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Study of the single-band Bloch oscillation effect with the pseudo-spectral method

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Abstract. Using the pseudo-spectral method for wave-packet evolution, we formulate and implement a *new* theoretical approach for studying the Bloch oscillation effect in a general number of dimensions. For this purpose, a novel recursive formula is obtained in the representation of Wannier functions for the infinitesimal time evolution of an electronic wave packet within the single-band approximation. This formula is valid for general position-dependent applied electric fields and arbitrary initial wave-packet shapes and crystal structures, and can also be generalized for time-dependent fields. For a tight-binding simple 'cubium' band, the infinitesimal time evolution can always be expressed in terms of Bessel functions of integer order; and for the 'empty-lattice model' band it can be expressed in terms of Fresnel functions for arbitrary electric fields also. As a further analytical application of our formalism, we derive an exact (finite-time) wave-packet evolution for the homogeneous and static electric field in the simple 'cubium' band. For this case, an estimate of the numerical error of the pseudo-spectral method is obtained for the mean position of the wave packet. As an illustrative example of the numerical implementation of our theoretical formalism, we present a simple one-dimensional numerical simulation for a Gaussian wave packet moving in a parabolic potential well. Finally, a general proof of the unitarity of the predicted time evolution is also presented, and different properties of our formalism pointed out.

1. Introduction

The electronic transport properties of semiconductor superlattice (SSL) structures have been the subject of intensive research in the last few years, both experimental and theoretical [1]. One of the main theoretical reasons for this has been the realization that such SSL structures constitute a physical framework within which the controversies [2] about the long-ago-predicted Bloch oscillation effect [3] could be settled. For studying the quantum dynamics of the electronic wave packet within the SSL structure, the most commonly used tool is the numerical simulation of the time-dependent Schrödinger equation by means of well known algorithms such as Cayley's or Crank-Nicholson's methods [4], in which the quantum evolution operator $\exp(-\mathrm{i}H\,\Delta t/\hbar)$ (described by (1) below) is approximated by the strictly unitary operator $(1+\mathrm{i}H\,\Delta t/2\hbar)^{-1}(1-\mathrm{i}H\,\Delta t/2\hbar)+\mathrm{O}(\Delta t^3)$, which ensures the norm conservation of the wavefunction at all times. If a physical model is assumed, such as the usual single-band tight-binding model [5], where a one-dimensional ($D=1$) infinite crystal is in the presence of a homogeneous external electric field, then the time-dependent Schrödinger equation can be represented by a system of coupled difference equations which can be solved exactly,

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thus allowing a thorough analytical formulation of the problem, where exact predictions for quantities such as the wave packet's position expectation value and its width parameter are possible for arbitrary times [5, 6]. Departures from this scheme are concerned mainly with the dynamical behaviour of the electronic wave packet within SSL structures in the presence of harmonically oscillating fields (giving rise to the well known phenomenon of 'dynamic localization' [7]), and SSL structures with isolated impurities either in the presence of combined homogeneous and harmonically oscillating electric fields in $D = 1$ dimensions [8] or homogeneous electric fields in $D = 2$ dimensions [9].

In this paper we set about developing a new theoretical approach for the study of the above-mentioned Bloch oscillation effect. This approach will yield a formula (equation (13) below) for the infinitesimal time evolution of an electronic wave packet defined in a general Bravais lattice in $D = 1, 2, 3$ dimensions, valid (within the single-band approximation, i.e., the subspace of Wannier functions of only one band [5]) for general position-dependent static (and time-dependent) electric fields, initial wave-packet shapes, and band structures, not being restricted, for instance, to the usual nearest-neighbour tight-binding model [5]. The above-mentioned new approach consists in the application of the pseudo-spectral method [10, 11] to the discrete nature of the Bravais lattice. Although spectral and pseudo-spectral methods (see [12] and references therein) have been widely used to study wave-packet evolution, they have not, to our knowledge, been previously applied to the Bloch oscillation effect. Hence the motivation for our approach. For a static and spatially homogeneous electric field, our formula can be iteratively evaluated exactly for an arbitrary time and be compared with well known tight-binding analytical results (recent reviews are given in [5, 8]); however, for an inhomogeneous field, we simulate numerically the time evolution of the wave packet without using, for example, any fast-Fourier-transform [4, 11] numerical routines. To this effect, as an interesting numerical example, we present an illustrative application for an electronic wave packet in the presence of a one-dimensional parabolic potential well [13], previously studied and discussed in the literature [13] within the context of the 'few-body problem on a lattice' [14]. Within this context [14], in which interband matrix elements are inconsequential, i.e., the single-band approximation, we shall develop our theoretical formalism below with an emphasis on analytical results. Although Cayley's or Crank-Nicholson's state-of-the-art numerical methods [4] yield 'effortless' solutions to the time-dependent Schrödinger equation, our pseudo-spectral theoretical formalism below also turns out to have interesting usefulness as an alternative and complementary numerical method. As such, we shall present it here.

2. Formalism

The formal solution of the time-dependent Schrödinger equation $\mathrm{i}\hbar\,\partial\Psi/\partial t = H\Psi$ for a general time-independent one-particle Hamiltonian H is given by [15]

$$\Psi(\boldsymbol{r}, t) = \mathrm{e}^{-\mathrm{i}H(t-t_0)}\Psi(\boldsymbol{r}, t_0) \tag{1}$$

(where $\hbar = 1$ for simplicity). Within the single-band approximation [14], let us separate the Hamiltonian H into a sum of a 'kinetic' energy (or band energy) $T(\boldsymbol{p})$ operator and an external potential energy $V(\boldsymbol{r})$ operator, $H = T(\boldsymbol{p}) + V(\boldsymbol{r})$. Here, the spatially periodic character of the superlattice (SSL) potential is incorporated within $T(\boldsymbol{p})$, while the external potential energy $V(\boldsymbol{r})$ describes any externally applied forces (such as electric field terms) not intrinsic to the superlattice. Now let the time t_0 be increased by an infinitesimal amount Δt, with $t = t_0 + \Delta t$; by the use of the *Baker–Campbell–Hausdorff* formula [16], the evolution operator $\exp(-\mathrm{i}H\,\Delta t)$ in (1) can be time split and approximated to order $(\Delta t)^3$ by

$$\Psi(\boldsymbol{r}, t_0 + \Delta t) = \mathrm{e}^{-\mathrm{i}\lambda V(\boldsymbol{r})}\mathrm{e}^{-2\mathrm{i}\lambda T(\boldsymbol{p})}\left[\mathrm{e}^{-\mathrm{i}\lambda V(\boldsymbol{r})}\Psi(\boldsymbol{r}, t_0)\right] + \mathrm{O}(\Delta t^3) \tag{2}$$

where $\lambda \equiv \Delta t/2$. If the bracketed term in (2) is expressed as the inverse of a spatial Fourier transform $\mathcal{F}$, then the operator $\exp(-2\mathrm{i}\lambda T(\boldsymbol{p}))$, which contains the spatial derivative operator through $\boldsymbol{p} = -\mathrm{i}\boldsymbol{\nabla}$, will act only on the spatial part of the transform resulting in $\exp(-2\mathrm{i}\lambda T(\boldsymbol{k}))\exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r})$. This is so for the class of kinetic energy operators $T(\boldsymbol{p})$ that we will use throughout this paper and that admit a power expansion as in (4) below. Thus, equation (2) can be written as a sequence of nested direct and inverse Fourier transforms:

$$\Psi(\boldsymbol{r}, t_0 + \Delta t) = \mathrm{e}^{-\mathrm{i}\lambda V(\boldsymbol{r})}\mathcal{F}^{-1}\left[\mathrm{e}^{-2\mathrm{i}\lambda T(\boldsymbol{k})}\mathcal{F}(\mathrm{e}^{-\mathrm{i}\lambda V(\boldsymbol{r})}\Psi(\boldsymbol{r}, t_0))\right] + \mathrm{O}(\Delta t^3). \tag{3}$$

Equation (3) is the basis of the pseudo-spectral method [10], to be applied in this paper to a quite general 'single-band' kinetic energy $T(\boldsymbol{k})$, which may, *for example*, be of the form [14]

$$T(\boldsymbol{k}) = \sum_{l,m} t_{lm}\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{R}_l - \boldsymbol{R}_m)} \tag{4}$$

where the $\boldsymbol{R}$s belong to a Bravais lattice, and $T(\boldsymbol{k})$ in (4), as the lattice Fourier transform of the 'hopping' matrix elements t_{lm}, has the periodicity of the corresponding reciprocal lattice with vectors $\boldsymbol{K}$, i.e., $T(\boldsymbol{k} + \boldsymbol{K}) = T(\boldsymbol{k})$. Consequently, $\exp(-2\mathrm{i}\lambda T(\boldsymbol{k}))$ in (3) is also a periodic function in the reciprocal space and can be expanded in a Fourier series [17] as

$$\mathrm{e}^{-2\mathrm{i}\lambda T(\boldsymbol{k})} = \sum_{\boldsymbol{R}'}\left[\frac{1}{v^*}\int_{1-\mathrm{BZ}}\mathrm{d}\boldsymbol{k}'\ \mathrm{e}^{-\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{R}'}\mathrm{e}^{-2\mathrm{i}\lambda T(\boldsymbol{k}')}\right]\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}'} \tag{5}$$

where v and $v^* = (2\pi)^D/v$ are respectively the volumes of the primitive cells in the direct and reciprocal lattices in $D = 1, 2, 3$ dimensions, and the integral in (5) is performed over the first Brillouin zone (1-BZ). Although the implementation of the pseudo-spectral method by (3) for a quadratic kinetic energy is well known [11], we have not found in the literature its application to a periodic kinetic energy. This periodicity in reciprocal space is sufficient for the validity of (5), *independently of the precise form of* $T(\boldsymbol{k})$.

The state $\Psi(\boldsymbol{r}, t)$ in (3) can be written [6, 8] as a linear combination of a complete set of orthonormal Wannier functions, whose properties are, for instance, known to be ideally suited for representing initial wavefunctions $\Psi(\boldsymbol{r}, t_0)$ that appear to arise in relevant experiments in SSL [18]. Thus, we can write

$$\Psi(\boldsymbol{r}, t) = \sum_{l,\boldsymbol{R}} C_{l,\boldsymbol{R}}(t)\Phi_l(\boldsymbol{r} - \boldsymbol{R}) \tag{6}$$

where the Wannier function $\Phi_l(\boldsymbol{r} - \boldsymbol{R})$ is typically localized about the lattice site $\boldsymbol{r} = \boldsymbol{R}$ with an extent of the order of the lattice constant [19]. Such a Wannier function is to be labelled with a band index denoted by l, but since we are considering in this work the electron's dynamics within a single band, the index l will be hereafter dropped. With the main possible exception of the case for extremely high electric fields, for which interband tunnelling does become relevant, this restriction in our formalism, namely, that of the single-band approximation, is known to be relatively unimportant [5, 6].

The substitution of (5) and (6) into (3) yields (up to $\mathrm{O}(\Delta t^3)$)

$$\begin{aligned}\Psi(\boldsymbol{r}, t_0 + \Delta t) = \mathrm{e}^{-\mathrm{i}\lambda V(\boldsymbol{r})}\frac{1}{v^* v}\int_{-\infty}^{\infty}\mathrm{d}\boldsymbol{k}\ \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}\int_{-\infty}^{\infty}\mathrm{d}\boldsymbol{r}'\ \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}'}\mathrm{e}^{-\mathrm{i}\lambda V(\boldsymbol{r}')}\\ \times\frac{1}{v^*}\sum_{\boldsymbol{R}'}\int_{1-\mathrm{BZ}}\mathrm{d}\boldsymbol{k}'\ \mathrm{e}^{-\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{R}'}\mathrm{e}^{-2\mathrm{i}\lambda T(\boldsymbol{k}')}\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}'}\sum_{\boldsymbol{R}} C_{\boldsymbol{R}}(t_0)\Phi(\boldsymbol{r}' - \boldsymbol{R}).\end{aligned} \tag{7}$$

By first performing the integration in the variable $\boldsymbol{k}$, and making use of

$$\int_{-\infty}^{\infty}\mathrm{d}\boldsymbol{k}\ \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{r} - \boldsymbol{r}' + \boldsymbol{R}')} = v^* v\delta(\boldsymbol{r} - \boldsymbol{r}' + \boldsymbol{R}') \tag{8}$$

and then integrating the Dirac delta function $\delta(\boldsymbol{r} - \boldsymbol{r}' + \boldsymbol{R}')$ in the variable $\boldsymbol{r}'$, equation (7) simplifies considerably to

$$\Psi(\boldsymbol{r}, t_0 + \Delta t) = \mathrm{e}^{-\mathrm{i}\lambda V(\boldsymbol{r})} \sum_{\boldsymbol{R}'\boldsymbol{R}} C_{\boldsymbol{R}}(t_0) F(\boldsymbol{R}') \mathrm{e}^{-\mathrm{i}\lambda V(\boldsymbol{r}+\boldsymbol{R}')} \Phi(\boldsymbol{r} + \boldsymbol{R}' - \boldsymbol{R}) \tag{9}$$

where $F(\boldsymbol{R}')$ has been defined as

$$F(\boldsymbol{R}') \equiv \frac{1}{v^*} \int_{1-\mathrm{BZ}} \mathrm{d}\boldsymbol{k}' \, \mathrm{e}^{-\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{R}'} \mathrm{e}^{-2\mathrm{i}\lambda T(\boldsymbol{k}')}. \tag{10}$$

It is now convenient to define $\boldsymbol{R}'' \equiv \boldsymbol{R} - \boldsymbol{R}'$, so as to be able to rewrite (9) in the form

$$\Psi(\boldsymbol{r}, t_0 + \Delta t) = \sum_{\boldsymbol{R}''} \left[\sum_{\boldsymbol{R}} C_{\boldsymbol{R}}(t_0) F(\boldsymbol{R} - \boldsymbol{R}'') \mathrm{e}^{-\mathrm{i}\lambda\left[V(\boldsymbol{r})+V(\boldsymbol{r}+\boldsymbol{R}-\boldsymbol{R}'')\right]} \right] \Phi(\boldsymbol{r} - \boldsymbol{R}''). \tag{11}$$

For the expression (11) to be of the appropriate necessary form of (6), i.e.,

$$\Psi(\boldsymbol{r}, t_0 + \Delta t) = \sum_{\boldsymbol{R}''} C_{\boldsymbol{R}''}(t_0 + \Delta t) \Phi(\boldsymbol{r} - \boldsymbol{R}'') \tag{12}$$

the expansion coefficients $C_{\boldsymbol{R}''}(t_0 + \Delta t)$ must be given by

$$C_{\boldsymbol{R}''}(t_0 + \Delta t) = \sum_{\boldsymbol{R}} C_{\boldsymbol{R}}(t_0) \mathrm{e}^{-\mathrm{i}\lambda(V(\boldsymbol{R})+V(\boldsymbol{R}''))} F(\boldsymbol{R} - \boldsymbol{R}'') \tag{13}$$

and are to be obtained from (11) by restricting the wavefunction $\Psi(\boldsymbol{r}, t_0 + \Delta t)$ to the Hilbert subspace of H [13, 14] which corresponds to that of the Bravais lattice points, around which the Wannier functions $\Phi(\boldsymbol{r} - \boldsymbol{R}'')$ are strongly localized; i.e., by setting $\boldsymbol{r} = \boldsymbol{R}''$ in (11) for the square-bracketed coefficients.

Equation (13), which gives the wave-packet coefficients defined on the lattice at a time infinitesimally later than the initial t_0, is valid for quite general external potentials $V(\boldsymbol{r})$ (associated with position-dependent constant electric fields and/or inhomogeneities), crystal lattices, initial wave-packet shapes, and single-band dispersions $T(\boldsymbol{k})$, thus limiting (13) to intraband dynamical evolutions only. Interestingly, the integral 'kernel' function $F(\boldsymbol{R}-\boldsymbol{R}'')$ in (10) does not depend upon the external potential $V(\boldsymbol{r})$. It is characteristically associated with the band and crystal structures *only*, as is obvious from its definition in (10) as an integral over the first Brillouin zone of the crystal lattice. Furthermore, although (13) is formally correct only to order $\mathrm{O}(\Delta t^3)$, it describes nevertheless a rigorously unitary time evolution as will be shown in appendix B. In the following we will apply (13) to some relevant cases.

3. Analytical applications

First, consider the dynamics of a single electron in the tight-binding three-dimensional band known as the 'cubium' band, with isotropic nearest-neighbour hopping matrix element A and primitive-cell constant a in a simple cubic lattice. Then, the integral in (13) is to be evaluated for a kinetic energy

$$T(\boldsymbol{k}) = -2A(\cos(ak_1) + \cos(ak_2) + \cos(ak_3)) \tag{14}$$

where k_1, k_3, k_3 are the components of $\boldsymbol{k}$ along the simple cubic crystal axes, leading to the result

$$C_{\boldsymbol{R}'}(t_0 + \Delta t) = \sum_{\boldsymbol{R}} C^0_{\boldsymbol{R}} \mathrm{e}^{-\mathrm{i}\lambda(V(\boldsymbol{R})+V(\boldsymbol{R}'))} \mathrm{i}^{n-n'+m-m'+p-p'} J_{n-n'}(z) J_{m-m'}(z) J_{p-p'}(z) \tag{15}$$

with $C^0_{\boldsymbol{R}} \equiv C_{\boldsymbol{R}}(t_0)$. In (15), the $J_n(z)$ are Bessel functions of the first kind and integer order n, with infinitesimal argument $z = 4A\lambda$, and given by the integral representation [20]

$$J_n(z) = \frac{\mathrm{i}^{-n}}{\pi} \int_0^{\pi} \mathrm{e}^{\mathrm{i}z\cos\theta} \cos(n\theta) \, \mathrm{d}\theta. \tag{16}$$

The integers n, m, p specify the direct lattice point $\boldsymbol{R} = n\hat{\boldsymbol{x}}_1 + m\hat{\boldsymbol{x}}_2 + p\hat{\boldsymbol{x}}_3$. Thus, the infinitesimal time evolution can be expressed for the cubium band in terms of Bessel functions for *quite arbitrary one-body potentials* $V(\boldsymbol{R})$ acting on the electron, in contrast with the finite-time evolution [5], wherein Bessel functions appear mostly for homogeneous electric fields. The infinitesimal evolution of a normalized wave packet within a single band can also be checked to be unitary from (15), i.e.,

$$\sum_{\boldsymbol{R}'} |C_{\boldsymbol{R}'}(t_0 + \Delta t)|^2 = \sum_{\boldsymbol{R}} |C^0_{\boldsymbol{R}}|^2 = 1$$

by using well known [20] analytical properties of Bessel functions.

For a constant and homogeneous force field of magnitude $\alpha = e|\boldsymbol{E}|$, the value of the potential energy operator $V(\boldsymbol{r})$ at the simple-cubic lattice point $\boldsymbol{R}$ is

$$V(\boldsymbol{R}) = \alpha(n\cos\Phi_1 + m\cos\Phi_2 + p\cos\Phi_3)$$

with Φ_1, Φ_2, Φ_3 the director angles of the associated vector electric field $\boldsymbol{E}$ (the lattice constant a has been set to $a = 1$ for simplicity, and $-e$ is the electronic electric charge). In this particular case, for a $t_0 = 0$ initial wave packet in $D = 3$ dimensions of the form $C^0_{\boldsymbol{R}} = C^0_n C^0_m C^0_p$, the sum over the lattice points in (15) can be decoupled into three individual sums. After some interesting algebra, we have found that (when $\Delta t \to 0$) each sum can be expressed exactly for any time by means of the addition theorem for Bessel functions used iteratively (Graf's formula [20]). As shown in appendix A, the final analytical result is

$$C_{\boldsymbol{R}'}(t) = \sum_{\boldsymbol{R}} C^0_{\boldsymbol{R}} \exp\left\{-\mathrm{i}\alpha\left[(n+n')\cos\Phi_1 + (m+m')\cos\Phi_2 + (p+p')\cos\Phi_3\right]t/2\right\} \times \mathrm{i}^{n-n'+m-m'+p-p'} J_{n-n'}(\xi_1) J_{m-m'}(\xi_2) J_{p-p'}(\xi_3) \tag{17}$$

where $\xi_j = (4A/(\alpha\cos\Phi_j))\sin(\frac{1}{2}\alpha t\cos\Phi_j)$; $j = 1, 2, 3$. It is worth checking that in $D = 3$ dimensions, equation (17) predicts the wave packet's periodic Bloch oscillation whenever the electric field $\boldsymbol{E}$ is oriented along the directions of the reciprocal-lattice vectors [17], that is, $\cos\Phi_1 = q/\gamma$, $\cos\Phi_2 = r/\gamma$, $\cos\Phi_3 = s/\gamma$, where q, r, s are non-zero, mutually prime integers, and $\gamma \equiv \sqrt{q^2 + r^2 + s^2}$; thus, one can verify that $C_{\boldsymbol{R}}(2\pi\gamma/\alpha) = C^0_{\boldsymbol{R}}$. For an electric field $\boldsymbol{E}$ with no components along a given lattice axis, some of the integers q, r, s will be zero, and the corresponding Bessel functions in (17) will approach zero with growing time t, giving rise to the well known dispersion effect of the wave packet in the direction of the absent electric field component [6]. An adaptation of (17) for $D = 1$, e.g. along the X-axis, follows from disallowing the propagation of the wave packet in the Y- and Z-axis directions, by taking the corresponding hopping matrix elements $A = 0$ in these directions. For the wave packet propagating only along the X-axis, equation (17) takes the form

$$C_{n'}(t) = \sum_n C^0_n \mathrm{e}^{-\mathrm{i}\alpha(n+n')t/2} \mathrm{i}^{n-n'} J_{n-n'}\left[\frac{4A}{\alpha}\sin\left(\frac{1}{2}\alpha t\right)\right] \tag{18}$$

which reproduces the most relevant features of the wave packet's dynamics for $D = 1$ under the influence of homogeneous and constant electric fields (see [5] and references therein), namely:

(a) if $t = \tau_B \equiv 2\pi/\alpha$ in (18), then $C_n(\tau_B) = C^0_n$ (Bloch oscillations with period τ_B);
(b) by taking C^0_n in (18) to be $C^0_n = J_{n-m}(2A/\alpha)$ and using Graf's addition formula for Bessel functions [20], the eigenfunctions of H can be shown from (18) to be given by

$$\sum_n J_{n-m}(2A/\alpha)\Phi(x-n)$$

with equidistant energy eigenvalues $E_m = \alpha m$ (the Wannier–Stark ladder), and time evolution for $C_n(t)$, given by $C_n(t) = \exp(-\mathrm{i}\alpha m t)C^0_n$.

To our knowledge, neither (17) nor (18) have been previously derived in the literature by making use of the pseudo-spectral method, as here presented in a novel manner (see, e.g., [5] and references therein). Another relevant case where the 'kernel' integral $F(\boldsymbol{R}-\boldsymbol{R}'')$ in (13) can be evaluated analytically is that of the 'empty-lattice model' band. As shown in appendix C, the corresponding kernel can then be easily expressed in terms of the Fresnel integrals [20]. Other analytical cases for different crystal and/or band structures might also be possible, but this remains here as an interesting open problem.

4. Numerical application and conclusions

Our numerical application is that of an inhomogeneous electric field for $D = 1$ (e.g., along the X-axis) derivable from a one-dimensional parabolic potential well of the form

$$V_n = \alpha n + \frac{1}{2}Kn^2 \tag{19}$$

at the nth lattice site. Such a potential has already been suggested in [13] and [14] so as to include the effects of a uniform and constant charge density on the dynamics of an electron in a lattice in a direction perpendicular to the surface of the crystal. In figure 1, we show some results of applying (15) to the case of the potential in (19), finding (where applicable) excellent numerical agreement with previous analytical work [13] concerning the dynamical (twofold) behaviour of a Gaussian wave packet in the presence of the parabolic potential of (19). These behaviours are the 'continuum regime' and the 'Bloch regime', depending upon the wave packet's initial position with respect to the equilibrium point of the 'harmonic oscillator on a lattice' [13] described by (19). In the first regime, the oscillator has (with $a = 1$) a simple-harmonic period given by $\tau = \pi\sqrt{2/(KA)}$, while in the second (or Bloch regime), it oscillates with a rather different period, $\tau_B = 2\pi/\alpha$, and amplitude, $|2A/\alpha|$, both associated with an effectively different potential well. The various properties of these two regimes, as well as the 'bifurcation' that links the two, are quite accurately described and explained by the corresponding 'semiclassical' model [17] approximation. For further details, the reader is here referred to reference [13], where the bifurcation, akin to that of a pendulum, is described at length. In fact, the entire problem can be made isomorphic to that of a simple pendulum by an appropriate canonical transformation [13,14]. The 'continuum regime' and the 'Bloch regime' then correspond to the 'oscillating' and to the 'rotating' pendulum behaviours, respectively. Some physical insight as regards such bifurcation might be worth mentioning: given a certain spatial charge density (i.e., a certain parabolic potential well) one can modulate the value of α by changing the external electric field, and thus, by going from the continuum over to the Bloch regime, the predicted oscillations should go through an irregular or highly non-periodic transitional state, as shown in figure 1(c).

In addition, our simulations show that the amplitude of the wave packet's mean position [5]

$$z(t) \equiv \langle x \rangle = \sum_n n|C_n(t)|^2$$

periodically recovers almost its initial value after damping intervals—a result not previously found by Gallinar and Chalbaud [13], because these authors did not consider the long-term time evolution of their wave packets. Near the bifurcation point predicted by the semiclassical model [13, 17], where the dynamical behaviour of the wave packet changes abruptly from the continuum to the Bloch regime, our quantum-mechanical simulations show that the periodic 'revival' behaviour of z simply begins to disappear and the wave packet does not recover its initial amplitude, thus entailing another interpretation of such a theoretical bifurcation point.

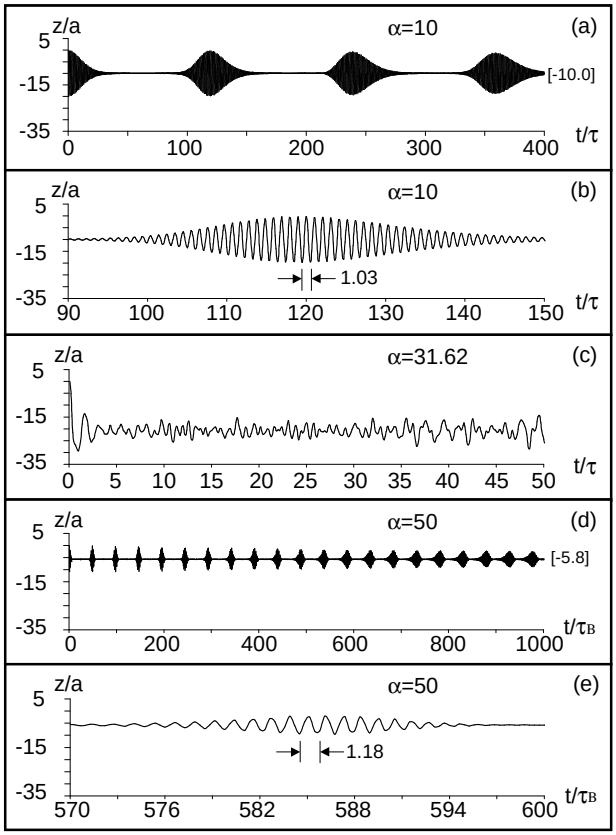

Figure 1. A sequence of numerical simulations of the wave packet's mean position $z(t) \equiv \langle x \rangle$ (in units of the cell constant a) versus time (in units of either τ or τ_B), where $\tau = \pi\sqrt{2/(Ka^2A)}$ is the period of the harmonic oscillator in the 'continuum regime' (in units of $\overline{h}$) and $\tau_B = 2\pi/(\alpha a)$ is the period of the Bloch oscillator (in units of $\overline{h}$). K is the 'spring' constant in the potential energy (19). The initial wave packet is the projection onto the lattice of the normalized $\Psi(t_0) = B\mathrm{e}^{-Cx^2}$ (where x is a continuous variable, $B = (Ka^2/(2\pi^2A))^{1/8}$, and $C = \sqrt{K/(8Aa^2)}$); the one-dimensional crystal model consists of 128 lattice sites for computational purposes. Each simulation was performed iteratively with an infinitesimal time increment $\Delta t = \tau/1000$; the sum in (15) was approximated by eleven Bessel functions ranging from J_{-5} up to J_5. For such approximations, the accumulated relative error in the probability amplitude $\sum_m |C_m|^2$ is 0.77% after a time $t = 400\tau$. For $A = 125\ Ka^2$ and unit values of K and a, we show the cases corresponding to the following force-field magnitudes α (in units of Ka): (a) 10, (c) 31.62, (d) 50. In (a) and (d), the visual profile of the peaks of the z-oscillations reveals the periodic 'revival' effect, after damping intervals where z 'rests' at the bottom of a potential well (centred at the position indicated inside brackets on the right-hand sides of the figures). The insets (b) of (a) and (e) of (d) show the details of the z-oscillations in the 'continuum' and 'Bloch' regimes respectively, with the indicated 'period' (arrows). In these plots, $\tau = 3.16\tau_B$. Case (c) shows a complete lack of both the oscillatory and the periodic revival behaviours of z; a finer simulation incorporating ten equidistant values of α in the interval (10, 50) would show that the critical value $\alpha = \sqrt{1000} = 31.6227\ldots$ predicted by the semiclassical model is indeed a 'bifurcation' point separating the 'continuum' regime from the 'Bloch' regime.

The revivals just described above show that the interference of the wave packet's components jumps alternatively from a destructive effect to a constructive one. It is interesting to notice that similar revival effects have been observed in numerical simulations using Cayley's

method [21] pertaining to quite different physical situations, where the wave packet is placed in a $D = 1$ SSL under the influence of a homogeneous and static electric field. In this case, the damping effect of z is attributed [21] to the interface roughness at the boundaries of the potential wells rather than to scattering mechanisms, and the revival effect (amplitude recovery) is related to the fact that only a few successive unit cells are initially occupied. Of course, in an actual crystal our revival effects for the parabolic potential might be masked—for example, by scattering and/or Coulomb interactions—because of the long-term nature of such revivals in terms of the Bloch oscillation period, making, thus, their eventual experimental observation extremely difficult, though theoretically possible.

As shown in appendix B, the extension of (13) to the case of time-dependent potentials is straightforward, and permits one to study easily the various effects associated with 'dynamic localization' [7]; an expanded version of our work [22] dealing also with such effects will be published elsewhere. Additionally, in a more general and wider-reaching scheme, the interest for our formulation (namely, equation (13)) of the intraband wave packet's dynamics under the influence of inhomogeneous fields is to be related to the 'few-body problem on a lattice' [14], where the 'quasiparticles' will move under the influence of their mutual position-dependent interactions. Few-body composites [14], such as the exciton [23] or the 'trion' [24] (an exciton plus a hole or plus an electron), moving in one dimension ($D = 1$), can thus be easily considered in our formalism [22] by suitable reinterpretation of equation (13) in a higher-dimensional ($D > 1$) space.

In summary, we have developed, in a representation of Wannier functions, a novel expression (13) for studying the intraband Bloch oscillation of an electronic wave packet as an application of the pseudo-spectral method. The validity and versatility of our expression was checked analytically for the homogeneous and static electric field in a simple cubic lattice. It was also checked numerically for a one-dimensional parabolic potential associated with a position-dependent electric field, as an illustrative example of its predictive power. In fact, it is possible that our pseudo-spectral approach would appear to provide [25], at least for short time intervals, an accurate approximate solution of the well known Houston differential equations [26] to the extent that interband transition terms can be totally discarded, when studying electronic motion in crystalline solids induced by electric fields [25]. Finally, we have also laid the groundwork for future studies along these lines, which should prove to be both interesting and fruitful.

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Appendix A

In this appendix we prove by iteration equation (17) in the text, making use of the pseudo-spectral result (13). We do this by first considering the time evolution of the $D = 1$ wave packet given by equation (18). We also give an estimate of the numerical error of the predicted wave packet's mean position

$$z(t) \equiv \langle x \rangle = \sum_n n|C_n(t)|^2.$$

The pseudo-spectral result (13) gives for $D = 1$ upon a first iteration that

$$C_n(\Delta t) = \sum_m C_m(0) \mathrm{e}^{-\mathrm{i}\lambda'(n+m)} \mathrm{i}^{m-n} J_{m-n}(\tau_1) \tag{A.1}$$

where $\tau_1 \equiv 4A\lambda$, and $\lambda' \equiv \alpha\lambda$, with $\lambda \equiv \Delta t/2$.

Let us now assume the inductive hypothesis, given by

$$C_n(l\ \Delta t) = \sum_m C_m(0) \mathrm{e}^{-\mathrm{i}l\lambda'(n+m)} \mathrm{i}^{m-n} J_{m-n}(\tau_l) \tag{A.2}$$

where τ_l is recursively given by

$$\tau_l = \tau_{l-1} \mathrm{e}^{\mathrm{i}\lambda'} + \tau_1 \mathrm{e}^{-\mathrm{i}\lambda'(l-1)} \tag{A.3}$$

with $\tau_0 \equiv 0$, and $l = 1, 2, 3, \ldots, p$.

We now show that (A.2) and (A.3) are also valid for $l = p + 1$. In effect,

$$\begin{aligned} C_n((p+1)\ \Delta t) &= \sum_m C_m(p\ \Delta t) \mathrm{e}^{-\mathrm{i}\lambda'(n+m)} \mathrm{i}^{m-n} J_{m-n}(\tau_1) \\ &= \sum_m \left\{ \sum_q C_q(0) \mathrm{e}^{-\mathrm{i}p\lambda'(q+m)} \mathrm{i}^{q-m} J_{q-m}(\tau_p) \right\} \mathrm{e}^{-\mathrm{i}\lambda'(n+m)} \mathrm{i}^{m-n} J_{m-n}(\tau_1) \end{aligned} \tag{A.4}$$

where (A.1) and (A.2) have been used.

From (A.4), we obtain

$$\begin{aligned} C_n((p+1)\ \Delta t) &= \sum_q C_q(0) \mathrm{i}^{q-n} \mathrm{e}^{-\mathrm{i}\lambda'(n+pq)} \sum_m \mathrm{e}^{-\mathrm{i}\lambda' m(p+1)} J_{m-n}(\tau_1) J_{q-m}(\tau_p) \\ &= \sum_q C_q(0) \mathrm{i}^{q-n} \mathrm{e}^{-\mathrm{i}\lambda'(n+pq)} \mathrm{e}^{-\mathrm{i}\lambda' n(p+1)} \mathrm{e}^{\mathrm{i}(q-n)\sigma} J_{q-n}(\tau_{p+1}). \end{aligned} \tag{A.5}$$

To sum over m in (A.5) we have used Graf's addition formula [20], according to which τ_{p+1} and σ must satisfy the single 'triangle' relationship

$$\tau_p = -\tau_1 \mathrm{e}^{-\mathrm{i}\lambda'(p+1)} + \tau_{p+1} \mathrm{e}^{\mathrm{i}\sigma}. \tag{A.6}$$

With the necessary identification $\sigma = -\lambda'$, given by Graf's addition formula [20], we finally obtain that

$$C_n((p+1)\ \Delta t) = \sum_q C_q(0) \mathrm{e}^{-\mathrm{i}(p+1)\lambda'(n+q)} \mathrm{i}^{q-n} J_{q-n}(\tau_{p+1}). \tag{A.7}$$

Equations (A.7) and (A.6) together prove the inductive hypothesis for $l = p + 1$.

The appropriate solution of the difference equation (A.3) for τ_l is

$$\tau_l = \frac{\tau_1}{\sin\lambda'} \sin l\lambda' \tag{A.8}$$

which when inserted in (A.2) with the identification $t = l\ \Delta t$, in the limit $l \to \infty$ and $\Delta t \to 0$, leads finally to the exact result

$$C_n(t) = \sum_m C_m(0) \mathrm{e}^{-\mathrm{i}\alpha(n+m)t/2} \mathrm{i}^{m-n} J_{m-n}\left[\frac{4A}{\alpha} \sin\left(\frac{1}{2}\alpha t \right) \right]$$

proving equation (18) in the text, and as a consequence, with the appropriate renormalizations $\alpha \to \alpha \cos \Phi j$ ($j = 1, 2, 3$) along the simple-cubic crystal axes, proving equation (17), too.

We now give an estimate of the error in the numerically predicted $z(t)$ by making use of the formal analogy between (A.2) and equation (18). As shown in [5], the exact $z_{ex}(t)$ calculated from (18) is given by

$$z_{ex}(t) = z_{ex}(0) + \frac{2A}{\alpha} |S_0| [\cos\theta_0 - \cos(\alpha t + \theta_0)] \tag{A.9}$$

where

$$S_0 \equiv \sum_m C_m^*(0) C_{m-1}(0) = |S_0|\, \mathrm{e}^{\mathrm{i}\theta_0}. \tag{A.10}$$

Since τ_l in (A.2) or (A.8) can be written as

$$\tau_l = \frac{\alpha\, \Delta t/2}{\sin(\alpha\, \Delta t/2)} \left[\frac{4A}{\alpha} \sin\left(\frac{1}{2} \alpha t \right) \right] \tag{A.11}$$

then it follows that the numerically predicted $z(t)$ calculated from (A.2) can be expressed as

$$z(t) - z(0) = \left[\frac{\sin(\alpha\, \Delta t/2)}{\alpha\, \Delta t/2} \right]^{-1} [z_{ex}(t) - z_{ex}(0)]\,. \tag{A.12}$$

In consequence, since $\Delta t \to 0$, the exact amplitude of the Bloch oscillation differs from the pseudo-spectral numerical one only by a 'diffracting' factor $\sin(\alpha\, \Delta t/2)/[\alpha\, \Delta t/2]$ close to unity, while the frequency and phase remain identical to the exact ones at all times.

Appendix B

In this appendix we generalize equation (13) so as to include the effects due to time-dependent external electric fields, and we also verify that the resulting expression yields a rigorously unitary time evolution of the wave packet.

The formal solution of the time-dependent Schrödinger equation $\mathrm{i}\hbar\, \partial\Psi/\partial t = H(t)\Psi$ for a general time-dependent one-particle Hamiltonian $H(t) = T(\boldsymbol{p}) + V(\boldsymbol{r}, t)$ is given by the time-ordered formula [15]

$$\Psi(\boldsymbol{r}, t) = T\left(\exp\left(-\mathrm{i} \int_{t_0}^{t} H(t')\, \mathrm{d}t' \right) \right) \Psi(\boldsymbol{r}, t_0) \tag{B.1}$$

(with $\hbar = 1$). For a time $t = t_0 + \Delta t$, with an infinitesimal Δt, the result of the time ordering T of the evolution operator

$$\exp\left(-\mathrm{i} \int_{t_0}^{t} H(t')\, \mathrm{d}t' \right)$$

in (B.1), when approximated up to the order of $(\Delta t)^4$, can be shown to be given by

$$T\left(\exp\left(-\mathrm{i} \int_{t_0}^{t_0+\Delta t} H(t')\, \mathrm{d}t' \right) \right) = \exp\left(-\mathrm{i} \int_{t_0}^{t_0+\Delta t} H(t')\, \mathrm{d}t' \right) + \frac{\Delta t^3}{12} [H_0, \dot{H}_0] + \mathrm{O}(\Delta t^4) \tag{B.2}$$

where the commutator $[H_0, \dot{H}_0] \equiv H_0 \dot{H}_0 - \dot{H}_0 H_0$ is, in general, different from zero given the non-commutativity of the operators $T(\boldsymbol{p})$ and $\partial V(\boldsymbol{r}, t)/\partial t$. We have defined $H_0 \equiv H(t_0)$ and $\dot{H}_0 \equiv [\partial H(t)/\partial t]_{t_0}$. A proof of (B.2) will be given after equation (B.5) below.

Using (B.2), we can write (B.1) (to order $(\Delta t)^3$) as

$$\begin{aligned} \Psi(\boldsymbol{r}, t_0 + \Delta t) &= \exp\left(-\mathrm{i}\, \Delta t\, T(\boldsymbol{p}) - \mathrm{i} \int_{t_0}^{t_0+\Delta t} V(\boldsymbol{r}, t')\, \mathrm{d}t' \right) \Psi(\boldsymbol{r}, t_0) + \mathrm{O}(\Delta t^3) \\ &= \exp\left(-(\mathrm{i}/2) \int_{t_0}^{t_0+\Delta t} V(\boldsymbol{r}, t')\, \mathrm{d}t' \right) \mathrm{e}^{-\mathrm{i}\, \Delta t\, T(\boldsymbol{p})} \\ &\quad \times \exp\left(-(\mathrm{i}/2) \int_{t_0}^{t_0+\Delta t} V(\boldsymbol{r}, t')\, \mathrm{d}t' \right) \Psi(\boldsymbol{r}, t_0) + \mathrm{O}(\Delta t^3) \end{aligned} \tag{B.3}$$

where the Baker–Campbell–Hausdorff formula [16] has been invoked. Equation (B.3) is the generalization of (2) for time-dependent electric fields. Since

$$\int_{t_0}^{t_0+\Delta t} V(\boldsymbol{r},t')\,\mathrm{d}t' = \Delta t\, V(\boldsymbol{r},t_0) + \frac{1}{2}(\Delta t)^2\,[\partial V(\boldsymbol{r},t)/\partial t]_{t_0} + \mathrm{O}(\Delta t^3) \tag{B.4}$$

with some additional manipulations, we finally obtain our corresponding generalization of equation (13), as the time-iterative formula given by

$$C_{\boldsymbol{R}''}^{n+1} = \sum_{\boldsymbol{R}} C_{\boldsymbol{R}}^{n} \exp\left\{-\mathrm{i}\left[\lambda(V_{\boldsymbol{R}}^{n} + V_{\boldsymbol{R}''}^{n}) + \lambda^2(\partial V_{\boldsymbol{R}}^{n}/\partial t + \partial V_{\boldsymbol{R}''}^{n}/\partial t)\right]\right\} F(\boldsymbol{R}-\boldsymbol{R}'') \tag{B.5}$$

where $C_{\boldsymbol{R}}^{n} \equiv C_{\boldsymbol{R}}(t_0 + n\,\Delta t)$, $V_{\boldsymbol{R}}^{n} \equiv V(\boldsymbol{R}, t_0 + n\,\Delta t)$, $\partial V_{\boldsymbol{R}}^{n}/\partial t \equiv [\partial V(\boldsymbol{R},t)/\partial t]_{t_0+n\,\Delta t}$ and $\lambda \equiv \Delta t/2$, for $n = 0, 1, 2, 3, \ldots$.

To conclude this demonstration, let us now prove the validity of (B.2). To this end let us develop the first few terms of the time-ordered evolution operator on the left-hand side of equation (B.2) as

$$\begin{aligned} T\left(\exp\left(-\mathrm{i}\int_{t_0}^{t_0+\Delta t} H(t')\,\mathrm{d}t'\right)\right) &= 1 + (-\mathrm{i})\int_{t_0}^{t_0+\Delta t}\mathrm{d}t'\,H(t') \\ &+ (-\mathrm{i})^2\int_{t_0}^{t_0+\Delta t}\mathrm{d}t'\,H(t')\int_{t_0}^{t'}\mathrm{d}t''\,H(t'') \\ &+ (-\mathrm{i})^3\int_{t_0}^{t_0+\Delta t}\mathrm{d}t'\,H(t')\int_{t_0}^{t'}\mathrm{d}t''\,H(t'')\int_{t_0}^{t''}\mathrm{d}t'''\,H(t''') \\ &+ (-\mathrm{i})^4\int_{t_0}^{t_0+\Delta t}\mathrm{d}t'\,H(t')\int_{t_0}^{t'}\mathrm{d}t''\,H(t'')\int_{t_0}^{t''}\mathrm{d}t'''\,H(t''')\int_{t_0}^{t'''}\mathrm{d}t''''\,H(t'''') + \ldots. \end{aligned} \tag{B.6}$$

Each of the above four multiple-integral terms in (B.6) can be calculated explicitly (up to $\mathrm{O}(\Delta t^4)$), i.e.,

$$\int_{t_0}^{t_0+\Delta t}\mathrm{d}t'\,H(t') = \frac{\Delta t}{1!}H_0 + \frac{\Delta t^2}{2!}\dot{H}_0 + \frac{\Delta t^3}{3!}\ddot{H}_0 \tag{B.7}$$

$$\int_{t_0}^{t_0+\Delta t}\mathrm{d}t'\left(H(t')\int_{t_0}^{t'}\mathrm{d}t''\,H(t'')\right) = \frac{\Delta t^2}{2!}H_0^2 + \frac{\Delta t^3}{3!}(2\dot{H}_0H_0 + H_0\dot{H}_0) \tag{B.8}$$

$$\int_{t_0}^{t_0+\Delta t}\mathrm{d}t'\left(H(t')\int_{t_0}^{t'}\mathrm{d}t''\,H(t'')\int_{t_0}^{t''}\mathrm{d}t'''\,H(t''')\right) = \frac{\Delta t^3}{3!}H_0^3 \tag{B.9}$$

$$\int_{t_0}^{t_0+\Delta t}\mathrm{d}t'\left(H(t')\int_{t_0}^{t'}\mathrm{d}t''\,H(t'')\int_{t_0}^{t''}\mathrm{d}t'''\,H(t''')\int_{t_0}^{t'''}\mathrm{d}t''''\,H(t'''')\right) = \mathrm{O}(\Delta t^4) \tag{B.10}$$

where $\ddot{H}_0 \equiv \left[\partial^2 H(t)/\partial t^2\right]_{t_0}$. Since (B.9) is the last significant term of the expansion of (B.6) up to $\mathrm{O}(\Delta t^4)$, we can write the left-hand side of (B.2) as

$$\begin{aligned} T\left(\exp\left(-\mathrm{i}\int_{t_0}^{t_0+\Delta t} H(t')\,\mathrm{d}t'\right)\right) &= 1 - \mathrm{i}\frac{\Delta t}{1!}H_0 + \frac{\Delta t^2}{2!}(-\mathrm{i}\dot{H}_0 - H_0^2) \\ &+ \frac{\Delta t^3}{3!}(-\mathrm{i}\ddot{H}_0 - 2\dot{H}_0H_0 - H_0\dot{H}_0 + \mathrm{i}H_0^3) + \mathrm{O}(\Delta t^4). \end{aligned} \tag{B.11}$$

On the other hand, we have the expansions

$$\exp\left(-\mathrm{i}\int_{t_0}^{t_0+\Delta t} H(t')\,\mathrm{d}t'\right) = \exp\left[-\mathrm{i}\left(\frac{\Delta t}{1!}H_0 + \frac{\Delta t^2}{2!}\dot{H}_0 + \frac{\Delta t^3}{3!}\ddot{H}_0\right)\right] + \mathrm{O}(\Delta t^4)$$
$$= 1 - \mathrm{i}\frac{\Delta t}{1!}H_0 + \frac{\Delta t^2}{2!}(-\mathrm{i}\dot{H}_0 - H_0^2) + \frac{\Delta t^3}{3!}\left(-\mathrm{i}\ddot{H}_0 - \frac{3}{2}\dot{H}_0 H_0 - \frac{3}{2}H_0\dot{H}_0 + \mathrm{i}H_0^3\right) + \mathrm{O}(\Delta t^4). \tag{B.12}$$

Equation (B.2) follows from comparing (B.11) with (B.12), thus achieving the aforementioned demonstration of (B.2), and concluding our proof.

Although we have already pointed out that equation (15) yields a unitary time evolution by using analytical properties of Bessel functions, we now present a formal general proof of unitarity starting from equation (B.5) above. To this end, let us introduce the compact notation

$$\langle C^{n+1}|C^{n+1}\rangle \equiv \sum_{\boldsymbol{R}'} |C_{\boldsymbol{R}'}(t_0 + (n+1)\,\Delta t)|^2 \tag{B.13}$$

and

$$f(V^n_{\boldsymbol{R}} + V^n_{\boldsymbol{R}''}) \equiv \lambda(V^n_{\boldsymbol{R}} + V^n_{\boldsymbol{R}''}) + \lambda^2(\partial V^n_{\boldsymbol{R}}/\partial t + \partial V^n_{\boldsymbol{R}''}/\partial t). \tag{B.14}$$

Assuming that our potential $V(\boldsymbol{r})$ is a real-valued function, by substituting (B.5) into (B.13) we obtain

$$\langle C^{n+1}|C^{n+1}\rangle = \sum_{\boldsymbol{R}\boldsymbol{R}''}(C^n_{\boldsymbol{R}})^* C^n_{\boldsymbol{R}''}\mathrm{e}^{-\mathrm{i}f(V^n_{\boldsymbol{R}''}-V^n_{\boldsymbol{R}})}\sum_{\boldsymbol{R}'} F^*(\boldsymbol{R}-\boldsymbol{R}')F(\boldsymbol{R}''-\boldsymbol{R}'). \tag{B.15}$$

The sum over the product of the 'kernel' integrals F in (B.15) is performed by substituting the explicit form for F given by (10), i.e.,

$$\sum_{\boldsymbol{R}'} F^*(\boldsymbol{R}-\boldsymbol{R}')F(\boldsymbol{R}''-\boldsymbol{R}') = \frac{1}{(v^*)^2}\int_{1-\mathrm{BZ}} \mathrm{d}\boldsymbol{k}'\,\mathrm{d}\boldsymbol{k}''\,\mathrm{e}^{2\mathrm{i}\lambda[T(\boldsymbol{k}')-T(\boldsymbol{k}'')]} \times \mathrm{e}^{\mathrm{i}(\boldsymbol{k}'\cdot\boldsymbol{R}-\boldsymbol{k}''\cdot\boldsymbol{R}'')}\sum_{\boldsymbol{R}'}\mathrm{e}^{\mathrm{i}\boldsymbol{R}'\cdot(\boldsymbol{k}''-\boldsymbol{k}')}. \tag{B.16}$$

From the identities related to Fourier analysis of periodic systems [17], it is known that

$$\sum_{\boldsymbol{R}'}\mathrm{e}^{\mathrm{i}\boldsymbol{R}'\cdot(\boldsymbol{k}''-\boldsymbol{k}')} = N\delta_{\boldsymbol{k}',\boldsymbol{k}''} \tag{B.17}$$

where $\boldsymbol{R}'$ runs through the N sites in the Bravais lattice of a crystal sample in $D = 3$ dimensions with volume $V = Nv$ (v being the volume of the primitive cell in the direct lattice); $\boldsymbol{k}'$, $\boldsymbol{k}''$ are arbitrary vectors in the first Brillouin zone (1-BZ) which are consistent with the Born–von Karman boundary conditions, and $\delta_{\boldsymbol{k}',\boldsymbol{k}''}$ is the Kronecker delta. By suitable interpretation of the 1-BZ integral [17], we now write

$$\int_{1-\mathrm{BZ}}\mathrm{d}\boldsymbol{k}''\,\mathrm{e}^{-2\mathrm{i}\lambda T(\boldsymbol{k}'')}\mathrm{e}^{-\mathrm{i}\boldsymbol{k}''\cdot\boldsymbol{R}''}\delta_{\boldsymbol{k}',\boldsymbol{k}''} = \frac{(2\pi)^3}{Nv}\sum_{\boldsymbol{k}''}\mathrm{e}^{-2\mathrm{i}\lambda T(\boldsymbol{k}'')}\mathrm{e}^{-\mathrm{i}\boldsymbol{k}''\cdot\boldsymbol{R}''}\delta_{\boldsymbol{k}',\boldsymbol{k}''}$$
$$= \frac{(2\pi)^3}{Nv}\mathrm{e}^{-2\mathrm{i}\lambda T(\boldsymbol{k}')}\mathrm{e}^{-\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{R}''}. \tag{B.18}$$

Substituting (B.18) into (B.16), we finally obtain [17]

$$\sum_{\boldsymbol{R}'} F^*(\boldsymbol{R}-\boldsymbol{R}')F(\boldsymbol{R}''-\boldsymbol{R}') = \frac{(2\pi)^3}{(v^*)^2 v}\int_{1-\mathrm{BZ}}\mathrm{d}\boldsymbol{k}'\,\mathrm{e}^{\mathrm{i}\boldsymbol{k}'\cdot(\boldsymbol{R}-\boldsymbol{R}'')} = \delta_{\boldsymbol{R},\boldsymbol{R}''} \tag{B.19}$$

which immediately yields

$$\langle C^{n+1}|C^{n+1}\rangle = \sum_{\boldsymbol{R}\boldsymbol{R}''}(C^n_{\boldsymbol{R}})^* C^n_{\boldsymbol{R}''}\mathrm{e}^{-\mathrm{i}f(V^n_{\boldsymbol{R}''}-V^n_{\boldsymbol{R}})}\delta_{\boldsymbol{R},\boldsymbol{R}''} = \langle C^n|C^n\rangle \tag{B.20}$$

thus ending our proof of unitarity.

Appendix C

In this appendix we will present another analytical application of our equation (13) for the infinitesimal time evolution of an electronic wave packet. In this case, let us consider the one-dimensional ($D = 1$) single-band kinetic energy $T(k) = k^2/2M$ representing the geometrical abstraction known as the 'empty-lattice' model [19], where $k \in [-\pi/a, \pi/a]$ (periodically extended over the reciprocal lattice) for a $D = 1$ crystal with a lattice constant a. Thus, $T(k)$ can be expressed as the Fourier series

$$T(k) = \frac{k^2}{2M} = \frac{1}{2a^2M}\left[\frac{\pi^2}{3} - 4\left(\frac{\cos ak}{1^2} - \frac{\cos 2ak}{2^2} + \frac{\cos 3ak}{3^2} - \cdots\right)\right] \tag{C.1}$$

which corresponds to the form of the single-band kinetic energy (4) with hopping matrix elements t_{lm} in one dimension given by

$$t_{lm} = (1 - \delta_{l,m})\frac{(-1)^{l-m}}{a^2M(l-m)^2} + \delta_{l,m}\frac{\pi^2}{6a^2M}$$

(with $\delta_{l,m}$ the Kronecker delta). The above represents a case where *all* of the intraband hopping matrix elements t_{lm} are taken into account, and not only the nearest-neighbour ones as is done in the kinetic energy model for $T(k)$ given by equation (14).

The substitution of $T(k) = k^2/2M$ into (10) leads to the evaluation of the integral

$$F(m) = \frac{a}{2\pi}\int_{-\pi/a}^{\pi/a} \mathrm{d}k\ \mathrm{e}^{-\mathrm{i}kma}\mathrm{e}^{-2\mathrm{i}\lambda k^2/2M} = \frac{1}{\pi}\int_0^{\pi} \mathrm{d}y\ \cos(my)\mathrm{e}^{-\mathrm{i}\eta y^2} \tag{C.2}$$

with $\eta \equiv \lambda/Ma^2 = \Delta t/2Ma^2$, where $y \equiv ka$ and m is an integer number. $F(m)$ in (C.2) can remarkably be expressed in terms of the Fresnel integrals [20]

$$\begin{aligned} C(x) &\equiv \int_0^x \mathrm{d}\xi\ \cos\left(\frac{\pi}{2}\xi^2\right) \\ S(x) &\equiv \int_0^x \mathrm{d}\xi\ \sin\left(\frac{\pi}{2}\xi^2\right) \end{aligned} \tag{C.3}$$

which are to be used in the expressions [20]

$$\begin{aligned} \int \mathrm{d}y\ \cos(\eta y^2 + my) &= \sqrt{\frac{\pi}{2\eta}}\left[\cos\left(\frac{m^2}{4\eta}\right)C_m^+(y,\eta) + \sin\left(\frac{m^2}{4\eta}\right)S_m^+(y,\eta)\right] \\ \int \mathrm{d}y\ \sin(\eta y^2 + my) &= \sqrt{\frac{\pi}{2\eta}}\left[\cos\left(\frac{m^2}{4\eta}\right)S_m^+(y,\eta) - \sin\left(\frac{m^2}{4\eta}\right)C_m^+(y,\eta)\right] \end{aligned} \tag{C.4}$$

where some of the auxiliary functions

$$\begin{aligned} C_m^{\pm}(y,\eta) &\equiv C\left(\frac{\eta y \pm m/2}{\sqrt{\eta\pi/2}}\right) \\ S_m^{\pm}(y,\eta) &\equiv S\left(\frac{\eta y \pm m/2}{\sqrt{\eta\pi/2}}\right) \end{aligned} \tag{C.5}$$

defined above have been introduced. Finally, combining the expressions given as (C.4), equation (C.2) can be written after some manipulations in the useful and compact form

$$F(m) = \frac{1}{\sqrt{8\pi\eta}}\mathrm{e}^{\mathrm{i}m^2/4\eta}\left[C_m^+(\pi,\eta) - \mathrm{i}S_m^+(\pi,\eta) + C_m^-(\pi,\eta) - \mathrm{i}S_m^-(\pi,\eta)\right]. \tag{C.6}$$

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