Fast transfer and efficient coherent separation of a bound cluster in the extended Hubbard model

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Abstract. We study the formation and dynamics of the bound pair (BP) in a strongly correlated extended Hubbard model for both the Bose and the Fermi system. The bound triple (BT) for the Bose system is also investigated. We find that the bandwidths of the BP and BT gain significantly when the on-site and nearest-neighbor interaction strengths reach the corresponding resonant points. This allows fast transfer and efficient coherent separation of the BP and BT. The exact result shows that the success probability of the coherent separation is unity in the optimal system. In the Fermi system, this finding can be applied to create distant entanglement without the need for temporal control and the measurement process.

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1. Introduction

Ultra-cold atoms have become an ideal playground for the testing of few-particle fundamental physics and have attracted attention because of their increasing technological applications. The experimental observation of an atomic bound pair (BP) in an optical lattice [1] has stimulated many experimental and theoretical investigations in strongly correlated boson systems [2–12]. The essential physics of the proposed BP is that the periodic potential suppresses single-particle tunneling across the barrier, a process that would lead to the decay of the pair. Such a type of BP therefore cannot get migration speed through the lattice. In addition, the dynamics of pair formation and separation is also of interest in both fundamental and application aspects. Concerning the cluster formation and separation in quantum chemistry and nuclear physics, the multi-photon bound state has been studied due to its potential applications in information processing and quantum device physics [13–16].

In this paper, we study the influence of the nearest-neighbor (NN) interaction on the few-boson bound state. We will show that the resonant NN interaction can also induce the BP and bound triple (BT) states. These bound states are distinct from known ones, as their bandwidths are comparable to that of a single particle. This feature allows full overlap between the scattering band of a single particle and the band of a BP or a BT, leading to the coherent separation and combination processes. We propose relatively simple schemes to implement such processes. The exact result shows that the success probability of coherent separation is unity for a BP whereas it approaches unity for a BT in optimal systems. Quantum entanglement is typically fragile to practical noise. Every external manipulation, however, inevitably induces noise in the system. Applying the results we obtained from the Bose–Hubbard system to the corresponding Fermi system, the coherent separation process can be utilized to create distant entanglement without the need for the temporal control and measurement process. This mechanism avoids possible errors arising from any additional external manipulation.

2. Fast bound pair (BP) dynamics

Let us start by analyzing in detail the two-particle problem in an extended Bose–Hubbard model, which is simpler than the Fermi one but shares similar features for the issue concerned. The Hamiltonian is written as follows:

\[ H_B = -t \sum_{i=1}^{N} (a_i^\dagger a_{i+1} + \text{h.c.}) + \frac{U}{2} \sum_{i=1}^{N} n_i (n_i - 1) + V \sum_{i=1}^{N} n_i n_{i+1}, \]  
(1)

where \( a_i^\dagger \) is the creation operator of the boson at the \( i \)th site; the tunneling strength, on-site and NN interactions between bosons are denoted by \( t \), \( U \) and \( V \). For the sake of clarity and simplicity, we only consider an odd-site system with \( N = 2N_0 + 1 \) and periodic boundary conditions \( a_{N+i} = a_i \). In this paper, we restrict ourselves to the one-dimensional system. Nevertheless the conclusion can be extended to the high-dimensional system.

First of all, a state in the two-particle Hilbert space, as shown in [10], can be written as \( |\psi_k\rangle = \sum_r f^k(r) |\phi_r^k\rangle \), where

\[ |\phi_0^k\rangle = \frac{1}{\sqrt{2N}} e^{ik/2} \sum_j e^{ikj} a_j^\dagger |\text{vac}\rangle, \]  
(2)
\[ |\phi_r^k \rangle = \frac{1}{\sqrt{N}} e^{i(k+1)/2} \sum_j e^{i k j} a_j^+ a_{j+r}^+ |\text{vac} \rangle. \]  

(3)

Here, \(|\text{vac} \rangle\) is the vacuum state for the boson operator \(a_i\). Here, \(k = 2\pi n/N, n \in [1, N]\) denotes the momentum, and \(r \in [1, N_0]\) is the distance between the two particles. Due to the translational symmetry of the present system, the Schrödinger equations for \(f^k(r), r \in [0, N_0]\) are easily shown to be

\[ T_r^k f^k(r+1) + T_{r-1}^k f^k(r-1) + [U \delta_{r,0} + V \delta_{r,1} + (-1)^n T_r^k \delta_{r,N_0} - \epsilon_k] f^k(r) = 0, \]  

(4)

where \(T_r^k = -2\sqrt{2} t \cos(k/2)\) for \(r = 0\) and \(-2t\cos(k/2)\) for \(r \neq 0\). Besides, we also have the boundary conditions \(f^k(-1) = f^k(N_0 + 1) = 0\). Note that for an arbitrary \(k\), the solution of (4) is equivalent to that of the single-particle \(N_0 + 1\)-site tight-binding chain system with NN hopping amplitude \(T_j^k\) and on-site potentials \(U, V\) and \((-1)^n 2t \cos(k/2)\) at the 0th, 1th and \(N_0\)th sites, respectively. Obviously, in each \(k\)-invariant subspace, there are three types of bound states arising from the on-site potentials under the following conditions. In the case when \(|U - V| \gg t\), the particle can be localized at either the 0th or 1th site, corresponding to (i) the on-site BP state or (ii) the NN BP state. Interestingly, in the case of resonance \(U = V\) and \(|U|, |V| \gg t\), the particle can be in the bonding state (or anti-bonding state) between the 0th and 1th sites, corresponding to a new BP state, called (iii) the resonant BP (RBP) state. In this paper, hereafter, we focus on this type of bound state and denote RBP as BP. All the \(N\) bound states of (iii), indexed by \(k\), constitute a BP band.

In previous works [10, 11], the bound states of (i) and (ii) were well investigated and the corresponding BP bandwidths are of order \(t^2/U\) and \(t^2/V\). Then they can be regarded as stationary compared to the single particle in the strongly correlated limit. In order to analyze the dynamics of the BP of type (iii), we pursue the solution of (4) in the case where \(U = V\) and \(|U|, |V| \gg t\) via the Bethe-ansatz method. We focus on the bound state solution of the Schrödinger equation (4) for a large system. The Bethe-ansatz wavefunction has the form \(f^k(j) = e^{-\epsilon_j \pi} (j \geq 1)\). The corresponding Schrödinger equation (4) can be reduced to

\[ -\sqrt{2} T^k f^k(1) + (U - \epsilon_k) f^k(0) = 0, \]  

(5a)

\[ -\sqrt{2} T^k f^k(0) - T^k f^k(2) + (V - \epsilon_k) f^k(1) = 0, \]  

(5b)

\[ \epsilon_k + 2T^k \cosh(\kappa) = 0, \]  

(5c)

with \(T^k = 2t \cos(k/2)\). After simplification, we obtain

\[ 2 \sinh(\kappa) + U' + V'[2 \cosh(\kappa) + U'][\cosh(\kappa) - \sinh(\kappa)] = 0. \]  

(6)

Taking \(U' = U/T^k, V' = V/T^k\) for simplicity, we note that (6) is similar to equation (7) of [11] after proper transformation. We can express (6) in another form,

\[ \cosh^3(\kappa) + \frac{V'}{2V'}(2U' + V') - 1 \cosh^2(\kappa) \frac{U'(U' + 2V') - 4}{4} \cosh(\kappa) \frac{U'^2 + (U'V' - 2)^2}{8V'} = 0, \]  

(7)

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which can be reduced to
\[
\cosh^3(\kappa) + \frac{(3U'^2 - 1)}{2U'} \cosh^2(\kappa) + \frac{(3U'^2 - 4)}{4} \cosh(\kappa) + \frac{U'^2 + (U'^2 - 2)^2}{8U'} = 0
\] (8)
in the case when \( U = V \). The approximate solution of (8) leads to the approximate BP solution in the form
\[
f^k(r) \simeq \eta_k \begin{cases} 
-\sqrt{2} \epsilon_k / (\epsilon_k - U), & (r = 0), \\
-\text{sgn}(U/\epsilon_k))^{(r-1)} \xi^{(r-1)}_k, 
\end{cases}
\] (9)
with the spectrum
\[
\epsilon_k \simeq U \pm \sqrt{2} \epsilon_k + \frac{\epsilon_k^2}{2U'},
\] (10)
where
\[
\eta_k^{-2} = \frac{|\epsilon_k|}{2\sqrt{\epsilon_k^2 - 4\epsilon_k^2}} + \frac{2\epsilon_k^2}{(\epsilon_k - U)^2} + \frac{1}{2},
\] (11)
\[
\xi_k = \left( |\epsilon_k| + \sqrt{\epsilon_k^2 - 4\epsilon_k^2} \right) / (2|\epsilon_k|),
\] (12)
and
\[
\epsilon_k = -2t \cos(k/2)
\] (13)
is the partial dispersion relation of a single particle. Neglecting the terms of order \( t^2/U \) in the eigenvalue and those of order \( t/U \) in the eigenfunction, the two branches of the BP spectrum can be rewritten as
\[
|\psi^{\text{BP}}_k\rangle = \sum_j \frac{\epsilon^{kj(j+1/2)}}{\sqrt{2N}} \left( a_j^{\dagger/2} / \sqrt{2} \mp e^{i(k/2)} a_{j+1}^{\dagger/2} \right) |\text{vac}\rangle,
\] (14)
\[
\epsilon^{\text{BP}}_k = U \pm 2\sqrt{2}t \cos(k/2).
\] (15)
Observing the above expressions, we find that they can be regarded as a plane wave of the composite particle, BP. Actually, this can be easily understood in terms of the equivalent effective Hamiltonian, which can be obtained in the quasi-invariant subspace spanned by the basis \( \{|l\rangle_p, l \in [1, 2N]\} \) with diagonal energy \( U \). The set of basis \( \{|l\rangle_p\} \) is defined as
\[
|l\rangle_p \equiv \begin{cases} 
a_{l/2}^{\dagger/2} / \sqrt{2} |\text{vac}\rangle, & (\text{mod} (l, 2) = 1), \\
a_{l/2}^{\dagger/2} a_{l/2+1}^{\dagger/2} |\text{vac}\rangle, & (\text{mod} (l, 2) = 0).
\end{cases}
\] (16)
The effective Hamiltonian of the ring, restricted to the basis \( \{|l\rangle_p\} \), reads
\[
\mathcal{H}_{\text{BP}} = -\sqrt{2}t \sum_{l=1}^{2N} (|l\rangle_p \langle l + 1| + \text{h.c.}),
\] (17)
which describes a free Bloch particle in a single band. However, this BP state is distinct from the previous on-site and NN BP because of its large bandwidth, \( 4\sqrt{2}t \). It shows that the speed of a BP wavepacket must be in the range of 0 to \( 2\sqrt{2}t \), which is the reason why we call it a
Figure 1. Plots of the BP solutions of the Schrödinger equation (4) for a system with $U = V$, all $U$ values are marked in units of $t$. The solid lines represent the exact numerical solutions. The dashed line represents the plot of (10), which is obtained in the strong coupling approximation. All the plots are shifted by $U$ from the original positive branch solutions.

fast BP. This is very significant for quantum technologies in the following two aspects: (i) the BP wavepacket can be a new choice as a quantum information carrier due to its fast speed. (ii) The bandwidth match between BP and a single particle may lead to the coherent separation of the BP.

The complete spectrum consists of a bound band and a scattering band. In the large-$U$ regime, these are separated by a gap. As $U$ decreases, the gap becomes smaller and disappears at $U = V$, $|U| = 6t$, which is determined by (8). Beyond this region the bound and scattering bands merge and are indistinguishable. In order to verify the validity of the BP solution and find the range of parameter values for the approximate expression of (10), numerical simulations are performed. We compute the solution of (4) in the case when $U = V$ for a wide range of values. It indicates that such a BP bound band can be well defined by (10) within the range $U = V$, $|U| > 6t$. Figure 1 shows the plots of the comparison of the approximate and numerical solutions. It shows that the approximate analytical result (10) agrees with the exact numerical result even for moderate $U$. It can be seen that the existence of the fast BP solution is simply due to the fact that there is no energy cost to go from an on-site pair configuration to an NN pair configuration.

Additionally, in the spirit of the above analysis, one can also construct a similar BP for the extended Hubbard model on a triangular lattice (or zigzag lattice), which can be written as

$$H_T = -t \sum_{\langle i,j \rangle} (a_i^\dagger a_j + \text{h.c.}) + V \sum_{\langle i,j \rangle} n_i n_j.$$  (18)
Here \((i, j)\) denotes the NN site pairs. We neglect the \(U\) term for simplicity under the condition that it is off-resonant from the \(V\) term. The corresponding BP is the NN pair, which consists of two neighbor particles.

3. Coherent separation of the BP

So far, we have proposed a new type of local BP, which propagates as a single particle in a uniform chain. It is known that a new-generation device is always based on new physical mechanisms. For the BP, we need to study its various properties and possible applications. It is worthy to note that, in such a system, the scattering band of a single particle fully overlaps the band of a BP (15). This fact indicates that a BP may break in the scattering process by a resonant impurity. In order to demonstrate a perfect process of BP separation, we propose an optimal system which is a uniform chain with a resonant impurity embedded in it. The uniform chain acts as a channel for the transport of a BP wave, under the conditions \(U = V\) and \(|V| \gg t\). The resonant impurity consists of two sites with the tunneling strength \(t_0\), one site of which has far-off resonant on-site interaction \(U_s\) satisfying \(|U_s| \gg |U|\) and the other site has resonant chemical potential \(\mu = U\).

This setup is described by the Hamiltonian

\[
H_{\text{BPS}} = -t \sum_{i=-\infty}^{+\infty} a_i^\dagger a_{i+1} - (t_0 - t) a_1^\dagger a_2 + \text{h.c.} + U \sum_{i=-\infty}^{+\infty} n_i \left( \frac{n_i - 1}{2} + n_{i+1} \right) + \frac{U_s - U}{2} n_1 (n_1 - 1) + U n_2. \tag{19}
\]

To investigate the scattering process of an input BP wavepacket from the left, one can establish an equivalent effective Hamiltonian in the quasi-invariant subspace with diagonal energy \(U\) spanned by the basis \(\{|l\rangle_{\text{ps}}, l \in \mathbb{Z}\}\) defined as

\[
|l\rangle_{\text{ps}} = \begin{cases} 
(16) & (l \leq 0), \\
1 - l + 1 & (l \geq 1).
\end{cases}
\tag{20}
\]

Acting \(H_{\text{BPS}}\) on the quasi-invariant subspace, the equivalent effective Hamiltonian reads

\[
\mathcal{H}_{\text{BPS}} = -t \left( \sqrt{2} \sum_{l=-\infty}^{l_0} + \sum_{l=1}^{+\infty} \right) |l\rangle_{\text{ps}} \langle l + 1| - t_0 |0\rangle_{\text{ps}} \langle 1| + \text{h.c.}, \tag{21}
\]

which describes two connected semi-infinite chains with different hopping constants. The on-site interaction \(U_s\) ascertains \(H_{\text{BPS}}\) to be a linear chain, which would be beneficial in enhancing the success probability of the coherent separation.

The separation process of a BP wavepacket is illustrated in figures 2(a) and (b). After scattering, a part of the BP wavepacket is reflected by the impurity, while the other part is separated into two independent particles: one of the particles resides at the site with chemical potential \(U\), while the other particle is reflected to the left with a higher speed than that of the reflected BP wavepacket. Figure 4(b) is a numerical simulation of such a process. With the aid of the effective Hamiltonian (21), the previous process can be reduced to a simple single-particle scattering problem: an incident wavepacket is scattered by the joint linking the two semi-infinite
chains. The reflecting wave represents the reflecting BP wave, while the transmitting wave represents the separated reflecting particle. In this sense, the coherent separation probability is equal to the transmission coefficient of the effective Hamiltonian, which can be obtained exactly via Green’s function or the Bethe-ansatz method \[17–19\].

For an incident plane wave of \(k_0\), the coherent separation probability \(P(k_0)\) for a chosen system at \(t_0 = \sqrt{2}t\) is

\[
P(k_0) = 2 \left( 1 + \frac{1 - \sqrt{2} \cos^2 k_0}{\sin k_0 \sqrt{\cos (2k_0)}} \right)^{-1}
\]

for \(k_0 \in (\pi/4, \pi/2]\) and \(P(k_0) = 0\) for \(k_0 \in (0, \pi/4]\). The sudden death of \(P(k_0)\) within the region \((0, \pi/4)\) is due to the mismatch between the energies of the two sides of the joint. On the other hand, \(P(k_0)\) also represents the particle resident population at the impurity. The profile of \(P(k_0)\) is plotted in figure 3. It indicates that \(P(k_0)\) can reach 1.0 at \(k_0 = \pi/2\).

In practice, this process can be implemented via an incident wavepacket instead of a plane wave. Actually, the typical wavepacket, a Gaussian wavepacket in the space \(\{|l\}_{ps}\) can be constructed as

\[
|\Phi(k_0, N_c)| = \frac{1}{\sqrt{\Omega}} \sum_l e^{-(\alpha^2/2)(l-N_c)^2+i\alpha l} |l|_{ps},
\]

where \(\Omega\) is the normalization factor. Here \(N_c\) is its center in the space \(\{|l\}_{ps}\) and \(k_0\) is its momentum. The corresponding group velocity in the space \(\{|l\}_{ps}\) is \(v_g = 2\sqrt{2}t \sin k_0\), which
Figure 3. Plots of the separation probability $P(k_0)$ (solid line) and the group velocity $v_g$ (dashed line) as functions of the momentum of the incident wavepacket. It shows that both of them reach their maxima at $\pi/2$.

is also plotted in figure 3. It shows that for the fastest wavepacket with momentum $\pm\pi/2$, the success probability of the coherent separation can approach unity. The fastest wavepacket with momentum $\pm\pi/2$ is also the one most robust against spreading [20]. We define it as the optimal BP wavepacket to demonstrate perfect coherent separation. In the original system, it can be written as

$$\left| \phi(\pm, h_c) \right\rangle \simeq \frac{1}{\sqrt{\Omega_2}} \sum_j (-1)^j e^{-2\alpha^2(j-h_c)^2} \times \left( a_j^{\dagger 2}/\sqrt{2} \pm ia_j^{\dagger} a_{j+1}^{\dagger} \right) \left| \text{vac} \right\rangle,$$

which is obtained from (23) with wide width ($\alpha \ll 1$) and $k_0 = \pm \pi/2$ by the mapping rule (20). Here symbols $\pm$ and $h_c$ denote the direction of movement (sgn($\pm \pi/2$)) and the center of the wavepacket. The corresponding single-particle wavepacket has the form

$$\left| \psi(\pm, h_c) \right\rangle = \frac{1}{\sqrt{\Omega_2}} \sum_j e^{-(\alpha^2/2)(j-h_c)^2} \pm i(\pi/2)j a_j^{\dagger} \left| \text{vac} \right\rangle.$$

Note that $\left| \phi(\pm, h_c) \right\rangle$ is slower than $\left| \psi(\pm, h_c) \right\rangle$. This is also illustrated in figures 2(b) and (c) and especially in figure 4(b).

Thus, in the optimal case, the perfect scattering process can be expressed as

$$\left| \phi(+, -\infty) \right\rangle \left| \text{vac} \right\rangle \Rightarrow r \left| \phi(-, -\infty) \right\rangle \left| \text{vac} \right\rangle + s \left| \psi(-, -\infty) \right\rangle a_2^{\dagger} \left| \text{vac} \right\rangle,$$

and the corresponding inverse process as

$$\left| \psi(+, -\infty) \right\rangle a_2^{\dagger} \left| \text{vac} \right\rangle \Rightarrow r \left| \phi(-, -\infty) \right\rangle a_2^{\dagger} \left| \text{vac} \right\rangle + s \left| \phi(-, -\infty) \right\rangle \left| \text{vac} \right\rangle,$$

where $\Rightarrow$ represents the time evolution. Equations (26) and (27) represent the reversibility of the two processes, coherent separation and combination, due to the time-reversal symmetry of the system. Here $r$ and $s$ represent the reflection and transmission amplitudes. Then the success probability of the coherent separation is $|s|^2$.  

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In order to verify the validity of the proposed scheme and find an appropriate range of the parameter values to realize coherent separation in practice, numerical simulations are performed. We compute the time evolution of an incident Gaussian wavepacket with the form of (23) in a finite system of (19) by the exact diagonalization technique. The incident wavepackets are taken with $\alpha = 0.1$ and $k_0 \in [0.3\pi, 0.5\pi]$. The corresponding success probability of coherent separation $|s|^2$ is plotted in figure 4(a) for the cases when $U_s/t = 200$, $U/t = 7, 15, 30$ and $\infty$ (which corresponds to the equivalent effective Hamiltonian (21)). The corresponding $P(k_0)$ (22) is also plotted for comparison. For the sake of illustration of the coherent separation process, we plot the profile of the evolving wave function in the form of a contour map (figure 4(b)). It shows that the equivalent effective Hamiltonian (21) is appropriate to describe the dynamics of the BP in the large $U$ limit. In the case of moderate $U$, the efficiency of the coherent separation is still high, especially for the wavepacket with $k_0 = \pi/2$. Hence we conclude that the coherent separation scheme is indeed very efficient due to its three advantages: fast transfer, robustness and high efficiency.

4. Creation of distant entanglement

Now we analyze a similar problem in the extended Fermi–Hubbard model. We will see that the obtained results for the Boson BP can be directly applied to the Fermi system. Furthermore, we develop a protocol to generate the entanglement for two distant fermions. Entanglement as a unique feature of quantum mechanics has been recognized to be a powerful resource in quantum information processing and communication. Numerous protocols for the preparation of distant entanglement have been proposed. Most of them utilize two types of processes: (i) the adiabatic passage via temporal control of the system [21]; (ii) the natural dynamic process associated with a subsequent measurement [22]. The experimental realization of such schemes requires a long
coherence time or accurate detection, which is still a challenge in practice. Moreover, quantum entanglement is typically fragile to practical noise. Every external manipulation inevitably induces noise in the system. Hence, it is better to diminish any possible additional external manipulation. In the following, we will propose a scheme based on the above-mentioned coherent separation. Its three advantages, fast transfer, robustness and high efficiency, may help us to avoid the difficulties associated with the temporal control and measurement process.

The corresponding fermionic Hamiltonian reads

$$H_F = -t \sum_{i=-\infty}^{+\infty} c_{i\sigma}^\dagger c_{i+1\sigma} + (t_0 - t) \sum_{\sigma} c_{1\sigma}^\dagger c_{2\sigma} + \text{h.c.}$$

$$+ U \sum_{i=-\infty}^{+\infty} (n_{i\uparrow}n_{i\downarrow} + n_{i\downarrow}n_{i+1\uparrow}) + (U_s - U) n_{1\uparrow}n_{1\downarrow} + Un_2,$$

where $c_{i\sigma}^\dagger$ is the creation operator of a fermion at site $i$ with spin $\sigma = \uparrow, \downarrow$ and $n_i = n_{i\uparrow} + n_{i\downarrow}$. For a similar two-particle problem, all the previous conclusions for the Bose system are also valid for the Fermi system under the following mapping rule:

$$a_j^\dagger / \sqrt{2} \langle \text{vac} \rangle \rightarrow c_{j\downarrow}^\dagger c_{j\uparrow}^\dagger \langle \text{vac} \rangle, \quad a_j^\dagger a_j^\dagger \langle \text{vac} \rangle \rightarrow (c_{j\downarrow}^\dagger c_{j\uparrow}^\dagger - c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger) / \sqrt{2} \langle \text{vac} \rangle. \quad (29)$$

It should be noted that the bound states of two fermions with opposite spins in an extended Hubbard system have been studied in [23]. They proposed three types of bound states. Type $U$ is bound by the on-site interaction, while type $V$ is bound by the NN interaction, which admits two kinds of NN pairs with spin one and zero, respectively. In this paper, the Fermi BP originating from (29) at $U = V$ can be regarded as the combination of two types of symmetric BPs proposed in [23] (symmetric bound states are mentioned as the $U$ type and $V$ type with spin zero). Nevertheless, if we consider the fermionic version of (18) on a triangular lattice, the corresponding mapping rule of (29) can be extended to a triplet (anti-symmetric) pair. In the following, we focus on the dynamics of the symmetric Fermi BP in a chain and analyze a similar process to that discussed in the Bose system.

Accordingly we represent the wavepacket as

$$|\phi(\pm, N_c)\rangle \rightarrow |\phi_{\uparrow\downarrow}(\pm, N_c)\rangle,$$

$$|\psi(\pm, N_c)\rangle \rightarrow |\psi_{\uparrow\downarrow}(\pm, N_c)\rangle. \quad (30)$$

Nevertheless, from the process

$$|\phi_{\uparrow\downarrow}(+, -\infty)\rangle \langle \text{vac} \rangle \rightarrow r |\phi_{\uparrow\downarrow}(-, -\infty)\rangle \langle \text{vac} \rangle$$

$$+ \frac{s}{\sqrt{2}} \left( |\phi(\pm, -\infty)\rangle c_{2\downarrow}^\dagger - |\psi(\pm, -\infty)\rangle c_{2\uparrow}^\dagger \right) \langle \text{vac} \rangle \quad (31)$$

and the corresponding inverse process

$$\left( |\phi(\pm, -\infty)\rangle c_{2\downarrow}^\dagger - |\psi(\pm, -\infty)\rangle c_{2\uparrow}^\dagger \right) \langle \text{vac} \rangle \rightarrow r \left( |\phi(\pm, -\infty)\rangle c_{2\downarrow}^\dagger - |\psi(\pm, -\infty)\rangle c_{2\uparrow}^\dagger \right) \langle \text{vac} \rangle$$

$$+ \sqrt{2} s |\phi_{\uparrow\downarrow}(-, -\infty)\rangle \langle \text{vac} \rangle, \quad (32)$$

we can see that the two separated fermions have characteristics distinct from those of the bosons, due to the fact that, after scattering, the state $a_i^\dagger a_i^\dagger \langle \text{vac} \rangle$ is a separable state, while the state $(c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger - c_{i\downarrow}^\dagger c_{i\uparrow}^\dagger) / \sqrt{2} \langle \text{vac} \rangle$ is the maximally entangled state. The process of (31)
with $r = 0$ shows that a local Einstein–Podolsky–Rosen pair can be converted to a distant Einstein–Podolsky–Rosen pair automatically in a short time. Utilizing this scheme, one can obtain a pair of almost maximally entangled nodes, shared by Alice and Bob. This can be used for perfect quantum transport via teleportation.

It is worth noting that the entanglement between two distant particles is not created via the impurity, but is transferred from a pre-existing local entangled state to a separated entangled state. The merit of the above scheme lies in the property of the natural time evolution process in an always on system without the need for the temporal control and measurement process.

However, we would like to point out that creating distant entangled pairs in an actual experiment requires precise control over the particle number in order to protect the stability of the BP. This is because the scheme is not robust when there is more than one BP present, since, unlike the situation in [1], here two BPs can scatter into a free particle plus an immobile bound quadruplet, which can scatter with another BP to produce a free particle plus an immobile bound quadruplet, and so on.

In addition, when we consider the combination process of two fermions with different spin orientations as illustrated in figure 2(c), it becomes a little complicated. We will start our analysis from the simplest case in the two-particle problem, two parallel fermions. It is equivalent to the two-spinless-fermion system, in which the BP no longer exists. The corresponding process is

$$\left| \varphi_1 (+, -\infty) \right| c_{2 \uparrow} \left| \text{vac} \right> \Longrightarrow \left| \varphi_1 (-, -\infty) \right| c_{2 \uparrow} \left| \text{vac} \right>, \quad (33)$$

which represents the complete reflection of the incident wavepacket. Due to the SU(2) symmetry of the Hamiltonian (19), we have

$$\left| \varphi_1 (+, -\infty) \right| c_{2 \uparrow} \left| \text{vac} \right> + \left| \varphi_1 (+, -\infty) \right| c_{2 \uparrow} \left| \text{vac} \right> \Longrightarrow \left| \varphi_1 (-, -\infty) \right| c_{2 \uparrow} \left| \text{vac} \right> + \left| \varphi_1 (-, -\infty) \right| c_{2 \uparrow} \left| \text{vac} \right>. \quad (34)$$

Equations (31), (33) and (34) lead to

$$\left[ \alpha \left| \varphi_1 (+, -\infty) \right> + \beta \left| \varphi_1 (+, -\infty) \right> \right] c_{2 \uparrow} \left| \text{vac} \right> \Longrightarrow \alpha \left| \varphi_1 (-, -\infty) \right| c_{2 \uparrow} \left| \text{vac} \right> - \frac{\beta S}{\sqrt{2}} \left| \phi_{1 \downarrow} (-, -\infty) \right> \left| \text{vac} \right>$$

$$+ \frac{\beta}{2} \left( \left| \varphi_1 (-, -\infty) \right| c_{2 \downarrow} + \left| \varphi_1 (-, -\infty) \right| c_{2 \downarrow} \right) \left| \text{vac} \right>$$

$$- \frac{\beta r}{2} \left( \left| \varphi_1 (-, -\infty) \right| c_{2 \downarrow} - \left| \varphi_1 (-, -\infty) \right| c_{2 \downarrow} \right) \left| \text{vac} \right>. \quad (35)$$

5. Bound triple (BT)

We now consider the three-particle bound state, BT, in the extended Bose–Hubbard model. For the sake of simplicity, we directly investigate the system in the limit $|V| \gg |U|$, where the perturbation method is applicable and provides a clear physical picture. The BT state is constructed by the three-particle cluster in the configurations $a_{1-1}^\dagger a_{1+1}^\dagger \left| \text{vac} \right>$ and $a_{12}^\dagger a_{13}^\dagger \left| \text{vac} \right>$, which possess the same diagonal energy $2V$. Since the transition strength between them (or the bandwidth of the new composite particle) is of the order of $t$, there may exist a fast transfer mode in such a system. Accordingly, its dynamics obeys the following effective Hamiltonian,

$$\mathcal{H}_{\text{BT}} = -\sqrt{2} t \sum_{i=1}^{N} \left( \sqrt{2} \left| 3i - 2 \right> \left( 3i - 1 \right) + \left| 3i - 1 \right> \left( 3i + 1 \right) + h.c. \right) \right) \quad (36)$$

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which is obtained based on the quasi-invariant subspace with diagonal energy $2V$ spanned by the basis $\{ |l\rangle, l \in [1, 3N]\}$:

$$
|l\rangle_1 = \begin{cases}
    a_{i/3}^\dagger a_{i+3}^\dagger a_{i+6}^\dagger |\text{vac}\rangle, & (\text{mod}(l, 3) = 0), \\
    a_{(i+2)/3}^\dagger a_{(i+5)/3}^\dagger \sqrt{2} |\text{vac}\rangle, & (\text{mod}(l, 3) = 1), \\
    a_{(i+1)/3}^\dagger a_{(i+4)/3}^\dagger \sqrt{2} |\text{vac}\rangle, & (\text{mod}(l, 3) = 2).
\end{cases}
$$

(37)

The effective Hamiltonian $H_{\text{BT}}$ depicts a period-3 or trimerized chain system, which can be further brought to a diagonal form,

$$
H_{\text{BT}} = \sum_k \Lambda_k |k\rangle \langle k|,
$$

(38)

where $k = 2\pi n/N, n \in [1, N]$ is the momentum and $|k\rangle$ is the eigenstate of $H_{\text{BT}}$. Here we have used the Fourier transformation

$$
|\lambda, k\rangle = \frac{1}{\sqrt{N}} \sum_{l=1}^{N} e^{-ikl} |3l - \lambda\rangle,
$$

(39)

to construct the secular equation

$$
\begin{pmatrix}
    0 & -2t & -\sqrt{2}te^{ik} \\
    -2t & 0 & -\sqrt{2}t \\
    -\sqrt{2}te^{ik} & -\sqrt{2}t & 0
\end{pmatrix}
\begin{pmatrix}
    \gamma_{1,k} \\
    \gamma_{2,k} \\
    \gamma_{3,k}
\end{pmatrix}
= \Lambda_k
\begin{pmatrix}
    \gamma_{1,k} \\
    \gamma_{2,k} \\
    \gamma_{3,k}
\end{pmatrix}
$$

(40)

for the eigenstate $|k\rangle = \sum_{\lambda=1}^{3} \gamma_{\lambda,k} |\lambda, k\rangle$. The spectrum $\Lambda_k$ is the solution of $\Lambda_k^3 - 8t^2 \Lambda_k + 8t^3 \cos k = 0$, which possesses gaps at $\pm \pi/3$ and $\pm 2\pi/3$ due to trimerization. Nevertheless, in the case of the weak trimerization, the eigenstates around $\pm \pi/2$ are hardly influenced by fast and robust against the spreading. Then the Gaussian wavepacket of the form (23) with $k_0 = \pm \pi/2$ should be still fast and robust against the spreading. The corresponding optimal three-particle wavepacket is denoted as $|\chi(\pm, N_c)\rangle$. The scheme to perform the coherent separation of a BT is based on the system depicted by the Hamiltonian

$$
H_{\text{BTS}} = -t \sum_{i=-\infty}^{+\infty} (a_i^\dagger a_{i+1} + \text{h.c.}) + V \sum_{i=-\infty}^{+\infty} n_in_{i+1} + \frac{U_s}{2} n_3(n_3 - 1) + V n_3.
$$

(41)

To investigate the scattering process of an input BT wave from the left, one can establish an effective Hamiltonian in the quasi-invariant subspace with diagonal energy $2V$ spanned by the basis $\{ |l\rangle_\text{ts}, l \in \mathbb{Z}\}$ defined as

$$
|l\rangle_\text{ts} = \begin{cases}
    (37), & (l \leq 2) \\
    a_0^\dagger a_1^\dagger a_3^\dagger |\text{vac}\rangle, & (l = 3) \\
    a_{4-l}^\dagger a_2^\dagger a_3^\dagger |\text{vac}\rangle, & (l \geq 4).
\end{cases}
$$

(42)

The corresponding equivalent effective Hamiltonian can be written as

$$
H_{\text{BTS}} = -t \left( \sqrt{2} \sum_{l=-\infty}^{+\infty} |l\rangle_\text{ts} \langle l + 1| - t |0\rangle_\text{ts} \langle 3| - (2 - \sqrt{2}) t \sum_{j=-\infty}^{0} |3j + 1\rangle_\text{ts} \langle 3j + 2| + \text{h.c.},
$$

(43)
which is illustrated in figure 5(c). An equivalent system is two connected semi-infinite chains with a side coupled two-site segment at the joint linking them. In the optimal case, the perfect separation (or combination) process in the real space can be expressed as

$$|\chi(+, -\infty)\rangle \langle \text{vac}| \implies r |\chi(-, -\infty)\rangle \langle \text{vac}| + s |\varphi(-, -\infty)\rangle a_2^\dagger a_3^\dagger \langle \text{vac}|,$$

and the corresponding inverse process as

$$|\varphi(+, -\infty)\rangle a_2^\dagger a_3^\dagger \langle \text{vac}| \implies r |\varphi(-, -\infty)\rangle a_2^\dagger a_3^\dagger \langle \text{vac}| + s |\chi(-, -\infty)\rangle \langle \text{vac}|.$$

This separation process of a BT wavepacket is illustrated in figures 5(a) and (b) and also in figure 6(b). It is a little different from that of the BP. An incident three-particle wavepacket leaves an NN pair at the impurity, while the other particle is reflected to the left with a higher speed than that of the reflected BT wavepacket.

In order to verify the validity of the proposed scheme and find an appropriate range of parameter values to realize the coherent separation in practice, numerical simulations are performed. We compute the time evolution of an incident Gaussian wavepacket with the form of (23) in a finite system of (41) by the exact diagonalization technique. The incident wavepackets are taken with $\alpha = 0.1$ and $k_0 \in [0.4\pi, 0.5\pi]$. The corresponding success probability of the coherent separation $|s|^2$ is plotted in figure 6(a) for the cases with $U_s/t = 200$, $V/t = 10, 30, 50, 100$ and $\infty$ (which corresponds to the equivalent effective Hamiltonian (43)). For the sake of illustrating the coherent separation process, we plot the profile of the evolving wave function in the form of a contour map (figure 6(b)). It shows that the equivalent effective Hamiltonian (43)
Figure 6. Plots of the numerical simulation for the coherent separation of a BT Gaussian wavepacket. (a) The success probability of the coherent separation of an incident wavepacket with $\alpha = 0.1$ and $k_0 \in [0.4\pi, 0.5\pi]$ in the systems with $V = 10, 30, 50, 100$ and $\infty$ ($H_{\text{BTS}}$) in units of $t$. (b) Contour plot of the profile of the wave function in the scattering process in the system with $V = 100$ for the incident BT Gaussian wavepacket with $\alpha = 0.1$ and $k_0 = \pi/2$.

is appropriate to describe the dynamics of the BT in the large $V$ limit. In the case of moderate $V$, the efficiency of the coherent separation is still high, especially for the broad wavepacket.

6. Summary

We studied the BP and BT states in the extended Hubbard model. We found that the resonant NN interaction can induce the BP and triple states. They are distinct from the known ones in previous work, as their bandwidths are comparable with those of a single particle. In other words, the bandwidths of the bound clusters can be drastically widened by the NN interaction. We proposed relatively simple schemes to realize the coherent separation of these bound clusters. The exact result showed that the success probability of coherent separation is unity for a BP whereas it approaches unity for a BT in the optimal systems. We also studied the singlet BP in the extended Fermi–Hubbard system. We showed that the corresponding coherent separation process can be utilized to create long-distance entanglement without the need for the temporal control and measurement process. Finally, we believe that our study will shed more light on directions for future research on the multi-particle bound state.

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