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Transient dynamics of super Bloch oscillations of a one dimensional Holstein polaron under the influence of an external AC electric field

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We extend our theoretical formalism for DC-field polaron dynamics to the dynamics of a one-dimensional Holstein polaron in an external AC electric field using the multiple Davydov trial states. Effects of carrier-phonon coupling on detuned and resonant scenarios are investigated for both zero phase and non-zero phase. For slightly off-resonant or detuned cases, a beat between usual Bloch oscillations and an AC driving force results in super Bloch oscillations, i.e., rescaled Bloch oscillations in both the spatial and the temporal space. Super Bloch oscillations are damped by carrier-phonon coupling. For resonant cases, if the carrier is created on two nearest-neighbouring sites, the carrier wave packet spreads with small-amplitude oscillations. Adding carrier-phonon coupling localizes the carrier wave packet. If an initial broad Gaussian wave packet is adopted, the centroid of carrier wave packet moves with a certain velocity and with its shape unchanged. Adding the carrier-phonon coupling broadens the carrier wave packet and slows down the carrier movement. Our findings may help provide guiding principles on how to manipulate the dynamics of super Bloch oscillations of carriers in superlattice semiconductors and optical lattices by modifying DC and AC field strengths, AC phases, and detuning parameters.

the whole system. However, when a uniform electrical field F is applied, all eigenstates of the single-electron tight-binding Hamiltonian become spatially localized Wannier-Stark states due to Bragg reflections, while electrons keep oscillating within a finite volume if scattering effects neglectable. The periodic motion occurs in real and in reciprocal space, and is known as the BOs [2]. The center-of-mass of electronic wave packets performs a periodic oscillation with an amplitude given by the Stark localization length $L = J/aF$, where J is a tunneling coefficient and a refers to the lattice constant along the field direction [3–6]. Since scattering processes induced by defects and environment effects, an experimental detection of the BOs is highly nontrivial. Until 1970s, Esaki *et al.* firstly proposed that the BOs are achievable in semiconducting superlattices [7]. By 1992, the first experiment observation of the BOs was reported by Feldmann *et al.* in superlattices under an external electric field [1]. More recently, cold atoms and Bose-Einstein condensates (BECs) in optical lattices have been revealed as a very convenient carrier to observe BOs since the scattering processes can be significantly reduced [8–10]. To probe the mechanism by which the BOs take place, the dynamics of the carrier wave packet has been extensively studied in various physical systems [11–21], including a semiconductor waveguide [22] and a thermo-optic polymer array subjected to a temperature gradient [23].

1 introduction

Since the first experimental observation of time-domain Bloch oscillations (BOs) in superlattices under an external electric field, the oscillation and dynamical localization of electrons in spatial and temporal domains have attracted great attention [1]. In perfect crystals, lattices generate a periodic potential and Bloch theorem predicts that electronic states can extend uniformly over

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In the last decade, there has emerged much interest in dynamics of a quasiparticle affected not only by a direct current (DC) field but also by a superimposed alternating current (AC) field [24–29]. Influences of the DC and AC field have been theoretical and experimentally reported for the BECs in optical lattice [30, 31], for charge carriers in organic materials [25], for light in periodic optical waveguide arrays [24, 32], and for [carriers](#) in a one-dimensional quantum-dot superlattice [33], and in a semiconductor superlattice [34]. It has been shown that particular AC fields result in the localized wave packet for certain AC frequencies [33, 35, 36]. This kind of localization is known as dynamical localization and it is conceptually different from Anderson localization [37, 38]. Dynamical localization has been experimentally reported in cold atoms and the BECs in one-dimensional optical lattices [39, 40]. Remarkably, it was demonstrated that a weakly interacting BEC in a harmonically driven tilted potential can support directed transport or large amplitude oscillations of the wave function, depending on the driven frequency [31, 41, 42]. In 2010, Haller *et al.* observed giant center-of-mass oscillations in real space with a displacement across hundreds of lattice sites when they added a periodic modulation to the force near the Bloch frequency, and firstly named the oscillations as super Bloch oscillations (SBOs) [43]. Kolovsky *et al.* soon followed up with a theoretical explanation: when the AC frequency is close to the Bloch frequency, the difference between the two frequencies leads to the SBOs, and a near resonant driving transforms Wannier-Stark states into new 'super' Wannier-Stark states with localization length $\tilde{L} \approx \tilde{J}/a\tilde{F}$, where $\tilde{J}$ is an effective tunneling coefficient, and $\tilde{F}$ corresponds to an effective field [44–46]. The term super refers to the fact that the amplitude in position space of such an oscillation is several orders of magnitude larger than for 'normal' BOs [24, 47].

Environmental effects are of essential importance to dynamics of the BOs and SBOs in target systems such as semiconductor superlattices, organic materials and quantum dots. Due to the complexity of system-bath interactions, it is difficult to devise exact analytical solutions to the dynamics of these systems under the influence of the external electric fields. Fröhlich's model of polaron was employed in 1970 by Feynman *et al.* to study the motion of an electron in a polar crystal in a strong electric field [48]. Later, much theoretical work focused on transition rate probabilities, which can be derived from the rate equations or the Boltzmann equation [49, 50]. In the 1990s, Holthaus *et al.* proposed to use AC fields to localize the [carrier](#) in disordered semiconductor superlattices [51], and carried out a systematic study on [carrier](#) localization in AC-driven tight-binding lattices

[37]. However, fully quantum mechanically modeling of polaron dynamics under the simultaneous presence of DC and AC fields have not received much-deserved attention over the last decades. Moreover, regardless of the rapid experimental progress on the SBOs [31, 43], few theoretical work have been devoted to study the dynamics of the SBOs [27, 52].

Despite extensive studies on the BOs, roles of the complex interplay between the carrier and its accompanying phonon cloud still remains an open question [53]. With respect to the BOs dynamics in the Su-Schrieffer-Heeger model for polymers [15, 16, 54, 55] and the Peyrard-Bishop-Holstein model for DNA [56], the phonon bath is treated classically and the associated carrier-phonon coupling semi-classically. In 1997, Bonča and Trugman used the one-dimensional Holstein molecular crystal model to study dynamics of an electron coupled to optical phonons under a strong electric field. Their work retained full quantum coherence in the description of nonequilibrium dynamics of a polaron [53, 57–59]. Recently, the crux of transient BOs dynamics was laid out in our previous study by employing the multiple Davydov trial states [13]. Since the dynamical control of the SBOs can be realized in the same experimental setup for the engineering of the BOs, it is necessary to extend the successful method for the BOs dynamics to study the influence of carrier-phonon coupling on the SBOs [37]. With respect to the SBOs, spatial and temporal dynamics affected by carrier-phonon interactions has not received adequate attention. In fact, very few literatures can be found to study the effects of system-bath interactions on the dynamics of the SBOs. Here, we continue our endeavor with an accurate theoretical treatment of the SBOs dynamics of the [carrier](#) coupled to the phonons.

In this work, we investigate the impact of diagonal [carrier](#)-phonon coupling on polaron dynamics in a ring system in the presence of the DC and AC electric fields using the multiple Davydov D_2 trial state with the Dirac-Frenkel variational principle. The rest of the paper is structured as follows. In Sec. 2, we present the Hamiltonian in the gauge transformed form and our trial wave function, the multi- D_2 *Ansatz*. Dynamics of the SBOs is examined in Sec. 3. Polaron dynamics for the detuned and resonant cases is examined in Sec. 3.1. Finally, polaron dynamics for non-zero AC phase is described in Sec. 3.2. Conclusions are drawn in Sec. 4.

2 methodology

2.1 Model

The Hamiltonian of the one-dimensional Holstein polaron reads

$$\hat{H} = \hat{H}_{ca} + \hat{H}_{ph} + \hat{H}_{ca-ph} \quad (1)$$

where $\hat{H}_{ca}$, $\hat{H}_{ph}$, and $\hat{H}_{ca-ph}$ are the **charge carrier** Hamiltonian, the bath (phonon) Hamiltonian, the **carrier-phonon** coupling Hamiltonian, respectively. An extra term

$$[F_{dc} + F_{ac} \cos(\omega_{ac} t + \phi_{ac})] \sum_n n a_n^\dagger a_n \quad (2)$$

is added to represent the scalar potential interactions induced by the external electric field. F_{dc} denotes a DC field and $F_{ac} \cos(\omega_{ac} t + \phi_{ac})$ serves as an AC field. In the presence of the external field, the potential of the field at the boundary of the system were found to become discontinuous if taking the periodic boundary conditions into consideration via bending a linear chain into a ring [60]. This problem can be solved by adopting a gauge transformed vector potential, i.e., $A(t) = -F_{dc}t - \frac{F_{ac}}{\omega_{ac}} \sin(\omega_{ac} t + \phi_{ac})$ [61, 62]. Then we can recast the Hamiltonian as a gauge transformed Hamiltonian for the ring system under the external electric field,

$$\begin{aligned} \hat{H}_{ca} &= -J \sum_n a_n^\dagger \left(e^{iA(t)} a_{n+1} + e^{-iA(t)} a_{n-1} \right), \\ \hat{H}_{ph} &= \omega_0 \sum_n b_n^\dagger b_n, \\ \hat{H}_{ca-ph} &= -g\omega_0 \sum_n a_n^\dagger a_n (b_n + b_n^\dagger), \end{aligned} \quad (3)$$

where $\hat{a}_n^\dagger$ ($\hat{a}_n$) and $\hat{b}_n^\dagger$ ($\hat{b}_n$) are the **carrier** and phonon creation (annihilation) operators for the n -th site, respectively. Written in the phonon momentum space,

$$\hat{H}_{ph} = \sum_q \omega_q \hat{b}_q^\dagger \hat{b}_q, \quad (4)$$

$$\hat{H}_{ca-ph} = -N^{-1/2} g \sum_{n,q} \omega_q \hat{a}_n^\dagger \hat{a}_n \left(e^{iqn} \hat{b}_q + e^{-iqn} \hat{b}_q^\dagger \right), \quad (5)$$

where ω_q is the phonon frequency with momentum q , and $\hat{b}_q^\dagger$ ($\hat{b}_q$) is the creation (annihilation) operator of a phonon with momentum q ,

$$\hat{b}_q^\dagger = N^{-1/2} \sum_n e^{iqn} \hat{b}_n^\dagger, \quad \hat{b}_n^\dagger = N^{-1/2} \sum_q e^{-iqn} \hat{b}_q^\dagger. \quad (6)$$

J and g are the transfer integral and the diagonal **carrier-phonon** coupling strength, respectively. There has been related theoretical work that takes the Holstein model describing an electron interacting locally with dispersionless optical phonons in a strong electric field to study the

inelastic quantum transport process [50]. The full quantum coherence was revealed to be retained in the model and dispersionless optical phonon was found to absorb the excess energy from the external field to avoid infinite drift velocity of the electron [53, 63]. In this work, we consider the Einstein dispersionless model, i.e., $\omega_q = \omega_0$. In the remainder of the paper, ω_0 is set to unity as the energy unit.

2.2 Multiple Davydov trial states

The multiple Davydov trial states with multiplicity M , which are essentially M copies of the corresponding single Davydov *Ansatz*, have been developed to investigate the time evolution of the Holstein polaron following the Dirac-Frenkel variational principle [64]. A series of multiple Davydov trial states, i.e., the multiple Davydov D_1 , $D_{1.5}$, and D_2 *Ansätze*, have been proposed, demonstrating significant improvements over single Davydov states in the flexibility and the accuracy of the trial states [65–67]. Recently, the multiple Davydov D_2 trial state, also known as the multi- D_2 *Ansatz*, has been successfully applied to obtain accurate dynamics of a variety of open quantum systems [68–70], including the singlet fission model [71] and the dissipative Landau-Zener model [73].

In this work, we employ the multi- D_2 *Ansatz*. It can be constructed as

$$\begin{aligned} |D_2^M(t)\rangle &= \sum_i^M \sum_n^N \psi_{in} |n\rangle_{ca} |\lambda_i\rangle, \\ &= \sum_i^M \sum_n^N \psi_{in} \hat{a}_n^\dagger |0\rangle_{ca} \exp \left\{ \sum_q \left[\lambda_{iq} \hat{b}_q^\dagger - \lambda_{iq}^* \hat{b}_q \right] \right\} |0\rangle_{ph}, \end{aligned} \quad (7)$$

where ψ_{in} and λ_{iq} are time-dependent variational parameters for the **carrier** probability and phonon displacement, respectively, n represents the site number, and i labels the coherent superposition state. If $M = 1$, the $|D_2^M(t)\rangle$ *Ansatz* is restored to the usual Davydov D_2 trial state. The equations of motion of the variational parameters ψ_{in} and λ_{iq} are then derived by adopting the Dirac-Frenkel variational principle,

$$\begin{aligned} \frac{d}{dt} \left(\frac{\partial L_2}{\partial \dot{\psi}_{in}^*} \right) - \frac{\partial L_2}{\partial \psi_{in}^*} &= 0, \\ \frac{d}{dt} \left(\frac{\partial L_2}{\partial \dot{\lambda}_{iq}^*} \right) - \frac{\partial L_2}{\partial \lambda_{iq}^*} &= 0. \end{aligned} \quad (8)$$

for the multi- D_2 *Ansatz*, and the Lagrangian L_2 is formulated as

$$\begin{aligned} L_2 &= \langle D_2^M(t) | \frac{i}{2} \frac{\partial}{\partial t} - \hat{H} | D_2^M(t) \rangle \\ &= \frac{i}{2} \left[\langle D_2^M(t) | \frac{\partial}{\partial t} | D_2^M(t) \rangle - \langle D_2^M(t) | \frac{\partial}{\partial t} | D_2^M(t) \rangle \right] \\ &\quad - \langle D_2^M(t) | \hat{H} | D_2^M(t) \rangle. \end{aligned} \quad (9)$$

where the first term yields

$$\begin{aligned} &\frac{i}{2} \left[\langle D_2^M(t) | \frac{\partial}{\partial t} | D_2^M(t) \rangle - \langle D_2^M(t) | \frac{\partial}{\partial t} | D_2^M(t) \rangle \right] \\ &= \frac{i}{2} \sum_{i,j} \sum_n \left(\psi_{jn}^* \dot{\psi}_{in} - \dot{\psi}_{jn}^* \psi_{in} \right) S_{ji} \\ &\quad + \frac{i}{2} \sum_{i,j} \sum_n \psi_{jn}^* \psi_{in} S_{ji} \sum_q \left[\frac{\dot{\lambda}_{jq}^* \lambda_{jq} + \lambda_{jq}^* \dot{\lambda}_{jq}}{2} \right. \\ &\quad \left. - \frac{\dot{\lambda}_{iq} \lambda_{iq}^* + \lambda_{iq} \dot{\lambda}_{iq}^*}{2} + \lambda_{jq}^* \dot{\lambda}_{iq} - \lambda_{iq} \dot{\lambda}_{jq}^* \right], \end{aligned} \quad (10)$$

and the second term takes the form

$$\begin{aligned} &\langle D_2^M(t) | \hat{H} | D_2^M(t) \rangle \\ &= \langle D_2^M(t) | \hat{H}_{ca} | D_2^M(t) \rangle + \langle D_2^M(t) | \hat{H}_{ph} | D_2^M(t) \rangle \\ &\quad + \langle D_2^M(t) | \hat{H}_{ca-ph} | D_2^M(t) \rangle \end{aligned} \quad (11)$$

where the Debye-Waller factor is formulated as

$$S_{ij} = \exp \left\{ \sum_q \lambda_{iq}^* \lambda_{jq} - \frac{1}{2} \left(|\lambda_{iq}|^2 + |\lambda_{jq}|^2 \right) \right\}. \quad (12)$$

Detailed derivations of the equations of motion for the variational parameters are given in the Supporting Information. In the numerical calculations, the fourth-order Runge-Kutta method is used to integrate the equations of motion.

It is noted that our multi- D_2 *Ansatz* is essentially the same as the *Ansatz* in the multi-configurational Ehrenfest (MCE) method proposed by Shalashilin *et al.* [74–76]. The formulation notations may be different. In the language of the MCE approach, λ_{iq} is called coherent state Z_{iq} , and the multiplicity M refers to the number of Ehrenfest configurations or simply the Ehrenfest basis set size. The two methods also differ in equations of motion. MCE approach relies on the predetermined equations of motion of the coherent state, which are chosen to be the Ehrenfest equations. In contrast, our variational method with the multi- D_2 *Ansatz* uses the fully variational principle and its equations of motion are more

computationally expensive and accurate. Validity of our approach has been extensively tested in the previous work, and calculations are performed with a sufficiently large multiplicity M in this work. For the details of the accuracy test, please refer to Ref. [13].

Time evolution of the *carrier* probability $P_{ca}(t, n)$ is also calculated

$$P_{ca}(t, n) = \langle D_2^M(t) | \hat{a}_n^\dagger \hat{a}_n | D_2^M(t) \rangle. \quad (13)$$

We further study the current of the system under external field,

$$\begin{aligned} j(t) &= \langle D_2^M(t) | i \left(\sum_n e^{iA(t)} \hat{a}_n^\dagger \hat{a}_{n+1} - H.c. \right) | D_2^M(t) \rangle \\ &= i \sum_{i,j} \sum_n \psi_{jn}^* (t) [e^{iA(t)} \psi_{i,n+1}(t) \\ &\quad - e^{-iA(t)} \psi_{i,n-1}(t)] S_{ji}. \end{aligned} \quad (14)$$

We further define a mean value $c(t)$ of the *carrier* wave packet as follows

$$\begin{aligned} c(t) &= \sum_i^n n P_{ca}(t, n) \\ \sigma(t)^2 &= \sum_i^n (n - c(t))^2 P_{ca}(t, n) \end{aligned} \quad (15)$$

where the mean value $c(t)$ describes the centroid of the *carrier* wave packet. It is noted that the mean value $c(t)$ is sensitive to the initial standard deviation σ_0 of the *carrier* wave packet.

3 Numerical results and discussions

In the absence of the *carrier*-phonon coupling, if the field $F_{dc} + F_{ac} \cos(\omega_{ac} t + \phi_{ac})$ is applied to the *carrier*, the inherent localization of the BOs and SBOs is circumvented for some suitable conditions of AC frequency ω_{ac} and phase ϕ_{ac} . Dignam *et al.* examined the conditions for dynamic localization of electrons in a periodic potential due to an applied AC electric field. Haller *et al.* investigated the particles transport in a lattice potential subjected to a harmonic driving and reported that the details of the motion depend on the ratio between the driving frequency ω_{ac} and the Bloch frequency ω_B [43]. If the AC field is absent ($F_{ac} = 0$), the BOs occur at the Bloch frequency $\omega_B = F_{dc}$, where $\omega_B = 2\pi/T_B$ with T_B denoting the time period of the BOs. When the AC frequency is detuned from the Bloch frequency, the SBOs arise. A small detuning $\omega_{ac} - \omega_B$ results in a beat between the Bloch cycle and

the drive, with a drastic change of the particle motion. On top of the BOs, the SBOs motion shows a much larger oscillation in position space that extends over hundreds of lattice sites. Those SBOs directly correspond to the motion of normal BOs, just rescaled in space and time. In other words, the SBOs are observed when ω_{ac} satisfies the condition

$$N_{\text{int}}\omega_{ac} = \omega_B(1 + \delta) = F_{dc}(1 + \delta) \quad (16)$$

for some nonvanishing integer N_{int} , where $|\delta| \ll 1$ is a small dimensionless detuning parameter, which will control the period of the SBOs. $N_{\text{int}} = 1$ was most commonly used in theoretical and experimental studies [27, 43, 45], and is thus adopted in this work as well. The time period of the SBOs is given by $T_{\text{SB}} = 2\pi/(\delta\omega_B) = 2\pi/(\delta F_{dc})$. When the detuning parameter δ vanishes, T_{SB} diverges [52].

3.1 Detuned and resonant cases

Experimental realizations of SBOs phenomenon are given by the BEC in modulated standing light waves or semiconductor superlattices in far-infrared laser fields [37]. Using BECs in optical lattice potentials generated by interfering laser waves, the BOs and SBOs can be engineered by a force that is provided by gravity or by acceleration of the lattice potential. Haller *et al.* observed the SBOs for the BEC subjected to harmonic driving, by changing the lattice tilt as an external force as well as lattice depth and spacing [43]. Alberti *et al.* managed to control the quantum transport of cold Sr atoms that are trapped in an optical lattice potential aligned along the Earth's gravity field [31]. The *carrier* motion will inevitably be influenced by the environmental fluctuation on the optical lattice potential or the lattice vibration in the semiconductor superlattice [8–10, 77]. The surrounding influence on the *carrier* can be modeled as phonons [1], and thus the key issue of this work is the effects of *carrier*-phonon coupling. As shown in Hamiltonian (1), *carrier*-phonon interactions included in the Holstein model are in the form of the diagonal coupling as a nontrivial dependence of the *carrier* site energies on the lattice coordinates [78].

We will study the influence of *carrier*-phonon coupling in two typical categories: resonant ($\delta = 0$) type and detuned ($\delta \neq 0$) type of *carrier* motion. These two types have been reported previously in the observation of SBOs of a BEC under superposed DC and AC forces [43]. After experimental investigation in one-dimensional optical lattice, the two types of movement has also been analyzed numerically using a semiclassical approach [47].

Generally, for a simple resonant AC field with frequency $\omega_{ac} = \omega_B$, the wave function of the carrier performs a directed motion with oscillatory features and drift velocity depending on the phase ϕ_{ac} . On the contrary, if the frequency of the AC field ω_{ac} is detuned with respect to ω_B , the wave packet exhibits a beating effect of the SBOs. These two scenarios were referred to as resonant and detuned types. In this work, we will focus on certain sets of parameters as representative values of these two different situations under the influence of *carrier*-phonon coupling.

Being strongly dependent on the initial conditions, the motion of the *carrier* wave packet subject to an AC and DC electric field has been found to exhibit a breathing mode or the typical BOs/SBOs [13, 43, 79], thus here we discuss the initial conditions before moving on to specific calculations. Effects of initial Gaussian wave packets have been investigated by Caetano *et al.* under the superposed DC and AC field [24, 47]. The outcomes of initial Gaussian wave packet of different widths σ_0 is speculated first [44]. For very narrow initial Gaussian wave packet, the excton is almost created on only one site and there are no typical oscillations for the centroid of the *carrier* wave packet, which is denoted by $c(t)$. The application of a DC field leads to a symmetric breathing mode with unchanged $c(t)$ and an oscillatory wave-packet width

$$\sigma(t) = \sqrt{\sigma_0^2 + 2 \left[2 \frac{J}{F_{dc}} \sin\left(\frac{\omega_B t}{2}\right) \right]^2}. \quad (17)$$

While the introduction of an AC field in the detuned cases leads to a symmetric motion of fixed $c(t)$ and a varying width

$$\sigma(t) = \sqrt{\sigma_0^2 + 2 |\chi(t)|^2}, \quad (18)$$

with

$$\chi(t) = 2J \sum_{n=-\infty}^{\infty} \mathcal{J}_n\left(\frac{F_{ac}}{\omega_{ac}}\right) \frac{1}{\delta\omega_B} \exp\left(-i\frac{\delta\omega_B}{2}t\right) \sin\left(\frac{\delta\omega_B}{2}t\right), \quad (19)$$

where $\mathcal{J}_n$ is the ordinary Bessel function of order n . For the resonant case, the AC field results in a symmetrically spreading wave packet with width

$$\sigma(t) = \sum_{n=-\infty}^{\infty} \mathcal{J}_n\left(\frac{F_{ac}}{\omega_{ac}}\right) \sqrt{2J}t. \quad (20)$$

As the initial width of the Gaussian wave packet increases, the oscillation amplitude of $c(t)$ converges to those of the semiclassical cases, in which the motion of wave packet centroid agrees with the movement of particles [24, 47]. Using a broad initial Gaussian wave packet, the *carrier* movement exhibits the typical SBOs in the

Figure 1 Time evolution of the **carrier** probability $P_{ca}(t, n)$ for detuned cases ($\delta \neq 0$) with two-site-centered initial condition. In the left panels, $\delta = 1/9$ and $F_{dc} = 0.45$. In the right panels, $\delta = -1/11$ and $F_{dc} = 0.55$. **Carrier**-phonon coupling is $g = 0$ in the upper panels, and $g = 0.5$ in the lower panels. Other parameters are $M = 16$, $N = 16$, $J = 0.1$, $F_{ac} = 1.0$, $\omega_{ac} = 0.5$, and $\phi_{ac} = 0$.

detuned scenario and a linear movement with superimposed small-amplitude oscillation in the resonant case, also defined as the directed motion of the **carrier** [43, 52].

When a two-site-centered initial state is adopted as the initial condition, the **carrier** is created on two nearest neighboring sites, $\psi_n(t=0) = (\delta_{n,N/2} + \delta_{n,N/2+1})/\sqrt{2}$ [64]. Using this initial condition, the **carrier** exhibits partially BOs in the presence of only the DC field, conveying the quantum feature of the **carrier** wave packet explicitly [13]. However, the influence of the AC field on the movement of the **carrier** wave packet using this initial condition has not been investigated. In this study, the two-site-centered state is used as the initial condition, and the phonon displacement $\lambda_{i,q}(t=0) = 0$ is set.

First, let us analyze how the polaron evolves when the field is applied. The time-domain evolution of the **carrier** wave packet is shown in Fig. 1 for the detuned cases. We fix $J = 0.1$, $F_{ac} = 1.0$, $\omega_{ac} = 0.5$, and $\phi_{ac} = 0$, and vary the set of δ and F_{dc} . Fig. 1(a) is for $\delta = 1/9$ and $F_{dc} = 0.45$, and the corresponding wave packet moves to the left-hand side. In opposite, the **carrier** wave packet shifts to the right-hand side with $\delta = -1/11$ and $F_{dc} = 0.55$, as shown in Fig. 1(b). Both detuned cases show that the **carrier** performs the SBOs. The oscillation amplitudes for the two-site-centered condition are smaller than those for the broad initial Gaussian wave packet, since the lat-

Figure 2 Currents for detuned cases of Fig. 1.

ter ones are the largest oscillation amplitudes among all types of initial conditions [44]. It can be also revealed that the direction of the **carrier** wave package centroid movement can be engineered by tuning δ and F_{dc} .

As presented in Figs. 1(c) and (d), a coupling strength of $g = 0.5$ is used. It is shown that by increasing the strength of the **carrier**-phonon coupling, the **carrier** states become more localized. Holthaus *et al.* has reported that the dynamical localization of the wave packet can be intentionally manipulated by varying the strength of the electric field in disordered semiconductor superlattices [51]. This conclusion has been well supported by several authors [39, 44], and is also in agreement with our simulations. Our findings imply that changing the **carrier**-phonon coupling strength is another promising way to engineer the dynamical localization of the SBOs.

In view of the oscillatory behavior of the **carrier** wave packet described in Fig. 1 for the detuned cases, it is reasonable to expect that the electric current behaves in a similar manner. An observable of interest, the current is numerically calculated according to Eq. (14). As shown in Fig. 2(a) and Fig. 2(b), currents $j(t)$ display well-defined oscillatory behavior in both detuned cases. Relevant movement directions and temporal periods of the currents match perfectly those obtained from the **carrier** wave packet. As presented in Fig. 1(a) and Fig. 2(a), $\delta = 1/9$ leads to $T_{SB} = 9T_B$. $T_{SB} = 11T_B$ in Fig. 1(b) and Fig. 2(b) results from $\delta = -1/11$. The current of DC cases in the previous study shows oscillations in a purely sine function form [13]. In comparison, the current in the simultaneous presence of AC and DC cases here have two features: low-frequency oscillation marked by dash-dotted line due to the AC field, and high-frequency oscillations induced by the DC field. Fig. 2(c) and Fig. 2(d)

Figure 3 Time evolution of the **carrier** probability $P_{ca}(t, n)$ for resonant cases ($\delta = 0$) with two-site-centered initial condition. In the left panels, $F_{dc} = 0.5$. In the right panels, $F_{dc} = -0.5$, denoting that electric field is an opposite direction of left panels. **Carrier**-phonon coupling is $g = 0$ in the upper panels, and $g = 0.5$ in the lower panels. Other parameters are $M = 16$, $N = 16$, $J = 0.1$, $F_{ac} = 1.0$, $\omega_{ac} = 0.5$, and $\phi_{ac} = 0$.

Figure 4 Currents for detuned cases of Fig. 3.

show the decay of amplitudes of the currents due to dissipation effects of the **carrier**-phonon coupling, in agreement with quenching of the BOs due to strong **carrier**-phonon coupling [17–20]. It can be found that both the high-frequency and low-frequency oscillations of the current are damped, in accord with the breakdown of the SBOs patterns of the **carrier** wave packet.

We proceed to the resonant case of $\delta = 0$ in this subsection. If the broad initial Gaussian wave packet is applied, the center of mass of the wave packet moves almost linearly with superimposed high-frequency and small-amplitude oscillations while its shape is essentially unchanged, that is to say, resonant modulation of detuning parameter causes directed motion of the wave packet's center of mass [47]. When the **carrier** is created at two nearest neighbouring sites, there is no directed motion observed. Instead, the **carrier** wave packet spreads over the ring at certain velocity with small-amplitude and high-frequency oscillations, as presented in Fig. 3(a) and Fig. 3(b), leading to negligible **carrier** wave package centroid movement from the initial positions. This movement can be denoted as bifurcated motion. After the **carrier**-phonon coupling of $g = 0.5$ is added, the wave packets become localized in shape and their averaged center substantially shift away during the evolution, as shown in Fig. 3(c) and Fig. 3(d). Because the external DC fields use opposite directions $F_{dc} = 0.5$ and $F_{dc} = -0.5$ in the left and right panels, respectively, the wave packet in Fig. 3(c) is found to shift to left hand side while that in Fig. 3(d) move to the right hand side. As shown in Fig. 4, the currents show corresponding oscillation features. In upper panels of Fig. 3 and Fig. 4, only values of T_B is listed because the T_{SB} approaches infinity. In the lower panels, the dissipation features are again observed after the addition of **carrier**-phonon interactions. Domínguez et al. have considered the Peyrard-Bishop-Holstein model of charge transport in DNA to study the SBOs of the charge carrier semiclassically, and the current oscillation in resonant cases was found to be modulated without decay in time [25]. In contrast, the periodicity is broken and the amplitude of the oscillatory current are smaller in our fully quantum mechanical results.

3.2 AC phase modulation

Recent observations include global motion of the atom cloud, pointing to the importance of AC phase correction [27]. By appropriate modulation of the phase, the **carrier** transport can be precisely engineered. Fig. 5. presents a quantitative study of the AC phase and time-dependent amplitudes of such SBOs. Figs. 5(a)-(b) show the time evolution of the **carrier** wave packet for ϕ_{ac} of 0 , $\pi/4$, $3\pi/8$, and $\pi/2$. In Fig. 5(e), we plot the time evolution of wave packet centroid for these AC phases. It can be found that the motion corresponding to each phase is shifted with unchanged temporal period.

Figure 5 Time evolution of the carrier probability $P_{ca}(t, n)$ for various phases (a) $\phi_{ac} = 0$, (b) $\phi_{ac} = \pi/4$, (c) $\phi_{ac} = 3\pi/8$, and (d) $\phi_{ac} = \pi/2$, in the absence of carrier-phonon coupling ($g = 0$). (e) Mean values $c(t)$ of the carrier wave packets. Two-site-centered initial condition is used. Other parameters are $M = 1$, $N = 16$, $J = 0.1$, $F_{dc} = 0.45$, $F_{ac} = 1.0$, $\omega_{ac} = 0.5$, and $\delta = 1/9$.

Effects of the carrier-phonon coupling for $\phi_{ac} = \pi/2$ are presented in Figs. 6 and 7. Fig. 6 shows the SBO features in two detuned cases of $\delta = 1/9$ and $-1/11$. It is worth noting that phase manipulations can lead to similar carrier motion patterns for different parameter sets, as shown in Figs. 6(a) and (b). This similarity is destroyed after adding the carrier-phonon coupling, as shown in Figs. 6(c) and (d). Since the DC field strength in Figs. 6(d) is larger than that in Figs. 6(c), the carrier wave packet in Figs. 6(c) becomes more localized than its counterpart in Figs. 6(d).

Fig. 7 is for the resonant cases of $\delta = 0$. Fig. 7(a) characterizes time evolution of the carrier wave packet between the bifurcated motion and the directed motion. As the phase ϕ_{ac} increases from 0 to $\pi/2$, the bifurcated motion

Figure 6 Time evolution of the carrier probability $P_{ca}(t, n)$ for detuned cases with the non-zero phase $\phi_{ac} = \pi/2$. In the left panels, $\delta = 1/9$ and $F_{dc} = 0.45$. In the right panels, $\delta = -1/11$ and $F_{dc} = 0.55$. Carrier-phonon coupling is $g = 0$ in the upper panels, and $g = 0.5$ in the lower panels. Two site initial condition is used. Other parameters are $M = 16$, $N = 16$, $J = 0.1$, $F_{ac} = 1.0$, and $\omega_{ac} = 0.5$.

of the carrier wave packet morphs into the directed motion, but can not turn into complete directed motion due to the two-site-centered initial condition. When a Gaussian wave packet of $\sigma_0 = 2.0$ is used initially, Fig. 7(b) shows the directed motion of the polaron as well as superimposed BOs. The center of mass of the carrier wave packet moves with a certain speed to the left-hand side and with its wave packet shape kept. It can be found that the velocity of the carrier in Fig. 7(b) agrees with that of the main branch in Fig. 7(a). The group velocity of the carrier is

$$v_g = -J \cos \left(k + \frac{F_{ac}}{\omega_{ac}} \cos \phi_{ac} - \phi_{ac} + \delta \omega t \right) \mathcal{J}_1 \left(\frac{F_{ac}}{\omega_{ac}} \right), \quad (21)$$

where k is the carrier momentum and $\mathcal{J}_1$ is the Bessel function of order $n = 1$ [27]. Due to $\delta = 0$ for the resonant cases, the group velocity becomes a time-independent constant value of $J \cos \left(k + \frac{F_{ac}}{\omega_{ac}} \cos \phi_{ac} - \phi_{ac} \right) \mathcal{J}_1 \left(\frac{F_{ac}}{\omega_{ac}} \right)$, leading to the directed motion of the carrier. By addition of the carrier-phonon coupling in the resonant cases with a non-zero AC phase, the wave packet is broadened during the evolution and the carrier motion becomes slower than the movement of the bare carrier. Haller *et al.* has reported that by varying the AC phases and detuning pa-

Figure 7 Time evolution of the carrier probability $P_{\text{ex}}(t, n)$ for resonant cases ($\delta = 0$) with the non-zero phase $\phi_{\text{ac}} = \pi/2$. Left panels with two-site-centered initial condition, and right panels with Gaussian initial condition of $\sigma_0 = 2$. Carrier-phonon coupling is $g = 0$ in the upper panels, and $g = 0.5$ in the lower panels. Other parameters are $M = 16$, $N = 16$, $J = 0.1$, $F_{\text{ac}} = 1.0$, and $\omega_{\text{ac}} = 0.5$

rameters, the wave shape can be greatly changed [43]. Haller's conclusion agrees with our findings in the absence of the carrier-coupling in this section. In addition, our study shows that the application of carrier-phonon coupling can also adjust the wave shape and shifting amplitude.

4 Conclusion

In our previous work [13], we studied the intriguing role played by the carrier-phonon coupling in dynamics of a Holstein polaron under the influence of a DC external field. In this work, we extend our formalism to investigate the influence of an AC external field. Following the Dirac-Frenkel time-dependent variational principle, the polaron dynamics under the AC field is probed by employing the multi- D_2 Ansatz. It is revealed that the direction of carrier wave package centroid movement can be engineered by tuning δ and F_{dc} under the two-site-centered initial condition. The carrier transport can also be modulated by varying the AC phase ϕ_{ac} . If $\phi_{\text{ac}} = 0$, SBOs appear in the detuned case of $\delta \neq 0$, while bifurcated motion of the wave packet is found in the resonant case of $\delta = 0$. After adding the carrier-phonon coupling, the carrier states become localized in the de-

tuned scenarios, leading to clear suppression of the carrier wave packet motion. For the resonant cases, the carrier-phonon coupling breaks the bifurcated motion of the carrier wave packet, and shifts the carrier away from the original positions. If $\phi_{\text{ac}} = \pi/2$, the carrier-phonon coupling destroys the modulated patterns of SBOs in the detuned case. Using a broad Gaussian wave packet as the initial state, the centroid of carrier wave packet moves with a certain velocity and with its shape unchanged in the resonant cases. Adding the carrier-phonon coupling broadens the carrier wave packet and slows down the carrier movement. A detailed understanding of the transport mechanism of multiple carriers under an external field is of great interest and awaits future investigations. In addition, the coherent superpositions of BOs and Zener tunneling between minibands of a binary lattice, also known as Bloch-Zener oscillations [80,81], have been experimentally demonstrated for light waves in curved femtosecond laser-written waveguide arrays [82]. Work on simulating Bloch-Zener dynamics is in progress.

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Key words. super Bloch oscillations, polaron dynamics, Davydov Ansatz, carrier-phonon coupling

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