

Interband coupling in Bloch electron dynamics: Application to the two-band model

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The theory of Bloch dynamics for a single electron in a homogeneous electric field of arbitrary time dependence is established. The complete density matrix formulation for the dynamics is developed, and the two-band model is extracted. The two-band model is studied with emphasis on the interband coupling. A standard “*s-p*” two-band model is utilized from the nearest-neighbor tight-binding approximation to study the dynamics. In the analysis, the interband coupling paradigm is developed whereby the momentum component of the interband coupling is evaluated parametrically by using an analytically established band-matching condition. This leads to an interband coupling dependence on the band structure alone, and a significant reduction in computational complexity. The interband coupling parameter is then used to evaluate the transition probability as a function of external electric field over a wide range of field values. Results for the two-band current composites and each separate Bloch band are derived and analyzed. The temporal nature of the transition probability and current for a uniform electric field scenario is demonstrated and discussed.

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I. INTRODUCTION

From the early development of quantum mechanics, it has been clear that the fundamentals of solid state physics and its application evolution would necessarily depend on a clear understanding of the Bloch electron response to electromagnetic fields. Historically, the first solid state studies detailed the fundamental development of electron motion in reciprocal space including the elucidation of Zener tunneling, the acceleration theorem, and effective mass dynamics [1–3]. Overtime, the development of modern fabrication technologies prompted novel transport research in the micro- and nanometer-spatial domain. This led to studies with band-engineered superlattices (SLs) and tailored periodic structures which brought to experimental realization the early-on developed notional concepts of the Bloch oscillations and Wannier-Stark localization [4–6]. Further, the latest discovery of 2D materials such as graphene and similar low-dimensional materials has opened remarkable new areas of exploration in solid state physics [7,8].

Most recently, there has been intense activity generated with the advent of pico-to-attosecond time resolved technologies [9,10]. This has opened the door to novel probe methods relevant to atomic and solid-state materials, and has stimulated the study of new phenomena including high harmonic

generation (HHG) [11–14]. The nature of HGG in solids is commonly ascribed [14] to a three-step process whereby a strong applied electric field excites an electron from the valence to the conduction band, creating a hole in the valence band; then, both electron and hole accelerate in the field gaining kinetic energy; and finally, the electron and hole recombine. It is suggested that this three-step process, which generates an interband and intraband current component, constitutes the total HHG current contribution; in addition, from studies [15] using the two-band model, it is further found that the HHG spectrum is dominated by the interband current, and that the cutoff properties are limited by the largest band-gap separation. Moreover, multiband Bloch electron dynamics [16,17] in electric fields is central to a wide variety of solid state applications where real band structure is implicitly included in the analysis [18–20].

In this work, we make use of our past approach with regard to treating homogeneous electric fields. The choice of vector potential gauge leads to a natural set of basis functions for describing Bloch electron dynamics in a homogeneous electric field of arbitrary time dependence. These basis functions are the instantaneous eigenstates of the time-dependent Schrödinger equation, and are frequently referred to as the accelerated Bloch representation (ABR), whereby the $u_{n\mathbf{k}(t)}(\mathbf{r})$ component of the total Bloch functions alone are time dependent through $\mathbf{k}(t) = \mathbf{K} + \frac{1}{\hbar} \int_{t_0}^t \mathbf{F}(t') dt'$. Using this ABR, we (J. B. Krieger and present coauthor G. J. Iafrate) have been able to develop [21] a one-electron quantum transport equation for solid state dynamics which fully describes intra- and interband dynamics, optical absorption, and the quantum inclusion of intercollisional field effects, that is, the effect of electron field-driven acceleration during the collision process,

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or, equivalently, optical transition processes. Today, ABR is a key representation for complementing the analysis of dynamical ultrafast processes arising from emergent imaging technologies [22–24].

However, in explicitly calculating the interband coupling parameter, $\mathbf{R}_{nn'}(\mathbf{k}(t))$, implicit in the theory, which is defined in terms of the matrix elements of cellular Bloch function, $u_{n\mathbf{k}(t)}(\mathbf{r})$, for bands n and n' , there is well known difficulty associated with calculations of such matrix elements [11, 15, 18–20, 25–27]. Thus we look to circumvent this burden by seeking an alternative approach to the evaluation of $\mathbf{R}_{nn'}(\mathbf{k}(t))$.

Therefore, in this work, we focus on the importance of interband coupling, first as it is developed in a general theoretical framework, and then, as an extraction from the general approach, in an illustrative two-band model example. A special feature of this work makes use of an analytical band matching condition to circumvent numerical difficulties inherent in the evaluating interband matrix elements. This is illustrated in the two-band model.

In Sec. II, as a framework for our analysis, the theory of Bloch electron dynamics in a homogeneous, but arbitrarily time-dependent, electric field is presented using instantaneous eigenstates of the Schrödinger equation. The transition amplitude and transition probability are established in terms of the interband coupling parameter and transition energy difference. In Sec. III, a two-band model is extracted from the general theory and analyzed in the light of interband coupling. In the analysis, the momentum component of the coupling parameter is evaluated parametrically using a band-matching condition developed by Krieger [28]. As such, the evaluation of the interband matrix element is greatly simplified so as to depend only on the band structure and band structure parameters. This simplicity more readily facilitates in the analytical and numerical evaluation of Bloch dynamical properties. In Sec. IV, the Bloch current is developed in the general density matrix formulation, and then reduced for the two-band model; further, this section develops the Bloch electron current in the two-band model, and details the temporal features of the diagonal and off-diagonal components of the current in a constant electric field. Appendix establishes the parametric evaluation of the transition probability within the two-band model.

II. BACKGROUND: DYNAMICS IN A HOMOGENEOUS ELECTRIC FIELD

The Hamiltonian describing the dynamics [16, 17] for a Bloch electron in a crystal potential, $V_c(\mathbf{r})$, subject to a time-dependent homogeneous electric field is

$$\hat{H}(\mathbf{r}, \hat{\mathbf{p}}, t) = \frac{1}{2m_0} \left[\hat{\mathbf{p}} - \frac{e}{c} \mathbf{A}(t) \right]^2 + V_c(\mathbf{r}); \quad (1)$$

here, m_0 is the free electron mass, $\hat{\mathbf{p}} = -i\hbar\nabla_{\mathbf{r}}$ is the electron momentum operator, e is the electron charge, c is the speed of light in a vacuum, $\mathbf{r}$ is the space coordinate, and $\mathbf{A}(\mathbf{r}, t)$ is the vector potential given by

$$\mathbf{A}(t) = -c \int_{t_0}^t \mathbf{E}(t') dt', \quad (2)$$

where t_0 is the time that the electric field, $\mathbf{E}(t)$, is turned on. For convenience, we define

$$-\frac{e}{c} \mathbf{A}(t) = e \int_{t_0}^t \mathbf{E}(t') dt' \equiv \mathbf{p}_c(t), \quad (3a)$$

thus noting that

$$\dot{\mathbf{p}}_c = \mathbf{F}(t), \quad (3b)$$

where $\mathbf{F}(t) = e\mathbf{E}(t)$ is the external force on the electron. We then insert Eq. (3a) into the Hamiltonian of Eq. (1) and write the Schrödinger equation for the dynamics as

$$i\hbar \frac{\partial}{\partial t} |\Psi(\mathbf{r}, t)\rangle = \left[\frac{1}{2m_0} (\hat{\mathbf{p}} + \mathbf{p}_c(t))^2 + V_c(\mathbf{r}) \right] |\Psi(\mathbf{r}, t)\rangle. \quad (4)$$

In seeking the solution to Eq. (1), we look to utilize the instantaneous eigenstates of the Schrödinger equation, Eq. (4). This means we look to solve

$$\left[\frac{1}{2m_0} (\hat{\mathbf{p}} + \mathbf{p}_c(t))^2 + V_c(\mathbf{r}) \right] |\tilde{\Psi}(\mathbf{r}, t)\rangle = \varepsilon(t) |\tilde{\Psi}(\mathbf{r}, t)\rangle, \quad (5)$$

where both $|\tilde{\Psi}(\mathbf{r}, t)\rangle$ and $\varepsilon(t)$ have an admitted time dependence due to presence of $\mathbf{p}_c(t)$. In seeking the solution to Eq. (5), we let

$$|\tilde{\Psi}(\mathbf{r}, t)\rangle = e^{-i\frac{\mathbf{p}_c}{\hbar} \cdot \mathbf{r}} |\Phi(\mathbf{r}, t)\rangle; \quad (6)$$

placing $|\tilde{\Psi}(\mathbf{r}, t)\rangle$ of Eq. (6) into Eq. (5), we find that

$$\left[\frac{1}{2m_0} \hat{\mathbf{p}}^2 + V_c(\mathbf{r}) \right] |\Phi(\mathbf{r}, t)\rangle = \varepsilon(t) |\Phi(\mathbf{r}, t)\rangle. \quad (7)$$

We note that the solutions to Eq. (7) are the Bloch functions and the energy-band functions, but as a function of time through the time dependence of the wave vector, $\mathbf{k}(t)$. Therefore we express $|\Phi(\mathbf{r}, t)\rangle$ and $\varepsilon(t)$ as

$$|\Phi_{n,k}(\mathbf{r}, t)\rangle = e^{i\mathbf{k}(t) \cdot \mathbf{r}} u_{n\mathbf{k}(t)}(\mathbf{r}) \quad (8a)$$

and

$$\varepsilon(t) = \varepsilon_n(\mathbf{k}(t)), \quad (8b)$$

where n is the energy-band index. To establishing the allowed values of $\mathbf{k}(t)$, we note that the Hamiltonian of Eq. (5) is invariant under lattice translation. Thus, imposing periodic boundary conditions on $|\tilde{\Psi}(\mathbf{r}, t)\rangle$ in Eq. (6), we find

$$\mathbf{k}(t) - \frac{1}{\hbar} \mathbf{p}_c(t) = \sum_{i=1}^3 \frac{g_i}{N_i} \mathbf{G}_i, \quad (9)$$

where $\mathbf{G}_i$ are the primitive reciprocal-lattice vectors (i denotes a dimension), N_i are the number of cells in the i direction, and g_i are integers with $-\frac{N_i}{2} < g_i < \frac{N_i}{2}$. It follows from Eq. (9) that

$$\hbar \dot{\mathbf{k}}(t) = \dot{\mathbf{p}}_c(t) = \mathbf{F}(t), \quad (10a)$$

which establishes the *acceleration theorem*. Therefore we can adopt the notation

$$\mathbf{k}(t) = \mathbf{K} + \mathbf{k}_c(t), \quad (10b)$$

where

$$\mathbf{k}_c(t) = \frac{1}{\hbar} \int_{t_0}^t \mathbf{F}(t') dt'. \quad (10c)$$

Thus the instantaneous eigenstates of Eq. (6) are

$$|\Psi_{n\mathbf{K}}(\mathbf{r}, t)\rangle = \frac{1}{\sqrt{\Omega}} e^{i\mathbf{K}\cdot\mathbf{r}} u_{n\mathbf{K}(t)}(\mathbf{r}), \quad (11)$$

with $(\Psi_{n\mathbf{K}}, \Psi_{n'\mathbf{K}'}) = \delta_{n,n'}\delta_{\mathbf{K},\mathbf{K}'}$, whereas the states of Eq. (8a) are

$$|\Phi_{n\mathbf{k}}(\mathbf{r}, t)\rangle = \frac{1}{\sqrt{\Omega}} e^{i\mathbf{k}(t)\cdot\mathbf{r}} u_{n\mathbf{k}(t)}(\mathbf{r}), \quad (12)$$

where Ω is the crystal volume. These states are the so-called *Houston states*. In comparing $\Phi_{n\mathbf{k}}$ and $\Psi_{n\mathbf{K}}$, we note that $\Phi_{n\mathbf{k}}$ are a total function of $\mathbf{k}(t)$; whereas in $\Psi_{n\mathbf{K}}$, the instantaneous eigenstates, the exponential phase factor in $\Psi_{n\mathbf{K}}$ of Eq. (11) depends on $\mathbf{K}$ alone, independent of time, whereas the cellular Bloch function, $u_{n\mathbf{k}(t)}(\mathbf{r})$, is dependent upon $\mathbf{k}(t)$, and therefore the electric field through Eq. (10b). We note that the instantaneous eigenstates of Eq. (5) are a natural set of complete states for treating the time evolution of the Schrödinger equation of Eq. (4) [29].

In seeking the solution to the Schrödinger equation of Eq. (4), we employ the complete set of instantaneous eigenstates of Eq. (11), $|\Psi_{n\mathbf{K}}\rangle$, to obtain

$$|\Psi(\mathbf{r}, t)\rangle = \sum_n \sum_{\mathbf{K}} a_{n\mathbf{K}}(t) \Psi_{n\mathbf{K}}(\mathbf{r}, t) e^{-\frac{i}{\hbar} \int_0^t \varepsilon_n(\mathbf{K}) d\tau}. \quad (13)$$

Putting Eq. (13) into Eq. (4) and using the orthogonality of $\Psi_{n\mathbf{K}}$ noting that $(\Psi_{n\mathbf{K}}, \Psi_{n'\mathbf{K}'}) = \delta_{n,n'}\delta_{\mathbf{K},\mathbf{K}'}$, we find

$$i \frac{\partial}{\partial t} a_{n\mathbf{K}}(t) = \sum_{n'} \frac{\partial P_{nn'}(t)}{\partial t} a_{n'\mathbf{K}}(t), \quad (14a)$$

where the sum is over all crystal bands at the same $\mathbf{K}$ in the Brillouin zone (BZ) and

$$\frac{\partial P_{nn'}(t)}{\partial t} = - \left(\Psi_{n\mathbf{K}}, \frac{\partial \Psi_{n'\mathbf{K}}}{\partial t} \right) e^{\frac{i}{\hbar} \int_0^t [\varepsilon_n(\mathbf{K}(\tau)) - \varepsilon_{n'}(\mathbf{K}(\tau))] d\tau}, \quad (14b)$$

the probability transition rate. In making use of the instantaneous eigenstates as noted in Eq. (6), and after calculating $(\Psi_{n\mathbf{K}}, \frac{\partial \Psi_{n'\mathbf{K}}}{\partial t})$ with $\hbar \dot{\mathbf{k}}(t) = \mathbf{F}(t)$, we find the probability transition

$$P_{nn'}(t) = \frac{1}{\hbar} \int_0^t dt' \mathbf{F}(t') \cdot \mathbf{R}_{nn'}(\mathbf{k}(t')) \times e^{\frac{i}{\hbar} \int_0^{t'} [\varepsilon_n(\mathbf{k}(\tau)) - \varepsilon_{n'}(\mathbf{k}(\tau))] d\tau}, \quad (15a)$$

where

$$\mathbf{R}_{nn'}(\mathbf{k}(t)) = \frac{i}{\Omega_c} \int_{\Omega_c} d\mathbf{r} u_{n\mathbf{k}(t)}^*(\mathbf{r}) \nabla_{\mathbf{k}} u_{n'\mathbf{k}(t)}(\mathbf{r}), \quad (15b)$$

the interband coupling parameter, with $\mathbf{R}_{nn'}(\mathbf{k}) = \mathbf{R}_{n'n}^*(\mathbf{k})$, and Ω_c is the volume of the unit cell. We note that Eq. (14a) along with Eq. (14b) are often referred [18–20] to as the K-I (Krieger-Iafrate) equation derived previously [16,17]; this term appears in an augmented form as

$$i\hbar \dot{a}_{n\mathbf{K}}(t) = \varepsilon_n(\mathbf{K}) a_{n\mathbf{K}}(t) - \mathbf{F}(t) \cdot \sum_{n'} \mathbf{R}_{nn'}(t) a_{n'\mathbf{K}}(t). \quad (16)$$

Here, Eqs. (14a) and (16) are equivalent, and are related by an integration factor. Yet Eq. (14a) is of central interest when considering electric-field-induced interband transitions [21,30], while Eq. (16) is in a form conducive to insertion

into high performance computation such as full-band Monte Carlo simulations [18]. We have historically [21,30,31] used the form embraced in Eqs. (14a) and (14b) since $P_{nn'}(t)$ of Eq. (15a) expresses the direct transition probability to make transitions between states n and n' under the influence of the electric field.

Lastly, we note that the phase of $|\Psi(\mathbf{r}, t)\rangle$ in Eq. (13) is typically chosen so that $\mathbf{R}_{nn} = 0$, a provision which assumes that a crystal possesses an inversion symmetry. If inversion symmetry is broken, then $\mathbf{R}_{nn}$ is nonzero and needs to be retained. This gives rise to Berry phase effects [32] which are included implicitly in part of the initial condition of $a_{n\mathbf{K}}(t)$ of Eq. (16) as $a_{n\mathbf{K}}(t) e^{-\frac{i}{\hbar} \int_0^t \bar{\varepsilon}_n(\mathbf{K}(\tau)) d\tau}$; here, $\bar{\varepsilon}_n(\mathbf{K}) = \varepsilon_n(\mathbf{K}) - \mathbf{F}(t) \cdot \mathbf{R}_{nn}(\mathbf{K})$, where the electric field and $\mathbf{k}(t)$ have the same temporal dependence.

Key to the evaluation of $P_{nn'}(t)$ or $a_{n\mathbf{K}}(t)$ using Eq. (14a) or Eq. (16) is knowledge of the Bloch bands, $\varepsilon_n(\mathbf{K})$, and the cellular wave functions, $u_{n\mathbf{K}}(\mathbf{r})$, for the given periodic potential, $V_c(\mathbf{r})$. The evaluation especially focuses on the properties of $\mathbf{R}_{nn'}(\mathbf{K})$ with regard to the cellular wave function phase and convergence. Therefore, in the next section, we will study interband coupling by analyzing a two-band model dynamics.

III. INTERBAND COUPLING; THE TWO-BAND MODEL

Central to Bloch dynamics in homogeneous electric fields is the probability transition $P_{nn'}(t)$ from state n to n' which we found to be given in Eq. (15a). For further analysis in this section, we specify that $\mathbf{F}(t) = F_0 \hat{\mathbf{x}}$, a constant in the $\hat{\mathbf{x}}$ direction ($F_0 = eE_0$), and $t_0 = 0$; then, we find

$$P_{nn'}(t) = \frac{F_0}{\hbar} \int_0^t dt' X_{nn'}(t') e^{\frac{i}{\hbar} \int_0^{t'} [\varepsilon_n(\mathbf{k}(\tau)) - \varepsilon_{n'}(\mathbf{k}(\tau))] d\tau}, \quad (17)$$

where $X_{nn'} = (\mathbf{R}_{nn'})_x$. Since $X_{nn'}$, ε_n , and $\varepsilon_{n'}$ are periodic in $\mathbf{G}$, the reciprocal lattice vectors, we let $t = N\tau_B$, where $\tau_B = 2\pi/\omega_B$ is the Bloch period, $\omega_B = F_0 a/\hbar$ is the Bloch frequency, $a = a_x$ is the lattice constant in the $\hat{\mathbf{x}}$ direction, and N is a positive integer. Then it follows [30] that $P_{nn'}(N\tau_B)$ can be summed to give

$$P_{nn'}(N\tau_B) = \frac{1 - e^{iN\beta_{nn'}}}{1 - e^{i\beta_{nn'}}} P_{nn'}(\tau_B), \quad (18a)$$

so that

$$|P_{nn'}(N\tau_B)|^2 = \frac{\sin^2(\beta_{nn'}/2)}{\sin^2(\beta_{nn'}/2)} |P_{nn'}(\tau_B)|^2, \quad (18b)$$

where

$$\beta_{nn'} = \frac{1}{F_0} \int_{-G/2}^{G/2} [\varepsilon_n(\mathbf{k}) - \varepsilon_{n'}(\mathbf{k})] dk_x, \quad (18c)$$

and

$$P_{nn'}(\tau_B) = \frac{F_0}{\hbar} \int_0^{\tau_B} dt' X_{nn'}(t') \times e^{\frac{i}{\hbar} \int_0^{t'} [\varepsilon_n(\mathbf{k}(\tau)) - \varepsilon_{n'}(\mathbf{k}(\tau))] d\tau}. \quad (18d)$$

Through the transformation to $\mathbf{k}$ -space using $k_x(t) = \hbar^{-1} F_0 t + K_x$, for $K_x = 0$ and $P_{nn'}(\tau_B) \rightarrow P_{nn'}(G)$

($G = G_x = 2\pi/a_x$), we get

$$P_{nn'}(G) = \int_{-G/2}^{G/2} dk_x X_{nn'}(k_x) e^{\frac{i}{\hbar} \int_0^{k_x} [\varepsilon_n(\mathbf{k}') - \varepsilon_{n'}(\mathbf{k}')] dk'_x}. \quad (18e)$$

Therefore

$$|P_{nn'}(N\tau_B)|^2 = \frac{\sin^2(\beta_{nn'}N/2)}{\sin^2(\beta_{nn'}/2)} |P_{nn'}(G)|^2. \quad (19a)$$

Importantly, for N large ($N \gg 1$), that is for long times ($t \gg \tau_B$), Eq. (19a) becomes

$$\frac{|P_{nn'}(N\tau_B)|}{N} = |P_{nn'}(G)|. \quad (19b)$$

Thus the probability transition (a dimensionless quantity) for one cycle over BZ is the probability “per unit time” and is therefore key to the dynamics of the periodic system under consideration. It is interesting to note from Eq. (18b) that maximum growth of the transition amplitude from states n to n' occurs after many cycles of τ_B , that is, as N becomes large. As N gets large in Eq. (18b), the N -dependent term limits as N^2 for N large with shrinking width $1/N$, provided $\beta_{n,n'} \rightarrow 2\pi(m + \delta)$, where m is a positive integer and δ is vanishingly small. Thus $\beta_{n,n'} = 2\pi m$ serves as a *selection rule* for $n \rightarrow n'$ transitions, affirming the Wannier-Stark quantization rule [16,17].

Next, we calculate $|P_{nn'}(G)|$ for a model two-band solid-state crystal in the nearest-neighbor tight-binding (NNTB) approximation. We use this model to examine the quality factors associated with $P_{nn'}(G)$ of Eq. (18e). In proceeding to calculate $P_{nn'}(G)$, we need $(\varepsilon_{n_c} - \varepsilon_{n_v})$ so as to calculate $\int_0^{k_x} [\varepsilon_{n_c}(\mathbf{k}') - \varepsilon_{n_v}(\mathbf{k}')] dk'_x$, and we need $X_{n_cn_v}(k_x)$ for representative “ s - p ” model bands in NNTB approximation. Here, we let “ s ” band represents the valence band “ n_v ” and “ p ” band represents the conduction band “ n_c .” Keeping the nearest-neighbor term from $\varepsilon_n(\mathbf{K}) = \sum_{\mathbf{l}} \varepsilon_n(\mathbf{l}) e^{i\mathbf{K} \cdot \mathbf{l}}$, we have to lowest order in $\mathbf{l} \approx \mathbf{a}$ ($\mathbf{a}$ is the primitive lattice vector),

$$\begin{aligned} \varepsilon_{n_c}(\mathbf{K}) &= \varepsilon_{n_c}(0) + W_c \sin^2(\mathbf{K} \cdot \mathbf{a}/2), \\ \varepsilon_{n_v}(\mathbf{K}) &= \varepsilon_{n_v}(0) - W_v \sin^2(\mathbf{K} \cdot \mathbf{a}/2), \end{aligned} \quad (20)$$

where W_c and W_v are the widths of n_c and n_v bands, respectively. This becomes

$$\begin{aligned} \varepsilon_{n_c}(\mathbf{K}) - \varepsilon_{n_v}(\mathbf{K}) &= A - B \cos(\mathbf{K} \cdot \mathbf{a}); \\ A &= \frac{1}{2}(E_g + \varepsilon_g), \quad B = \frac{1}{2}(E_g - \varepsilon_g), \end{aligned} \quad (21)$$

where $\varepsilon_g = \varepsilon_{n_c}(\mathbf{K} = 0) - \varepsilon_{n_v}(\mathbf{K} = 0)$ and $E_g = \varepsilon_{n_c}(\mathbf{K} \cdot \mathbf{a} = \pi) - \varepsilon_{n_v}(\mathbf{K} \cdot \mathbf{a} = \pi)$.

In considering the long-time limit ($t \gg \tau_B$), we let $t = N\tau_B$, with N equal to a positive integer, and let N become large ($N \gg 1$). Then, for the two-band model assumed in Eq. (20), we find that $\beta_{n_cn_v}$ becomes

$$\beta_{n_cn_v} = \pi \frac{E_g + \varepsilon_g}{\hbar\omega_B}. \quad (22)$$

It then follows from Eq. (19a) that

$$\begin{aligned} \frac{|P_{n_cn_v}(N\tau_B)|^2}{|P_{n_cn_v}(\tau_B)|^2} &= \frac{\sin^2[N\pi(E_g + \varepsilon_g)/2\hbar\omega_B]}{\sin^2[\pi(E_g + \varepsilon_g)/2\hbar\omega_B]} \\ &\equiv \eta(N, \hbar\omega_B). \end{aligned} \quad (23)$$

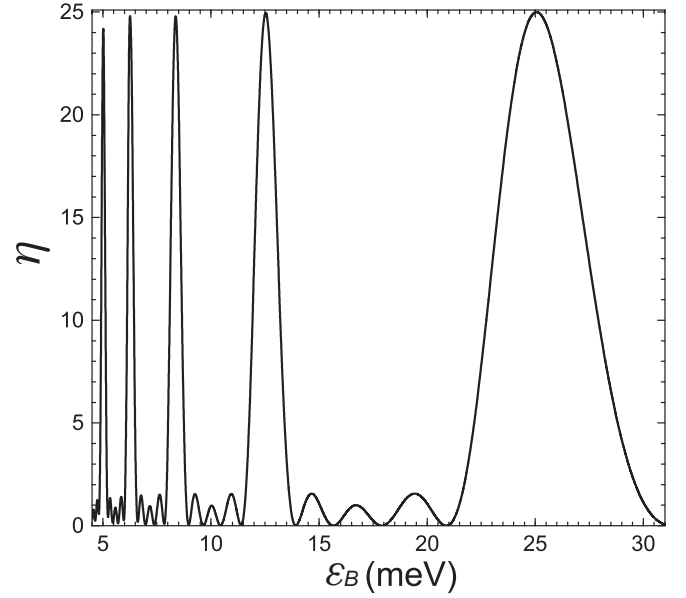


FIG. 1. Relative probability transition $\eta(N, \varepsilon_B)$ vs $\varepsilon_B = \hbar\omega_B$ calculated from Eq. (23): $N = 5$, $W_v = 10$ meV, and $W_c = 40$ meV.

Thus, in accordance with the general selection rule that $\beta_{nn'} = 2\pi m$, maximum growth is achieved from Eq. (23) when $(E_g + \varepsilon_g)/2 = m\hbar\omega_B$. Then, it follows from Eq. (21) that $A_1 \equiv A/\hbar\omega_B = m$ under the condition of maximum growth. As well, $\eta(N, \hbar\omega_B)$ scales with N as $\eta(N, \hbar\omega_B) = N^2$.

As an example, Fig. 1 graphically displays the behavior of Eq. (23) for $N = 5$, plotting $\eta(N, \hbar\omega_B)$ versus $\varepsilon_B = \hbar\omega_B$ for five sharp peaks corresponding to “quantum” numbers from $m = 1$ to 5, calculated for SL band parameters $W_p = 10$ meV, $W_c = 40$ meV, and $a = 10^{-6}$ cm. The peak width broadens with increasing electric field, $\varepsilon_B \propto E$. Table I details the peak positions for different m as displayed in Fig. 1, together with the corresponding frequencies, ν_B , and electric field strengths, E . Note that the function $\eta(N, \hbar\omega_B)$ at a fixed N can take values less than unity for $\hbar\omega_B$ lying in between the adjacent peaks of maximum growth. Then, depending on $\hbar\omega_B$, the value of $|P_{n_cn_v}(N\tau_B)|$ for many periods of τ_B can be larger or less than that for one period. This determines the characteristic electron dynamics in electric field within the two-band model as in effectively or weakly coupled bands relative to interband transitions. Also this suggests the possibility for control the interband coupling with the applied electric field.

Figure 2 illustrates the dependence of $|P_{n_cn_v}(\tau_B)|$ on Bloch electron energy ε_B , calculated for two regions of the

TABLE I. Characteristics of peak positions of the relative probability transition shown in Fig. 1 ($W_v = 10$ meV, $W_c = 40$ meV, and $a = 10^{-6}$ cm).

m	$\hbar\omega_B$ (meV)	ν_B (THz)	E (kV/cm)
1	5	1.2	5
2	6.25	1.5	6.25
3	8.33	2	8.33
4	12.5	3	12.5
5	25	6	25

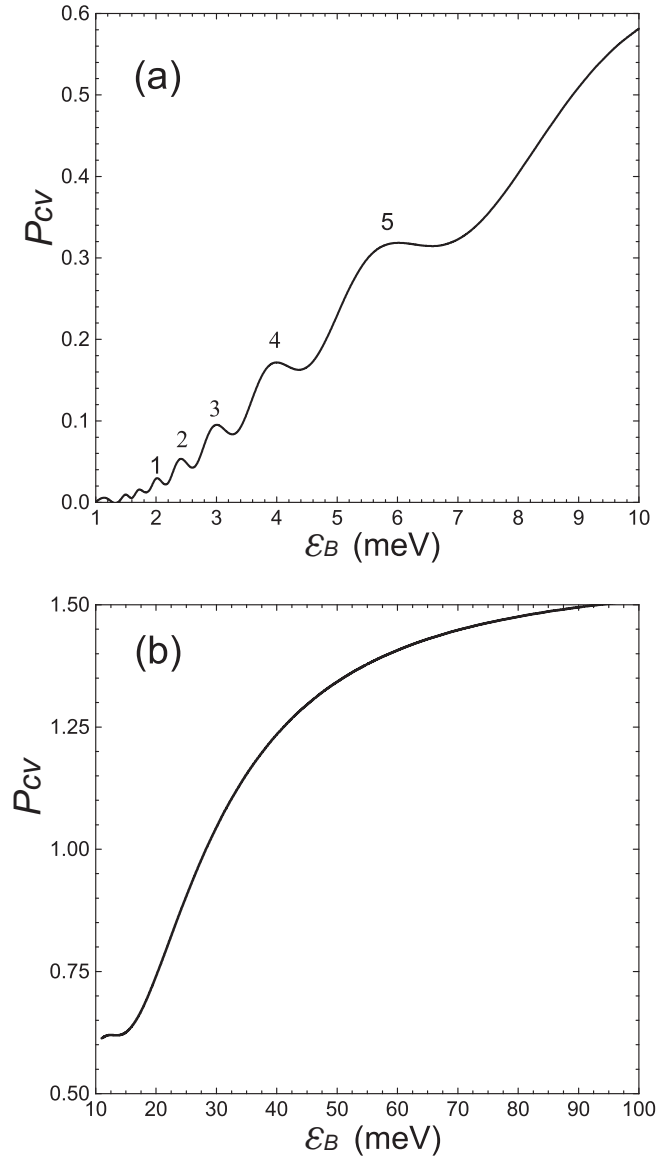


FIG. 2. $P_{cv} = |P_{n_c n_v}|$ vs $\varepsilon_B = \hbar\omega_B$ calculated from 1 to 10 meV (a), and from 10 to 100 meV (b); $W_v = 10$ meV, $W_c = 40$ meV. In (a), the curve maximums 1–5 correspond to the condition of maximum growth: 1. $m = 12$; 2. $m = 10$; 3. $m = 8$; 4. $m = 6$; and 5. $m = 4$; even values of m correspond to maximums, while odd m to minimums.

energy ε_B . As seen in Fig. 2(a), $|P_{n_c n_v}(\tau_B)|$ exhibits the oscillatory behavior for $\varepsilon_B \leq 10$ meV, while in Fig. 2(b) it becomes monotonically increasing function of ε_B . In Fig. 2(a), the positions of maximums and minimums correlate with even and odd m -values, reflected in the condition of maximum growth.

Temporal behavior of the probability transition during one Bloch cycle is shown in Fig. 3, where we plot $|P_{n_c n_v}(N\tau_B)|^2$ as a parametrical function of time using $\zeta = (2t - \tau_B)/\tau_B$; the initial time $t = 0$ corresponds to $\zeta = -1$ and $t = \tau_B$ to $\zeta = 1$. Figure 3 also details relative contributions of the integrals $I_1(\zeta)$ and $I_2(\zeta)$ into the monotonically increasing probability transition with the increase of time.

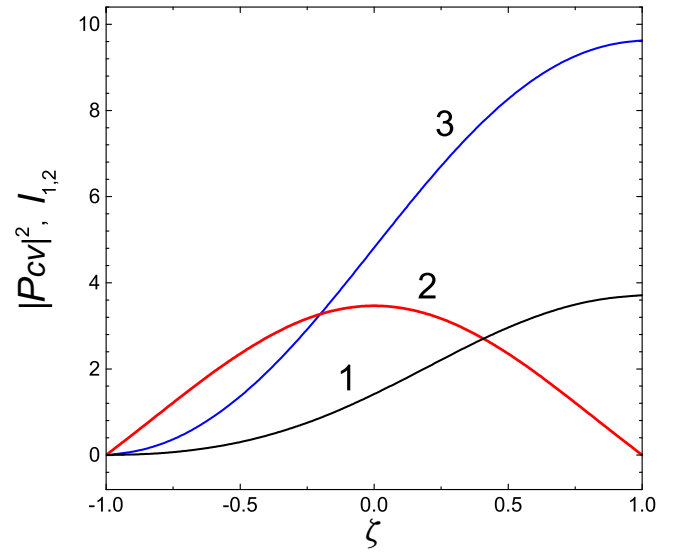


FIG. 3. Probability transition $|P_{n_c n_v}(\zeta)|^2$ as a function of normalized time $\zeta = (2t - \tau_B)/\tau_B$ calculated for one Bloch cycle: $t = 0$ ($\zeta = -1$), $t = \tau_B$ ($\zeta = 1$); $\hbar\omega_B = 8$ meV. Curves: 1 (black) $|P_{n_c n_v}(\zeta)|^2$, 2 (red) $[-I_2(\zeta)]$, and 3 (blue) $I_1(\zeta)$ [Eqs. (A6)–(A8) of Appendix].

We also note here that $P_{n_c n_v}$ scales when considering the comparative analysis of bulk and SL materials. A scaling analysis is provided in Appendix.

For $X_{n_c n_v}(k_x)$, we note that $\hat{p}_x = (m_0/i\hbar)[x, \hat{H}]$. For the conduction and valence bands of $\hat{H}$, we can write

$$\langle n_c, \mathbf{k} | \hat{p}_x | n_v, \mathbf{k} \rangle = \frac{m_0}{i\hbar} X_{n_c n_v}(\mathbf{k}) [\varepsilon_{n_c}(\mathbf{k}) - \varepsilon_{n_v}(\mathbf{k})] \quad (24a)$$

so that

$$X_{n_c n_v}(\mathbf{k}) = \frac{i\hbar}{m_0} \frac{(\hat{p}_x)_{n_c n_v}}{\varepsilon_{n_c}(\mathbf{k}) - \varepsilon_{n_v}(\mathbf{k})}. \quad (24b)$$

Now generally, for the instantaneous eigenstates $\langle \Psi_{n' \mathbf{K}} | \hat{\mathbf{p}} | \Psi_{n \mathbf{K}} \rangle = [\hbar \mathbf{K} \delta_{n', n} + \hat{\mathbf{p}}_{n' n}(\mathbf{k})] \delta_{\mathbf{K}', \mathbf{K}}$, with $\hat{\mathbf{p}}_{n' n}(\mathbf{k}) = \langle u_{n' \mathbf{k}} | \hat{\mathbf{p}} | u_{n \mathbf{k}} \rangle = \frac{1}{\Omega_c} \int_{\Omega_c} u_{n' \mathbf{k}}^* \hat{\mathbf{p}} u_{n \mathbf{k}} d\mathbf{r}$. In NNTB, with $n_c \neq n_v$, $\hat{\mathbf{p}}_{n_c n_v}(\mathbf{k}) = \langle u_{s \mathbf{k}} | \hat{\mathbf{p}} | u_{p \mathbf{k}} \rangle$, where subindex $s(p)$ corresponds to the $s(p)$ state of an atomic orbital function,

$$\begin{aligned} |u_{s \mathbf{K}}(\mathbf{r})\rangle &= \frac{1}{\sqrt{N_0}} \sum_{\mathbf{l}} e^{i\mathbf{K} \cdot \mathbf{l}} \Phi_s(\mathbf{r} - \mathbf{l}), \\ |u_{p \mathbf{K}}(\mathbf{r})\rangle &= \frac{1}{\sqrt{N_0}} \sum_{\mathbf{l}} e^{i\mathbf{K} \cdot \mathbf{l}} \Phi_p(\mathbf{r} - \mathbf{l}), \end{aligned} \quad (25)$$

and N_0 is the normalization number. Then

$$\begin{aligned} \langle u_{s \mathbf{k}} | \hat{\mathbf{p}} | u_{p \mathbf{k}} \rangle &= \frac{1}{N_0} \sum_{\mathbf{l}} \sum_{\mathbf{l}'} e^{i\mathbf{K} \cdot (\mathbf{l}' - \mathbf{l})} \\ &\times \langle \Phi_s(\mathbf{r} - \mathbf{l}) | \hat{\mathbf{p}} | \Phi_p(\mathbf{r} - \mathbf{l}') \rangle. \end{aligned} \quad (26)$$

In the spirit of NNTB for (s, p) states, we assume that $\langle \Phi_s(\mathbf{r} - \mathbf{l}) | \hat{\mathbf{p}} | \Phi_p(\mathbf{r} - \mathbf{l}') \rangle \equiv \mathbf{p} \delta_{\mathbf{l}, \mathbf{l}'}$, parametrically, so that

$$\langle u_{s \mathbf{k}} | \hat{\mathbf{p}} | u_{p \mathbf{k}} \rangle = \mathbf{p}, \quad (27a)$$

a c number, independent of $\mathbf{k}$. Thus

$$X_{n_c n_v}(\mathbf{k}) = i\hbar \frac{p_x}{m_0[\varepsilon_{n_c}(\mathbf{k}) - \varepsilon_{n_v}(\mathbf{k})]}. \quad (27b)$$

The parameter p_x , a c number in this NNTB model, is now determined by application of a theorem developed by Krieger [28], which states that near the *connection point* of the bands n_c and n_v , the interband coupling parameter limits as

$$X_{n_c n_v}(K_x, \mathbf{K}_\perp)|_{K_x \sim q_x} \simeq \frac{1}{4(K_x - q_x)}, \quad (28)$$

where the connection point of the bands is determined by the auxiliary condition

$$\varepsilon_{n_c}(q_x, \mathbf{q}_\perp) = \varepsilon_{n_v}(q_x, \mathbf{q}_\perp); \quad (29)$$

here, q_x is generally complex for two nonoverlapping bands. Using ε_{n_c} , ε_{n_v} of Eq. (20), the connection condition gives $q_x = i|q_x|$, with

$$\sinh(a_x |q_x|) = 2 \frac{\sqrt{\varepsilon_g E_g}}{E_g - \varepsilon_g}. \quad (30)$$

In order to calculate p_x from Eq. (27a), we expand $[\varepsilon_{n_c}(\mathbf{K}) - \varepsilon_{n_v}(\mathbf{K})]$ about $\mathbf{q}$ to order $(\mathbf{K} - \mathbf{q})$, and we obtain for Eq. (21)

$$\varepsilon_{n_c}(\mathbf{K}) - \varepsilon_{n_v}(\mathbf{K}) = (\varepsilon_{n_c} - \varepsilon_{n_v})_{\mathbf{K}=\mathbf{q}} + \nabla_{\mathbf{K}}(\varepsilon_{n_c} - \varepsilon_{n_v})_{\mathbf{K}=\mathbf{q}} \cdot (\mathbf{K} - \mathbf{q}) + \mathcal{O}(\mathbf{K} - \mathbf{q})^2. \quad (31a)$$

From the condition of Eq. (29), the first term of the expansion is zero. For the second term, we note that from Eq. (21)

$$\nabla_{\mathbf{K}}(\varepsilon_{n_c} - \varepsilon_{n_v})_{\mathbf{K}=\mathbf{q}} = \mathbf{a}B \sin(\mathbf{q} \cdot \mathbf{a}), \quad (31b)$$

and from the connection condition, Eq. (21) provides $\cos(\mathbf{q} \cdot \mathbf{a}) = A/B$, so that $\sin(\mathbf{q} \cdot \mathbf{a}) = \sqrt{B^2 - A^2}/B$. Thus

$$[\varepsilon_{n_c}(\mathbf{K}) - \varepsilon_{n_v}(\mathbf{K})]_{\mathbf{K}=\mathbf{q}} = \mathbf{a} \cdot (\mathbf{K} - \mathbf{q})B \sin(\mathbf{q} \cdot \mathbf{a}).$$

Taking into account that A, B are given in Eq. (21), with $E_g > \varepsilon_g$, then $\sin(\mathbf{q} \cdot \mathbf{a}) = i\sqrt{\varepsilon_g E_g}/B$, we obtain

$$[\varepsilon_{n_c}(\mathbf{K}) - \varepsilon_{n_v}(\mathbf{K})]_{\mathbf{K}=\mathbf{q}} = i\sqrt{\varepsilon_g E_g} \mathbf{a} \cdot (\mathbf{K} - \mathbf{q}).$$

For the field in the $\hat{\mathbf{x}}$ direction, with $\mathbf{q} = q_x \hat{\mathbf{x}} + \mathbf{q}_\perp$, we find

$$[\varepsilon_{n_c}(\mathbf{k}) - \varepsilon_{n_v}(\mathbf{k})]_{k_x=q_x} = i\sqrt{\varepsilon_g E_g} a_x (k_x - q_x). \quad (31c)$$

Putting (31c) into Eq. (27b) and comparing it with Eq. (28), we find that p_x must be

$$p_x = \frac{1}{4} \frac{m_0}{\hbar} a_x \sqrt{E_g \varepsilon_g}. \quad (32)$$

Thus $X_{n_c n_v}(\mathbf{k})$ of Eq. (27b) becomes

$$X_{n_c n_v}(\mathbf{k}) = \frac{i}{4} \frac{a_x \sqrt{\varepsilon_g E_g}}{\varepsilon_{n_c}(\mathbf{k}) - \varepsilon_{n_v}(\mathbf{k})}. \quad (33)$$

We note that since $\mathbf{k}$ is real in our analysis, $X_{n_c n_v}(\mathbf{k}) = X_{n_v n_c}^*(\mathbf{k})$ does not suffer from an unspecified phase factor in accordance with Krieger's findings [28].

Thus, by use of the band-matching condition and the subsequent parametrization of the momentum matrix elements, we have simplified the interband matrix elements so as to depend on the band structure and band gap parameters alone.

The detail evaluation of this interband matrix element for the two-band model is given in Appendix with the transition probability, $P_{n_c n_v}$; its use follows in the remainder of the analysis.

IV. CURRENT FLOW IN THE DENSITY MATRIX FORMULATION; TWO-BAND MODEL

A. General formulation [21,30]

In the density matrix formulation, the current is evaluated as

$$\mathbf{j}(t) = e \sum_{n, \mathbf{k}} \sum_{n', \mathbf{k}'} \hat{Q}_{n\mathbf{k}, n'\mathbf{k}'}(t) \hat{\mathbf{v}}_{n'\mathbf{k}', n\mathbf{k}}(t), \quad (34)$$

where the density matrix operator $\hat{Q}(t)$ obeys the Liouville equation

$$i\hbar \frac{\partial \hat{Q}}{\partial t} = [\hat{H}, \hat{Q}], \quad (35)$$

and the Hamiltonian $\hat{H}$ for our problem is given by Eq. (1) with $\mathbf{p}_c(t)$ defined in Eq. (3a). The matrix elements of the velocity operator $\hat{\mathbf{v}}$ are governed by the relation

$$\hat{\mathbf{v}} = \frac{1}{i\hbar} [\mathbf{r}, \hat{H}]. \quad (36)$$

It then follows using the instantaneous eigenstates of $\hat{H}$ that

$$\hat{\mathbf{v}}_{n\mathbf{k}, n\mathbf{k}} = \frac{1}{\hbar} \nabla_{\mathbf{k}} \varepsilon_n(\mathbf{k}) \quad (37)$$

for band n and wave vector $\mathbf{k}(t) = \mathbf{K} + \mathbf{p}_c(t)/\hbar$. Also

$$\hat{\mathbf{v}}_{n\mathbf{k}, n'\mathbf{k}'} = \frac{1}{m_0} \hat{\mathbf{p}}_{n\mathbf{k}, n'\mathbf{k}'}, \quad (38)$$

where

$$\frac{\hat{\mathbf{p}}_{n\mathbf{k}, n'\mathbf{k}'}}{m_0[\varepsilon_{n'}(\mathbf{k}) - \varepsilon_n(\mathbf{k})]} = \frac{1}{i\hbar} \mathbf{R}_{nn'}(\mathbf{k}), \quad n' \neq n. \quad (39)$$

Here, $\hat{\mathbf{p}}_{n\mathbf{k}, n'\mathbf{k}'}$ are momentum matrix elements with respect to Bloch cellular functions,

$$\mathbf{R}_{nn'}(\mathbf{k}) = \frac{i}{\Omega_c} \int_{\Omega_c} u_{n\mathbf{k}}^*(\mathbf{r}) \nabla_{\mathbf{k}} u_{n'\mathbf{k}'}(\mathbf{r}) d\mathbf{r}, \quad (40)$$

with $\mathbf{R}_{nn'}(\mathbf{k}) = \mathbf{R}_{n'n}^*(\mathbf{k})$.

In $\mathbf{j}(t)$, the terms can be easily expressed in terms of diagonal, $\mathbf{j}_d(t)$, and off-diagonal, $\mathbf{j}_{od}(t)$, elements

$$\begin{aligned} \mathbf{j}(t) &= \mathbf{j}_d(t) + \mathbf{j}_{od}(t) = e \sum_{n, \mathbf{k}} \hat{Q}_{n\mathbf{k}, n\mathbf{k}}(t) \hat{\mathbf{v}}_{n\mathbf{k}, n\mathbf{k}}(t) \\ &+ e \sum_{n' \neq n} \sum_{n, \mathbf{k}} \hat{Q}_{n\mathbf{k}, n'\mathbf{k}'}(t) \hat{\mathbf{v}}_{n'\mathbf{k}', n\mathbf{k}}(t). \end{aligned} \quad (41)$$

We note that in the matrix elements with respect to $\mathbf{k}$, we always assume that $\mathbf{k}' = \mathbf{k}$ since all matrix elements of interest generate a Kronecker delta $\delta_{\mathbf{k}, \mathbf{k}'}$ in the resolvent. Since the elements of $\hat{\mathbf{v}}$ have been established in Eqs. (37) and (38), we now seek to determine the density matrix from Eq. (35).

Taking the matrix elements of the Liouville equation (35) with respect to the instantaneous eigenstates, we find

$$i\hbar \left(\frac{\partial \hat{Q}}{\partial t} \right)_{n\mathbf{k}, n'\mathbf{k}'} = [\hat{H}, \hat{Q}]_{n\mathbf{k}, n'\mathbf{k}'} = [\varepsilon_n(\mathbf{k}) - \varepsilon_{n'}(\mathbf{k})] \hat{Q}_{n\mathbf{k}, n'\mathbf{k}'}. \quad (42)$$

The instantaneous eigenstates are time dependent and satisfy

$$i\hbar \frac{\partial \psi_{n\mathbf{K}}(\mathbf{r}, t)}{\partial t} = \mathbf{F}(t) \cdot \sum_{n'} \mathbf{R}_{n'n}(\mathbf{k}(t)) \psi_{n'\mathbf{K}}(\mathbf{r}, t), \quad (43)$$

it then follows that

$$\left(\frac{\partial \hat{\rho}}{\partial t} \right)_{n\mathbf{k}, n'\mathbf{k}} = \frac{\partial}{\partial t} \hat{\rho}_{n\mathbf{k}, n'\mathbf{k}} - \frac{1}{i\hbar} \mathbf{F}(t) \cdot \sum_{n''} [\mathbf{R}_{n''n'}(\mathbf{k}) \hat{\rho}_{n\mathbf{k}, n''\mathbf{k}} - \mathbf{R}_{nn''}(\mathbf{k}) \hat{\rho}_{n''\mathbf{k}, n'\mathbf{k}}].$$

Therefore the density matrix of Eq. (42) becomes

$$i\hbar \frac{\partial \hat{\rho}_{n\mathbf{k}, n'\mathbf{k}}}{\partial t} - \mathbf{F}(t) \cdot \sum_{n''} [\mathbf{R}_{n''n'}(\mathbf{k}) \hat{\rho}_{n\mathbf{k}, n''\mathbf{k}} - \mathbf{R}_{nn''}(\mathbf{k}) \hat{\rho}_{n''\mathbf{k}, n'\mathbf{k}}] = [\varepsilon_n(\mathbf{k}) - \varepsilon_{n'}(\mathbf{k})] \hat{\rho}_{n\mathbf{k}, n'\mathbf{k}}. \quad (44)$$

In Eq. (44), breaking up the sum over n'' so as to retain only the terms with $n'' = (n, n')$ while dropping all other terms of order $n'' \neq (n, n')$, we get

$$i\hbar \frac{\partial \hat{\rho}_{n\mathbf{k}, n'\mathbf{k}}}{\partial t} = [\bar{\varepsilon}_n(\mathbf{k}) - \bar{\varepsilon}_{n'}(\mathbf{k})] \hat{\rho}_{n\mathbf{k}, n'\mathbf{k}} + \mathbf{F}(t) \cdot \mathbf{R}_{nn'}(\mathbf{k}) (\hat{\rho}_{n\mathbf{k}} - \hat{\rho}_{n'\mathbf{k}}), \quad (45a)$$

where

$$\bar{\varepsilon}_n(\mathbf{k}) \equiv \varepsilon_n(\mathbf{k}) - \mathbf{F}(t) \cdot \mathbf{R}_{nn}(\mathbf{k}), \quad (45b)$$

and $\hat{\rho}_{n\mathbf{k}} \equiv \hat{\rho}_{n\mathbf{k}, n\mathbf{k}}$. Therefore Eq. (45a) represents an approximate expression for the off-diagonal elements, $\hat{\rho}_{n\mathbf{k}, n'\mathbf{k}}$, in terms of the diagonal elements. On the other hand, when $n = n'$ in Eq. (44), we find

$$i\hbar \frac{\partial \hat{\rho}_{n\mathbf{k}}}{\partial t} = \mathbf{F}(t) \cdot \sum_{n' \neq n} [\mathbf{R}_{nn'}^*(\mathbf{k}) \hat{\rho}_{n\mathbf{k}, n'\mathbf{k}} - \mathbf{R}_{nn'}(\mathbf{k}) \hat{\rho}_{n'\mathbf{k}, n\mathbf{k}}], \quad (46)$$

which is an exact expression relating the diagonal elements, $\hat{\rho}_{n\mathbf{k}}$, to the off-diagonal elements, $\hat{\rho}_{n\mathbf{k}, n'\mathbf{k}}$. Thus, in integrating Eq. (45a) subject to the initial condition $\hat{\rho}_{n\mathbf{k}, n'\mathbf{k}}(t_0) = 0$ ($n' \neq n$), we obtain

$$\hat{\rho}_{n\mathbf{k}, n'\mathbf{k}}(t) = \frac{1}{i\hbar} \int_{t_0}^t dt' \mathbf{F}(t') \cdot \mathbf{R}_{nn'}(\mathbf{k}(t')) [\hat{\rho}_{n\mathbf{k}}(t') - \hat{\rho}_{n'\mathbf{k}}(t')] e^{\frac{i}{\hbar} \int_{t'}^t [\bar{\varepsilon}_n(\mathbf{k}) - \bar{\varepsilon}_{n'}(\mathbf{k})] d\tau}, \quad (47)$$

the equation for off-diagonal elements in terms of the diagonal elements. Then putting $\hat{\rho}_{n\mathbf{k}, n'\mathbf{k}}(t)$ of Eq. (47) into Eq. (46) thereby eliminating the off-diagonal elements, we obtain an integro-differential equation for $\hat{\rho}_{n\mathbf{k}}$ alone

$$\begin{aligned} \frac{\partial}{\partial t} \hat{\rho}_{n\mathbf{k}}(t) &= 2\text{Re} \sum_{n' \neq n} Q_{nn'}^*(t) \int_{t_0}^t dt' Q_{nn'}(t') \\ &\times [\hat{\rho}_{n'\mathbf{k}}(t') - \hat{\rho}_{n\mathbf{k}}(t')]; \end{aligned} \quad (48a)$$

here

$$\begin{aligned} Q_{n\mathbf{k}, n'\mathbf{k}}(t) &\equiv \frac{\partial P_{nn'}(t)}{\partial t} \\ &= \frac{1}{\hbar} \mathbf{F}(t) \cdot \mathbf{R}_{nn'}(\mathbf{k}(t)) e^{\frac{i}{\hbar} \int_{t_0}^t [\varepsilon_n(\mathbf{k}(\tau)) - \varepsilon_{n'}(\mathbf{k}(\tau))] d\tau}, \end{aligned} \quad (48b)$$

where $P_{nn'}(t)$ is defined in Eq. (15a).

B. Two-band model

In applying the general formulation to a two-band model, we designate $n = n_c$, $n' = n_v$, representing the conduction and valence bands, respectively. Below we use these designations in calculating the density matrix and electron velocity matrix elements.

Calculation of the density matrix. For each band, n_c and n_v , Eq. (48a) becomes

$$\frac{\partial}{\partial t} \hat{\rho}_{n_c\mathbf{k}}(t) = \int_{t_0}^t dt' \Gamma(t, t') [\hat{\rho}_{n_v\mathbf{k}}(t') - \hat{\rho}_{n_c\mathbf{k}}(t')] \quad (49a)$$

and

$$\frac{\partial}{\partial t} \hat{\rho}_{n_v\mathbf{k}}(t) = \int_{t_0}^t dt' \Gamma(t, t') [\hat{\rho}_{n_c\mathbf{k}}(t') - \hat{\rho}_{n_v\mathbf{k}}(t')], \quad (49b)$$

where

$$\Gamma(t, t') = Q_{n_c n_v}^*(t) Q_{n_c n_v}(t') + Q_{n_c n_v}(t) Q_{n_c n_v}^*(t'), \quad (49c)$$

with $\Gamma(t, t') = \Gamma^*(t, t')$. It then follows from Eqs. (49a) and (49b) that

$$\frac{\partial}{\partial t} [\hat{\rho}_{n_c\mathbf{k}}(t) + \hat{\rho}_{n_v\mathbf{k}}(t)] = 0, \quad (50a)$$

which yields

$$\hat{\rho}_{n_c\mathbf{k}}(t) + \hat{\rho}_{n_v\mathbf{k}}(t) = \hat{\rho}_{n_c\mathbf{k}}(t_0) + \hat{\rho}_{n_v\mathbf{k}}(t_0) = 1; \quad (50b)$$

also

$$\begin{aligned} \frac{\partial}{\partial t} [\hat{\rho}_{n_c\mathbf{k}}(t) - \hat{\rho}_{n_v\mathbf{k}}(t)] \\ = -2 \int_{t_0}^t dt' \Gamma(t, t') [\hat{\rho}_{n_c\mathbf{k}}(t') - \hat{\rho}_{n_v\mathbf{k}}(t')]. \end{aligned} \quad (51)$$

Integrating the right-hand side of Eq. (51) by parts while noting $\Gamma(t, t')$ of Eq. (49c), we find

$$\begin{aligned} \frac{\partial}{\partial t} [\hat{\rho}_{n_c\mathbf{k}}(t) - \hat{\rho}_{n_v\mathbf{k}}(t)] &= -2 \left\{ [\hat{\rho}_{n_c\mathbf{k}}(t) - \hat{\rho}_{n_v\mathbf{k}}(t)] \gamma(t) \right. \\ &\quad \left. - \int_{t_0}^t dt' \frac{\partial}{\partial t'} [\hat{\rho}_{n_c\mathbf{k}}(t') - \hat{\rho}_{n_v\mathbf{k}}(t')] \gamma(t') \right\}, \end{aligned} \quad (52a)$$

where

$$\gamma(t) \equiv \int_{t_0}^t dt' \Gamma(t, t') = \frac{\partial}{\partial t} |P_{n_c n_v}(t)|^2, \quad (52b)$$

with $P_{n_c n_v}(t)$ defined in Eq. (15a). Ignoring the integral term of the residual integration by parts as higher order, we approximate Eq. (52a) as

$$\frac{\partial}{\partial t} [\hat{\rho}_{n_c\mathbf{k}}(t) - \hat{\rho}_{n_v\mathbf{k}}(t)] = -2\gamma(t) [\hat{\rho}_{n_c\mathbf{k}}(t) - \hat{\rho}_{n_v\mathbf{k}}(t)], \quad (53)$$

It then follows from Eqs. (53) and (52b) that, to lowest order,

$$\hat{\rho}_{n_c\mathbf{k}}(t) - \hat{\rho}_{n_v\mathbf{k}}(t) = [\hat{\rho}_{n_c\mathbf{k}}(t_0) - \hat{\rho}_{n_v\mathbf{k}}(t_0)] e^{-2|P_{n_c n_v}(t)|^2}. \quad (54)$$

Combining Eq. (54) with Eq. (50b), we can solve for $\hat{\rho}_{n_c\mathbf{k}}(t)$ and $\hat{\rho}_{n_v\mathbf{k}}(t)$ separately as

$$\begin{aligned} \hat{\rho}_{n_c\mathbf{k}}(t) &= \frac{1}{2} [\hat{\rho}_{n_c\mathbf{k}}(t_0) (1 + e^{-2|P_{n_c n_v}(t)|^2}) \\ &\quad + \hat{\rho}_{n_v\mathbf{k}}(t_0) (1 - e^{-2|P_{n_c n_v}(t)|^2})] \end{aligned} \quad (55a)$$

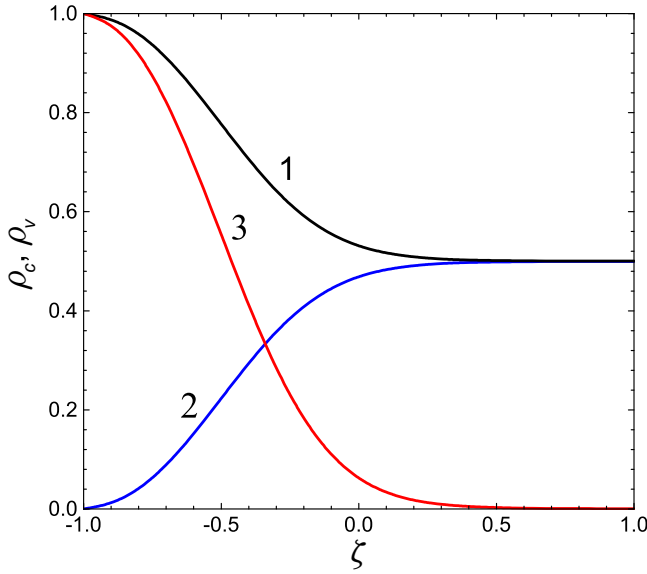


FIG. 4. Diagonal elements of density matrix $\rho_c \equiv \hat{\rho}_{n_c\mathbf{k}}$, $\rho_v \equiv \hat{\rho}_{n_v\mathbf{k}}$ as a function of normalized time $\zeta = (2t - \tau_B)/\tau_B$ calculated for one Bloch cycle: $t = 0$ ($\zeta = -1$), $t = \tau_B$ ($\zeta = 1$); initial conditions: $\rho_v(t = 0) = 1$, $\rho_c(t = 0) = 0$; $\hbar\omega_B = 8$ meV. Curves: 1 (black) $\rho_v(\zeta)$, 2 (blue) $\rho_c(\zeta)$, and 3 (red) $[\rho_v(\zeta) - \rho_c(\zeta)]$.

and

$$\hat{\rho}_{n_v\mathbf{k}}(t) = \frac{1}{2} [\hat{\rho}_{n_c\mathbf{k}}(t_0)(1 - e^{-2|P_{n_cn_v}(t)|^2}) + \hat{\rho}_{n_v\mathbf{k}}(t_0)(1 + e^{-2|P_{n_cn_v}(t)|^2})]. \quad (55b)$$

Equations (54)–(55b) are plotted in Fig. 4 for one Bloch cycle.

The diagonal matrix elements $\hat{\rho}_{n_c\mathbf{k}}(t)$ and $\hat{\rho}_{n_v\mathbf{k}}(t)$ can be expanded to order $|P_{n_cn_v}(t)|^2$ by expanding the exponents in Eqs. (55a) and (55b); as such

$$\begin{aligned} \hat{\rho}_{n_c\mathbf{k}}(t) &= \hat{\rho}_{n_c\mathbf{k}}(t_0) - [\hat{\rho}_{n_c\mathbf{k}}(t_0) - \hat{\rho}_{n_v\mathbf{k}}(t_0)]|P_{n_cn_v}(t)|^2, \\ \hat{\rho}_{n_v\mathbf{k}}(t) &= \hat{\rho}_{n_v\mathbf{k}}(t_0) + [\hat{\rho}_{n_c\mathbf{k}}(t_0) - \hat{\rho}_{n_v\mathbf{k}}(t_0)] \\ &\quad \times |P_{n_cn_v}(t)|^2. \end{aligned} \quad (56)$$

In considering the off-diagonal elements of Eq. (47) for the two-band model, we find

$$\begin{aligned} \hat{\rho}_{n_c\mathbf{k},n_v\mathbf{k}}(t) &= \frac{1}{i\hbar} \int_{t_0}^t dt' \mathbf{F}(t') \cdot \mathbf{R}_{n_cn_v}(\mathbf{k}(t')) \\ &\quad \times e^{\frac{i}{\hbar} \int_{t_0}^{t'} [\varepsilon_{n_c}(\mathbf{k}(\tau)) - \varepsilon_{n_v}(\mathbf{k}(\tau))] d\tau} [\hat{\rho}_{n_c\mathbf{k}}(t') - \hat{\rho}_{n_v\mathbf{k}}(t')]. \end{aligned} \quad (57a)$$

Here, we assume that $\mathbf{R}_{nn} = 0$ so that $\bar{\varepsilon}_n = \varepsilon_n$. In Eq. (57a), factoring out the exponential term $e^{-\frac{i}{\hbar} \int_{t_0}^{t'} [\varepsilon_{n_c}(\mathbf{k}(\tau)) - \varepsilon_{n_v}(\mathbf{k}(\tau))] d\tau}$ and utilizing the notation of Eq. (48b) together with Eq. (54), we can reexpress Eq. (57a) as

$$\begin{aligned} \hat{\rho}_{n_c\mathbf{k},n_v\mathbf{k}}(t) &= e^{-\frac{i}{\hbar} \int_{t_0}^t [\varepsilon_{n_c}(\mathbf{k}(\tau)) - \varepsilon_{n_v}(\mathbf{k}(\tau))] d\tau} \\ &\quad \times [\hat{\rho}_{n_c\mathbf{k}}(t_0) - \hat{\rho}_{n_v\mathbf{k}}(t_0)] \frac{1}{i} \\ &\quad \times \int_{t_0}^t dt' \frac{\partial P_{n_cn_v}}{\partial t'} e^{-2|P_{n_cn_v}(t')|^2}. \end{aligned} \quad (57b)$$

Noting that $P_{n_cn_v}(t_0) = 0$, we can establish $\hat{\rho}_{n_c\mathbf{k},n_v\mathbf{k}}(t)$ of Eq. (57b) to order $|P_{n_cn_v}(t)|^2$ as

$$\begin{aligned} \hat{\rho}_{n_c\mathbf{k},n_v\mathbf{k}}(t) &= e^{-\frac{i}{\hbar} \int_{t_0}^t [\varepsilon_{n_c}(\mathbf{k}(\tau)) - \varepsilon_{n_v}(\mathbf{k}(\tau))] d\tau} [\hat{\rho}_{n_c\mathbf{k}}(t_0) - \hat{\rho}_{n_v\mathbf{k}}(t_0)] \\ &\quad \times \frac{1}{i} P_{n_cn_v}(t) + \mathcal{O}(|P_{n_cn_v}(t)|^2). \end{aligned} \quad (58)$$

Here, we see that $P_{n_cn_v}(t)$ is given by

$$\begin{aligned} P_{n_cn_v}(t) &= \frac{1}{\hbar} \int_{t_0}^t dt' \mathbf{F}(t') \cdot \mathbf{R}_{n_cn_v}(\mathbf{k}(t')) \\ &\quad \times e^{\frac{i}{\hbar} \int_{t_0}^{t'} [\varepsilon_{n_c}(\mathbf{k}(\tau)) - \varepsilon_{n_v}(\mathbf{k}(\tau))] d\tau}. \end{aligned} \quad (59)$$

Calculation of the electron current. The current in the two-band model can be written directly from Eq. (41) as

$$\begin{aligned} \mathbf{j} &= \mathbf{j}_d + \mathbf{j}_{od} \equiv e \sum_{\mathbf{k}} \left[(\hat{\rho}_{n_c\mathbf{k}} \hat{\mathbf{v}}_{n_c\mathbf{k}} + \hat{\rho}_{n_v\mathbf{k}} \hat{\mathbf{v}}_{n_v\mathbf{k}}) \right. \\ &\quad \left. + \left(\hat{\rho}_{n_c\mathbf{k},n_v\mathbf{k}} \frac{\hat{\mathbf{p}}_{n_v\mathbf{k},n_c\mathbf{k}}}{m_0} + \hat{\rho}_{n_c\mathbf{k},n_v\mathbf{k}}^* \frac{\hat{\mathbf{p}}_{n_v\mathbf{k},n_c\mathbf{k}}^*}{m_0} \right) \right], \end{aligned} \quad (60)$$

where $\hat{\mathbf{v}}_{n_c\mathbf{k}}$, $\hat{\mathbf{v}}_{n_v\mathbf{k}}$ are given for bands n_c , n_v in Eq. (37), and the off-diagonal velocities are given by Eqs. (38) and (39). The diagonal and off-diagonal matrix elements of the density matrix have been determined in terms of the interband coupling parameter $P_{n_cn_v}$ in Eqs. (55a), (55b), and (57b), respectively.

We now calculate $\mathbf{j}(t)$ of Eq. (60) considering separately $\mathbf{j}_d$ and $\mathbf{j}_{od}$. For the current diagonal (d) and off-diagonal (od) matrix elements contributions, we have from Eq. (60)

$$\mathbf{j}_d = e \sum_{\mathbf{k}} (\hat{\rho}_{n_c\mathbf{k}} \hat{\mathbf{v}}_{n_c\mathbf{k}} + \hat{\rho}_{n_v\mathbf{k}} \hat{\mathbf{v}}_{n_v\mathbf{k}}), \quad (61)$$

$$\begin{aligned} \mathbf{j}_{od} &= \frac{e}{m_0} \sum_{\mathbf{k}} (\hat{\rho}_{n_c\mathbf{k},n_v\mathbf{k}} \hat{\mathbf{p}}_{n_v\mathbf{k},n_c\mathbf{k}} + \hat{\rho}_{n_c\mathbf{k},n_v\mathbf{k}}^* \hat{\mathbf{p}}_{n_v\mathbf{k},n_c\mathbf{k}}^*) \\ &= 2 \frac{e}{m_0} \text{Re} \sum_{\mathbf{k}} \hat{\rho}_{n_c\mathbf{k},n_v\mathbf{k}} \hat{\mathbf{p}}_{n_v\mathbf{k},n_c\mathbf{k}}. \end{aligned} \quad (62)$$

Substituting $\hat{\rho}_{n_c\mathbf{k}}$, $\hat{\rho}_{n_v\mathbf{k}}$ from Eqs. (55a), (55b) and $\hat{\mathbf{v}}_{n_c\mathbf{k}}$, $\hat{\mathbf{v}}_{n_v\mathbf{k}}$ from Eq. (37), we obtain

$$\begin{aligned} \mathbf{j}_d(t) &= \frac{e}{2} \sum_{\mathbf{k}} \left\{ [\hat{\rho}_{n_c\mathbf{k}}(t_0)(1 + e^{-2|P_{n_cn_v}(k_x(t))|^2}) \right. \\ &\quad \left. + \hat{\rho}_{n_v\mathbf{k}}(t_0)(1 - e^{-2|P_{n_cn_v}(k_x(t))|^2})] \frac{1}{\hbar} \nabla_{\mathbf{k}} \varepsilon_{n_c}(\mathbf{k}) \right. \\ &\quad \left. + [\hat{\rho}_{n_v\mathbf{k}}(t_0)(1 + e^{-2|P_{n_cn_v}(k_x(t))|^2}) \right. \\ &\quad \left. + \hat{\rho}_{n_c\mathbf{k}}(t_0)(1 - e^{-2|P_{n_cn_v}(k_x(t))|^2})] \frac{1}{\hbar} \nabla_{\mathbf{k}} \varepsilon_{n_v}(\mathbf{k}) \right\}. \end{aligned} \quad (63)$$

In further developing $\mathbf{j}_d(t)$ and $\mathbf{j}_{od}(t)$ using the parameters from the adopted “s–p” model, we note from $\varepsilon_{n_c}(\mathbf{k})$ and $\varepsilon_{n_v}(\mathbf{k})$ of Eq. (20) that

$$\begin{aligned} \mathbf{v}_{n_c} &= \frac{1}{\hbar} \nabla_{\mathbf{k}} \varepsilon_{n_c}(\mathbf{k}) = \mathbf{a} \frac{W_c}{2\hbar} \sin(\mathbf{k} \cdot \mathbf{a}), \\ \mathbf{v}_{n_v} &= \frac{1}{\hbar} \nabla_{\mathbf{k}} \varepsilon_{n_v}(\mathbf{k}) = -\mathbf{a} \frac{W_v}{2\hbar} \sin(\mathbf{k} \cdot \mathbf{a}), \end{aligned} \quad (64)$$

where $\mathbf{k}(t) = (F_0 t + K_x)\hat{\mathbf{x}} + \mathbf{K}_\perp$. Then, in terms of the two-band model parameters, $\mathbf{j}_d(t)$ becomes

$$\begin{aligned} \mathbf{j}_d(t) = \mathbf{a} \frac{e}{4\hbar} \sum_{\mathbf{k}} \{ & [\hat{\varrho}_{n_c\mathbf{k}}(t_0)(1 + e^{-2|P_{n_c n_v}(k_x(t))|^2}) \\ & + \hat{\varrho}_{n_v\mathbf{k}}(t_0)(1 - e^{-2|P_{n_c n_v}(k_x(t))|^2})] W_c \\ & - [\hat{\varrho}_{n_v\mathbf{k}}(t_0)(1 + e^{-2|P_{n_c n_v}(k_x(t))|^2}) \\ & + \hat{\varrho}_{n_c\mathbf{k}}(t_0)(1 - e^{-2|P_{n_c n_v}(k_x(t))|^2})] W_v \} \sin(\mathbf{k} \cdot \mathbf{a}). \end{aligned} \quad (65)$$

Noting that $\hat{\varrho}_{n_c\mathbf{k}}(t_0) + \hat{\varrho}_{n_v\mathbf{k}}(t_0) = 1$, we can rewrite (65) as

$$\begin{aligned} \mathbf{j}_d(t) = \mathbf{a} \frac{e}{4\hbar} \sum_{\mathbf{k}} \{ & [1 + (\hat{\varrho}_{n_c\mathbf{k}}(t_0) - \hat{\varrho}_{n_v\mathbf{k}}(t_0)) \\ & \times e^{-2|P_{n_c n_v}(k_x(t))|^2}] W_c \\ & - [1 - (\hat{\varrho}_{n_c\mathbf{k}}(t_0) - \hat{\varrho}_{n_v\mathbf{k}}(t_0)) e^{-2|P_{n_c n_v}(k_x(t))|^2}] W_v \} \\ & \times \sin(\mathbf{k} \cdot \mathbf{a}), \end{aligned} \quad (66)$$

or

$$\begin{aligned} \mathbf{j}_d(t) = \mathbf{a} \frac{e}{4\hbar} \sum_{\mathbf{k}} [& W_c - W_v + (W_c + W_v) \\ & \times (\hat{\varrho}_{n_c\mathbf{k}}(t_0) - \hat{\varrho}_{n_v\mathbf{k}}(t_0)) e^{-2|P_{n_c n_v}(k_x(t))|^2}] \\ & \times \sin(\mathbf{k} \cdot \mathbf{a}). \end{aligned} \quad (67)$$

To evaluate the off-diagonal part of $\mathbf{j}(t)$ in Eq. (62), we use Eqs. (57b), (59), and (39); thus, we obtain

$$\begin{aligned} \mathbf{j}_{od}(t) = -\frac{2e}{\hbar} \text{Re} \sum_{\mathbf{k}} [& \hat{\varrho}_{n_c\mathbf{k}}(t_0) - \hat{\varrho}_{n_v\mathbf{k}}(t_0) \\ & \times \mathbf{R}_{n_c n_v}^*(\mathbf{k}(t)) [\varepsilon_{n_c}(\mathbf{k}) - \varepsilon_{n_v}(\mathbf{k})] \\ & \times e^{-\frac{i}{\hbar} \int_{t_0}^t (\varepsilon_{n_c} - \varepsilon_{n_v}) d\tau} \int_{t_0}^t dt' \frac{\partial P_{n_c n_v}}{\partial t'} e^{-2|P_{n_c n_v}(t')|^2}]. \end{aligned} \quad (68)$$

Letting $\mathbf{F}(t) = F_0 \hat{\mathbf{x}}$, and $[\mathbf{R}_{n_c n_v}(\mathbf{k}(t))]_x = X_{n_c n_v}(\mathbf{k}(t))$ as derived using Eqs. (59) and (33), we obtain

$$\begin{aligned} P_{n_c n_v}(t) = i \frac{F_0}{\hbar} \frac{a \sqrt{\varepsilon_g E_g}}{4} \\ \times \int_{t_0}^t dt' \frac{e^{\frac{i}{\hbar} \int_{t_0}^{t'} [\varepsilon_{n_c}(\mathbf{k}(\tau)) - \varepsilon_{n_v}(\mathbf{k}(\tau))] d\tau}}{\varepsilon_{n_c}(\mathbf{k}(t')) - \varepsilon_{n_v}(\mathbf{k}(t'))}. \end{aligned} \quad (69)$$

For $[\mathbf{j}_{od}]_x(t) \equiv j_{od}(t)$ in Eq. (68), we find

$$\begin{aligned} j_{od}(t) = -\frac{2e}{\hbar} \text{Re} \sum_{\mathbf{k}} [& \hat{\varrho}_{n_c\mathbf{k}}(t_0) - \hat{\varrho}_{n_v\mathbf{k}}(t_0)] X_{n_c n_v}^*(\mathbf{k}(t)) \\ & \times [\varepsilon_{n_c}(\mathbf{k}) - \varepsilon_{n_v}(\mathbf{k})] e^{-\frac{i}{\hbar} \int_{t_0}^t [\varepsilon_{n_c}(\mathbf{k}(\tau)) - \varepsilon_{n_v}(\mathbf{k}(\tau))] d\tau} \\ & \times \int_{t_0}^t dt' \frac{\partial P_{n_c n_v}}{\partial t'} e^{-2|P_{n_c n_v}(t')|^2}. \end{aligned} \quad (70)$$

Noting from Eq. (33) that

$$X_{n_c n_v}^*(\mathbf{k}) [\varepsilon_c(\mathbf{k}) - \varepsilon_v(\mathbf{k})] = -i \frac{a}{4} \sqrt{\varepsilon_g E_g}, \quad (71)$$

we find that $j_{od}(t)$ of Eq. (70) becomes

$$\begin{aligned} j_{od}(t) = \frac{e}{2\hbar} a \sqrt{\varepsilon_g E_g} \text{Re} \sum_{\mathbf{k}} i [& \hat{\varrho}_{n_c\mathbf{k}}(t_0) - \hat{\varrho}_{n_v\mathbf{k}}(t_0)] \\ & \times e^{-\frac{i}{\hbar} \int_{t_0}^t [\varepsilon_{n_c}(\mathbf{k}(\tau)) - \varepsilon_{n_v}(\mathbf{k}(\tau))] d\tau} \\ & \times \int_{t_0}^t dt' \frac{\partial P_{n_c n_v}}{\partial t'} e^{-2|P_{n_c n_v}(t')|^2}. \end{aligned} \quad (72)$$

We now calculate $\mathbf{j}(t)$ of Eq. (60) to lowest order in $P_{n_c n_v}$; we use Eq. (67) to evaluate the diagonal part of $\mathbf{j}(t)$ and Eq. (72) for the off-diagonal part. Making use of the appropriate expansion in the exponential term $e^{-2|P_{n_c n_v}|^2} \simeq 1 - 2|P_{n_c n_v}|^2$, we find

$$\begin{aligned} \mathbf{j}_d(t) = \mathbf{a} \frac{e}{2\hbar} \sum_{\mathbf{k}} \{ & W_c \hat{\varrho}_{n_c\mathbf{k}}(t_0) - W_v \hat{\varrho}_{n_v\mathbf{k}}(t_0) \\ & - (W_c + W_v) [\hat{\varrho}_{n_c\mathbf{k}}(t_0) - \hat{\varrho}_{n_v\mathbf{k}}(t_0)] |P_{n_c n_v}(t)|^2 \} \\ & \times \sin(\mathbf{k} \cdot \mathbf{a}) \end{aligned} \quad (73)$$

and

$$\begin{aligned} \mathbf{j}_{od}(t) = \frac{e}{2\hbar} a \sqrt{\varepsilon_g E_g} \text{Re} \sum_{\mathbf{k}} i [& \hat{\varrho}_{n_c\mathbf{k}}(t_0) - \hat{\varrho}_{n_v\mathbf{k}}(t_0)] \\ & \times e^{-\frac{i}{\hbar} \int_{t_0}^t [\varepsilon_{n_c}(\mathbf{k}(\tau)) - \varepsilon_{n_v}(\mathbf{k}(\tau))] d\tau} P_{n_c n_v}(t), \end{aligned} \quad (74)$$

where $P_{n_c n_v}(t)$ is given in Eq. (69).

For $\mathbf{j}_d(t)$ of Eq. (73) and $\mathbf{j}_{od}(t)$ of Eq. (74), we now convert the $\sum_{\mathbf{k}}$ to an $\int d\mathbf{k}$, and convert the integrands to functions of $\mathbf{k}$. In this regard, use is made of the acceleration theorem $\hbar \dot{\mathbf{k}} = \mathbf{F}(t)$, which gives the explicit rate of change of $\mathbf{k}(t)$ with time, so that we can write

$$\frac{1}{\hbar} \int_0^t \varepsilon(\mathbf{k}(t')) dt' = \frac{1}{F} \int_0^{\mathbf{k}(t)} \varepsilon(\mathbf{k}') d\mathbf{k}'. \quad (75)$$

Also $\sum_{\mathbf{k}} \rightarrow \frac{\Omega}{(2\pi)^3} \int d\mathbf{k}$, where Ω , the crystal volume, is equal to the number of primitive cells, N_c , times the volume of a primitive cell, Ω_c . Then, we find that $\mathbf{j}_d(t)$ of Eq. (73) and $\mathbf{j}_{od}(t)$ of Eq. (74) become

$$\begin{aligned} \mathbf{j}_d(t) = \mathbf{a} \frac{e}{2\hbar} \frac{\Omega}{(2\pi)^3} \int d\mathbf{k} \{ & W_c \hat{\varrho}_{n_c\mathbf{k}}(t_0) - W_v \hat{\varrho}_{n_v\mathbf{k}}(t_0) \\ & - (W_c + W_v) [\hat{\varrho}_{n_c\mathbf{k}}(t_0) - \hat{\varrho}_{n_v\mathbf{k}}(t_0)] |P_{n_c n_v}(t)|^2 \} \\ & \times \sin(\mathbf{k} \cdot \mathbf{a}) \end{aligned} \quad (76)$$

and

$$\begin{aligned} j_{od}(t) = \frac{e}{\hbar} \frac{a}{2} \sqrt{\varepsilon_g E_g} \text{Re} \frac{\Omega}{(2\pi)^3} i \int d\mathbf{k} [& \hat{\varrho}_{n_c\mathbf{k}}(t_0) - \hat{\varrho}_{n_v\mathbf{k}}(t_0)] \\ & \times e^{-\frac{i}{\hbar} \int_{t_0}^t [\varepsilon_{n_c}(\mathbf{k}') - \varepsilon_{n_v}(\mathbf{k}')] d\mathbf{k}'} P_{n_c n_v}(\mathbf{k}), \end{aligned} \quad (77)$$

where from Eq. (69)

$$\begin{aligned} P_{n_c n_v}(\mathbf{k}(t)) = i \frac{a \sqrt{\varepsilon_g E_g}}{4} \\ \times \int_{K_x}^{k_x(t)} dk'_x \frac{e^{\frac{i}{\hbar} \int_{K_x}^{k'_x} [\varepsilon_{n_c}(k'') - \varepsilon_{n_v}(k'')] dk''_x}}{\varepsilon_{n_c}(k'_x) - \varepsilon_{n_v}(k'_x)}. \end{aligned} \quad (78)$$

The behavior of $P_{cv} \equiv |P_{n_c n_v}|$ on the Bloch electron energy $\varepsilon_B = \hbar \omega_B$ is illustrated by Fig. 2.

C. Evaluation of electron current in the two-band model

1. Current components $j_d(t)$ and $j_{od}(t)$

The electron current is evaluated from Eqs. (73) and (74). To provide the initial conditions, we assume that at $t_0 = 0$ the electron is in the valence band with $K_x = K_x^{(0)}$ so that $k_x(t) = K_x^{(0)} + F_0 t / \hbar$; then $\hat{Q}_{n_v \mathbf{k}}(t_0 = 0) = \delta_{K_x, K_x^{(0)}}$ and $\hat{Q}_{n_c \mathbf{k}}(t_0 = 0) = 0$ for all K_x in the BZ.

For the diagonal matrix elements contribution, we have

$$j_d(t) = e \frac{a}{2\hbar} \sum_{\mathbf{k}} \{ W_c \hat{Q}_{n_c \mathbf{k}}(t_0) - W_v \hat{Q}_{n_v \mathbf{k}}(t_0) - (W_c + W_v) [\hat{Q}_{n_c \mathbf{k}}(t_0) - \hat{Q}_{n_v \mathbf{k}}(t_0)] |P_{n_c n_v}(t)|^2 \} \times \sin(k_x(t)a). \quad (79)$$

Using the initial conditions, we obtain after summation in Eq. (79) over wave vectors

$$j_d(t) = -e \frac{a W_v}{2\hbar} \left\{ 1 - \left(1 + \frac{W_c}{W_v} \right) |P_{n_c n_v}(k_x(t))|^2 \right\} \times \sin(k_x(t)a). \quad (80)$$

Since in Eq. (64) $(\mathbf{v}_{n_v})_x \equiv v_{n_v} = -a \frac{W_v}{2\hbar} \sin(k_x a)$ and $(\mathbf{v}_{n_c})_x \equiv v_{n_c} = a \frac{W_c}{2\hbar} \sin(k_x a)$, we can rewrite Eq. (80) as

$$j_d(t) = e v_{n_v}(k_x(t)) [1 - |P_{n_c n_v}(k_x(t))|^2] + e v_{n_c}(k_x(t)) |P_{n_c n_v}(k_x(t))|^2, \quad (81)$$

with $k_x(t) = K_x^{(0)} + \omega_B t / a$.

To evaluate the off-diagonal contribution to electron current of Eq. (74), we use the chosen initial conditions to obtain

$$j_{od}(t) = e \frac{a}{2\hbar} \sqrt{\varepsilon_g E_g} \text{Re} \left\{ i e^{-\frac{i}{\hbar} \int_0^t [\varepsilon_{n_c}(k_x(t')) - \varepsilon_{n_v}(k_x(t'))] dt'} \times P_{n_c n_v}(k_x(t)) \right\}. \quad (82)$$

The integral in exponent can be evaluated using Eq. (21) as

$$\int_0^t [\varepsilon_{n_c}(k_x(t')) - \varepsilon_{n_v}(k_x(t'))] dt' = At - \frac{B}{\omega_B} [\sin(k_x(t)a) - \sin(K_x^{(0)}a)], \quad (83)$$

and substituting (83) into (82), we find

$$j_{od}(t) = e \frac{a}{2\hbar} \sqrt{\varepsilon_g E_g} \times \text{Re} \left\{ i e^{-\frac{i}{\hbar} \left[At - \frac{B}{\omega_B} [\sin(k_x(t)a) - \sin(K_x^{(0)}a)] \right]} \times P_{n_c n_v}(k_x(t)) \right\}. \quad (84)$$

Now, letting for the initial state $K_x^{(0)} = -\pi/a$ and using $\tau = \omega_B t$ in Eqs. (81) and (84), we obtain

$$j_d(\tau) = e v_{n_v}^{(0)} \left\{ 1 - \left(1 + \frac{W_c}{W_v} \right) |P_{n_c n_v}(\tau)|^2 \right\} \sin \tau; \quad (85)$$

here, $v_{n_v}^{(0)} = a W_v / 2\hbar$ is the amplitude of the electron velocity $v_{n_v}(k_x(t))$. Having calculated $\text{Re}\{\dots\}$ in Eq. (84), we

find

$$\begin{aligned} j_{od}(\tau) = & e v_{n_v}^{(0)} \frac{\varepsilon_g}{2(1+r)W_v} \left\{ \cos \left[A_1 \left(\tau + \frac{B}{A} \sin \tau \right) \right] \right. \\ & \times \int_0^\tau d\tau' \frac{\cos \left[A_1 \left(\tau' + \frac{B}{A} \sin \tau' \right) \right]}{1 + \frac{B}{A} \cos \tau'} \\ & + \sin \left[A_1 \left(\tau + \frac{B}{A} \sin \tau \right) \right] \\ & \times \left. \int_0^\tau d\tau' \frac{\sin \left[A_1 \left(\tau' + \frac{B}{A} \sin \tau' \right) \right]}{1 + \frac{B}{A} \cos \tau'} \right\}. \quad (86) \end{aligned}$$

2. Periodic features of currents $j_d(t)$ and $j_{od}(t)$

Here, we explore the temporal features of $j_d(t)$ and $j_{od}(t)$ in the long-time limit for $t \gg \tau_B$. Since $\varepsilon_n(\mathbf{k})$ and $\mathbf{R}_{nn'}(\mathbf{k})$ are periodic functions of $\mathbf{k}$ in the BZ, and $\mathbf{k}(t) = (F_0 t / \hbar) \hat{\mathbf{x}} + \mathbf{K}$, we then observe that the natural temporal period for the system is $\tau_B = 2\pi / \omega_B = \hbar G / F_0$, where $G = 2\pi / a$.

Therefore we examine the behavior of $j_d(t)$ [Eq. (73)] and $j_{od}(t)$ [Eq. (74)], where use has been made of the exponential expansion of $\exp(-2|P_{n_c n_v}|^2)$ to $\mathcal{O}(|P_{n_c n_v}|^2)$ letting $t = N\tau_B$ (N is a positive integer), so that

$$\begin{aligned} j_d(N\tau_B) = & e \frac{a}{2\hbar} \sum_{\mathbf{k}} \{ W_c \hat{Q}_{n_c \mathbf{k}}(t_0) - W_v \hat{Q}_{n_v \mathbf{k}}(t_0) \\ & - (W_c + W_v) [\hat{Q}_{n_c \mathbf{k}}(t_0) - \hat{Q}_{n_v \mathbf{k}}(t_0)] |P_{n_c n_v}(N\tau_B)|^2 \} \\ & \times \sin[(K_x + N\tau_B F_0 / \hbar)a]. \quad (87) \end{aligned}$$

Noting that $|P_{n_c n_v}(N\tau_B)| = N |P_{n_c n_v}(G)|$ from Eq. (19b), then $j_d(N\tau_B)$, in the large N limit, becomes

$$\begin{aligned} j_d(N\tau_B) = & e \frac{a}{2\hbar} \sum_{\mathbf{k}} \{ W_c \hat{Q}_{n_c \mathbf{k}}(t_0) - W_v \hat{Q}_{n_v \mathbf{k}}(t_0) \\ & - (W_c + W_v) [\hat{Q}_{n_c \mathbf{k}}(t_0) - \hat{Q}_{n_v \mathbf{k}}(t_0)] N^2 |P_{n_c n_v}(G)|^2 \} \\ & \times \sin[(K_x + N\tau_B F_0 / \hbar)a]. \quad (88) \end{aligned}$$

For $j_{od}(N\tau_B)$, from Eq. (74), we find

$$\begin{aligned} j_{od}(N\tau_B) = & e \frac{a}{2\hbar} \sqrt{\varepsilon_g E_g} \text{Re} \sum_{\mathbf{k}} i [\hat{Q}_{n_c \mathbf{k}}(t_0) - \hat{Q}_{n_v \mathbf{k}}(t_0)] \\ & \times e^{-\frac{i}{\hbar} \int_0^{N\tau_B} [\varepsilon_{n_c}(\mathbf{k}(\tau)) - \varepsilon_{n_v}(\mathbf{k}(\tau))] d\tau} P_{n_c n_v}(N\tau_B). \quad (89) \end{aligned}$$

Since

$$\begin{aligned} & \int_0^{N\tau_B} [\varepsilon_{n_c}(\mathbf{k}(\tau)) - \varepsilon_{n_v}(\mathbf{k}(\tau))] d\tau \\ & = N \int_0^{\tau_B} [\varepsilon_{n_c}(\mathbf{k}(\tau)) - \varepsilon_{n_v}(\mathbf{k}(\tau))] d\tau \end{aligned}$$

and

$$\begin{aligned} & \exp \left\{ -\frac{i}{\hbar} \int_0^{N\tau_B} [\varepsilon_{n_c}(\mathbf{k}(\tau)) - \varepsilon_{n_v}(\mathbf{k}(\tau))] d\tau \right\} \\ & = \exp \{ -iN\beta_{n_c n_v} \}, \end{aligned}$$

where $\beta_{n_c n_v}$ is defined in Eq. (18c), the off-diagonal current component $\mathbf{j}_{\text{od}}(N\tau_B)$ can be reexpressed as

$$\mathbf{j}_{\text{od}}(N\tau_B) = e \frac{a}{2\hbar} \sqrt{\varepsilon_g E_g} \text{Re} \sum_{\mathbf{k}} i [\hat{\rho}_{n_c \mathbf{k}}(t_0) - \hat{\rho}_{n_v \mathbf{k}}(t_0)] \times e^{-iN\beta_{n_c n_v}} P_{n_c n_v}(N\tau_B). \quad (90)$$

We note that the term $\exp\{-iN\beta_{n_c n_v}\} P_{n_c n_v}(N\tau_B)$ has the same property expressed in Eq. (18b), that is,

$$|e^{-iN\beta_{n_c n_v}} P_{n_c n_v}(N\tau_B)|^2 = \frac{\sin^2(\beta_{n_c n_v} N/2)}{\sin^2(\beta_{n_c n_v}/2)} |P_{n_c n_v}(\tau_B)|^2. \quad (91)$$

Thus, for the two-band model, we find that the diagonal component of the current, j_d in Eq. (88) is periodic with $N\tau_B$, but with increasing amplitude N^2 , depending upon $(W_c + W_v)$ and the initial conditions. For j_{od} , we find from Eq. (90) that the off-diagonal current component is driven by the transition amplitude, $P_{n_c n_v}(N\tau_B)$, at $N\tau_B$ and the initial conditions; this parameter, as depicted in Figs. 2(a) and 2(b), oscillates between the two states, eventually saturating at high enough field, at about $\hbar\omega_B/(\varepsilon_{n_c} - \varepsilon_{n_v}) \simeq 1$. For $\hbar\omega_B/(\varepsilon_{n_c} - \varepsilon_{n_v}) \ll 1$, $P_{n_c n_v}(N\tau_B)$ is sufficiently small and negligible such that the Bloch oscillation term dominates.

V. SUMMARY AND CONCLUSIONS

Bloch electron dynamics has been developed for a single electron accelerating in a constant electric field described in a vector potential gauge. A standard “*s-p*” two-band model was utilized based on the nearest-neighbor tight-binding approximation to analyze the interband dynamics. The momentum component of the interband coupling has been evaluated based on analytically derived band-matching condition and used to evaluate the transition probabilities. Bloch intra- and interband currents, and other observables relevant to the multiband dynamics have been calculated over a wide range of electric field values. The analysis makes use of the periodic nature of the system to derive selection rules based on the maximum growth of the transition probability thus affirming Wannier-Stark quantization. The graphical analysis of the transition probability demonstrates the oscillatory and broadening characteristics of the transitions with electric field.

The use of the vector potential gauge to describe the electric field preserves the periodicity of the system Hamiltonian. In addition, it is found that the diagonal and off-diagonal components of the Bloch current derived from the density matrix are discerned in terms of the Bloch period in the long-time limit; the periodic nature of the single-band and the two-band dynamics are displayed. Detailed results show that the diagonal component of the current is periodic with the Bloch period, but with increasing temporal amplitudes; the off-diagonal component is oscillatory between the bands due to dependence on the transition probability.

DATA AVAILABILITY

The data that support the findings of this article are not publicly available upon publication because it is not technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this

research project. The data are available from the authors upon reasonable request.

APPENDIX: EVALUATION OF $P_{n_c n_v}(t)$ IN THE TWO-BAND MODEL

We evaluate $P_{n_c n_v}(t)$ of Eq. (69) for an arbitrary time t within one Bloch cycle $t_0 \leq t \leq t_0 + \tau_B$ (for a longer time $t > \tau_B$, the evaluation can be carried out in the similar way)

$$P_{n_c n_v}(t) = i \frac{F_0 a \sqrt{\varepsilon_g E_g}}{\hbar} \frac{4}{4} \times \int_{t_0}^t dt' e^{\frac{i}{\hbar} \int_{t_0}^{t'} [\varepsilon_{n_c}(\mathbf{k}(\tau)) - \varepsilon_{n_v}(\mathbf{k}(\tau))] d\tau} \frac{1}{\varepsilon_{n_c}(\mathbf{k}(t')) - \varepsilon_{n_v}(\mathbf{k}(t'))}. \quad (A1)$$

Using $k_x(t) = K_x + F_0(t - t_0)/\hbar$, where $K_x = k_x(t = t_0)$ is the initial value of $k_x(t)$ in the BZ, we rewrite (A1) as

$$P_{n_c n_v}(k_x) = i \frac{a \sqrt{\varepsilon_g E_g}}{4} \times \int_{K_x}^{k_x} dk'_x \frac{e^{\frac{i}{\hbar} \int_{K_x}^{k'_x} [\varepsilon_{n_c}(k'_x) - \varepsilon_{n_v}(k'_x)] dk'_x}}{\varepsilon_{n_c}(k'_x) - \varepsilon_{n_v}(k'_x)}, \quad (A2)$$

where $K_x \leq k_x \leq K_x + 2\pi/a$. Letting $\vartheta = ak_x$, we reduce $P_{n_c n_v}(k_x)$ of Eq. (A2) for the two-band model [Eqs. (20) and (21)] as

$$P_{n_c n_v}(\vartheta) = ie^{-iA_1(\vartheta_0 - \frac{B}{A} \sin \vartheta_0)} \times \frac{\sqrt{r}}{2(1+r)} \int_{\vartheta_0}^{\vartheta} d\vartheta' \frac{e^{iA_1(\vartheta' - \frac{B}{A} \sin \vartheta')}}{1 - \frac{B}{A} \cos \vartheta'}, \quad (A3)$$

where $r = \varepsilon_g/E_g$, $\vartheta_0 = aK_x$, $\vartheta_0 \leq \vartheta \leq \vartheta_0 + 2\pi$, and

$$A_1 = \frac{(1+r)E_g}{2\hbar\omega_B}, \quad \frac{B}{A} = \frac{1-r}{1+r}. \quad (A4)$$

Considering the initial condition $K_x = 0$, then $\vartheta_0 = 0$, we get

$$P_{n_c n_v}(\vartheta) = i \frac{\sqrt{r}}{2(1+r)} \int_0^{\vartheta} d\vartheta' \frac{e^{iA_1(\vartheta' - \frac{B}{A} \sin \vartheta')}}{1 - \frac{B}{A} \cos \vartheta'}, \quad (A5a)$$

$\vartheta \in [0, 2\pi]$; while for $K_x = -\pi/a$, then $\vartheta_0 = -\pi$, we get

$$P_{n_c n_v}(\vartheta) = ie^{iA_1\pi} \frac{\sqrt{r}}{2(1+r)} \int_{-\pi}^{\vartheta} d\vartheta' \frac{e^{iA_1(\vartheta' - \frac{B}{A} \sin \vartheta')}}{1 - \frac{B}{A} \cos \vartheta'}, \quad (A5b)$$

with $\vartheta \in [-\pi, \pi]$.

The terms responsible for interband coupling enter into the total current $j(t)$ through the off-diagonal $j_{\text{od}}(t)$ and diagonal $j_d(t)$ contributions as $P_{n_c n_v}$ and $|P_{n_c n_v}|^2$, respectively. Thus we obtain

$$|P_{n_c n_v}(\vartheta)|^2 = \frac{r}{4(1+r)^2} [I_1^2(\vartheta) + I_2^2(\vartheta)], \quad (A6)$$

where

$$I_1(\vartheta) = \int_{\vartheta_0}^{\vartheta} d\vartheta' \frac{\cos[A_1(\vartheta' - \frac{B}{A} \sin \vartheta')]}{1 - \frac{B}{A} \cos \vartheta'},$$

$$I_2(\vartheta) = \int_{\vartheta_0}^{\vartheta} d\vartheta' \frac{\sin[A_1(\vartheta' - \frac{B}{A} \sin \vartheta')]}{1 - \frac{B}{A} \cos \vartheta'}. \quad (A7)$$

In the integrals of Eq. (A7), the integration can be reduced to a “unit” interval by the substitution $\vartheta = \pi\zeta$ to obtain

$$\begin{aligned} I_1(\zeta) &= \pi \int_{\zeta_0}^{\zeta} d\zeta' \frac{\cos[A_1(\pi\zeta' - \frac{B}{A} \sin \pi\zeta')]}{1 - \frac{B}{A} \cos \pi\zeta'}, \\ I_2(\zeta) &= \pi \int_{\zeta_0}^{\zeta} d\zeta' \frac{\sin[A_1(\pi\zeta' - \frac{B}{A} \sin \pi\zeta')]}{1 - \frac{B}{A} \cos \pi\zeta'}, \end{aligned} \quad (\text{A8})$$

where $\zeta_0 = \vartheta_0/\pi$, and $(aK_x/\pi) \leq \zeta \leq (aK_x/\pi) + 2$.

Now, we evaluate $P_{n_c n_v}(\tau_B)$ defined in Eq. (18d). Letting $t = t_0 + \tau_B$ in Eq. (A1) [$\vartheta = \vartheta_0 + 2\pi$ in Eq. (A3)], and using the initial conditions specified in Eqs. (A5a) and (A5b), we obtain for $\vartheta_0 = 0$

$$\begin{aligned} P_{n_c n_v}(\tau_B) &= i \frac{\sqrt{r}}{2(1+r)} \left\{ \int_0^\pi d\vartheta \frac{e^{A_1(\vartheta - \frac{B}{A} \sin \vartheta)}}{1 - \frac{B}{A} \cos \vartheta} \right. \\ &\quad \left. + e^{i2\pi A_1} \int_0^\pi d\vartheta \frac{e^{-A_1(\vartheta - \frac{B}{A} \sin \vartheta)}}{1 - \frac{B}{A} \cos \vartheta} \right\} \end{aligned} \quad (\text{A9a})$$

and for $\vartheta_0 = -\pi$, respectively,

$$P_{n_c n_v}(\tau_B) = i e^{i\pi A_1} \frac{\sqrt{r}}{1+r} \int_0^\pi d\vartheta \frac{\cos[A_1(\vartheta - \frac{B}{A} \sin \vartheta)]}{1 - \frac{B}{A} \cos \vartheta}. \quad (\text{A9b})$$

Further, under the condition of *maximum growth*, that is $A_1 = m$, a positive integer as noted below Eq. (23), it follows from (A9a) and (A9b), respectively, that

$$P_{n_c n_v}^{(mg)}(\tau_B) = i \frac{\sqrt{r}}{1+r} \int_0^\pi d\vartheta \frac{\cos[m(\vartheta - \frac{B}{A} \sin \vartheta)]}{1 - \frac{B}{A} \cos \vartheta} \quad (\text{A10a})$$

and

$$P_{n_c n_v}^{(mg)}(\tau_B) = i e^{im\pi} \frac{\sqrt{r}}{1+r} \int_0^\pi d\vartheta \frac{\cos[m(\vartheta - \frac{B}{A} \sin \vartheta)]}{1 - \frac{B}{A} \cos \vartheta}. \quad (\text{A10b})$$

Note that the exponential factor $e^{im\pi}$ in Eq. (A10b) becomes equal to 1 for $m = 2n$ and (-1) for $m = 2n - 1$ ($n = 1, 2, \dots$). Thus, in calculating $|P_{n_c n_v}^{(mg)}(\tau_B)|$, we get

$$|P_{n_c n_v}^{(mg)}(\tau_B)| = \frac{\sqrt{r}}{1+r} \int_0^\pi d\vartheta \frac{\cos[m(\vartheta - \frac{B}{A} \sin \vartheta)]}{1 - \frac{B}{A} \cos \vartheta}. \quad (\text{A11})$$

We note that the probability transition $P_{n_c n_v}$ and $|P_{n_c n_v}|^2$ depend parametrically on the electric field E through the dependence of ω_B on E ; also, they depend on the energy bands parameters ε_g and E_g . The results of calculation of $|P_{n_c n_v}(\zeta)|^2$ are shown in Fig. 3 for $\hbar\omega_B = 8$ meV; other parameters are $W_v = 10$ meV, $W_c = 40$ meV ($r = 0.25$), $A_r = r/4(1+r)^2 = 0.04$, $A_1 = 3.1$, and $B/A = 0.6$. The interval $\zeta \in [-1, 1]$ corresponds to one cycle for the electron to traverse the BZ. Indeed, $t - t_0 = (\zeta + 1)\tau_B/2$, so that $t = t_0$ corresponds to $\zeta = -1$, and $t - t_0 = \tau_B$ to $\zeta = 1$.

The analysis shows that $P_{n_c n_v}(\tau_B)$ scales when considering comparative analysis for bulk and SL materials. Given A_1 , the ratio $B/A = (1-r)/(1+r)$ will scale from bulk to SL magnitudes. This means that the main difference in $P_{n_c n_v}(\tau_B)$ values is determined by A_1 . The brief illustrative chart compares key parameters that determine A_1 and the ratio B/A . We assume for bulk (b) $a = 10^{-8}$ cm, $\varepsilon_g = 1$ eV, $E_g = 4$ eV; and for SL: $a = 10^{-6}$ cm, $\varepsilon_g = 10$ meV, $E_g = 40$ meV. Then, it follows that $G_{\text{SL}} = 10^{-2} G_b$, $\hbar\omega_{\text{SL}}^{\text{SL}} = 10^2 \hbar\omega_b^b$, and $\tau_B^{\text{SL}} = 10^{-2} \tau_B^b$; also, $A_1^{\text{SL}} = 10^{-4} A_1^b$, $B^{\text{SL}}/A^{\text{SL}} = B^b/A^b = 0.6$. In scaling from bulk to SL dimensions, the ratio of B/A preserved in magnitude, but A_1 scales as noted in $A_1^{\text{SL}} = 10^{-4} A_1^b$. So the phase of the integral is markedly affected by the scaling from bulk to SL dimensions.

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