Dynamics of spin–orbit-coupled cold atomic gases in a Floquet lattice with an impurity

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Abstract
In this work, we have studied the quantum tunneling of a single spin–orbit-coupled atom held in a periodically modulated optical lattice with an impurity. As a result we find that the dynamical localization takes place globally at the collapse points of quasienergy spectrum, even when the impurity potential is far off-resonant with the driving field. Meanwhile, two types of local second-order tunneling processes appear beyond expectation between the two nearest-neighbor sites of the impurity, with the spin unchanged and with the impurity site population negligible. Though tunneling behaviors of the two types seem to be the same, they are believed to involve two distinct mechanisms: one is related to spin-independent process, while the other is to spin-dependent tunneling process. The two types of second-order processes can be identified by means of resonant tunneling with or without spin flipping by tuning the impurity potential to be in resonance with the driving field. In the Floquet picture, the system with the localized impurity develops a fine structure of avoided crossings of quasienergies near the collapse point, which is crucial to understand the so-called second-order tunneling dynamics. These results are confirmed analytically on the basis of effective three-site model and multiple-time-scale asymptotic perturbative method, and may be exploited for engineering the spin-dependent quantum transport in realistic experiments.

Keywords: dynamical localization, spin–orbit coupling, second-order tunneling

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

1. Introduction
Spin–orbit coupling (SOC) effect, ubiquitous in condensed matter physics, lies at the heart of fundamental phenomena such as spin Hall effect [1], topological insulators [2], Majorana fermions [3], as well as practical applications such as spintronic devices [4]. Recently, artificial SOC has been successfully engineered in the laboratory with both neutral bosonic and fermionic ultracold atoms [5–10], which not only exhibits many exotic phases [11–18] (some of which have no direct analog in conventional condensed matter systems), but also provides an ideal platform to recreate and explore novel SOC physics with an unprecedented level of tunability of experimental parameters. Motivated by the ongoing experimental achievements, scholars have put extensive efforts toward understanding the static properties of the SO-coupled atomic gases [17–26], as well as gaining insight into their intriguing dynamics, including unconventional collective...
dipole oscillations [27, 28], relativistic dynamics with analogs of Zitterbewegung [29] and Klein tunneling [30], spin Josephson effects in a double-well potential [31–33], spin-dependent tunneling and spin transportation in Floquet systems of SO-coupled ultracold atom systems [34, 35], non-equilibrium dynamics of SO-coupled lattice bosons [36], tunable Landau–Zener transitions [37] and chaos-driven dynamics [38] in SO-coupled atomic gases, localization of a SO-coupled particle or Bose–Einstein condensate moving in a 1D quasiperiodic potential [39, 40] and random potential [41, 42], entanglement [43, 44] and dynamical phase transition [44] in a SO-coupled Bose–Einstein condensate, and so on.

When SOC is combined with optical lattices, a spin-flip term is produced in Bose–Hubbard Models, in addition to the standard spin-conserving tunneling between nearest-neighbor lattice sites. In recent experiments, SO-coupled bosonic systems in an optical lattice have been successfully realized [45], which promises a testbed for theoretical studies of diverse new phases and SOC-related spin-dependent transportations. Typically, defects play a prominent role in the dynamical properties of the realistic lattice systems. A large number of papers have been devoted to theoretical investigation of the behaviors of quantum particles without SOC hopping on a defective lattice, such as the existences of bound state in the continuum (BIC) [46] and Floquet bound states [47] in the one-dimensional two-particle Hubbard model with an impurity, the resonant tunneling of a single particle [48] and correlated pair tunneling [49, 50] in driven one-dimensional lattices with an impurity, to name only a few. By contrast, the physics of a single SO-coupled ultracold atom in a driven one-dimensional optical lattice with an impurity remains an unexplored frontier. On the other hand, for controlling more favorably spin-dependent tunneling and spin transportation in lattices, disorder and external driving field may be intentionally introduced. From this point of view, it would be worthwhile to study the dynamics of a SO-coupled particle moving in a periodically driven lattice with an impurity.

This paper is principally aimed to understand how the interplay between impurity, SOC and periodic driving determines the novel tunneling dynamics of a single SO-coupled atom moving in an optical lattice. As we find it, the dynamical localization (DL) is not destroyed when considering tunneling dynamics of a single SO-coupled atom with only spin-conserving coupling or with only spin-flipping coupling in the driven optical lattice with an impurity, but the local dynamics of the system is remarkably affected when the competition among impurity, SOC and periodic driving is introduced. Specifically, there are two scenarios. In the resonant regime, where the impurity potential is equal to a multiple of the driving frequency, the dynamics of the system is dominated by resonant tunneling between the impurity and its two nearest-neighbor sites. Such a system with only coupling between states with the same spin will exhibit resonant tunneling without spin flipping, while the one with only coupling between states with different spins demonstrates resonant tunneling with spin flipping. In the non-resonant regime, where the impurity potential is far off-resonant with the driving field, the second-order tunneling process emerges surprisingly even under the DL conditions when either only the spin-conserving tunneling term or only the spin-flipping tunneling term is presented; in either case, a single spin-up (down) atom tunnels back and forth between the two nearest-neighbor sites of the impurity in such a way that the spin remains unchanged and the impurity site population is negligible over all the evolution time. For the single SO-coupled atom with either only spin-conserving coupling or with only spin-flipping coupling term, the second-order tunneling processes exhibit remarkable resemblance, though, they are generated via different virtual intermediate states and therefore should be interpreted in the context of two distinct mechanisms. The first mechanism involves a spin-independent tunneling process in which the virtual intermediate state without spin-flipping is eliminated, thereby yielding a spin-independent effective tunneling rate. The second one stems from a second-order transition via elimination of the virtual intermediate state with spin flipping and actually involves a spin-dependent tunneling process, thus second-order transition of this type has a spin-dependent effective tunneling rate.

2. Model system and Floquet-quasienergy spectrum

The tunneling dynamics in ultracold bosonic system has been a subject of active research efforts for many years. One primary and prototype example is the tunneling of bosons in double well, which has been extensively studied and understood (for example, see [51–56] and references therein). Nevertheless, to date not much is known about the tunneling dynamics of spin–orbit-coupled bosons in optical lattices with periodic modulation of on-site energy and a localized impurity. In this work, we consider a single ultracold atom with internal up and down pseudospin states [1] and [1] trapped in a spin-independent one-dimensional periodically driven optical lattice with an impurity at site \( n = 0 \). The effective SOC can be implemented simultaneously experimentally using two counter-propagating Raman lasers which generate a momentum-sensitive coupling between the two internal hyperfine states of the same atom. In the most general tight-binding description, the single-particle Hamiltonian governing this system is of the following form [34, 35, 39]

\[
H = \sum_n \left[ -\hbar \omega_n \hat{c}_n \hat{c}_{n+1} + \h.c. + \varepsilon(t) \hat{c}_n \hat{c}_n^\dagger + \frac{\Omega}{2} \hat{c}_n \hat{\sigma}_z \hat{c}_n^\dagger \right] + \varepsilon_0 \hat{c}_0 \hat{c}_0^\dagger,
\]

(1)

where \( \hat{c}_n = (\hat{c}_{n,1}^\dagger, \hat{c}_{n,1}^\dagger, \hat{c}_{n,2}, \hat{c}_{n,2})^T \) (hereafter superscript \( T \) stands for the transpose) and \( \hat{c}_n \hat{c}_n^\dagger \) (\( \hat{\sigma}_{n,\sigma} \)) creates (annihilates) a boson with pseudospin \( \sigma = \uparrow, \downarrow \) at site \( n = 0, \pm 1, \pm 2, \ldots \), \( \hat{\sigma}_{n,\sigma} \) are the usual \( 2 \times 2 \) Pauli matrices, \( \Omega \) is the effective Zeeman field intensity, and \( \varepsilon_0 \) the impurity potential strength. We are considering a localized impurity at a single site. Due to the high degree of controllability of the optical lattice in the cold atom experiments, it is possible to produce the single-site impurity potential with arbitrary strength in a controllable way, for example, by introducing irregularities in the height or width.
of the single well, \( \mathcal{T} \) is the time-ordering operator. 

The diagonal terms of \( \mathcal{T} \) describe spin-conserving hopping while off-diagonal spin-flip terms describe the SO coupling arising from a two-photon Raman process. In our model, we assume that the driving field take the form \( \dot{\epsilon}(t) = F \cos(\omega t) \) with amplitude \( F \) and frequency \( \omega \).

For simplicity, we have set \( \hbar = 1 \) and adopted the parameter \( \nu \) as a unit to scale the other parameters \( \Omega, F, \omega, \varepsilon_0 \) so that they become dimensionless. In realistic experiment, the Zeeman field \( \Omega \) is on the order of recoil frequency \( \nu = \hbar k^2/(2m) \sim 22.5 \text{KHz} \) \[5\]. \( \nu \sim 0.1 \nu, / \hbar, \) and the driving frequency \( \omega \) can be adjusted between \( 0 \sim 30 \text{ KHz} \) \[57\]. Thus, the system parameters can be tuned experimentally in a wide range as follows \( \Omega / \nu \sim 10, \dot{F} / \nu \sim \varepsilon_0 / \omega \sim 0 \sim 10 \nu \). In our discussion, what is essential is the ratios between these parameters \( \nu, \Omega, F, \omega, \varepsilon_0 \).

In Hilbert space with a complete set of Fock basis \( \{n, \sigma\} \), where \( [n, \sigma] \) represents the state of a spin-\( \sigma \) particle occupying a lattice site \( n \), the state vector of the SO-coupled system at any time \( t \) can be expanded as

\[
|\psi(t)\rangle = \sum_{n,\sigma} a_{n,\sigma}(t)|n, \sigma\rangle,
\]

where \( a_{n,\sigma}(t) \) indicates the time-dependent probability amplitude of the atom being in state \( [n, \sigma] \), and the corresponding probabilities read \( P_{n,\sigma} = |a_{n,\sigma}(t)|^2 \), conserving the normalization condition \( \sum_{n,\sigma} P_{n,\sigma} = 1 \). Substituting equations (1) and (2) into Schrödinger equation \( i\hbar \partial_t |\psi(t)\rangle = \mathcal{H}|\psi(t)\rangle \), one obtains the following coupled equations for the probability amplitude \( a_{n,\sigma} \)

\[
\begin{aligned}
\dot{a}_{n,1} &= -\nu [\cos \alpha (a_{n+1,1} + a_{n-1,1})] \\
&+ \sin \alpha (-a_{n+1,1} - a_{n-1,1}) + \dot{\epsilon}(t)a_{n,1} + \varepsilon_0 b_{n,1}a_{n,1} + \frac{\Omega}{2} a_{n,1}, \\
\dot{a}_{n,-1} &= -\nu [\cos \alpha (a_{n+1,-1} + a_{n-1,-1})] \\
&+ \sin \alpha (-a_{n+1,-1} - a_{n-1,-1}) + \dot{\epsilon}(t)a_{n,-1} + \varepsilon_0 b_{n,-1}a_{n,-1} - \frac{\Omega}{2} a_{n,-1}.
\end{aligned}
\]

Throughout our paper, the overdots represents a derivative with respect to the time variable \( t \), unless stated otherwise. From equations (3) and (4), it is easy to observe that the couplings between states with the same (different) spin are proportional to cosine (sine) functions of the SOC strength. The terms proportional to \( \cos \alpha \) are the usual spin-conserving tunneling, while those proportional to \( \sin \alpha \) are the spin-flipping tunneling. When \( \alpha = \pi, I = 0, 1, 2, \ldots \), only the usual tunneling is presented; When \( \alpha = (2l + 1)\pi/2, I = 0, 1, 2, \ldots \), the usual tunneling vanishes and only the spin-flipping tunneling is kept. Otherwise, the spin-conserving and spin-flipping tunnelings will coexist. Thus the quantum transport with or without spin flipping can be manipulated by adjusting the SO coupling strength \( \alpha \). In what follows, we will illustrate how the tunneling dynamics of a single SO-coupled atom in an optical lattice is governed by interplay between impurity and periodic driving, with focus on the usual spin-conserving tunneling (\( \sin \alpha = 0 \)) and the purely spin-flipping tunneling (\( \cos \alpha = 0 \)) case.

Before investigating the corresponding quantum tunneling dynamics, we first discuss the quasienergies and Floquet states of the considered system (1). According to Floquet theory, the time-periodicity of Hamiltonian allows to write solutions of the Schrödinger equations (3) and (4) in the form of \( a_{n,\sigma}(t) = \tilde{a}_{n,\sigma}(t) \exp(-i\epsilon t) \), where \( \epsilon \) are the quasienergies and \( \tilde{a}_{n,\sigma}(t) \), to which we shall refer as Floquet modes, are periodic with the driving period \( \mathcal{T} = 2\pi/\omega \). Due to the periodicity in space (apart from the single-site impurity and the boundary effects), the quasienergies for the allowed quantum states of the tight-binding lattice will group together, thus forming quasienergy band.

In figure 1, we plot quasienergy spectrum versus the driving parameter \( F/\omega \) for the usual spin-conserving tunneling (\( \sin \alpha = 0 \)) (upper row) and the purely spin-flipping tunneling (\( \cos \alpha = 0 \)) (lower row) cases, by direct diagonalization of the evolution operator over one period \( U(T, 0) = T \exp \left[ -i \int_0^T \mathcal{H}(t) \, dt \right] \), where \( T \) is the time-ordering operator. In all the numerical calculations, we have set the size of lattice to be \( N = 21 \) and \( \Omega = \omega \). The reason for our choice of the special value of the Zeeman field intensity is that the narrowing (collapse) of quasienergy spectrum for the purely spin-flipping tunneling case occurs only when the Zeeman field intensity is an integer multiple of the driving frequency. As can be seen in the left column of figure 1, in the resonant...
case of $\varepsilon_0 = \omega$, for $\sin \alpha = 0$ (upper left), the quasienergies make up a miniband and exhibit a set of band collapses at $F/\omega = 2.405, 5.5201, \ldots$, the zeros of Bessel $J_0$ function, while two pairs of doubly degenerate quasienergies deviate from the rest of miniband near the collapse regions; however, for $\cos \alpha = 0$ (lower left), the quasienergy band shows a similar set of collapses when $F/\omega = 3.8317, 7.0156, \ldots$, the zeros of Bessel $J_1$ function, accompanied by four non-degenerate quasienergies deviating from the rest in the vicinity of the collapse regions.

It is obvious that the quasienergy spectrums corresponding to the case $\sin \alpha = 0$, for which only the spin-conserving couplings are presented, have the same structure of that in the case of their spinless atom counterpart reported in [48], where the band collapses have been observed at the zeros of Bessel $J_0$ function. It is because in this situation the results are spin-independent and thus the quasienergy band corresponding to the spin-up states is exactly the same as that corresponding to the spin-down states. By contrast, for $\cos \alpha = 0$ (only the spin-flipping couplings are presented), the spin-flipping tunneling is associated with an energy cost of $\Omega$. When the effective Zeeman field intensity matches a multiple of the driving frequency, that is, when this condition $\Omega = m_0 \omega$ with positive integer $m$ is satisfied, the system is able to exchange energy of $m$ quanta with the driving field to bridge the energy difference $\Omega$ created by the spin-flipping tunneling. In this case, the driven SO-coupled system behaves approximately, in a time-averaged sense, like an undriven one with the rescaled hopping matrix element $v_{in} (F/\omega)$. In our situation, where $\Omega = \omega$, the collapses of quasienergy band accordingly become located at the zeros of Bessel $J_1$ function, rather than the zeros of Bessel $J_0$ function as in the spin-independent tunneling case. Due to the existence of an impurity, there is a corresponding energy difference created by a static tilt between the impurity and its two nearest-neighbor sites, which results in four associated quasienergies distinguished from quasienergy flatness (narrowing) in the vicinity of the collapse point, in stark contrast to the case of perfect optical lattice in which all the quasienergies will collapse into a single value.

As shown in the right column of figure 1, in the off-resonant case of $\varepsilon_0 = 1.2 \omega$, except that two quasienergy levels (which for the usual spin-conserving tunneling $\sin \alpha = 0$ case are identical and exactly overlapped, as shown in figure 1(b)) remain isolated from the rest of the miniband for all the values of $F/\omega$, there also exist a series of band collapses just as in the resonant case. The quasienergy levels separated markedly from the rest correspond to localized states for which an atom with spin up or down is captured by the impurity. Particularly interesting, the region of the level collapse is in fact a region with several avoided crossings as shown in the insets of figures 1(b) and (d). As we shall show in the next section, these fine structures of avoided level crossings near the pseudocollapse points can be conveniently exploited for engineering the spin-dependent transportation. The pseudocollapse herein refers to a phenomenon that all quasienergy levels seem to, but really do not, collapse into a point.

To gain more insight into the behaviors of quasienergies at the collapse points, we plot in figure 2 quasienergies within one Brillouin zone $0 \leq \varepsilon \leq \omega$ of quasienergies as functions of $\varepsilon_0/\omega$. (a) The usual spin-conserving tunneling ($\sin \alpha = 0$) case, $F/\omega = 2.4045$. (b) The purely spin-flipping tunneling ($\cos \alpha = 0$) case, $F/\omega = 3.8317$. The other parameters are $n = 1, \omega = 20, \Omega = 20$.

3. Tunneling dynamics with or without spin flipping

In this section, we will present a comprehensive analysis of the tunneling physics underlying the quasienergy spectrum of the considered system (1). As is well known, the crossing (collapse) of the quasienergies of the underlying time-periodic system is always associated with a celebrated quantum phenomenon called DL [38], in which a localized particle periodically returns to its initial state following the periodic change of the field. Upon occurrence of DL, the initial localized quantum state will not diffuse. To study the
system’s time evolution quantitatively, we have plotted the time dependence of the mean-square displacement \(\langle n^2 \rangle\), as illustrated in figure 3, by numerically solving equations (3) and (4) with the size of lattice \(N = 21\). Clearly, for the off-resonance case, if we start the system with a single spin-up (or spin-down) atom in the impurity site \((n = 0)\), the system will be frozen in the initial state, which is suggested by the structure of two levels isolated from the rest of miniband in figures 1(b) and (d). The frozen dynamics arises from the fact the particle is captured by impurity. Thus, in order to illustrate the physical significance of the miniband collapses, we assume in the following calculations that the system be initialized in state \([-1, 1]\), that is, with a spin-up atom in the left-side neighbor of impurity site \((-1)\). For this initial state, if there is a diffusive (spatially delocalized) propagation through the whole optical lattice, the mean-square displacement \(\langle n^2 \rangle\) will increase without bound. By comparison of figures 3(a), (b) and (c), (d), it can be readily seen that the behaviors of time dependence of the mean-square displacement are similar between the usual spin-conserving tunneling \(\sin \alpha = 0\) (top) and the purely spin-flipping tunneling \(\cos \alpha = 0\) (bottom) case, whether the driving parameters are located on (the solid lines) or off (the dashed lines) the band collapse points. As is apparent in figure 3, for both \(F/\omega = 2.405\) (solid lines in the top row) and \(F/\omega = 3.8317\) (solid lines in the bottom row) corresponding to the collapse points in the cases of \(\sin \alpha = 0\) and \(\cos \alpha = 0\), respectively, the mean-square displacements are seen to be bounded and the celebrated DL [58] occurs, whereas in the case of \(F/\omega = 1.5\) (dashed lines) the mean-square displacements grow without bound and the particle initially occupying site \(-1\) delocalizes. Detailed examination of the bounded solutions (evidence of DL) reveals that the mean-square displacement varies between 1 and 0.5 for the resonant case (see insets in left column), indicating that the particle propagates through several lattice spacings and returns repeatedly to the initial location, while the mean-square displacement remains near unity for the off-resonant case (see insets in right column), seeming to be a frozen dynamics. The seemingly frozen dynamics, as we will show below, is actually a second-order tunneling between the two nearest-neighbor sites of the impurity.

For a clearer observation of the tunneling dynamics presented above, we show in figure 4 the time evolution of occupation probabilities \(P_{n,\sigma}\) for the resonant case \(\varepsilon_0/\omega = 1\) via direct integration of equations (3) and (4) with the size of lattice \(N = 21\), assuming that a spin-up atom is initially prepared in the site \(-1\) and that the driving parameters are properly set at the band collapse points. Under such assumptions, though the DL dominates globally, resonant oscillations with (without) spin flipping can take place between the impurity and its two nearest-neighbor sites, as depicted in figures 4(a) and (b) respectively. For the same set of parameters as in inset of figure 3(a), where \(\sin \alpha = 0\) and \(F/\omega = 2.405\), the occupation probabilities \(P_{1,\uparrow}\) (\(P_{1,\downarrow}\) oscillate between 1 and \(-1\), at the same time, the occupation probability \(P_{0,\uparrow}\) varies between 0 and 0.5, which indicates that the dynamics of system is dominated by the spin-conserving tunneling only between the impurity and its two nearest-neighbor sites and thus can be understood in an effective three-site model with three localized basis functions \(\{0, \uparrow\}\) and
and \( \cos \alpha = 0 \) case at the band collapse point \( F/\omega = 2.405 \). (b) The purely spin-flipping tunneling \( \sin \alpha = 0 \) case at the first collapse point \( F/\omega = 3.8317 \). The circles in (a) and (b), respectively, represent the second-order perturbative results from equations (10) and (16). Lower panels in (c) and (d) are schematic representations of the tunneling dynamics in (a) and (b) respectively. Red crosses indicate suppression of tunneling through that barrier, and the dashed-line arrows indicate the virtual first-order tunneling process, whereas the solid-line arrows indicate the allowed second-order tunneling which actually occurs. The other system parameters and initial state are the same as in figure 4.

\(|\pm 1, \uparrow\rangle\), see figure 4(a) and its inset. Likewise, for the same values of the parameters as in inset of figure 3(c), where \( \cos \alpha = 0 \) and \( F/\omega = 3.8317 \), a complete oscillation between the sites 0 and \( \pm 1 \), same as in figure 4(a) but with spin flipping and longer oscillation period, is observed in figure 4(b), in which case the system dynamics is limited in a subspace spanned by states \(|0, \downarrow\rangle\) and \(|\pm 1, \uparrow\rangle\) and thus can be described in an effective three-site model (the inset in figure 4(b)). These resonant oscillations (shown in figures 4(a) and (b)) between the impurity and its two nearest-neighbor sites are strongly reminiscent of multiple-photon resonances, which manifest themselves in the avoided crossings of quasienergy spectrum at the band collapse points (shown in figures 1(a) and (c)) and under the circumstances the system will exchange energy of an integer number of photons with the oscillating field to overcome the energy offset created by the impurity, thus offering a possible means for control of single-spin transportation with or without spin flipping. Noticing that the results are physically similar if we instead start the system with a single spin-down atom in the site \( -1 \), without loss of generality we restrict ourselves to the case of initial spin-up atom throughout our paper.

Now we turn to the off-resonant case with the same set of parameters and initial conditions as in insets of figures 3(b) and (d) where the DL takes place globally. In this case, the transition between the impurity and its two nearest-neighbor sites is non-resonant and is therefore suppressed when the strength of the impurity potential is comparatively far from any integer multiple of \( \omega \). To our surprise, the considered system actually performs Rabi oscillation between the localized states \(|-1, \uparrow\rangle\) and \(|1, \uparrow\rangle\) with negligible population at all the remaining sites \((n = \pm 1)\) for both the usual spin-conserving tunneling (figure 5(a)) and the purely spin-flipping tunneling (figure 5(b)) cases. These two Rabi oscillations shown in figures 5(a) and (b) correspond to the very similar observable tunneling behaviors where a single spin-up atom tunnels back and forth between the two nearest-neighbor sites of the impurity in a manner that the spin \( \uparrow \rangle \) remains unchanged and the impurity site population is negligible over all the evolution time, and thus their corresponding mean-square displacements as illustrated in the insets of figures 3(b) and (d) apparently will keep unchanged because of the symmetry of lattice. Obviously, the tight-binding model (1) can only give rise to the first-order transition between two adjacent sites, so that these tunneling processes between the two sites \(-1 \) and \( 1 \) are possible only due to the second-order transition. As we shall show in the next section in detail, two distinct physical mechanisms are believed to be involved. The first one is due to the second-order transition \(|-1, \uparrow\rangle \rightarrow |1, \uparrow\rangle\) via the virtual intermediate state \(|0, \uparrow\rangle\). The second one is induced by the second-order transition \(|-1, \uparrow\rangle \rightarrow |1, \downarrow\rangle\) via a different virtual intermediate state \(|0, \downarrow\rangle\). The respective tunneling dynamics can be summarized schematically in lower panels in figures 5(c) and (d), where crosses indicate suppression of tunneling through that barrier, the dashed-line arrows indicate the virtual first-order tunneling process, whereas the solid-line arrows indicate the second-order tunneling allowed.

In a nutshell, there are two types of second-order tunneling processes despite of very similar observable tunneling behaviors, which are interpreted in the context of two different mechanisms as schematically shown in figures 5(c) and (d). Actually, the aforementioned second-order tunneling processes are the direct consequences of the subtle avoided level crossings presented in the insets of figures 1(b) and (d), which can not be captured by the first-order perturbation and needs to be explained in the framework of the second-order perturbative theory.

4. Analysis of the tunneling dynamics

According to the above numerical results, we preliminarily come to a conclusion that the DL of the two-component atomic gas with SO coupling is non-destroyed by the impurity for both the usual spin-conserving tunneling and the purely spin-flipping tunneling cases, however, the local dynamics of the system are dramatically tuned by the ratio of the impurity potential to the driving frequency. Under the DL condition, in other words, when the driving parameters are properly chosen at the band collapse points, the occurrences of resonant tunneling as well as the second-order tunneling have been observed, in which the single atom can move only among the three sites \(0 \) and \( \pm 1 \) while all other inter-site tunneling passages are shut off. In both cases, the tunneling dynamics can be understood by an effective three-site model and the time evolution of quantum state of a spin-1/2 particle should be
confined in the truncated Hilbert spaces spanned by six Fock states. Next, we will try to substantiate our numerical calculations by the analytical method.

To proceed, we begin with equations (3) and (4) and introduce the following new amplitudes:

\[
b_{n,\uparrow}(t) = a_{n,\uparrow}(t) \exp \left\{ i (\Omega t + \frac{\Omega}{2} + \varepsilon_0 \delta_{n,0} t) \right\},
\]

(5)

\[
b_{n,\downarrow}(t) = a_{n,\downarrow}(t) \exp \left\{ i (\Omega t - \frac{\Omega}{2} + \varepsilon_0 \delta_{n,0} t) \right\},
\]

(6)

where we have set \( \Phi(t) = \int_0^t d\tau \varepsilon(\tau) = \frac{\Omega}{2} \sin \omega t \).

In terms of the new amplitudes \( b_{n,\sigma}(t) = \langle 0 \mid \hat{a}_{n,\sigma} \rangle \) and \( b_{n,\sigma}(t) = \langle 1 \mid \hat{a}_{n,\sigma} \rangle \), we can rewrite equations (3) and (4) in the form

\[
ib_{n,\uparrow} = -v \cos \alpha [b_{n+1,\uparrow} e^{i \delta n/\omega} - 2 b_{n,\uparrow} e^{i \delta n/\omega} - b_{n-1,\uparrow} e^{-i \delta n/\omega}]
\]

+ \( v \sin \alpha [b_{n+1,\uparrow} e^{i \delta n/\omega} - 2 b_{n,\uparrow} e^{i \delta n/\omega} - b_{n-1,\uparrow} e^{-i \delta n/\omega}] \),

\[
ib_{n,\downarrow} = -v \cos \alpha [b_{n+1,\downarrow} e^{-i \delta n/\omega} - 2 b_{n,\downarrow} e^{-i \delta n/\omega} - b_{n-1,\downarrow} e^{i \delta n/\omega}]
\]

+ \( v \sin \alpha [b_{n+1,\downarrow} e^{-i \delta n/\omega} - 2 b_{n,\downarrow} e^{-i \delta n/\omega} - b_{n-1,\downarrow} e^{i \delta n/\omega}] \).

(7)

Given the on-site energy at site \( n = 0 \) modified by the impurity, as can be seen in equation (7) (due to the property of the Kronecker delta function, the terms containing \( \varepsilon_0 \) in the exponential function vanish for \( n \neq 0, \pm 1 \)), the equations of motion describing the system with a spin-1/2 particle in sites \( n = 0, \pm 1 \) are in form different from those in other sites, which will lead to a remarkable change in the local dynamics of the sites \( n = 0, \pm 1 \).

By obtaining a close correspondence in analytic and numerical results, here we typically assume that the model (1) is in high-frequency (\( \omega \gg \nu \)) limits and \( \Omega = m \omega, \varepsilon_0 = m \omega + u \) for \( |u| \leq \omega/2 \), \( m, m' = 1, 2, \ldots \) with \( u \) being the reduced impurity strength.

By means of high-frequency approximation method, in which the rapidly oscillating exponential functions in the equation (7) are replaced by their time average and the formula \( \exp \{ \pm i F \sin(\omega t)/\omega \} = \sum J_0(F/\omega) \exp \{ \pm i k_0 t \} \) is utilized, we easily figure out that the hopping amplitude \( v \) between the states with the same (different) spins and across the neighboring sites \( i \) and \( j \) (i.e., \( i = 0 \) or \( j = 0 \)) is renormalized by the high-frequency periodic driving \( \nu J_m(F/\omega) \) and \( \nu J_m(F/\omega) \), respectively. Nevertheless, the effective hopping amplitudes between the neighboring sites \( i \) and \( j \) (either \( i = 0 \) or \( j = 0 \)) are determined by the reduced impurity strength as well as the ratio of the impurity potential to the driving frequency. Thus, the DL, also referred to as coherent destruction of tunneling (CDT) in the high-frequency limit [59], occurs at distinct values of the scaled driving amplitude \( F/\omega \), which satisfies either \( J_0(F/\omega) = 0 \) for the usual spin-conserving tunneling (\( \sin \alpha = 0 \)) case or \( J_m(F/\omega) = 0 \) for the purely spin-flipping tunneling (\( \cos \alpha = 0 \)) case. When DL (CDT) occurs, the dynamics of sites \( 0, \pm 1 \) is decoupled from that of other sites, and only tunneling among sites \( 0, \pm 1 \) is allowed.

### 4.1. Tunneling dynamics with only spin-conserving coupling

In this subsection, we will analyze the case of the usual spin-conserving tunneling (\( \sin \alpha = 0 \)), where the DL condition is given by \( J_0(F/\omega) = 0 \). Under the DL condition \( J_0(F/\omega) = 0 \), the system dynamics of spin-1/2 particle will be limited in two independent subspaces: \( \{1, \downarrow \}, \{0, \uparrow \}, \{1, \uparrow \} \} \) and \( \{1, \uparrow \}, \{0, \downarrow \}, \{1, \downarrow \} \} \). In this case, however, the tunneling dynamics among sites \( 0, \pm 1 \) are partially restored and tuned by the value of the impurity potential relative to the driving frequency.

Let us first consider the resonant case, namely, \( \varepsilon_0 = m \omega, m' = 1, 2, \ldots \). By averaging the rapidly oscillating exponential terms in equations of \( b_{n,\sigma}(t) \) for \( n = 0, \pm 1 \), we have the effective three-site model in the truncated subspaces

\[
i \dot{b}_{-1,\sigma} = -v \cos \alpha J_{-m}(F/\omega) b_{0,\sigma},
\]

\[
i \dot{b}_{0,\sigma} = -v \cos \alpha J_m(F/\omega) b_{1,\sigma} + J_m(F/\omega) b_{-1,\sigma},
\]

\[
i \dot{b}_{1,\sigma} = -v \cos \alpha J_m(F/\omega) b_{0,\sigma},
\]

(8)

with \( \cos \alpha = \pm 1 \). As can be seen in equation (8), the hopping matrix for nearest neighbors is spin independent and the dynamics of the system in the subspace \( \{1, \downarrow \}, \{0, \uparrow \}, \{1, \downarrow \} \} \) is exactly the same as in the subspace \( \{1, \uparrow \}, \{0, \downarrow \}, \{1, \uparrow \} \} \). It explains why in this case the quasienergies corresponding to the Floquet states with spin up are exactly overlapped with those with spin down. The combined actions of the impurity and the high-frequency periodic driving are expected to create Floquet-quasienergy spectrum, in which the hopping matrix between the impurity and any one of its nearest neighbors is renormalized to an effective hopping parameter \( v J_m(F/\omega) \) rather than to \( v J_0(F/\omega) \) such that avoided level crossings appear at the band collapse points \( J_0(F/\omega) = 0 \) as shown in figure 1(a). In the resonant case, the system dynamics is dominated by the resonant tunneling between the impurity and its two nearest-neighbor sites as shown in figure 4(a) despite in the presence of strong tilt, which is the familiar \( m' \)-photon assisted tunneling for \( m' = 1, 2, \ldots \).

It should be born in mind that the commonly used high-frequency (averaging) approximation, which has also been exploited for derivation of the above equation (8), corresponds to the first-order perturbation approximation. In this perturbation approximation treatment, for relatively strong values of the reduced impurity strength \( u \), the oscillation of the functions \( e^{i \omega t} \) in equation (7) becomes moderately fast and should be replaced by their average value (zero) such that the first-order transitions between sites 0 and 1 (or 1) are frozen approximately. Obviously, this remarkable second-order tunneling effect on the basis of the numerical result is missed in the high-frequency approximation analysis. A more accurate perturbative analysis is therefore needed for the correct study of the dynamical behaviors.

Now we continue with the off-resonant regime, \( \varepsilon_0 = m \omega + u, m' = 1, 2, \ldots \) with moderate value of \( |u| \), so as
to investigate the tunneling dynamics of the system with only spin-conserving coupling at the collapse point $J_d(F/\omega) = 0$, by means of the multiple-time-scale asymptotic analysis [60–62]. Equipped with the effective three-site model in a truncated Hilbert space spanned by the Fock basis set \{−1, 0, 1\}, we start by introducing $\epsilon = \nu / \omega$ as a small parameter for high-frequency driving and the normalized time variable $\tau = \omega t$, and by writing $b_{n,\sigma}(n = 0, \pm 1, \sigma = \uparrow, \downarrow)$ as a power-series expansion in $\epsilon$,

$$b_{n,\sigma}(\tau) = b_{n,\sigma}^{(0)}(\tau) + \epsilon b_{n,\sigma}^{(1)}(\tau) + \epsilon^2 b_{n,\sigma}^{(2)}(\tau) + \ldots. \tag{9}$$

Because the high-order terms can be neglected in the high-frequency regime, the probability amplitudes $b_{n,\sigma}$ can be approximately rewritten as the zeroth order $b_{n,\sigma}(\tau) = b_{n,\sigma}^{(0)}(\tau) = A_{n,\sigma}(\tau)$. By definition, $|A_{n,\sigma}|^2 (n = 0, \pm 1)$ refers to the occupation probability for a single particle with spin $\sigma$ in site $n$. According to the standard multiple-scale asymptotic perturbation method [60], we obtain the following equations for the amplitudes $A_{n,\sigma} (n = 0, \pm 1)$ up to the second-order $\epsilon^2$ for the usual spin-conserving tunneling ($\sin \alpha = 0$) case

$$i \frac{dA_{1,\sigma}}{dt} = -\epsilon^2(\chi_1 A_{1,\sigma} + \chi_2 A_{-1,\sigma}),$$

$$i \frac{dA_{0,\sigma}}{dt} = 2\epsilon^2\chi_2 A_{0,\sigma},$$

$$i \frac{dA_{-1,\sigma}}{dt} = -\epsilon^2(\chi_1 A_{-1,\sigma} + \chi_2 A_{1,\sigma}), \tag{10}$$

where we have set

$$\chi_1 = \sum_p \frac{J_p(F)}{-p - m' + u'}, \quad \chi_2 = \sum_p \frac{J_p(F)}{p + m' + u'} \tag{11}.$$

Equation (10) provides a correct description of the dynamics of the original system with only spin-conserving coupling under DL condition up to the second-order time scale $\sim 1/\epsilon^2$. In deriving equation (10), the intermediate state $|0, \sigma\rangle$ is eliminated and accordingly an effective tunneling rate between sites $|−1, \sigma\rangle$ and $|1, \sigma\rangle$ is given by $\omega_0^2 \chi_1 \equiv \nu^2 \chi_1 / \omega \ll \nu$, through returning to the original time variable $t$. From equation (10), we immediately note that the dynamics of the impurity is decoupled from that of its two neighbors and therefore the particle will be captured by the impurity if the system is initially prepared with a single particle in the impurity site. Considering that the temporal evolution equations for amplitude $A_{n,\sigma} (n = 0, \pm 1)$ are the same for any spin, as can be seen from equation (10), we thus have the spin-independent second-order tunneling between the two nearest-neighbor sites of the impurity with the population at the impurity site. In figure 5(a), we have calculated the time evolution of occupation probabilities $P_{n,\sigma}$ via integration of equation (10)—the second-order perturbative results, and compared them (circles) with the numerical results obtained from the original model (1) for the usual spin-conserving tunneling ($\sin \alpha = 0$) case with the initial state $|\psi(t = 0)\rangle = |−1, \uparrow\rangle$. A good agreement is found.

According to the Floquet theorem, we can construct the analytical Floquet solutions of the system by setting $a_{n,\sigma} = a_{n,\sigma}(t)$

$$\exp(-i\epsilon t) = A_{n,\sigma}(t)\exp\left\{ -i[n\Phi(t) + (-1)^n \frac{\Omega}{2} t + \epsilon_0 \delta_{n,0} \sigma]\right\} = A'_{n,\sigma}\exp\left\{ -i[n\Phi(t) + (-1)^n \frac{\Omega}{2} t + \epsilon_0 \delta_{n,0} \sigma]\right\}\exp(-iEt) (k = 0, 1 \text{ for } \sigma = \uparrow, \downarrow, \text{ respectively})$$

with the help of equations (5) and (6), where constants $A'_{n,\sigma}$ and $E$ are the eigenvector components and the eigenvalue of the time-independent version of equation (10) respectively. By inserting $A_{n,\sigma}(t) = A'_{n,\sigma}\exp(-iEt)$ into equation (10), and employing the transformations (5) and (6), we obtain the quasienergies for the off-resonant case with moderate value of $u$,

$$\begin{align*}
\varepsilon_{1,\sigma} &= -\frac{\nu^2\chi_2 + \nu^2\chi_1}{\omega} + (−1)^n \frac{\Omega}{2}, \\
\varepsilon_{2,\sigma} &= \frac{2\nu^2\chi_2}{\omega} + u + (−1)^n \frac{\Omega}{2}, \\
\varepsilon_{3,\sigma} &= -\frac{\nu^2\chi_2 - \nu^2\chi_1}{\omega} + (−1)^n \frac{\Omega}{2},
\end{align*} \tag{12}$$

where we have decomposed $\epsilon_0$ into a form of $\epsilon_0 = m'\omega + u, m' = 1, 2, \ldots$, and formulated the Floquet modes $|\psi_{j,\sigma}(t)\rangle \equiv (a_{−1,\sigma}, a_{0,\sigma}, a_{1,\sigma})^\text{T}$ for $j = 1, 2, 3$. Note that the functions of $\exp[\pm i\Phi(t)]$ and $\exp(im'\omega t)$ are $T$-periodic and hence that the Floquet modes inherit the period of the driving. The two sets of quasienergies ($k = 0, 1$) are for different spins $\sigma = \uparrow, \downarrow$ respectively, which are almost equal but displaced by a constant amount $\Omega$. Due to the fact that the quasienergies possess Brillouin zonelike structure with one zone width being $\omega$, when $\Omega = m\omega, m = 1, 2, \ldots$, the two sets of quasienergies can be mapped to one Brillouin zone and become identical if one set of quasienergies are all shifted by a constant amount $\Omega$. In this case, when falling into one Brillouin zone, $0 < \epsilon \leq \omega$, the two sets of quasienergies for different spins are equal to each other and given by

$$\begin{align*}
\varepsilon_{1,\sigma} &= -\frac{\nu^2\chi_2 + \nu^2\chi_1}{\omega} + \frac{\omega}{2}, \\
\varepsilon_{2,\sigma} &= \frac{2\nu^2\chi_2}{\omega} + u + \frac{\omega}{2}, \\
\varepsilon_{3,\sigma} &= -\frac{\nu^2\chi_2 - \nu^2\chi_1}{\omega} + \frac{\omega}{2}. \tag{14}
\end{align*}$$

4.2. Tunneling dynamics with only spin-flipping coupling

Now we are in a position to consider the case of the purely spin-flipping tunneling ($\cos \alpha = 0$), where the DL condition is given by $J_0(F/\omega) = 0$ when $\Omega = m\omega$ with $m$ positive integers. In this case, when the DL condition $J_0(F/\omega) = 0$ is satisfied, the spin evolution of the single-particle will be
limited in the following two independent subspaces: \{ \{ -1, \uparrow \}, \{ 0, \downarrow \}, \{ 1, \uparrow \} \} and \{ \{-1, \uparrow \}, \{ 0, \uparrow \}, \{ 1, \downarrow \} \}. Next, we will perform qualitative analysis on the resonant tunneling and second-order tunneling for the system with only spin-flipping coupling under DL condition, as follows.

When the impurity potential strength is in resonance with the driving field, \( \varepsilon_0 = m' \omega \), \( m' = 1, 2, \ldots \), the high-frequency averaging approximation of equation (7) yields the temporal evolution equation governing the local dynamics of the three sites \( 0, \pm 1 \).

\[
\begin{align*}
ib_{-1,1} &= v \sin \alpha J_{m-m'} F_0 b_{0,1}, \\
ib_{0,0} &= -v \sin \alpha \left[ J_{m-m'} F_0 b_{1,1} - J_{m-m} F_0 b_{-1,1} \right], \\
ib_{1,1} &= -v \sin \alpha J_{m-m'} F_0 b_{0,1}, \\
ib_{-1,1} &= -v \sin \alpha J_{m-m} F_0 b_{0,1}, \\
ib_{0,0} &= -v \sin \alpha [-J_{m+m'} F_0 b_{1,1} + J_{m-m'} F_0 b_{-1,1}], \\
ib_{1,1} &= v \sin \alpha J_{m-m'} F_0 b_{0,1},
\end{align*}
\]

where \( \sin \alpha = \pm 1 \). We again encounter the familiar multiphoton resonances, for which the system is able to exchange energy of an integer number of photons with the oscillating field to bridge the energy difference created by both the impurity potential and the spin-flipping tunneling due to SOC, and thus the tunneling is partly restored. This is witnessed by the fact that we have non-zero renormalized tunneling rate \( J_{m-m'}(F/\omega) \neq 0 \) and \( J_{m+m'}(F/\omega) = 0 \) in equation (15) even at the collapse points corresponding to the zeros of \( J_{m}(F/\omega) \). As the effective hopping rates are distinct when the dynamics is confined in the two independent subspaces: \{ \{-1, \uparrow \}, \{ 0, \downarrow \}, \{ 1, \uparrow \} \} and \{ \{-1, \downarrow \}, \{ 0, \uparrow \}, \{ 1, \downarrow \} \} respectively, equation (15) describes the spin-dependent resonant tunneling with spin flipping among the three sites \( 0, \pm 1 \), which is consistent with the numerical results presented in figure 4 where we have set \( m = m' = 1 \) and the initial state \( | -1, \uparrow \rangle \).

Turning to the off-resonant case, \( \varepsilon_0 = m' \omega + u \), \( m' = 1, 2, \ldots \), with moderate value of \( |u| \), where the second-order tunneling between the two nearest-neighbor sites of the impurity will emerge even under the DL condition. In the truncated Hilbert space, we still proceed with expanding the amplitudes \( b_{n,\sigma} \) by a power-series of \( \varepsilon \), \( b_{n,\sigma}(\varepsilon) = b_{n,\sigma,0}(\tau) + \varepsilon b_{n,\sigma,1}(\tau) + \varepsilon^2 b_{n,\sigma,2}(\tau) + \cdots \), where \( \tau = \omega \tau, \varepsilon = v/\omega \), and approximate the probability amplitudes \( b_{n,\sigma} \) as the leading order \( b_{n,\sigma,0}(\tau) = b_{n,\sigma,0}(\tau) = b_{n,\sigma}(\tau) \). It should be noted that the other amplitudes \( b_{n,\sigma}(n = 0, \pm 1) \) do not change in time, due to the frozen dynamics of lattice sites for \( n = 0, \pm 1 \) under the DL condition. The basis of the multiple-time-scale asymptotic analysis of equation (7) [60], we obtain the evolution equations for the amplitudes \( A_{n,\sigma} \) \( (n = 0, \pm 1) \) up to the second-order \( \varepsilon^2 \) for the purely spin-flipping tunneling (\( \cos \alpha = 0 \)) case, from equation (16), we observe that the dynamics of a particle initially occupying the impurity site is frozen in the second-order approximation, whereas the transition \( | -1, \uparrow \rangle \rightarrow | 1, \uparrow \rangle \) \( (| -1, \downarrow \rangle \rightarrow | 1, \downarrow \rangle) \) is generated by a second-order transition process via the virtual intermediate state \( | 0, \downarrow \rangle \) \( (| 0, \uparrow \rangle) \). This second-order transition describes such a physical process, in which a single spin-up (down) particle can only tunnel back and forth between the two nearest-neighbor sites of the impurity in a manner that the spin is nonetheless kept unchanged. This spin-invariant behavior exhibits remarkable resemblance to the usual spin-conserving tunneling case. However, in contrast to the usual spin-conserving tunneling case, the second-order tunneling process described by equation (16) is essentially spin-dependent and has distinct physical mechanisms, which can be viewed from the fact that two types of second-order transition processes \( | -1, \uparrow \rangle \rightarrow | 0, \downarrow \rangle \rightarrow | 0, \uparrow \rangle \) \( (| -1, \downarrow \rangle \rightarrow | 0, \uparrow \rangle \rightarrow | 0, \downarrow \rangle \) are generated through elimination of different virtual intermediate states \( | 0, \downarrow \rangle \) \( (| 0, \uparrow \rangle) \) and thus have distinct effective tunneling rates given by \( \omega^2 \chi_2 \) and \( \omega \varepsilon^2 \chi_2 \) respectively. Clearly, the tunneling dynamics (circles in figure 5(b)) obtained from the second-order perturbative results (equation (16)) are in consistency with those on the basis of a full numerical analysis of the original model (1) for the purely spin-flipping tunneling (\( \cos \alpha = 0 \)) case, see the curves in figure 5(b).
Fig. 6. Comparison between the numerically computed quasienergies (solid lines) from the original model (1) and the analytical quasienergies (open circles) based on the second-order perturbative results (equations (14) and (18)) for the non-resonant case $\varepsilon_0/\omega = 1.2$, at (a) $\sin \alpha = 0$ and (b) $\cos \alpha = 0$. The other parameters are $v = 1, \omega = 20, \Omega = 20$. The main panels show the enlargements of four analytical quasienergies (which are doubly degenerate for the $\sin \alpha = 0$ case) around $\varepsilon = 10$, and the insets show the two quasienergies (the analytical correspondences $\varepsilon_{2,\sigma}$ in equation (14) and $\varepsilon_3, \varepsilon_4$ in equation (18)) which are separated widely from the rest of band.

$A_{n,\sigma}(t) = A'_{n,\sigma}(t) \exp(-iEt)$ into equation (16), we have the resulting time-independent form of equation (16) which gives the eigenvector components $A'_{n,\sigma}$ and the eigenvalue $E$. With the help of equations (5) and (6), the analytical Floquet solutions of the considered system can be constructed as $\tilde{a}_{n,\sigma} = A_{n,\sigma}(t) \exp(-iEt) = A_{n,\sigma}(t) \exp \left\{ -i[n\Phi(t) + (-1)^{n+1}t + \varepsilon_0 \delta_{n,0}] \right\} = A'_{n,\sigma} \exp \left\{ -i[n\Phi(t) + (-1)^{n+1}t + \varepsilon_0 \delta_{n,0}] \right\} \exp(-iEt) (k = 0, 1$ for $\sigma = 1, 1$). Imposing the $T$-periodic boundary condition on these states $\tilde{a}_{n,\sigma}(t)$ reveals the corresponding quasienergies (modulo $\omega$) to be

$$
\varepsilon_1 = \frac{-v^2 \chi_4 + v^2 \chi_3}{\omega} + \frac{\omega}{2},
$$

$$
\varepsilon_2 = \frac{2v^2 \chi_4}{\omega} + u + \frac{\omega}{2},
$$

$$
\varepsilon_3 = \frac{-v^2 \chi_4 - v^2 \chi_3}{\omega} + \frac{\omega}{2},
$$

$$
\varepsilon_4 = \frac{-v^2 \chi_6 + v^2 \chi_5}{\omega} + \frac{\omega}{2},
$$

$$
\varepsilon_5 = \frac{2v^2 \chi_6}{\omega} + u + \frac{\omega}{2},
$$

$$
\varepsilon_6 = \frac{-v^2 \chi_6 - v^2 \chi_5}{\omega} + \frac{\omega}{2},
$$

(18)

where the identities $\Omega = m\omega, \varepsilon_0 = m'\omega + u, m, m' = 1, 2, \ldots$ have been used.

Our analytical quasienergies based on the second-order perturbative results of equations (14) and (18) are plotted as open circles in figures 6(a) and (b), corresponding to the usual spin-conserving tunneling ($\sin \alpha = 0$) and the purely spin-flipping tunneling ($\cos \alpha = 0$) case respectively. The six analytical Floquet states, with corresponding quasienergies given by either equations (14) or (18), originate from the localized impurity effect and behave differently from the rest of miniband state. It is noteworthy that the six analytical quasienergies are doubly degenerate for the usual spin-conserving tunneling case and this degeneracy breaks up for the purely spin-flipping tunneling case. Under the DL conditions, all the other quasienergies collapse into one single value (the value is $\omega/2 = 10$ for our selected parameters, as the other terms in each analytical expression of quasienergies (equations (14) and (18)) represent the corrections caused by the off-resonant single-site impurity). Because two quasienergies (the analytical correspondences $\varepsilon_{2,\sigma}$ in equation (14) and $\varepsilon_3, \varepsilon_4$ in equation (18)) are far separated from the rest of band, incorporation of them into the main panel will render the content of figure too small to be visible. Thus, we plot the well-separated analytical points in the insets of figure 6, making them bigger and easily readable for the reader. As clearly shown in figure 6, the analytical quasienergies given by equations (14) and (18) are in good agreement with the direct numerical results obtained from the original model (1), which again verifies the existence of avoided level crossings for the off-resonant case with moderate reduced impurity strength $u$.

5. Discussion and experimental aspects

Here, we first justify the validity of the effective three-site model approximation and the multiple-time-scale asymptotic perturbative approximation used in this work. To this end, we define two related variables: one is the time-averaged total probability of finding the single particle in sites $0, \pm 1$, $\langle S_1 \rangle = \frac{1}{\Delta t} \int_0^{\Delta t} \sum_\sigma \langle P_{1,\sigma} + P_{0,\sigma} + P_{1,\sigma} \rangle dt$; the other is the time-averaged total probability of finding the single particle in sites $\pm 1$, $\langle S_2 \rangle = \frac{1}{\Delta t} \int_0^{\Delta t} \sum_\sigma \langle P_{1,\sigma} + P_{0,\sigma} + P_{1,\sigma} \rangle dt$. The former is used to quantify the validity of the effective three-site model approximation: if $\langle S_1 \rangle \approx 1$ lasts for a long-enough averaging time interval $\Delta t$, the effective three-site model approximation is valid, otherwise it breaks down. The latter is to measure the validity of the multi-time-scale asymptotic analysis. If the average of the occupation probabilities of sites $\pm 1$ over a long-enough time interval $\Delta t$ is approximately equal to one, $\langle S_2 \rangle \approx 1$, it means that the single atom only tunnels between the two nearest-neighbor sites of the impurity with negligible impurity site population. When $\langle S_2 \rangle \approx 1$, the second-order tunneling occurs and the validity of the multi-time-scale asymptotic analysis can be justified. To delineate the validity regime of the effective three-site model approximation and the multi-time-scale asymptotic perturbative approximation, we numerically give $\langle S_1 \rangle$ (solid lines) and $\langle S_2 \rangle$ (dashed lines) as the function of the driving frequency $\omega$, for
the usual spin-conserving tunneling ($\sin \alpha = 0$) case with the parameters $v = 1$, $\epsilon_0 = 1.2 \omega$, $\Omega = \omega$, $F/\omega = 2.405$, as in figure 7(a), and for the purely spin-flipping tunneling ($\cos \alpha = 0$) case with the parameters $v = 1$, $\epsilon_0 = 1.2 \omega$, $\Omega = \omega$, $F/\omega = 3.8317$, as in figure 7(b). In our numerical calculations we have always assumed that the system is initialized in $|{-1}, \uparrow \rangle$ and we have shown the second variable $\langle S_2 \rangle$ by actually computing $\langle S_2 \rangle = \frac{1}{\Delta \tau} \int_{0}^{\Delta \tau} (P_{-1, \uparrow} + P_{1, \downarrow}) dt$ for $\Delta \tau = 200(\upsilon^{-1})$ because of $P_{1, \uparrow} = P_{-1, \downarrow} = 0$. It can be seen from figure 7 that the driving frequency $\omega$ on the order of or larger than $10v$ can be regarded safe for observing our theoretical predictions.

In the numerical calculations above, we have set that the size of the lattice is $N = 21$. Our numerical results (not shown) demonstrate that the magnitude of the driving frequency for validity of both approximations employed will decrease with the decrease of lattice size, and the effective three-site model approximation and the second-order perturbative approximation are still applicable even when the driving frequency is much smaller than $10v$ if we treat relatively small systems of up to $N > 3$. This indicates that our results are more realistic in the systems of up to relatively small numbers of sites, because the validity of single-band tight-binding description of the original model requires moderately small driving frequency.

Before concluding, we present some remarks on experimental aspects of our theoretical predictions. In our work, we only address the tunneling dynamics of the usual spin-conserving tunneling ($\sin \alpha = 0$) and the purely spin-flipping tunneling ($\cos \alpha = 0$) case. For the coexistence of the spin-conserving tunneling and the spin-flipping tunneling case, the simultaneous DL does not occur, because the collapse of

6. Conclusion

In summary, we have identified two types of second-order tunneling processes for a single SO-coupled atom placed in a driven optical lattice with an impurity, provided that the impurity potential strength is in far-off-resonance with the driving field. The two types of second-order tunneling seem to show up in the same way that an initially spin-up (down) atom only tunnels between the two nearest-neighbor sites of the impurity, in which the spin remains unchanged and the impurity site population is negligible during the evolution time. Nevertheless, it has been found that two distinct mechanisms are responsible for the two second-order tunneling processes: one is related to a spin-independent tunneling process in which the virtual intermediate state without spin-flipping is eliminated, the other is to a spin-dependent tunneling process in which the second-order transition is generated via elimination of a virtual intermediate state with spin-flipping. Fortunately, the two types of second-order tunneling processes can be distinguished by tuning the ratio of the impurity potential to the driving frequency. When the ratio becomes an integer, the spin-independent second-order tunneling is tuned to the resonant oscillation without spin-flipping between the impurity and its two nearest-neighbor sites, while the spin-dependent second-order tunneling is to the resonant oscillation with spin-flipping.

By means of the direct quasienergy-band computation, we evidence that all the resonant and second-order tunneling processes are reflected by the avoided level crossings near the pseudocollapse points of quasienergy bands. Furthermore, the very subtle and fine avoided level crossing in the quasienergy spectrum, which manifests itself dynamically in the second-order tunneling and is easily neglected in exact numerical simulations, has been fully understood in the framework of the second-order perturbative theory. These results may be
relevant to engineering the spin-dependent quantum transport in experiments and find some possible applications in the design of novel spintronics devices.

Recently, the spin-1 spin–orbit-coupled system has been successfully realized in experiment [66]. In such spin-1 system, treating any two hyperfine states as spin up and down component, we can study the spin-dependent tunneling dynamics of the spin–orbit-coupled atoms, as we have done for the pseudospin-1/2 case. However, the spin-1 system actually contains three spin components and includes the spin-dependent interaction [67–69], which makes its dynamics richer and more complex. An interesting direction for future work is to analyze the tunneling dynamics of spin-1 system in the presence of a localized impurity or random disorder uniformly distributed over the lattice [70–72].

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