Perfect coherent shift of bound pairs in strongly correlated systems

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In the present work we extend the concept of coherent shift for the extended Bose-Hubbard model and Fermi-Hubbard model. We present two types of local bound pair (BP) for Bose system and one type for Fermi system. It is shown exactly that the perfect coherent shift can be achieved in such models. We find that for a Bose on-site BP, the perfect coherent shift condition depends on the nearest-neighbor interaction strength and the momentum of the incident single particle wavepacket, while for the other two types of BPs, it is independent of the initial state in the proposed systems.

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I. INTRODUCTION

Bound pair (BP) state and its dynamics are interesting recent topics in quantum physics and quantum information [1][11]. In a previous work [10], we studied the dynamics of a BP and the interaction between a single particle and a BP. Within the large U regime, we first found an interesting scattering process, coherent shift, between them. We believed that, this phenomenon should not be exclusive and could be applied to quantum device design. In addition, M. Valiente et al. performed a comprehensive numerical simulation of such a scattering process, which is useful to understand this phenomenon [12]. It was pointed that a perfect coherent shift is hardly realized in such a uniform Bose-Hubbard system. In this paper, we present three examples to demonstrate how to realize the perfect coherent shift in both boson and fermion systems. We present two types of local BP for Bose system and one type for Fermi system. It is shown exactly that the perfect coherent shift can be achieved in such models. We find that for a Bose on-site BP, the perfect coherent shift condition depends on the nearest-neighbor (NN) interaction strength and the momentum of the incident single particle wavepacket, while for the other two types of BPs, it is independent of the initial state in the proposed systems. Our results indicate that the coherent shift phenomenon has a great potential for future applications.

The article is organized as follows: In Sec. II, we introduce an extended Bose-Hubbard and the formation of the two particle bound state. In Sec. III, we investigate the coherent shift process for an on-site BP in the case of weak NN interaction. Sec. IV is devoted to the same discussion for the NN BP. In Sec. V, we introduce the on-site BP in the Fermi system and demonstrate how to perform a perfect coherent shift. Sec. VI is the conclusion and a short discussion.

II. EXTENDED BOSE-HUBBARD MODEL

We begin with the Bose on-site BP, considering the scattering process between it and a single boson in an extended Bose-Hubbard model. The Hamiltonian reads

\[ H^B = -\kappa \sum_i \left( a_i^\dagger a_{i+1} + \text{H.c.} \right) + \frac{U}{2} \sum_i n_i (n_i - 1) + V \sum_i n_i n_{i+1}, \]

where \( a_i^\dagger \) \((a_i)\) is the particles creation (annihilation) operator and \( n_i = a_i^\dagger a_i \) is the number operator at the \( i \)th lattice site. The tunneling strength and the on-site interaction between bosons are denoted by \( \kappa \) and \( U \). Hamiltonian Eq. (1) has an additional NN interaction \( V \) in comparison to the original Hamiltonian Eq. (1) in previous paper [10].

First of all, a state in the two-particle Hilbert space, as shown in Ref. [10], can be written as

\[ |\psi_k \rangle = \sum_{k,r} f_k(r) |\varphi_{r}^k \rangle, \quad (2) \]

with

\[ |\varphi_{0}^k \rangle = \frac{1}{\sqrt{2N}} \sum_{j} e^{ikj} a_j^\dagger |\text{vac}\rangle, \quad (3) \]

\[ |\varphi_{r}^k \rangle = \frac{1}{\sqrt{N}} e^{ikr/2} \sum_{j} e^{ikj} a_j^\dagger a_{j+r}^\dagger |\text{vac}\rangle, \]

here |\text{vac}\rangle is the vacuum state for the boson operator \( a_i \). \( k = 2\pi n/N, n \in [1, N] \) denotes the momentum with \( N = 2N_0 + 1 \), and \( r \in [1, N_0] \) is the distance between the two particles. The matrix representation for the Hamiltonian operator \( H^B \) in the basis \( \{ |\varphi_{j}^k \rangle \} \) is

\[ H^k = \begin{pmatrix} U & \sqrt{2} T^k & T^k & \cdots & \cdots \\ \sqrt{2} T^k & V & T^k \ & & \ \ T^k \ & & \cdots & \cdots \\ \cdots \ & & \cdots & \cdots \\ \cdots \ & & \cdots & \cdots \\ T^k \ & & \cdots & \cdots \ \ T^k \ & & \cdots & \cdots \ \end{pmatrix}, \quad (4) \]
where $T^k = -2\kappa \cos (k/2)$, and $T^k_N = (-1)^n T^k$. Note that for an arbitrary $k$, the eigenvalues of $T^k$ are equivalent to that of the single-particle $N_0+1$-site tight-binding chain system with one abnormal NN hopping amplitude $\sqrt{2}T^k$ between 0th ($|\phi^k_0\rangle$) and 1st site ($|\phi^k_1\rangle$), and the on-site potentials $U$, $V$ and $T^k_N$ at 0th, 1st and $N_0$th sites respectively. It follows that 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 with $|U - V| \gg |\kappa|$, the particle can be localized at either 0th or 1st site, corresponding to (i) the on-site BP state, or (ii) the NN BP state. Interestingly, in the case of $U = V$, and $|U|, |V| \gg |\kappa|$, the particle can be in the bonding state (or anti-bonding state) between 0th and 1st sites, which was discussed in Ref. [13]. In previous works [10, 11], the bound states of (i) and (ii) were well investigated. In Ref. [10], it was shown that the coherent shift of an on-site BP occurs when it meets a single particle. In the following we focus on the scattering process between a BP and a single particle in the presence of the NN interaction. We will show exactly that the NN interaction can lead to the perfect coherent shift.

III. ON-SITE BOUND PAIR IN BOSE SYSTEM

Now we start with the on-site BP state. The formation of bound pair state in the Bose-Hubbard system was studied in Ref. [1, 9, 11]. Here in the extended Bose-Hubbard model, the on-site BP corresponds to the BP bounded by $U$ in the case of large $U$ but weak $V$, with $|U| \gg |\kappa| \sim |V|$. In this case, the solution of $f^k(r)$ has the form

$$f^k(r) \simeq \begin{cases} 1, & (r = 0), \\ 0, & (r \neq 0). \end{cases}$$

with eigenenergy

$$\varepsilon_k \simeq U + \frac{4\kappa^2}{U} (\cos k + 1).$$

One can see that the on-site BP state acts as a composite particle with effective hopping strength being $2\kappa^2/U$. According to Ref. [10], the effective Hamiltonian for a single on-site BP and a single particle in the extended Bose-Hubbard system can be obtained in the form

$$H^U_{\text{eff}} = -\kappa \sum_i (\tilde{a}^\dagger_i \tilde{a}_{i+1} + 2\tilde{b}^\dagger_i \tilde{b}_{i+1} \tilde{a}^\dagger_i \tilde{a}_{i+1} + \text{H.c.})$$

$$+ \frac{2\kappa^2}{U} \sum_i (\tilde{b}^\dagger_i \tilde{b}_{i+1} + \text{H.c.})$$

$$+ \left(2V - \frac{7\kappa^2}{2U}\right) \sum_i \tilde{b}^\dagger_i \tilde{b}_i \left(\tilde{a}_{i-1}^\dagger \tilde{a}_{i-1} + \tilde{a}_{i+1}^\dagger \tilde{a}_{i+1}\right)$$

$$+ \left(U + \frac{4\kappa^2}{U}\right) \sum_i \tilde{b}^\dagger_i \tilde{b}_i,$$

where $\tilde{a}_i$ and $\tilde{b}_i$ denote the hardcore bosons satisfying the following commutation relations $[\tilde{a}_j, \tilde{a}_i^\dagger] = [\tilde{b}_j, \tilde{b}_i^\dagger] = [\tilde{b}_j, \tilde{b}_i] = [\tilde{a}_j, \tilde{a}_i] = 0$, $(i \neq j)$; $\{\tilde{a}_i, \tilde{a}_j^\dagger\} = \{\tilde{b}_i, \tilde{b}_j^\dagger\} = 1$; $\{\tilde{b}_i, \tilde{a}_j\} = \{\tilde{a}_i, \tilde{b}_j\} = 0$. The former two terms of $H^U_{\text{eff}}$ depict the hoppings while the last two terms depict the interaction between the two kinds of particles. Considering the scattering problem without loss of generality, we set the particle $\tilde{b}_i^\dagger |\text{vac}\rangle$ at the 0th site and incident the particle $\tilde{a}_i^\dagger |\text{vac}\rangle$ from $-\infty$ at the beginning. For the scattering process between them within short duration, the particle $\tilde{b}_i^\dagger |\text{vac}\rangle$ is static compared to the single particle $\tilde{a}_i^\dagger |\text{vac}\rangle$. Then the whole scattering process dominantly governed by

$$H^U_{\text{eff}} = -\kappa \sum_{i=-\infty}^{0} \tilde{a}^\dagger_i \tilde{a}_{i+1} - 2\kappa \tilde{b}^\dagger_{-1} \tilde{b}_0 \tilde{a}^\dagger_0 \tilde{a}_{-1} + \text{H.c.}$$

$$+ 2V(\tilde{a}^\dagger_1 \tilde{a}_{-1} \tilde{b}^\dagger_0 \tilde{b}_0 + \tilde{b}^\dagger_{-1} \tilde{b}_1 \tilde{a}^\dagger_0 \tilde{a}_0)$$

$$+ U \tilde{b}^\dagger_0 \tilde{b}_0 + U \tilde{b}^\dagger_{-1} \tilde{b}_{-1},$$

at the condition $|U| \gg |\kappa| \sim |V|$. Here we neglected the terms with $\kappa^2/U$ and $\kappa^2/V$. The swapping process between a single particle and an on-site BP is the key of the coherent shift, which is schematically illustrated in Fig. 1(a). The scattering process is represented in the form

$$\tilde{a}^\dagger_{-\infty} \tilde{b}^\dagger_0 |\text{vac}\rangle \rightarrow r \tilde{a}^\dagger_{-\infty} \tilde{b}^\dagger_0 |\text{vac}\rangle + t \tilde{a}^\dagger_0 \tilde{b}^\dagger_{-1} |\text{vac}\rangle,$$

where $r$ and $t$ are the reflection and transmission (coherent shift) amplitudes, respectively.
The process of Eq. (9) can be rewritten as

In order to investigate the above Hamiltonian Eq. (8), we define a new set of basis \( \{|l\>\} \) as

\[
|l\> = \begin{cases} \tilde{a}^\dagger_l |0\rangle |\text{vac}\rangle, & (l < 0), \\ \tilde{a}^\dagger_{l+1} |1\rangle |\text{vac}\rangle, & (l \geq 0), \end{cases} \tag{10}
\]

and then reduce the two-body problem to a single particle problem. Actually, acting the Hamiltonian of Eq. (8) or the original Hamiltonian Eq. (1) on the basis (10), we obtain the equivalent single particle Hamiltonian

\[
H_{sp} = -\kappa \left( \sum_{l=0}^{\infty} + \sum_{l=-\infty}^{-2} \right) |l\> \langle l + 1| - 2\kappa |1\> \langle 0| + \text{H.c.}
+ 2\kappa |1\> \langle 1| + |0\> \langle 0|. \tag{11}
\]

The physics of the equivalent Hamiltonian is obvious, which describes a particle in the chain with an embedded impurity. The impurity consists of two neighboring sites with identical on-site potentials \( 2V \) and the tunneling strength \( 2\kappa \) between them. Fig. 2 is a schematic illustration of the equivalent effective Hamiltonian arising from the interaction of the central system with the leads

\[
\sum^R = \begin{pmatrix} -\kappa e^{ik} & 0 \\ 0 & -\kappa e^{ik} \end{pmatrix}. \tag{15}
\]

The transmission probability is given by

\[
|t|^2 = T_{12} = \text{Tr} \left[ \Gamma_1 G^R \Gamma_2 G^A \right]. \tag{16}
\]

Then we can obtain the transmission probability as,

\[
T_{12} = \frac{16 \sin^2 k}{\left( 4 (V/\kappa + l)^2 + 4 (V/\kappa + l) \cos k + 1 \right)}. \tag{18}
\]

Noting that the transmission coefficient is \( k \) dependent, we calculate the resonant transmission or perfect coherent shift. For \( T_{12} = 1 \), we have the NN coupling constant \( V = V_R \), where

\[
V_R = \frac{\kappa}{2} \left( -\cos k \pm \sqrt{\cos^2 k + 3} \right). \tag{19}
\]

It is worth noting that Eq. (19) is available for any \( k \), since \( V_R \) is always in the order of \( \kappa \). In practice, this process can be implemented via a broad wavepacket. For the case of \( k = \pi/2 \), which corresponds to the stabllest and fastest wave packet (17), we can generate a unitary swap between an on-site BP and a single particle under the condition \( V_R = \pm \sqrt{3}\kappa/2 \). In this condition, the \( k \) dependent transmission coefficient \( T_{12} (k) = 4 \sin^2 k / (4 - \cos^2 k) \). Then we get the conclusion that the perfect coherent shift can be achieved in the large \( U \) Bose-Hubbard model with weak NN interaction.

IV. NN BOUND PAIR IN BOSE SYSTEM

Now we consider another kind of bound pair in the extended Bose-Hubbard model (1). This bound pair is bounded by the NN interaction \( V \) rather than the on-site interaction \( U \). In large \( V \) limit, \( |V|, |V - U| \gg |\kappa| \), a pair of hardcore bosons can be bounded by the NN interaction \( V \). This was pointed out by M. Valiente et al. in their work (11). In such condition, the dynamics
of a single boson and an NN BP can be depicted by the following effective Hamiltonian

\[
H_\text{eff} = -\kappa \sum_i \left( a_i^\dagger a_{i+1} + B_i^\dagger B_{i+2} a_{i+3} a_i + \text{H.c.} \right) + \left( \frac{\kappa}{V} + \frac{2\kappa^2}{V - U} \right) \sum_i (B_i^\dagger B_{i+1} + \text{H.c.}) - \frac{2\kappa^2}{V} \sum_i (B_i^\dagger B_{i+2} a_{i-2} + B_{i+1}^\dagger B_i a_{i+3} a_{i+3}) + \left( V + \frac{2\kappa^2}{V} + \frac{4\kappa^2}{V - U} \right) \sum_i B_i^\dagger B_i,
\]

where the NN pair operator is defined as \( B_i^\dagger = a_i^\dagger a_{i+1}. \)

For the scattering process between the NN BP and the single particle within short duration, it is dominantly governed by the first term, which includes the hopping of a single particle and the swapping between them. The swapping process is schematically illustrated in Fig. 1(b). We consider the scattering problem between a single particle and an NN BP. Initially, an NN BP \( B_2^\dagger \) \( |\text{vac}\rangle \) is located at the dimer of sites 2 and 3, while a single particle \( a^\dagger |\text{vac}\rangle \) is located at the left. Similarly, we can define a set of basis \( \{ |l\rangle \}_v \) as

\[
|l\rangle_v = \begin{cases} a_i^\dagger B_i^\dagger |\text{vac}\rangle = a_i^\dagger a_{i+1}^\dagger |\text{vac}\rangle, & (l \leq 0) \\ B_0^\dagger a_i^\dagger |\text{vac}\rangle = a_i^\dagger a_{i+2}^\dagger |\text{vac}\rangle, & (l > 0) \end{cases}
\]

Acting the Hamiltonian Eq. \( \text{29} \) on the basis Eq. \( \text{21} \), after neglecting the high order terms \( \kappa^2/V \) and \( \kappa^2/(V - U) \), we obtain a uniform tight-binding chain. Obviously, such a system can realize the perfect coherent shift for any incident single particle wave with the shift distance being two lattice spacings. Comparing to the previous on-site BP, the perfect coherent shift of the NN BP is \( k \) independent.

V. ON-SITE BOUND PAIR IN FERMI SYSTEM

As pointed out in Ref. \( \text{12} \), the nonzero reflection of a single incident particle in the coherent shift process \( \text{10} \) is attributed to the swapping strength being \( 2\kappa \) rather than \( \kappa \). Essentially, this arises from the identity of two particles of the bound pair. Consequently, for a system with the bound pair consists of two particles with opposite spins, the unexpected reflection should be avoidable.

Now we turn to the Fermi system. A one-dimensional Fermi-Hubbard Hamiltonian reads

\[
H^F = -\kappa \sum_{i,\sigma} (c_i^\dagger c_{i+1,\sigma} + \text{H.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow},
\]

where \( c_i^\dagger \) is the creation operator of the fermion at the site \( i \) with spin \( \sigma = \uparrow, \downarrow \) and \( U \) is the on-site interaction. Similarly, there also exists bound pair state in such a system. Actually, a state in the two-particle Hilbert space with spin zero can be written as the form of Eq. \( \text{2} \), where we redefine the corresponding basis as

\[
|\phi^F_0\rangle = \frac{1}{\sqrt{N}} \sum_j e^{ik_0 j} c_{j,\uparrow}^\dagger c_{j,\downarrow}^\dagger |\text{vac}\rangle,
\]

\[
|\phi^F_c\rangle = \frac{1}{\sqrt{2N}} \sum_j e^{ik_0 j} \left( c_{j+1,\uparrow}^\dagger c_{j,\downarrow}^\dagger + c_{j,\uparrow}^\dagger c_{j+1,\downarrow}^\dagger \right) |\text{vac}\rangle.
\]

Then all the analysis for the formation of a Bose on-site BP can be applied completely on that of a Fermi on-site BP. Besides, in the large \( U \) limit, the effective Hamiltonian describing the dynamics of a single particle and a Fermi on-site BP has the form

\[
H_{\text{eff}}^F = -\kappa \sum_{i,\sigma} (\tilde{c}_{i,\sigma}^\dagger \tilde{c}_{i+1,\sigma} + \tilde{c}_{i,\sigma}^\dagger \tilde{c}_{i+1,\sigma} d_{i+1}^\dagger d_i + \text{H.c.}) + \frac{2\kappa^2}{U} \sum_i \left( d_i^\dagger d_{i+1} + \text{H.c.} \right) + \frac{2\kappa^2}{U} \sum_i \tilde{c}_{i,\sigma}^\dagger \tilde{c}_{i,\sigma} \left( d_{i-1}^\dagger d_{i-1} + d_{i+1}^\dagger d_{i+1} \right) + \left( U + \frac{4\kappa^2}{U} \right) \sum_i d_i^\dagger d_i,
\]

where \( \tilde{c}_{i,\sigma} = c_{i,\sigma} (1 - n_{i-\sigma}) \) is the projected fermion creation operator, \( d_i = c_{i,\uparrow} c_{i,\downarrow} \) is the on-site BP operator. The projector \( (1 - n_{i-\sigma}) \) allows to create an electron with spin \( \sigma \) at the site \( i \) only if there is no other electron on that site. For the scattering process between \( \tilde{c}_{i,\sigma} \) and \( d_i \) within short duration, it is dominantly governed by the first term, which includes the hopping of the single particle and the swapping between them. The swapping process is schematically illustrated in Fig. 1(c). We note that the swapping operation \( \tilde{c}_{i,\sigma}^\dagger \tilde{c}_{i+1,\sigma} d_{i+1}^\dagger d_i \) has the same coupling strength with the term \( \tilde{c}_{i,\sigma}^\dagger \tilde{c}_{i+1,\sigma} \). This allows the perfect coherent shift. In addition, such a process is independent of the momentum of the incident particle and the spin polarization, since the bound pair is singlet.

VI. CONCLUSION

In summary, we present three kinds of bound pairs and the corresponding optimal systems, which can avoid unexpected reflection in the coherent shift process. It is shown exactly that the perfect coherent shift can be achieved in the simply engineered systems. For a Bose on-site BP, the perfect coherent shift requires the resonant condition, which depends on the NN interaction strength and the momentum of the incident single particle wavepacket. For a Bose NN BP and a Fermi on-site BP, the perfect coherent shifts occur for an arbitrary initial state in the simple chain systems. We believe that our findings have a great potential for future applications.
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