field ground state. This is a general relation that is also present in other fragmented systems. For example, in the antiferromagnetic ground state of spin-1 Bose gases [26–28], the quantum ground state is unique while its effective ground state has infinite degeneracy due to the intrinsic SU(2) symmetry. Thus the quantum

ground state also corresponds to a fragmented condensate. Fragmented condensate is usually unstable against perturbations that breaks the symmetry and will evolve into one simple condensate, which is one of the effective ground states.

Distinct to the Bose–Hubbard model previously studied, one can define two kinds of order parameters for the quantum ground state in this model. One is the ordinary single particle order parameter $\langle \hat{a} \rangle$, and the other is the pair order parameter $\langle \hat{a}\hat{a} \rangle$. Both order parameters change with pair tunneling strength (figure 5(b)). One immediately sees that in the strong pair tunneling limit, the single particle order parameter $\langle \hat{a} \rangle$ almost vanishes, while the pair order parameter $\langle \hat{a}\hat{a} \rangle$ approaches a saturation value $-N/2$. This behavior indicates that for strong pair tunneling the condensate is no longer the usual single particle condensate, but a *pair condensate*. The pair order parameter changes sign during the increase of pair tunneling strength as a result of minimization of the pair tunneling energy. By tuning the ratio of pair tunneling to single particle tunneling, the system experiences a quantum phase transition from the single particle condensate to the pair condensate.

The pair condensate defined in this way can be extended into the case of optical lattice with periodic boundary condition, where a *pair superfluid* can be defined similarly. In this lattice system, the quantum ground state is still unique while the mean field one becomes hugely degenerate due to the large quasi-degeneracy in the quantum energy levels. From the analysis of the double-well model, it is clear that this pair superfluid is unstable and may decay into one of the mean field ground states, which is a simple superfluid. Among all the mean field ground states, two of them are of special interest. Denote the phase difference between two neighboring wells as $\pm\theta$, and then there are states with consecutive $+\theta$ or $-\theta$ phase accumulation between neighboring wells, satisfying $L\theta = 2q\pi$ (L is the number of wells, and q is the winding number of order parameter). They correspond to superfluids flowing clockwisely or counter-clockwisely. Thus these two ground states carry nonzero mass current, which is unconventional.

Note that the meaning of the pair superfluid here is different from that defined in BCS pairing or boson dimer for attractive interaction [29–34]. As the pair superfluid resides in the repulsive interaction regime, no bound state or dimer is formed here. Similar order parameter also exists elsewhere [24], where a *trion superfluid* is defined.

5. Experimental realization

We now turn to the experimental method of tuning the ratio between pair tunneling and single particle tunneling. It is worth noting that recently there has been an experiment which observed the density-dependent tunneling term in a one-dimensional optical lattice [35]. Although our result above is based on the study of a double well potential, it can be easily generalized to the case of optical lattice. We will take the case of optical lattice as an example to illustrate our experimental

scheme. For the convenience of following discussion, we split the original Hamiltonian for an optical lattice into three parts,

$$
\begin{aligned}
\hat{H}_0 = & -\sum_i \Big[t - U_3 \big(\hat{n}_i + \hat{n}_{i+1} - 1 \big) \Big] \big(\hat{a}_i^\dagger \hat{a}_{i+1} + \hat{a}_{i+1}^\dagger \hat{a}_i \big) \\
& + \frac{U_2}{2} \sum_i \big(\hat{a}_i^\dagger \hat{a}_i^\dagger \hat{a}_{i+1} \hat{a}_{i+1} + \hat{a}_{i+1}^\dagger \hat{a}_{i+1}^\dagger \hat{a}_i \hat{a}_i \big) \\
& + \frac{U_0}{2} \sum_i \hat{n}_i \big(\hat{n}_i - 1 \big) + \big(U_1 + U_2 \big) \sum_i \hat{n}_i \hat{n}_{i+1} \\
= & \ \hat{H}_{\text{tun}}^1 + \hat{H}_{\text{tun}}^2 + \hat{H}_{\text{int}},
\end{aligned} \tag{4}
$$

where $\hat{H}_{\text{tun}}^1$, $\hat{H}_{\text{tun}}^2$ and $\hat{H}_{\text{int}}$ denote the single particle tunneling, pair tunneling and the interaction terms, respectively.

For usual systems, the pair tunneling is much weaker than the single particle tunneling, but their ratio can be tuned experimentally with the method of shaking the optical lattice [36–39]. The idea is to renormalize the tunneling matrix element by adding a periodically oscillating linear force to the original system. Such a method has been utilized to tune the single particle tunneling in previous experiments. In actual fact, it can also be used to tune the pair tunneling strength, as will be demonstrated below. Assume the added linear force has frequency ω and amplitude K, then the Hamiltonian of the optical lattice after shaking becomes

$$
\hat{H}(t) = \hat{H}_0 + K \cos(\omega t) \sum_j j \hat{n}_j, \tag{5}
$$

where $\hat{H}_0$ is the original Hamiltonian before shaking the lattice and $\hat{n}_j$ is the particle number operator on site j.

Since the Hamiltonian is periodic in time with period $T = 2\pi/\omega$, according to the quantum Floquet theory [40], the solution of the periodically driven Schrödinger equation has the form $|\psi_n(t)\rangle = |u_n(t)\rangle \times \exp(-i\varepsilon_n t/\hbar)$, where $|u_n(t)\rangle = |u_n(t+T)\rangle$ and it satisfies the eigenvalue equation

$$
\Big[\hat{H}(t) - i\hbar \partial_t \Big] |u_n(t)\rangle = \varepsilon_n |u_n(t)\rangle, \tag{6}
$$

with ε_n being the quasienergies. In general, $|u_n(t)\rangle$ can be obtained by expansion in terms of the basis $\exp(im\omega t)$. By diagonalizing equation (6), one can find the Floquet functions $|u_n(t)\rangle$ and quasienergies ε_n.

Define the time-average inner product by

$$
\langle\langle \cdot | \cdot \rangle\rangle = \frac{1}{T} \int_0^T \mathrm{d}t \, \langle \cdot | \cdot \rangle, \tag{7}
$$

where $\langle \cdot | \cdot \rangle$ is the ordinary inner product. Then in the Floquet basis

$$
\begin{aligned}
\Big| \{ n_j \}, m \Big\rangle = \Big| \{ n_j \} \Big\rangle \exp \Bigg[& -i \frac{K}{\hbar\omega} \sin(\omega t) \\
& \times \sum_j j n_j + im\omega t \Bigg],
\end{aligned} \tag{8}
$$

with $|\{ n_j \}\rangle$ denoting the Fock state with n_j particles on the jth

site, the matrix element of equation (6) reads,

$$
\begin{aligned}
& \Big\langle\!\Big\langle \big\{ n_j' \big\}, m' \big| \hat{H}(t) - i\hbar \partial_t \big| \{ n_j \}, m \Big\rangle\!\Big\rangle \\
& = \delta_{m', m} \Big[\big\langle \big\{ n_j' \big\} \big| \, \hat{H}_{\text{int}} \, \big| \{ n_j \} \big\rangle + m\hbar\omega \Big] \\
& \quad + s^{m'-m} \mathcal{J}_{m'-m}(K/(\hbar\omega)) \big\langle \big\{ n_j' \big\} \big| \, \hat{H}_{\text{tun}}^1 \, \big| \{ n_j \} \big\rangle \\
& \quad + p^{m'-m} \mathcal{J}_{m'-m}(2K/(\hbar\omega)) \big\langle \big\{ n_j' \big\} \big| \, \hat{H}_{\text{tun}}^2 \, \big| \{ n_j \} \big\rangle,
\end{aligned} \tag{9}
$$

where $s = 1 \ (-1)$ for single particle tunneling from site j to $j+1$ $(j+1$ to $j)$, and $p = 1 \ (-1)$ for pair tunneling from site j to $j+1$ $(j+1$ to $j)$. $\mathcal{J}_n(x)$ is the nth order Bessel function of the first kind, given by the definition

$$
\mathcal{J}_n(x) = \frac{1}{2\pi} \int_0^{2\pi} e^{-i(n\tau - x \sin(\tau))} \mathrm{d}\tau. \tag{10}
$$

Matrix (9) has a block structure with respect to m, and in the case of high driving frequencies $\hbar\omega \gg \max\{J_i, U_i\}$, the coupling between different blocks can be neglected, so we only restrict to the block $m = 0$. Here the total single particle tunneling term J_i is defined as $J_i = t - U_3(n_i + n_{i+1} - 1)$, with n_i being the occupation number of site i. Then one can see that the original single particle tunneling matrix element is now replaced by $J_{\text{eff}}^1 = J_i \mathcal{J}_0(K/(\hbar\omega))$ [41], and the pair tunneling matrix element is replaced by $J_{\text{eff}}^2 = U_2 \mathcal{J}_0(2K/(\hbar\omega))$, respectively. So in the case of high driving frequencies, by restricting only to the block $m = 0$, the basis $|\{ n_j \}\rangle$ satisfy a time-independent Bose–Hubbard Hamiltonian with effective tunneling matrix elements J_{eff}^1 and J_{eff}^2, up to an overall phase factor $\exp\left[-i \frac{K}{\hbar\omega} \sin(\omega t) \sum_j j n_j \right]$ in time. Since the modulation of single particle tunneling and pair tunneling matrix elements depends on different functions, the ratio between the two tunneling matrix elements can be tuned by adjusting the driving frequency ω and the force strength K.

6. Conclusion

In summary, we have investigated both the quantum and mean field ground states of the extended Bose–Hubbard model for a double-well potential with pair tunneling. Firstly, we find that when the pair tunneling is strong enough, the mean field ground state of the system becomes complex and two-fold degenerate, while the quantum counterpart is always real and unique. The quantum ground state can be regarded as a superposition of two mean field states. Secondly, we have also discussed SSB in the perspective of effective ground state. The model serves as an example where the true ground state (quantum ground state) is quite different from the effective ground state (mean field ground state) that we really observe in experiments. We show that the degeneracy of the effective ground state is closely related to SSB, the quasi-degeneracy of the quantum spectrum and the stability of the quantum ground state. For large particle number, the quantum ground state is very sensitive to infinitesimal perturbations breaking the time reversal symmetry, resulting in one symmetry breaking effective ground state. Finally, we find that in

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the strong pair tunneling limit, the quantum ground state in fact corresponds to a fragmented condensate. In terms of the defined pair order parameter, it is also a pair condensate. We then propose an experimental scheme to tune the pair tunneling strength, and the conclusion drawn here can be tested within the current experimental techniques.

Acknowledgments

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