Hybrid atom-molecule quantum walks in one-dimensional optical lattice

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We study hybrid atom-molecule quantum walks in one-dimensional optical lattices with two interacting bosonic atoms which may be converted into a molecule. The hybrid atom-molecule energy bands include a continuum band and two isolated bands, which respectively correspond to scattering states and dressed bound states (DBS’s). Because of the atom-molecule coupling, the DBS’s may appear even in the absence of atom-atom interaction. From an initial state of two atoms occupying the same site, in addition to independent quantum walks which correspond to scattering states, correlated quantum walks appear as a signature of DBS’s. Even if the atom-atom interaction and the atom-molecule coupling are much stronger than the tunneling strengths, independent quantum walks may still appear under certain resonant conditions. The correlated quantum walks show two light-cones with different propagation velocities, which can be analytically explained by the effective tunneling strengths of the two different DBS’s.

I. INTRODUCTION

Quantum walks (QWs) [1], a direct result of quantum interference of different paths, have been extensively studied in both theory and experiments [2–5]. QWs can be exploited to various fields, from universal quantum computing [6], efficient quantum algorithm [7–11], energy transfer [12], to topological state detection [13, 14]. Single-particle QWs have already been implemented by various systems including ultracold atoms [15], ultracold ions [16], photonic waveguides [17] and atomic spin-impurities [18] etc. Moreover, it has also been demonstrated that single-particle QWs can be implemented via classical waves [19].

Beyond single-particle QWs, two-particle QWs have attracted extensively interests in recent years. The nonclassical correlation between non-interacting particles, i.e., the bunching and anti-bunching behavior, are found to depend strongly on the quantum statistical properties [20–22]. On the other hand, interaction between particles in a lattice is believed to be beneficial to universal quantum computation [23]. The interacting two-particle QWs have been discussed and implemented [24–26]. The interaction is found to strongly affect the spatial correlations [27]. Particularly, the repulsively or attractively interacting (quasi-)particles can form a bound pair [28, 29]. Therefore, besides the independent QWs, there is the co-walking of the bound pair [24, 27, 30].

Although the QWs of interacting particles have been extensively studied, it still remains unclear about the QWs involving atom-molecule coupling. According to the two-channel theory [31–34], a pair of atoms can be converted into a molecule. For two bosons in optical lattices, due to the atom-molecule coupling, their energy spectrum includes two isolated bands and a continuum one [31–34]. The states in isolated bands are in superposition of atomic bound state and molecular state, which are called the dressed bound states (DBS’s) in the following context. Under specific conditions, the DBS’s can be tuned to enter the continuum band and thus lead to so-called scattering resonance [32]. Therefore, it is intriguing to explore the signature of DBS’s in QWs.

In this article, by considering a one-dimensional (1D) Bose-Hubbard model with atom-molecular coupling, we study the QWs from two interacting Bose atoms occupying the same lattice site. We focus on exploring the interplay among atom-molecule coupling, atom-atom interaction and atom-molecule energy detuning. Without the atom-atom interaction, there are two kinds of DBS’s supported by pure atom-molecule coupling. Such an atom-molecule coupling may play the role of atom-atom interaction and then result in the correlated QWs. Due to the atom-molecule energy difference, the atom-atom interaction can be balanced under certain resonant conditions and so that the DBS’s are broken into scattering states. Under strong interactions, the QWs show two light-cones corresponding to the two DBS bands. By using the many-body degenerate perturbation theory, we give the effective models for the QWs of DBS’s, in which the effective tunneling strengths of DBS’s can be tuned by the atom-molecule energy difference. Specifically, the interplay between tunnelings of atoms and molecule can suppress the nearest-neighbor (NN) tunneling of DBS’s.

The paper is organized as follows. In Sec. II, we introduce our hybrid atom-molecule system and solve its energy bands. In Sec. III, we present the QWs from two atoms occupying the same site. In particular, we discuss how the QWs are affected by the pure atom-atom interaction (III A), the pure atom-molecule coupling (III B) and

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the interplay between atom-atom interaction and atom-molecule coupling (III C). In Sec. IV, we derive effective models for the QWs of DBS’s. At last, we make a brief summary and discussion of our results.

II. HYBRID ATOM-MOLECULE ENERGY BANDS

We consider two interacting Bose atoms in 1D optical lattices, where the two atoms can be converted into a molecule state via atom-molecule coupling. The system obeys the Hamiltonian,

$$\hat{H} = - \sum_{l=-L}^{L} \left( J_a \hat{\alpha}_l^\dagger \hat{\alpha}_{l+1} + J_m \hat{\mu}_l^\dagger \hat{\mu}_{l+1} + H.c. \right) \\
+ \frac{U}{2} \sum_{l=-L}^{L} \left( \hat{\mu}_l^a (\hat{\mu}_l^a - 1) + g \sum_{l=-L}^{L} \left( \hat{\alpha}_l^a \hat{\alpha}_{l+1}^a \hat{\mu}_l + H.c. \right) \\
+ \sum_{l=-L}^{L} \left( \varepsilon_a \hat{\mu}_l^a + \varepsilon_m \hat{\mu}_l^m \right) \right). \tag{1}$$

Here, $g$ is on-site atom-molecule coupling strength, $U$ is on-site background atom-atom interaction, $J_a(J_m)$ is the atomic(molecular) tunneling strength, $\varepsilon_a(\varepsilon_m)$ is the atomic(molecular) on-site energy, the lattice site index $l$ ranges from $-L$ to $L$, the total number of lattice sites is $L_1 = 2L + 1$ and the periodic boundary condition (PBC) is imposed. The bosonic operators $\hat{\alpha}_l^a (\hat{\mu}_l^a)$ and $\hat{\alpha}_l (\hat{\mu}_l)$ create and annihilate an atom (molecule) on the $l$-th site, respectively. Compared with the atomic tunneling strength $J_a$, the molecular tunneling strength $J_m$ is much smaller and so that it can be neglected [33, 35, 36]. Thus we set $J_m = 0$ in our numerical calculations, but still keep it in our analytical calculations. The atom-molecule coupling $g$ can be realized by applying magnetoassociation [37] or photoassociation [38, 39] technique. The on-site energies $\varepsilon_{a,m}$ can be tuned by applying external magnetic field.

The hybrid atom-molecule Hilbert space can be spanned by a complete set of orthogonal basis,

$$\mathcal{H}^{(2)} = \{ |l_1 l_2\rangle_a \oplus |j\rangle_m \}. \tag{2}$$

Here, $|j\rangle_m = \hat{\mu}_j^\dagger |0\rangle (-L \leq j \leq L)$ denotes the state of one molecule in the $j$-th lattice site, while $|l_1 l_2\rangle_a = (1 + \delta_{l_1 - l_2})^{-1/2} \hat{\alpha}_{l_1}^\dagger \hat{\alpha}_{l_2}^\dagger |0\rangle (-L \leq l_1 \leq l_2 \leq L)$ denotes the state of one atom in the $l_1$-th site and one atom in the $l_2$-th site, where $\delta_{l_1 - l_2}$ is Kronecker delta function. Hence, one can expand the eigenstates as, $|\Phi\rangle = \sum_{l_1 \leq l_2} \phi_{l_1 l_2} |l_1 l_2\rangle_a + \sum_{j} \varphi_j |j\rangle_m$. Thus, the eigenstate problem $\hat{H} |\Phi\rangle = E |\Phi\rangle$ is described by the coupled equations

$$\sum_{l_1 \leq l_2} \phi_{l_1 l_2} |l_1 l_2\rangle_a \langle l_1 l_2 | \hat{H} |l_1 l_2\rangle_a + \sum_{j} \varphi_j |l_1 l_2\rangle_a \langle l_1 l_2 | \hat{H} |j\rangle_m = E \phi_{l_1 l_2},$$

$$\sum_{j \neq j'} \varphi_{j'} |j\rangle \langle j' | + \sum_{l_1 \leq l_2} \phi_{l_1 l_2} |j\rangle \langle j | \hat{H} |l_1 l_2\rangle_a + E \varphi_j. \tag{3}$$

For simplicity, we define $\psi_{l_1 l_2} = (1 + \delta_{l_1 l_2})^{1/2} \phi_{l_1 l_2}$ and so that the normalization coefficient is eliminated. After some algebraic calculation, using commutation relations of bosonic operators, one can obtain

$$E \psi_{l_1 l_2} = -J_a (\psi_{l_1 l_2 + 1} + \psi_{l_1 - 1 l_2} + \psi_{l_1 l_2 + 1} + \psi_{l_1 l_2 - 1}),$$

$$+ \delta_{l_1 - l_2} U \psi_{l_1 l_2} + 2 \varepsilon_m \psi_{l_1 l_2} + 2 g \delta_{l_1 \delta_{l_2} j' \varphi_j}. \tag{4a}$$

$$E \varphi_j = -J_m (\varphi_{j + 1} + \varphi_{j - 1} + \varepsilon_m \varphi_j + g \delta_{l_1 \delta_{l_2} j' \varphi_j}. \tag{4b}$$

Obviously, Eq. (4a) and Eq. (4b) show the hybridization of atomic and molecular states. To solve these equations, we adopt the ansatz

$$\psi_{l_1 l_2} = C_a e^{iK_a R_a \xi(r)},$$

$$\varphi_j = C_m e^{iK_m R_m}. \tag{5}$$

Here, $K_a, R_a = (l_1 + l_2)/2$ and $r = l_2 - l_1$ are respectively the center-of-mass (c.o.m.) quasi-momentum, c.o.m. position and relative position of atoms. Correspondingly, $K_m$ and $R_m = j$ are the molecular quasi-momentum and position, respectively. The coefficients $C_a$ and $C_m$ are the normalization constants. The function $\xi(r)$ is independent of $K_a$ and $R_a$,

$$\xi(r) = C_e e^{ik|r|} + C_- e^{-ik|r|}, \tag{6}$$

where $k$ can be real or complex and $C_\pm$ are unknown coefficients. From the physical point of view, the states of atoms $\psi_{l_1 l_2}$ can be expressed as Bloch-like function with independent c.o.m. part and relative motion part.

Before we go further, let us prove that $K_a = K_m = K$ for eigenstates. When $l_1 = l_2 = j \ (R_m = R_a = R)$, combining Eq. (4b) and Eqs. (5), we have

$$E + 2J_m \cos(K_m) - \varepsilon_m C_m e^{i(K_m - K_a)R} = \xi(0) C_a. \tag{7}$$

Because Eq. (7) holds for all $R \in [-L, L]$, we have $K_m = K_a$. For simplicity, we denote $K_m = K = K$ and restrict it in the first Brillouin zone from now on. Since the PBC requires $\psi_{l_1 l_2 + 1} = \psi_{l_1 l_2}, \varphi_{j + 1} = \varphi_j$, the c.o.m. quasi-momentum obeys $K = 2\pi n/L$, with $n = -L, -L + 1, \ldots, L$.

From Eqs. (4) and (5), introducing $\hat{E} = E - 2\varepsilon_a$ and $\Delta = \varepsilon_m - 2\varepsilon_a$, one can obtain

$$\hat{E} \xi(r) = J^K_a \xi(r + 1) + \xi(r - 1) + \delta_{r,0} U_{e\xi} \xi(r), \tag{8}$$

where $U_{e\xi} = U + 2g^2/($$\hat{E} - \Delta - J^K_a$) and $J^K_a = -2 J_a \cos(K/2)$, $J^K_m = -2 J_m \cos(K)$. Obviously, the atom-molecule coupling contributes an additional energy-dependent term in the effective interaction $U_{e\xi}$. This indicates that the atom-molecule coupling $g$ may play the role of atom-atom interaction $U$ and therefore DBS’s may appear even the atom-atom interaction is absent.

In the case of $\Delta \to \infty$ or $U \to \infty$, Eq. (8) can be approximated as

$$\hat{E} \xi(r) = J^K_a \xi(r + 1) + \xi(r - 1) + \delta_{r,0} U \xi(r), \tag{9}$$

which reduces to the case of no atom-molecule coupling [40].
and $L$ each dot represents the proportion of molecular states, which
k Eq. (\ref{eq:1})). Here, the value of
Furthermore, according to the PBC, $\xi(r)$ obeys $\xi(r+L)$ = $e^{iKL_r/2}\xi(r)$ and therefore one can obtain the
coefficients $C_{\pm}$

$$C_{\pm} = \frac{-J_aK^2i\sin k + \left(U + \frac{2g^2}{2J_a \cos k - \Delta - J_m}\right)(1)}{J_aK^2i\sin k + \left(U + \frac{2g^2}{2J_a \cos k - \Delta - J_m}\right)(1)}.$$

Furthermore, according to the PBC, $\xi(r)$ obeys $\xi(r+L) = e^{iKL_r/2}\xi(r)$ and therefore one can obtain the coefficients $C_{\pm}$

$$\left.C_{\pm} = \frac{-J_aK^2i\sin k - \left(U + \frac{2g^2}{2J_a \cos k - \Delta - J_m}\right)(1)}{-J_aK^2i\sin k + \left(U + \frac{2g^2}{2J_a \cos k - \Delta - J_m}\right)(1)}\right).$$

Combining Eqs. (\ref{eq:11}) and (\ref{eq:12}), one can determine $k$ by solving the following equation,

$$J_aK^2i\sin k - \left(U + \frac{2g^2}{2J_a \cos k - \Delta - J_m}\right) = (-1)^{KL_r/2}e^{-ikL_r}.$$

This equation is invariant under the transformation $k \rightarrow -k$ and thus $k$ can be restrained in $[0, \pi]$. Substituting the values of $k$ into Eq. (10), we obtain the eigenenergies of scattering states, which are denoted by the circular dots in Fig. 1. The explicit expression of $\xi(r)$ is given as

$$\xi(r) \sim (-1)^{KL_r/2}e^{-ikL_r}e^{ik|r|} + e^{-ik|r|},$$

which has the same form as the one of no atom-molecule coupling [27, 40].

B. Isolated bands

Isolated bands correspond to the states of complex values of $k$. If the atom-molecule coupling is absent, i.e. $g = 0$, the atomic and molecular states are decoupled and there appears an isolated band corresponding to the molecular states, see Fig. 1 (a). When $J_m = 0$, the isolated molecular band is exactly given as $\tilde{E} = \Delta$.

For non-zero atom-molecule couplings $g$, the isolated bands correspond to DBS’s, whose $k$ can be assumed as $k = \beta + i\eta$ (where $\beta$ and $\eta$ are both real numbers). Noting that the wavefunction must remain finite when $r \rightarrow \infty$, Eq. (6) can be rewritten as

$$\xi(r) = e^{(i\beta - \eta)|r|}.$$

For simplicity, we introduce $e^{i\beta - \eta} \equiv \alpha$, which satisfies $\alpha \in \mathbb{C}$ and $0 < |\alpha| < 1$. Thus $\xi(r)$ can be rewritten as

$$\xi(r) = \alpha^{|r|}.$$

This expression indicates that the wavefunctions of atomic states decay exponentially when the relative distance increases [40]. Combining Eqs. (8) and (16), one can obtain

$$\tilde{E} = 2J_aK^2 + \left(U + \frac{2g^2}{E - \Delta - J_m}\right)$$

for $r = 0$, and

$$\tilde{E} = J_aK^2(\alpha^{-1} + \alpha)$$

for $r > 0$. Here, $\tilde{E}$ and $\alpha$ are unknown parameters. To ensure real eigenenergies $\tilde{E}$, the parameter $\alpha$ must be real as well and so that we have $\beta = m\pi$ and $m \in \mathbb{N}$. By numerically solving Eqs. (17) and (18), we obtain two isolated bands for DBS’s, see the triangular dots in Fig. 1. The two isolated bands are consistent with the ones given by other methods [31–33]. From Eqs. (17) and (18), when $J_m = U = \Delta = 0$, we find that if $(\tilde{E}, \alpha)$ are their solutions, then $(-\tilde{E}, -\alpha)$ are also their solutions. This means that these two isolated bands are symmetric with respect to $\tilde{E} = 0$ when $J_m = U = \Delta = 0$. 

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig1.png}
\caption{Energy bands for different atom-molecule coupling strengths: (a) $g = 0$, (b) $g = 1$, (c) $g = 2$ and (d) $g = 4$. The parameters are set as $J_a = 1$, $J_m = 0$, $U = 0$, $\Delta = 0$ and $L_t = 21$. The circular and triangular dots denote the scattering states and the DBS’s, respectively. The color of each dot represents the proportion of molecular states, which is given by $P_m = \sum_j |\varphi_j|^2$.}
\end{figure}
C. Interplay among the atom-molecule coupling, the atom-atom interaction and the atom-molecule energy difference

Below, given $g = 4J_m = 4$ and $J_m = 0$, we will show how the atom-atom interaction ($U$) and the atom-molecule energy difference ($\Delta$) affect the energy spectrum.

To explore the interplay of $g$ and $U$, we choose $\Delta = 0$. For simplicity, we concentrate our discussion on the case of $U > 0$. Actually, the following discussion can be easily applied to the case of $U < 0$. We present the energy bands for different values of $U/g$ in Fig. 2. Clearly, the repulsive interaction gradually lifts the energy of isolated bands. Under strongly repulsive interaction, the lower isolated band enters into the continuum band and results in the resonance between scattering and bound states [31, 32], see Fig. 2 (d). Around resonance, the states display strong hybridization than other states in continuum band. When $U$ approaches to infinity, from Eq. 8, the eigenenergies for the lower and upper isolated bands are given as $\tilde{E} = \Delta$ and $\tilde{E} = U$, respectively. In this instance, the lower isolated band purely corresponds to the bare molecule, while the upper isolated band corresponds to the bounded atomic pair.

To explore the interplay of $g$ and $\Delta$, we choose different values of $\Delta \neq 0$ and fix $U = 0$. We show the energy bands for $\Delta/g = -5$ and $\Delta/g = 5$ in Fig. 3. Compared with Fig. 1 (d), one can find that the isolated bands are shifted by $\Delta$. The two isolated bands for DBS’s always sandwich the continuum band. We have proved that there are two DBS solutions for a given $K$ if $U = 0$ and $g \neq 0$, see Appendix. A for more details. When $\Delta \to +\infty (\Delta \to -\infty)$, the lower (upper) isolated band gradually approaches to the bottom (above) boundary of the continuum band, see Fig. 4 (a). As stated in the previous subsection, when $|\Delta|$ tends to infinity, the atomic and molecular states are gradually decoupled. Therefore, there is only one isolated band that corresponds to the bare molecular states. In the case of nonzero atom-atom interaction ($U \neq 0$), the atom-atom interaction will shift the two DBS levels up (or down) for $U > 0$ (or $U < 0$), see Fig. 4 (b).

To explore the interplay between the atom-molecule energy difference ($\Delta$) and the atom-molecule coupling ($g$), we choose different values of $\Delta$ and fix $U = 2g = 8$, see Fig. 5. When $\Delta/g \ll -1$, the upper and lower isolated bands are respectively dominated by the bounded atomic pairs and the molecular states, see Fig. 5 (a). With the increase of $\Delta$, the lower isolated band is gradually shifted from the bottom to the upper of the continuum band, see Fig. 5 (b) and (c). Particularly, for certain values of $\Delta$, the lower isolated band may completely merge into the continuum band, see Fig. 5 (d).
For a given $B$ (b), the separated atomic states are degenerate when $\Delta = 0$. Under this condition, a tiny atomic tunneling will immediately make the separated atomic scattering states and DBS's. If $J_m = 0$, from Eq. (19), one can find that there is only one DBS solution for all $K$ when $\Delta = 2g^2/U$, see Fig. 5 (b).

This can be understood by the atom-molecule coupling in the limit of $J_a = J_m = 0$, see Appendix. B. By solving the eigen-equation, one can obtain three different kinds of eigenstates. One kind of the eigenstates corresponds to the doped-molecule states, which are in superposition of atomic and molecular states $|d_i\rangle = A_\sigma |l_i\rangle_m + B_\sigma |l_i\rangle_a$. Here $A_\sigma$ and $B_\sigma$ are the coefficients of lower ($\sigma = 1$) and upper ($\sigma = 2$) doped-molecule states. The lower doped-molecule states and the separated atomic states are degenerate when $\Delta = 2g^2/U$ ($U > 0$). Under this condition, a tiny atomic tunneling will immediately make the separated atomic states into the atomic scattering states, and then the atomic scattering states couple with the doped-molecule states. That is why the degenerate condition is identical to condition where the lower isolated band merges into the continuum band.

D. Resonance between scattering states and DBS's

In this subsection, we discuss the resonance between scattering states and DBS's and give the resonant conditions. From Eqs. (17) and (18), one can give the energies for two isolated bands of DBS's. However, for non-zero atom-atom interaction $U$, we have proved that there may be only one solution under some specific conditions (see Appendix. A for more details). For a given $K$, the condition of only one solution of DBS's is given as

$$\frac{2g^2}{U} - 2|J_a^K| - J_m^K < \Delta < \frac{2g^2}{U} + 2|J_a^K| - J_m^K.$$  \hfill (19)

This indicates that there exists resonance between scattering states and DBS's. If $J_m = 0$, from Eq. (19), one can find that there is only one DBS solution for all $K$ when $\Delta = 2g^2/U$, see Fig. 5 (b).

III. HYBRID ATOM-MOLECULE QUANTUM WALKS

In this section, we analyze the QWs in our atom-molecule Hubbard system (1). The initial state is chosen as $|\Psi(0)\rangle = |0,0\rangle_a$, in which both two atoms occupy the 0-th lattice site. The time-evolution is governed by the Schrödinger equation,

$$|\Psi(t)\rangle = e^{-i\hat{H}t}|\Psi(0)\rangle.$$  \hfill (20)

The atomic and molecular density distributions are respectively defined as

$$n_{a,i}(t) = \langle \Psi(t)|a_i^\dagger a_i|\Psi(t)\rangle,$$

$$n_{m,i}(t) = \langle \Psi(t)|m_i^\dagger m_i|\Psi(t)\rangle.$$  \hfill (21)

The spatial correlation of atoms is characterized by a second-order correlation function,

$$\Gamma_{l_1l_2}(t) = \langle \Psi(t)|a_{l_1}^\dagger a_{l_2}^\dagger a_{l_2} a_{l_1}|\Psi(t)\rangle,$$  \hfill (22)

which relates to the probability $P_{l_1l_2}(t) = |\langle l_1, l_2|\Psi(t)\rangle|^2$ via $\Gamma_{l_1l_2}(t) = (1 + \delta_{l_1, l_2})P_{l_1l_2}(t)$. Thus $\Gamma_{l_1l_2}(t)$ gives the
probability of detecting one particle at \( l_1 \)-th site and the other particle at \( l_2 \)-th site in the meantime. The diagonal terms \( \Gamma_{l_1=l_2}(t) \) describes the correlated QWs of two atoms, in which the two atoms walk as a whole. The non-diagonal terms \( \Gamma_{l_1 \neq l_2}(t) \) describes the independent QWs of two atoms.

### A. QWs without atom-molecule coupling

If there is no atom-molecule coupling, the time evolution from the initial state \( |0,0\rangle_a \) will evolve only in the subspace of the atomic states. Since the molecule subspace is not involved, the QWs of atoms is expected to only depend on \( J_a/U \). When the atom-atom interaction is weak, the initial state has large overlaps with the atomic scattering states and so that the time-evolution is dominated by independent QWs [27]. When the atom-atom interaction is strong, the two atoms in the same site will form stable bound state and so that the time-evolution is dominated by correlated QWs [27, 29, 33, 40].

In Fig. 6, we show the density distribution \( n_a(t) \) and the correlation function \( \Gamma_{l_1,l_2} \). The parameters are chosen as \( J_a = 1, J_m = 0, \Delta = 0, U = 20, g = 0 \) and \( L_t = 21 \). Indeed, under strong interaction, two atoms do perform correlated QWs, that is, the correlation function is dominated by the diagonal terms which recovers the results in Ref. [27].

**FIG. 6.** The correlated QWs under strong atom-atom interaction and zero atom-molecule coupling. (a) Time-evolution of the atomic density distribution. (b) Two-particle correlation function of the final state. The parameters are chosen as \( J_a = 1, J_m = 0, \Delta = 0, U = 20, g = 0 \) and \( L_t = 21 \).

### B. QWs with atom-molecule coupling

Since the atom-molecule coupling may play the role of effective interaction, to show how the atom-molecule coupling affects the QWs, we turn off the atom-atom interaction \( (U = 0) \) and the atom-molecule energy difference \( (\Delta = 0) \).

We first consider the QWs in the case of weak atom-molecule coupling \( g \ll J_a, J_m \). The parameters are chosen as \( J_a = J_m = 1, \Delta = 0, U = 0, g = 0.1 \) and \( L_t = 21 \).

The time-evolution of atomic density distribution and the final correlation function are shown in Fig. 7 (a) and (b). The correlation function is dominated by the off-diagonal terms, which indicates that the two atoms walk independently. This is because the effective interaction is weak, \( U_{\text{eff}} = 2g^2/(E - \Delta - J_m^K) \ll J_a \). On the other hand, the atom-molecule coupling may induce the atom-molecule Rabi oscillations [41, 42]. However, due to the weakness of the atom-molecule coupling, the atoms would walk away before they are converted to a molecule.

**FIG. 7.** The hybrid atom-molecule QWs with atom-molecule coupling and zero atom-atom interaction \( (U = 0) \) and zero atom-molecule energy difference \( (\Delta = 0) \). (a) and (b) for weak atom-molecule coupling \( g = 0.1 \). (c) and (d) for strong-molecule coupling \( g = 10 \). The other parameters are chosen as \( J_a = J_m = 1 \) and \( L_t = 21 \). The left column show the time-evolution of atomic density distribution and the right column show the final correlation functions of atoms.

However, even for strong atom-molecule coupling, correlated QWs disappear when the atom-molecule energy difference \( \Delta \) is much larger than the atom-molecule coupling \( g \). In such a situation, the larger atom-molecule energy difference makes the atom-molecule conversion negligible. Therefore, atomic and molecular states are nearly decoupled and the two atoms walk independently since
there is negligible effective atom-atom interaction from the atom-molecule conversion.

C. QWs near the resonance between scattering states and DBS’s

In above, we show that the time-evolution are either dominated by independent QWs or correlated ones. We wonder whether independent and correlated QWs may coexist. As mentioned in Sec. II, under the conditions of $g \gg J_{a,m}$ and $U \gg J_{a,m}$, the resonance between scattering states and DBS’s takes place around $\Delta \approx 2g^2/U$. Below we will show the coexistence of independent and correlated QWs near the resonance between scattering states and DBS’s.

In Fig. 8, we show the QWs with $J_a = J_m = 1$, $g = 10$, $\Delta = 40$ and $U = 5$ which satisfy the resonant condition $\Delta \approx 2g^2/U$. In the atomic density distribution, there appear clear oscillation stripes which are signatures of atom-molecule conversion, see Fig. 8 (a). In the final correlation function, in addition to significant off-diagonal elements near the boundaries, there are significant diagonal elements on the diagonal line, see Fig. 8 (b). This indicates the coexistence of independent and correlated QWs, although the propagation speed of correlated QWs is smaller than the one of independent QWs.

IV. EFFECTIVE SINGLE-PARTICLE MODEL FOR STRONGLY CORRELATED QUANTUM WALKS

The strongly correlated QWs can be described by a single-particle model. By employing the many-body quantum degenerate perturbation theory [43], we derive an effective single-particle Hamiltonian for the strongly correlated QWs.

To avoid the breakdown of DBS’s near the resonance between scattering states and DBS’s, we suppose $|\Delta - 2g^2/U| \gg 0$. When $J_{a,m} \ll g$ or $J_{a,m} \ll U$, the tunneling term $\hat{T} = -\sum (J_{a}^{\dagger}J_{m}^{\dagger} + J_{m}J_{a}) + H.c.$ in Hamiltonian (1) can be treated as a perturbation. Defining the subspace $\mathcal{H}_a^d = \{|d_{\sigma,l}\rangle, -L \leq l \leq L\}$ for DBS’s (see Appendix. B), the projection operator is given by projecting the full Hilbert space $\mathcal{H}^{(2)}$ onto the unperturbed subspace $\mathcal{H}_a^d$,

$$\hat{P}_\sigma = \sum_l |d_{\sigma,l}\rangle\langle d_{\sigma,l}|,$$

where $\sigma = \{1, 2\}$ denotes the index for two different kinds of DBS’s. Besides, the projection onto the orthogonal complement of $\mathcal{H}_a^d$ reads as

$$\hat{S}_\sigma = \sum_{E_{1,l_2}^{(0)} \neq E_{l_1,l_2}^{(0)}} \frac{1}{E_{1,l_2}^{(0)} - E_{l_1,l_2}^{(0)}} |l_1l_2\rangle\langle l_1l_2|$$

$$+ \sum_{l_1,\sigma',\sigma} \frac{1}{E_{\sigma}^{(0)} - E_{\sigma'}^{(0)}} |d_{\sigma',l_1}\rangle\langle d_{\sigma,l}|.$$ (24)

Therefore, according to the perturbation theory [43] up to second order, we have

$$\hat{H}_a^{\text{eff}} = \hat{h}_{\sigma,0} + \hat{h}_{\sigma,1} + \hat{h}_{\sigma,2}$$

$$= E_\sigma \hat{P}_\sigma + \hat{P}_\sigma \hat{T} \hat{P}_\sigma + \hat{P}_\sigma \hat{T} \hat{S}_\sigma \hat{T} \hat{P}_\sigma.$$ (25)

Substituting the projection operators and perturbation term into the above equation, we can obtain

$$\hat{h}_{\sigma,0} = E_\sigma \sum_l |d_{\sigma,l}\rangle\langle d_{\sigma,l}|,$$ (26)

$$\hat{h}_{\sigma,1} = -J_m A_\sigma^2 \sum_l (|d_{\sigma,l}\rangle\langle d_{\sigma,l+1}| + |d_{\sigma,l+1}\rangle\langle d_{\sigma,l}|),$$ (27)

$$\hat{h}_{\sigma,2} = \frac{2J_m^2 B_\sigma^2}{E_\sigma^{(0)} - E_{l_1,l_2}^{(0)}} \sum_l \left( 2 |d_{\sigma,l}\rangle\langle d_{\sigma,l}| + |d_{\sigma,l+1}\rangle\langle d_{\sigma,l}| \right)$$

$$+ \frac{J_m^2 A_\sigma^2 B_\sigma^2}{E_\sigma^{(0)} - E_{l_1,l_2}^{(0)}} \sum_l \left( 2 |d_{\sigma,l}\rangle\langle d_{\sigma,l}| + |d_{\sigma,l+2}\rangle\langle d_{\sigma,l}| \right).$$ (28)

Here, the coefficients $A_\sigma$ and $B_\sigma$ are given by calculating the unperturbed time-independent Schrödinger equation (see Appendix. B).

By introducing the mapping: $|d_{l}\rangle\langle d_{l}| \leftrightarrow |d_{l}^{\dagger}d_{l}\rangle\langle d_{l+1}| \leftrightarrow |d_{l}^{\dagger}d_{l+1}\rangle\langle d_{l}| \leftrightarrow |d_{l+1}^{\dagger}d_{l}\rangle$, the effective single-particle Hamiltonian can be written as

$$\hat{H}_a^{\text{eff}} = \sum_l \left( E_\sigma + \frac{4J_m^2 B_\sigma^2 B_{l_1,l_2}^2}{E_{l_1,l_2}^{(0)} - E_{l_1,l_2}^{(0)}} + 2 \frac{J_m^2 A_\sigma^2 A_{l_1,l_2}^2}{E_{l_1,l_2}^{(0)} - E_{l_1,l_2}^{(0)}} \right) |d_{l}\rangle\langle d_{l}|$$

$$+ \left( \frac{2J_m^2 B_\sigma^2}{E_\sigma^{(0)} - E_{l_1,l_2}^{(0)}} - J_m A_\sigma^2 \right) \sum_j \left( |d_{l}^{\dagger}d_{l+1}\rangle\langle d_{l}^{\dagger}d_{l}| + h.c. \right)$$

$$+ \left( \frac{J_m^2 A_\sigma^2 B_\sigma^2}{E_\sigma^{(0)} - E_{l_1,l_2}^{(0)}} \right) \sum_l \left( |d_{l}^{\dagger}d_{l+2}\rangle\langle d_{l}^{\dagger}d_{l}| + h.c. \right).$$ (29)
In addition to the nearest-neighbor (NN) tunneling, there appears the next-nearest-neighbor (NNN) tunneling, which originates from the effects of molecular tunneling. Since $|E_{1(0)}^{(0)} - E_{2(0)}^{(0)}| \gg |E_{1(0)}^{(0)} - E_{0(0)}^{(0)}|$ or $|E_{2(0)}^{(0)} - E_{0(0)}^{(0)}|$, the NNN tunneling term is generally negligible compared with other terms. By implementing a Fourier transformation, the above single-particle Hamiltonian can be easily diagonalized and the eigenenergies are given as

$$ E_{\sigma}^{\text{eff}} = \left( \frac{8J_0^2B^2_{\sigma}}{E_{\sigma}^{(0)} - E_{l_1l_2}^{(0)}} - 4J_mA_{\sigma}^2 \right) \cos^2 \left( \frac{K}{2} \right) + 4\frac{J_m^2A_{l_1l_2}^2}{E_{\sigma}^{(0)} - E_{l_1l_2}^{(0)}} \cos^2 K + E_{\sigma}^{(0)} + J_mA_{\sigma}^2, \quad (30) $$

which are well consistent with the ones from numerical diagonalization of the original Hamiltonian.

In the effective single-particle Hamiltonian (29), the effective NN tunneling strength is given as $J_{\text{eff},\sigma}^{NN} = 2J_0^2B_{\sigma}^2/(E_{\sigma}^{(0)} - E_{l_1l_2}^{(0)}) - J_mA_{\sigma}^2$. Obviously, $J_{\text{eff},\sigma}^{NN}$ also depends the atom-molecule energy difference $\Delta$. In Fig. 9 (a), we plot $J_{\text{eff},\sigma}^{NN}$ as a function of $\Delta$, in which the solid and dashed lines respectively correspond to the upper and lower DBS bands. The parameters are chosen as $J_0 = J_m = 1$, $g = 10$ and $U = 0$. The effective tunneling strengths for the upper and lower DBS bands are always different except for the crossing point. The different effective tunneling strength will result in different propagation speeds in QWs. In Fig. 9 (b), we show the atomic density distribution with $\Delta = -10$ and other parameters as same as the ones for Fig. 9 (a). Since the initial state mostly occupies the two DBS bands, there appear two light-cones: the inner light cone and the outer one respectively correspond to the QWs of DBS’s in the upper and lower bands.

From Fig. 9 (a), near $\Delta = -19.125$, the effective tunneling strength of the DBS’s in the upper band is almost zero, i.e. $J_{\text{eff},\sigma}^{NN} \approx 0$. Given $\Delta = -19.125$, we plot the energy bands in Fig. 9 (c). The upper DBS’s band is very flat, which indicates very small tunneling strength, while the lower DBS’s band is not. This is concordant with the results of effective model in Fig. 9(a). Noticing that $J_{\text{eff},\sigma}^{NN} \approx 0$, there is only the NNN tunneling term ($J_{NNN}^{NN} \approx 0.005$) in the effective Hamiltonian (29). Therefore, the odd sites are never occupied in the QWs from the 0-th site, which is a clear significant of the NNN tunneling, see Fig. 9 (d).

On the other hand, in the effective Hamiltonian (29), the effective tunneling induced by the molecular tunneling is of 1st order, while the effective tunneling induced by atomic tunneling is of 2nd order. This means that, as the molecular tunneling may has considerable effects, it should be treated carefully in realistic systems.

![FIG. 9. (a) The effective nearest-neighbor tunneling strength $J_{\text{eff},\sigma}^{NN}$ versus the atom-molecule energy difference $\Delta$. The parameters are chosen as $J_0 = J_m = 1$, $g = 10$ and $U = 0$. (b) Time-evolution of molecular density distribution with $\Delta = -10$ and the same parameters with (a). (c) The 21-site energy bands with $\Delta = -19.125$ and other parameters given for (a). The blue-dotted lines and the red dots correspond to the bands of DBS’s and atomic scattering states respectively. (d) Long time-evolution of atomic density distribution with $\Delta = -19.125$ and other parameters given for (a).]

V. SUMMARY AND DISCUSSIONS

In summary, we study the energy bands and hybrid atom-molecule QWs of a 1D coupled atom-molecule Hubbard system. We find that the atom-molecule coupling can play the role of effective atom-atom interaction. Unlike the conventional bounded atomic pair, the cooperation of the atom-atom interaction and the atom-molecule coupling induces two kinds of DBS’s, which are the dressed molecule states in superposition of bounded atomic pair and bare molecule. Even if the atom-atom interaction is absent, one can observe correlated QWs induced by the atom-molecule coupling. Tuning the parameters (the atom-molecule energy difference $\Delta$, the atom-atom interaction $U$ and the atom-molecule coupling $g$) to satisfy the resonant condition, one of the DBS’s will enter the continuum band and break into atomic scattering states. Thus, one can observe the coexistence of independent and correlated QWs near the resonance between scattering states and DBS’s. Away from the resonant condition, we employ many-body quantum degenerate perturbation theory to derive the effective single-particle Hamiltonian for the two DBS bands. The nearest-neighbor tunneling strength in the effective single-particle model can be turned off by tuning the atom-molecule energy difference $\Delta$. Due to the two DBS’s have different effective tunneling strengths, the QWs show two light cones with different propagation speeds.
Our study not only provides a full description for the hybrid atom-molecule QWs with atom-molecule coupling, but also will shine some light on the two-photon QWs with spontaneous parametric down-conversion (SPDC) [44-46]. In such a waveguide array, the near-degenerate signal and idler photons correspond to two identical atoms, the pump photon acts as the molecule, and the SPDC play the role of the atom-molecule coupling. The difference is that, in the waveguide array, the energy of signal and idler photons always equal to the pump photon, and there is no interaction between photons if the Kerr effects are absent. According to our study, the idler and signal photons may have effective on-site interaction induced by the SPDC even if there are no Kerr effects [47]. Furthermore, the idler and signal photons can form dressed bound states with the pump photon when the SPDC is sufficiently strong. Therefore, there will appear two different kinds of dressed photonic bound states with different effective hopping strengths between waveguides.

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Appendix A: Graphical illustration for solutions of DBS’s

To give the DBS’s, one has to determine the parameter $\alpha$ by solving Eqs. (17) and (18). From Eq. (18), we have

$$\alpha^\pm(\bar{E}) = \left(\bar{E} \pm \sqrt{\bar{E}^2 - (2J^K_a)^2}\right)/2J^K_a, \quad (A1)$$

and $|\bar{E}| > 2J^K_a$. Therefore, Eq. (17) can be rewritten as

$$\frac{-2g^2}{\bar{E} - \Delta - J^K_m} = \frac{2J^K_a}{\sqrt{\bar{E}^2 - (2J^K_a)^2}} + U. \quad (A2)$$

Because $|\alpha| < 1$, we have $\alpha = \alpha^-$ when $\bar{E} > 0$ and $\alpha = \alpha^+$ when $\bar{E} < 0$. Thus Eq. (A2) is equivalent to

$$\frac{-2g^2}{\bar{E} - \Delta - J^K_m} = \pm \sqrt{\bar{E}^2 - (2J^K_a)^2} + U. \quad (A3)$$

Introducing

$$\begin{align*}
E_1^{(0)} &= \left(U + \Delta - \sqrt{8g^2 + (U - \Delta)^2}\right)/2, \\
C_1 &= A_1/B_1 = (\Delta - U - \sqrt{8g^2 + (U - \Delta)^2})/2\sqrt{2}g,
\end{align*} \quad (B3a)$$

$$\begin{align*}
E_2^{(0)} &= \left(U + \Delta + \sqrt{8g^2 + (U - \Delta)^2}\right)/2, \\
C_2 &= A_2/B_2 = (\Delta - U + \sqrt{8g^2 + (U - \Delta)^2})/2\sqrt{2}g.
\end{align*} \quad (B3b)$$

In Fig. 10, given $g = 10$, $U = 20$, $J_a = 1$, $J_m = 0$ and $\Delta = 50$. Clearly, there are always two intersections if $U = 0$, while there might be only one intersection if $U \neq 0$ for some values of $\Delta$.
where $A_{\sigma} = \pm \frac{C_{\sigma}}{\sqrt{1 + C_{\sigma}^2}}$, $B_{\sigma} = \pm \frac{1}{\sqrt{1 + C_{\sigma}^2}}$ with $\sigma = \{1, 2\}$. Thus, the two eigenstates read as $|d_{\sigma,i}\rangle = A_{\sigma}|i\rangle_m + B_{\sigma}|i\rangle_a$. These two states correspond to two isolated DBS bands.

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