Preparation of stable excited states in an optical lattice via sudden quantum quench

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We study how stable excited many-body states of the Bose-Hubbard model, including both the gas-like state for strongly attractive bosons and bound cluster state for repulsive bosons, can be produced with cold bosonic atoms in an one-dimensional optical lattice. Starting from the initial ground states of strongly interacting bosonic systems, we can achieve stable excited states of the systems with opposite interaction strength by suddenly switching the interaction to the opposite limit. By exactly solving dynamics of the Bose-Hubbard model, we demonstrate that the produced excited state can be a very stable dynamic state. This allows the experimental study of excited state properties of ultracold atoms system in optical lattices.

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I. INTRODUCTION

Recent experiments with ultracold atoms have offered exciting opportunities to study quantum many-body physics in a highly controlled manner [1–4]. Beyond simulating the ground state (GS) properties of various many-body systems, the uniqueness of cold atomic system, such as the low dissipation rate and the Feshbach resonance technique, has led to the experimental realization of stable excited states, as demonstrated by recent observation of a one-dimensional (1D) stable excited state called super-Tonks-Girardeau (STG) gas [5] and repulsively bound atom pairs [6]. In general, a stable excited state is hard to be realized in traditional solid state systems since a pure excited state is not stable due to the energy dissipation between the system and the environment. The STG gas provides one of the counterintuitive examples realized in cold atom systems with no analog in solid state systems. It describes the lowest gas-like phase of the attractive Bose gas [2, 5], which is however a highly excited state against its cluster-like GS. The stability of the STG gas could be understood from the dynamics of the 1D integrable Bose gas [9]. Another example, i.e., the repulsively bound atom pairs, is also counterintuitive at first glance since two atoms with strongly repulsive on-site interaction usually repel each other. Theoretical studies have revealed the existence of exotic repulsively bound pairs in optical lattices [12–15].

The experimental realization of stable excited states provides a promising new area for searching novel quantum states in cold atom systems [16, 17]. However, the diversity and mechanism of realizing stable exited many-body states are still not well understood. Questions arise whether the STG gas can also be realized in a lattice system as the Tonks-Girardeau (TG) gas [4] and whether the two independent experiments [5, 6] can be understood in the same theoretical framework. In this work, we study how to prepare specific stable excited states, including both the gas-like excited state in attractive regime and repulsively bound cluster of atoms, for a Bose gas in a 1D optical lattice described by the basic Bose-Hubbard model (BHM). By exactly solving quench dynamics problem of BHM, we first show that a stable gas-like phase for the Bose gas with strongly attractive on-site interaction can be realized in the 1D optical lattice by suddenly switching interactions from the strongly repulsive regime to the attractive regime. Such an excited gas-like state avoids collapsing to the atom-cluster GS even under very strongly attractive interaction and could be viewed as a realization of STG gas in optical lattices. Furthermore, we show that a stable repulsively bound cluster state composed of N-atoms can be also realized by sudden switch of the interactions from the attractive side to the repulsive side. The existence of the repulsively bound cluster in optical lattice is closely related to the phenomenon of repulsively bound pairs. Our study suggests that the two seemingly unconnected phenomena [4, 6] could be understood in a unified theoretical framework, i.e., they could be explained by calculating the sudden quench dynamics of the BHM with different initial states.

II. SYSTEM AND SCHEME

We consider the system of ultracold bosonic atoms in a 1D deep optical lattice, which can be described by the BHM [18, 19]

\[
\hat{H} = -J \sum_i \left( \hat{b}_i^\dagger \hat{b}_{i+1} + \hat{b}_{i+1}^\dagger \hat{b}_i + \frac{1}{2}U \sum_i \hat{n}_i (\hat{n}_i - 1) \right), \tag{1}
\]

where \( \hat{b}_i^\dagger \) is the creation operator of bosons at the ith site, \( J \) and \( U \) denote the hopping strength and on-site interaction, respectively. The ratio \( U/J \) can be tuned by varying the depth of the optical lattice and using Feshbach resonance [18]. For convenience, we set \( J = 1 \) as the energy

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scale. Despite the BHM having been studied by various methods \cite{14,21}, the model is generally not exactly solvable by analytical method \cite{22}. As the GS properties have been extensively studied, the properties of excited state and related non-equilibrium physics based on the Hubbard model have recently attracted lots of attentions \cite{14,17,22,23,24,25}. In this work, we propose a scheme of preparing stable highly excited states of the BHM via a sudden switch of interactions from the strongly repulsive regime to the attractive regime and vice versa. Similar kind of quench has previously been used to create metastable states in other systems \cite{2,3,17}. We shall demonstrate how an initially prepared GS translates to a highly excited state by solving the quantum dynamics of BHM.

Suppose that the initial state $|\Psi_{ini}(t=0)\rangle = |\psi_0(U_0)\rangle$ is prepared in the strongly interacting regime with either $U_0 > 0$ or $U_0 < 0$, after a sudden switch to the opposite regime with interaction strength $U$, the wave-function $|\Psi(t)\rangle = e^{-iH(U)t} |\Psi_{ini}(U_0)\rangle$ can be calculated via

$$|\Psi(t)\rangle = \sum_n e^{-iE_n} c_n |\psi_n(U)\rangle,$$

(2)

where $c_n = \langle \psi_n(U) | \psi_0(U_0) \rangle$ with $|\psi_n(U)\rangle$ representing the $n$-th eigenstate of the BHM with on-site interaction $U$. It is straightforward that $|c_n|^2$ is the transition probability from the initial state to the $n$-th eigenstate of $H(U)$. To study the quench dynamics of the BHM, we shall scrutinize the full spectra and eigenstates of the BHM both analytically and numerically.

III. BETHE-ANSATZ SOLUTION FOR TWO-PARTICLE BHM

We begin with the two-particle problem of the BHM which is exactly solvable with the aid of Bethe-ansatz (BA) method. Although the two-particle problem is quite simple, its analytical result can provide us quite instructive understanding to many-particle systems as we shall discuss later. The BA wavefunction takes the form of $|\Psi\rangle = \sum_{x_1,x_2} \Psi(x_1,x_2) |x_1,x_2\rangle$ with

$$\Psi(x_1,x_2) = A_{12} e^{i(k_1 x_1 + k_2 x_2)} + A_{21} e^{i(k_2 x_1 + k_1 x_2)}$$

(3)

defined in the domain $x_1 \leq x_2$. The wavefunction in the other region $x_2 \leq x_1$ can be obtained by the symmetry of wavefunction. Explicitly, the coefficients are given by $A_P = (-1)^P \sin k_{p_2} - \sin k_{p_1} - iU/2$, where $P = \{p_1, p_2\}$ is one of the permutations of 1, 2 and $(-1)^P = 1$ or $-1$ for even or odd permutation. Under periodic boundary condition, the quasi-momenta $k_j$ ($j = 1, 2$) fulfill the Bethe-ansatz equations (BAE)

$$\exp (i k_j L) = \frac{\sin k_1 - \sin k_j - iU/2}{\sin k_1 - \sin k_j + iU/2}.$$  

The total momenta of the system is given by $K = k_1 + k_2$ and the eigenenergies are given by $E = -2 \sum_{i=1}^N \cos k_i$.

\[ k_j L = 2\pi I_j + 2 \arctan \frac{\sin k_1 - \sin k_j}{U/2} \]  

(4)

with $I_j = -(L-1)/2, \ldots, (L-1)/2$ and $I_1 < I_2$. While the bound states correspond to the string solution with the form of $k_1 = k + i\Lambda$ and $k_2 = k - i\Lambda$, where $k$ and $\Lambda$ are real. In this case the total momenta and eigenenergy take the form of $K = 2k$ and $E = -4J \cos k \sinh \Lambda$, respectively. In terms of $k$ and $\Lambda$ the original BAE transform into finding root of

$$\cos (kL) \exp (\Lambda L) = \frac{2 \cos k \sinh \Lambda - U/2}{2 \cos k \sinh \Lambda + U/2},$$  

(5)

where $k = I_j \pi/L$ with $I_j = 0, \pm 1, \pm 2, \ldots, \pm L/2 - 1$. Besides these $L-1$ bound states the $L$th one corresponds to $K_L = \pi$ and $E_L = U/J$. We obtain all eigenstates by solving (4) and (5). Full spectra for example systems with $U = \pm 10$ and $L = 50$ are displayed in Fig. 1. Taking advantage of analytical results for the two-particle case, we can calculate the transition probabilities exactly. First, we consider the case in which the initial state is prepared as the GS of the BHM in the repulsive side. After suddenly switching the on-site interaction to the attractive regime, we calculate the overlap of the initial wavefunction with the eigenstates of the attractive BHM. In the left inset, we show the transition probability...
from an initial GS (marked by the cross in the left Fig.1) with \( U_0 = 80 \), to the lowest scattering state (marked by the cross in the right Fig.1) with different values \( U < 0 \). Here the transition probability from the initial scattering GS to the final lowest scattering state is denoted by \( P_{sa} \) which is very close to one after switching to the strongly attractive regime. On the other hand, the probability for dynamically falling into the attractively bound state (denoted by \( P_{sb} \)) is almost zero. In the right inset, it is shown that after switching to the strongly repulsive regime, the initial attractively pair state (marked by the star in the right Fig.1) is transformed to the repulsively bound state (marked by the star in the left Fig.1) with the transition probability close to 1. Here the symbols \( P_{ba} \) and \( P_{bb} \) represent the transition probabilities from the initial bound state to final scattering state and the initial bound state to final bound state, respectively.

IV. MANY-PARTICLE SYSTEM

For the many-particle system with \( N \geq 3 \), the BHM is no longer exactly solvable by the BA method which can not properly treat the multi-occupation case \cite{[22]}. Nevertheless, for a finite size system, we can resort to the full exact diagonalization (ED) method to calculate the full energy spectra and eigenstates. Consequently the transition probabilities from the initial GS to arbitrary final states are straightforward to be calculated. In general, it is a formidable task to get the full spectra of a large system as the basis dimension of a \( N \)-particle BHM with size \( L \) is given by \( D = (N + L - 1)!/[N!(L - 1)!] \).

Despite the full spectra becoming very complicated as the particle number increases, we can still find some common characteristics of the spectra for systems with different sizes. When \( |U| \gg J \), the spectra is split into a series of separated bands. For the repulsive case, the lowest band is a scattering continuum of \( N \) asymptotically free particles, whereas the top band is a narrow band formed by the \( N \)-particle repulsively bound state. Between the top and bottom bands, there exists a series of scattering continua formed by bound cluster states or formed by bound state and free particle. To give a concrete example which may guide us to understand the structure of the spectra, we display the energy-momentum spectra for a system with \( N = 4 \), \( L = 30 \) and \( U = \pm 15 \). As shown in Fig.2, the bound states on the top band have the energies about \( 6U \), and the lowest band is a scattering continuum of 4 free particles. In between, the energies of three separated bands are approximately given by \( 3U \), \( 2U \) and \( U \), which suggests that these bands correspond to, respectively, the scattering continuum of a trimer and a free particle, two dimers, and a dimer and two free particles. The spectra for system with attractive interactions has a similar structure in reverse order. The zero-momentum \( N \)-particle attractively bound state is the GS, whereas the scattering continuum of \( N \) free particles is on the top of the spectra corresponding to highly excited states of the attractive system. We note that these separated bands are no longer discernable when the interaction strength is comparable to the band width.

For a sudden switch of the interaction from the strongly repulsive regime to the attractive side, we evaluate the transition probabilities from the initial repulsively GS to the final states. As displayed in Fig.3, the transition probability to the lowest excited state in the top scattering band is very close to 1 in the strongly attractive regime, whereas the probability for falling into the attractively cluster GS is almost completely suppressed. Since the transition rate to the scattering phase is very close to 1 in the strongly interacting regime, we expect that one can prepare such a highly excited state experimentally through switching the interaction from strong repulsion into strong attraction following the same way in the experiment of the STG gas. Actually, the stable excited scattering state prepared in this way can be viewed as a realization of STG gas in optical lattices. The gas-like excited state is no longer stable and decays quickly if the system enters to the weakly interacting regime.

We can understand the stability of the lowest scattering state in the strongly attractive limit from the analytical BA solution. We note that the BAE solutions for the repulsive case and that for the STG gas correspond to the same set of \( \{I_j\} \) according to \cite{[3]}. In the limit \(|U| \to \infty \), the solutions given by \( k_j = I_j 2\pi / L \) are exactly the same, which means that the repulsive GS state and the lowest scattering state in the attractive side are identical in the infinitely interacting limit.
by the two methods agree very well with, for example, BA solution and ED (see Fig. 4a). The energies obtained the initial GS of the same system with switch to attractive side. (b) The transition probability from the initial GS of the same system with $U > 0$ to the GS ($P_{bb}$) and the repulsively cluster state ($P_{bb}$) for various repulsive $U$.

In the strongly interacting regime with $|U| \gg 1$, the quasi-momentum distributions for the repulsive TG gas and the STG gas approach the free fermion distribution from different sides, and consequently the overlap between the repulsive GS and the STG state is close to 1, i.e., $|\langle \psi_{\text{STG}}(-U)|\psi_0(U)\rangle| \to 1$ as $|U| \to \infty$. The above exact discussion for 2-particle system can be directly extended to the many-particle systems. This is based on the observation that, in the strongly interacting regime, the extended BA solutions [22] can be used to describe the properties of scattering states very precisely for both the repulsive and attractive cases, although the solution is not an exactly analytical solution for the many-particle system in the rigorously integrable meaning [22]. Here the many-body BA wavefunction takes the form of $\Psi(x_1, \ldots, x_N) = \sum_P A_P e^{i \sum_j k_{\text{BA}} x_j}$, where the coefficients $A_P = (-1)^{P} \prod_{j=1}^{N} \left( \sin k_{p_j} - \sin k_{p_j} - iU/2 \right)$, $P = \{p_1, p_2, \ldots, p_N\}$ is one of the permutations of $1, \ldots, N$, and $\sum_P$ is the sum of all permutations. The quasimomenta are determined by the BAE

$$k_j L = 2\pi I_j + 2 \sum_{i=1}^{N} \arctan \frac{\sin k_i - \sin k_j}{U/2}. \quad (6)$$

Both the GS solution for $U > 0$ and the STG solution for $U < 0$ are determined by the same set of $\{I_j\} = \{-N/2, \ldots, (N+1)/2\}$. To confirm that, we calculate and compare the GS energy for the $U > 0$ case and energy of the lowest scattering state for the $U < 0$ case by both the BA solution and ED (see Fig. 3). The energies obtained by the two methods agree very well, for example, $E_{\text{BA}} < E_{\text{ED}}$ and ED results suggests that the BA solutions can give very good results consist with the ED results in the strongly interacting regime. (c) The local two-particle correlation function $g_2(U) = \partial E(U)/\partial U$ vs interaction.

\[ \delta = |E_{\text{ED}} - E_{\text{BA}}|/|E_{\text{ED}}| < 10^{-5} \text{ for } |U| = 100 \text{ as shown in the Fig. 4b. As } |U| \to \infty, \text{ we have } E_{\text{STG}} = E_{\text{STG}}. \text{ Such a gas-like state shares similar characteristics with its continuum correspondence. For example, the STG phase exhibits stronger local correlation than the repulsive Bose gas as displayed in the Fig. 4b.} \]

Finally, we turn to the case in which the initial state is chosen to be the GS of the BHM in the strongly attractive interaction limit, i.e., the cluster-type bound state with all the atoms tending to stay together due to the strongly on-site attractive interaction. After the on-site attraction is suddenly switched to the strongly repulsive regime, we also find that the cluster-type bound state is stable and the initial system translates to the repulsively cluster state as marked by star in Fig. 2b. In Fig. 3c, we show the transition probabilities from the initial attractively bound state to the repulsively bound state and the scattering GS in the repulsive side. We find that the transition probability to the repulsively bound state is close to 1 whereas the transition to the scattering GS is almost completely suppressed in a wide range of interaction.
V. SUMMARY

In summary, we have studied the transition from the GS of strongly repulsive or attractive bosons to the gas-like highly excited state of attractive bosons or the repulsively bound state through a switch of interaction. By calculating the transition probabilities, we have shown that the gas-like excited state and repulsively bound state are stable in the strongly interacting regime and thus are possible to be observed with cold atoms in optical lattices.

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