Time evolution of Bloch electrons in a homogeneous electric field

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(Received 8 July 1985)

The theory of a Bloch electron moving in the presence of a homogeneous electric field is reviewed and objections to the conventional derivations are discussed. A new derivation of the time development of a Bloch electron moving in a homogeneous, but time-dependent, electric field is presented using a vector potential to describe the field rather than the usual scalar potential. This new treatment avoids all the basic assumptions of the conventional derivations and demonstrates that a Bloch electron will oscillate in a single band with the Bloch period if a homogeneous electric field is abruptly turned on, with a tunneling probability into other bands given by the conventional expression. It is also shown that the calculated optical absorption will have the same ladderlike structure that would be obtained if Wannier-Stark quantized energy levels are assumed, although the present calculation makes no such assumption. The previous objections to the existence of Bloch oscillations for electrons in a perfect periodic potential are examined and found to be irrelevant provided the tunneling probability per Bloch oscillation period is much less than one, a condition that is generally satisfied for typical elemental and compound semiconductors for electric fields smaller than 10^6 V/cm.

I. INTRODUCTION

Ever since the initial application of quantum mechanics to the dynamics of electrons in solids, the analysis of Bloch electrons moving in a homogeneous electric field has been of central importance.

By employing quasiclassical considerations, Bloch[1] demonstrated that a wave packet composed of a superposition of states from a single band peaked about some quasimomentum, $\hbar\mathbf{k}$, moves with a group velocity given by the gradient of the energy-band function with respect to the quasimomentum and that the time rate of change of the quasimomentum is equal to $\mathbf{F}$, the force on the electron due to the external field which is present in addition to the crystal periodic potential. Thus, neglecting interband transitions, the quasimomentum of a Bloch electron in a homogeneous electric field will be uniformly accelerated into the next Brillouin zone in a repeated zone scheme (or equivalently undergoes an umklapp process back into the first zone) with the Bloch period of oscillation given by $\hbar G/F$, where G is the length of the reciprocal-lattice vector in the direction of the field with a corresponding oscillation of the electron wave packet in configuration space.

Early calculations of the tunneling probability into other bands in which the electric field is represented by a time-independent scalar potential were made by Zener[2] using a Wentzel-Kramers-Brillouin (WKB) generalization of Bloch functions, by Houston[3] using accelerated Bloch states (Houston states), and subsequently by Kane[4] and Argyres[5] who employed the crystal-momentum representation (CMR) which leads to Wannier-Stark[6] quantized energy levels. Their calculations lead to the conclusion that the tunneling rate per Bloch period is $\ll 1$ for electric fields $\lesssim 10^6$ V/cm for typical band parameters corresponding to elemental or compound semiconductors.[7]

Despite the apparent agreement among these calculations, the validity of employing the CMR or Houston functions to describe electrons moving in a periodic potential and an applied electric field potential has been disputed. Some of the main criticisms may be summarized as follows.

(a) The eigenvalues of the energy of the time-independent Schrödinger equation are not quantized but are continuous with all values of E allowed.

(b) Since the Hamiltonian is not periodic on the boundaries of a (finite) crystal, it is not clear that one can employ the CMR or Houston functions since Bloch functions are periodic on the boundary, i.e., a superposition of Bloch functions to represent the wave function ψ will automatically yield a ψ which is periodic on the boundary, but the solution of the time-dependent Schrödinger equation, including the nonperiodic scalar potential, $\phi = -e\mathscr{E}\cdot\mathbf{r}$, may not have this property.

(c) The CMR of the operator x which enters in the calculation may not be well defined because $x\phi_{n\mathbf{k}}$ cannot be represented as a linear combination of Bloch states, i.e., $\int |x\phi_{n\mathbf{k}}|^2 d\tau$ diverges as the crystal approaches infinite extent in the x direction.

We give below a brief historical account concerning these controversies.

In a series of papers, Wannier[6] and collaborators[8,9] have argued that in the presence of a homogeneous electric field, one can modify the Bloch functions in such a way that there is no interband coupling and an electron in a crystal will move within one band with its $\mathbf{k}$ changing in time according to Bloch's theory. Furthermore, if $\mathbf{k}(t=0)$ is in the direction of a reciprocal-lattice vector,

the periodic motion in k space gives rise to an energy quantization with $\Delta E = Fa$ where a is the lattice constant in the direction of the field, the so-called Wannier-Stark ladders. "The basis for this idea is that energy bands arise from the translational symmetry of the crystalline field and this symmetry is not removed physically by the presence of the applied field,"[8] i.e., the force on the electron is periodic with the lattice period.

These arguments have been refuted by Zak,[10] who shows that although it immediately follows from the one-dimensional time-independent Schrödinger equation for the infinite crystal with lattice constant a, that if E is an eigenvalue, so is $E + naF$ an eigenvalue, the spectrum of E is continuous with $-\infty < E < \infty$, so the ladders in energy do not exist. Zak also points out that for a finite crystal, the use of periodic boundary conditions arising from the idea of bending the string of atoms into a chain is no longer valid because the potential of the field will become discontinuous so the end points cannot be considered equivalent. Wannier[11] has argued that Zak's critique of his proof is not valid, but concedes that the Stark ladders may be metastable resonant states limited by interband tunneling, as are the electron states in the hydrogen atom in the presence of a constant electric field. However, Wannier's arguments were immediately rejected by Zak,[12] who claims that Wannier's original equation was incorrect as shown using the kq representation.

Rabinovitch[13] has further rigorously shown that if the usual Born—von Kármán periodic boundary conditions are employed for a finite one-dimensional crystal, i.e., $\psi(x+L)=\psi(x)$, then there are no solutions of the time-independent Schrödinger equation if the potential includes the effect of the electric field. He also argues that if one employs the less restrictive periodic boundary conditions $\psi(0)=\psi(L)$ and $\partial\psi(0)/\partial x = \partial\psi(L)/\partial x$, then the symmetry argument that leads to the Stark ladders is no longer valid. Thus, in either case, for a finite crystal, no Stark ladders are obtained.

Rabinovitch and Zak[14] have numerically solved the Schrödinger equation for the energy eigenvalues and eigenfunctions for a Mathieu-type model crystal in an electric field of finite range. They find that the energy eigenfunctions are drastically affected by the addition of boundary conditions, whereas the energy eigenvalues are not significantly affected. These eigenvalues show a complete absence of the Stark ladder spectrum.

Rabinovitch and Zak[15] have extended Zak's[10] earlier arguments to the question of Bloch oscillation. They argue that since neglecting the interband coupling terms in the time-independent Schrödinger equation in the CMR leads incorrectly to energy quantization, then the interband terms cannot be neglected in the lowest approximation because they are the same order as the terms retained. Applying the same reasoning to the time-dependent equation, they conclude (without offering a proof) that neglecting the interband terms as a first approximation, as done by Houston, is incorrect for times equal to or longer than the period of one Bloch oscillation. On the basis of treating the problem in the kq representation,[16] they conclude that the electron does not execute a Bloch oscillation because the eigenvalue E is continuous and therefore cannot be assigned a band index.

Nevertheless, shortly before these latter arguments appeared, experimental results were obtained by Koss and Lambert,[17] which were interpreted as supporting the existence of Wannier-Stark levels. They found that the observed low-temperature optical absorption of GaAs in a strong electric field ($\mathscr{E} \approx 10^5$ V/cm) closely followed the theoretical predictions of Callaway,[18] which were based on employing Kane's wave function and Wannier-Stark quantized energy levels. The "staircase" in the optical absorption as a function of incident photon energy was both qualitatively and quantitatively in agreement with theoretical predictions assuming quantized energy levels.

More recently, Churchill and Holmstrom[19] have reviewed the theory of Bloch oscillations. They argue that, since for free electrons, an electron wave packet is uniformly accelerated by a constant electric field, they conclude "that the Bloch oscillation model, in which interband transitions are discounted, gives an unrealistic picture, since it requires a discontinuous change in the form $v(t)$ from a linear to an oscillating function of time when even a small lattice potential is added." They then show that if transitions into adjacent bands take place at every Brillouin-zone (BZ) edge, then the resulting velocity converges to the empty lattice case as the strength of the periodic potential approaches zero. They conclude that the whole question of electron motion under the simultaneous influence of a periodic lattice potential and an applied field ought to be thoroughly reviewed.

In a subsequent paper,[20] they construct exact solutions $\psi(x,t)$ of the time-dependent Schrödinger equation by taking linear combinations of the solutions of the time-independent Schrödinger equation with energies corresponding to a Stark ladder, i.e., $E_n = \varepsilon + naF$, $-\infty < n < \infty$ for a one-dimensional model. Assuming this series converges, they show that the wave function can be written as a Bloch-like state with a time-dependent wave vector in agreement with Wannier's result.[6] However, here all values of ε are allowed in agreement with Zak.[10] They also show that the solutions $\psi(x,t)$ repeat after a period of one Bloch oscillation. However, although the $\psi(x,t)$ are Bloch-like they do not reduce to the usual Bloch state for $F=0$, i.e., these functions are not adiabatically connected to the zero-field state in agreement with the results of Wannier and Van Dyke.[9] Furthermore, they show these solutions do not satisfy Born—von Kármán boundary conditions, since the latter would require

$$k(t) = k' + \frac{Ft}{\hbar} = \frac{2\pi s}{na} ,$$

where s is some integer, which is clearly impossible since t is a continuous variable.

Finally, they argue that $\psi(x,t)$ is actually a standing wave and thus the solutions of the time-dependent equation carry *no* current and hence no Bloch oscillations exist. They conclude that "diagrams which are sometimes used to portray trajectories of $k(t)$ superimposed upon the constant-energy contours within the Brillouin zone are incorrect and misleading."

The fact that these "accelerated Bloch functions"[20] do

not reduce to the usual Bloch functions as $F\to 0$ is related to the fact that even for an infinitesimal F, the potential $-Fx$ diverges as $|x|\to\infty$, so

$$\lim_{F\to 0}\lim_{x\to\infty} Fx \neq \lim_{x\to\infty}\lim_{F\to 0} Fx \ .$$

Thus if we consider the solutions for the infinite crystal, they will not reduce to the usual Bloch functions as $F\to 0$ because the potential due to the field becomes infinite as $|x|\to\infty$ and makes the eigenfunctions nonanalytic functions of the field.[21]

The difficulty of treating the operator x in the CMR also poses some mathematical problems as already noted in (c) above. However, Blount[22] has argued that these difficulties can be surmounted and that the operator x can, in the right context, be given a Bloch-state representation.

In order to clarify our understanding of the behavior of Bloch electrons moving in a homogeneous electric field, it would be of considerable value to develop a procedure that would be valid for a finite crystal (thus avoiding the difficulties inherent in treating the potential $-Fx$ in an infinite crystal), employing periodic boundary conditions only on solutions of equations that are explicitly periodic (thus avoiding the problem pointed out by Rabinovitch), without any assumption about the nature of the allowed energy spectrum (thus avoiding the controversy about Wannier-Stark levels). In Sec. II we shall do so. Then, in Sec. III we shall discuss the validity of the objections to the possibility of Bloch oscillations raised in Refs. 15, 19, and 20.

II. BLOCH ELECTRON IN A HOMOGENEOUS ELECTRIC FIELD DESCRIBED BY A VECTOR POTENTIAL

We consider the time evolution of an electron in a Bloch state for $t\leq 0$ under the influence of an electric field, $\mathscr{E}(t)$, turned on at $t=0$. The time-dependent Schrödinger equation may then be written

$$H\psi(\mathbf{r},t)=\left[\frac{[\mathbf{p}-(e/c)\mathbf{A}]^2}{2m}+v(\mathbf{r})\right]\psi=i\hbar\frac{\partial\psi}{\partial t} \ , \tag{1}$$

where

$$\mathbf{A}=-c\int_0^t \mathscr{E}(t')dt' \tag{2}$$

and $v(\mathbf{r})$ is the crystal periodic potential.

It is convenient to obtain $\psi(\mathbf{r},t)$ from $\psi(\mathbf{r},t=0)$ by employing an eigenfunction expansion whose elements are the instantaneous solutions of the same Hamiltonian, i.e.,

$$\left[\frac{[\mathbf{p}-(e/c)\mathbf{A}]^2}{2m}+v(\mathbf{r})\right]\phi_i'(\mathbf{r},t)=\varepsilon_i(t)\phi_i'(\mathbf{r},t) \ , \tag{3}$$

where the $\varepsilon_i(t)$ are, in general, time dependent because $\mathbf{A}=\mathbf{A}(t)$. Then for each t the set $\{\phi_i'\}$ can be chosen to be C—O—N and can be used as a basis in which to expand ψ. (After this paper was completed we learned that Kittel[23] has considered the motion of an electron in a homogeneous time-dependent electric field by employing a vector potential. His treatment is primarily concerned with proving the acceleration theorem for an electron confined to a single band, whereas we shall include an analysis of the effects of interband coupling.)

Now, for each t, H is invariant under a crystal lattice translation because $v(\mathbf{r})$ is periodic and $\mathbf{A}$ is independent of $\mathbf{r}$ for a homogeneous electric field. This is the fundamental advantage of treating the effect of the field in terms of a vector potential instead of a scalar potential, i.e., the Hamiltonian maintains its periodicity as does the force on the electron. The apparent disadvantage is that even if $\mathscr{E}$ is time independent for $t>0$, the vector potential is still time dependent, so the eigenvalues, $\varepsilon_i(t)$, will be time dependent.

The solutions of Eq. (3) are easily obtained by substituting

$$\phi_i'(\mathbf{r},t)=e^{ie\chi'/\hbar c}\phi_i(\mathbf{r},t) \tag{4}$$

into Eq. (3) with $\chi'=\mathbf{A}\cdot\mathbf{r}$. The resulting equation for ϕ_i is

$$\left[\frac{p^2}{2m}+v(\mathbf{r})\right]\phi_i=\varepsilon_i\phi_i \tag{5}$$

with solutions

$$\phi_i=\phi_{n\mathbf{k}}(\mathbf{r})$$

and

$$\varepsilon_i=\varepsilon_n(\mathbf{k}) \ , \tag{6}$$

i.e., the Bloch functions with $\varepsilon_n(\mathbf{k})$, the energy band functions of the unperturbed crystal. Then from Eqs. (4) and (6)

$$\phi_i'(\mathbf{r},t)=e^{ie\mathbf{A}\cdot\mathbf{r}/\hbar c}\phi_{n\mathbf{k}}(\mathbf{r}) \ . \tag{7}$$

Furthermore, since H is invariant under a lattice translation, we can define the allowed values of $\mathbf{k}$ using periodic boundary conditions on the ϕ_i'. The result is

$$\frac{e\mathbf{A}}{\hbar c}+\mathbf{k}=\sum_i \frac{n_i}{N_i}\mathbf{G}_i \ , \tag{8}$$

where $\mathbf{G}_i$ $(i=1,2,3)$ are the primitive reciprocal-lattice vectors, N_i are the number of cells in the i direction, and n_i are integers with $-N_i/2<n_i\leq N_i/2$ in order to avoid redundant solutions.

Therefore, in order for periodic boundary conditions to be satisfied, the $\mathbf{k}$ must be functions of t which satisfy

$$\hbar\dot{\mathbf{k}}=\frac{-e}{c}\dot{\mathbf{A}}=\frac{-e}{c}(-c\mathscr{E})=e\mathscr{E}=\mathbf{F} \ . \tag{9}$$

Thus the $\phi_{n\mathbf{k}(t)}$ are precisely the Houston functions which are derived here without making any assumption about the neglect of interband matrix elements but arise instead as the exact time-dependent eigenfunctions of the time-dependent Hamiltonian of the system. In this system it follows from Eq. (8) and the time dependence of $\mathbf{A}(t)$ that the BZ describing the allowed $\mathbf{k}(t)$ values is itself time dependent, i.e., the periodic boundary conditions lead to BZ boundaries that move in time so as time increases the electron wave vector does not undergo an umklapp process back to the other side of the BZ, but continues with continuous values of $\mathbf{k}(t)$ in the time-dependent zone.

Thus, the problem of employing periodic boundary conditions on the eigenfunctions to be used in an expansion and simultaneously maintaining $\hbar\dot{\mathbf{k}}=\mathbf{F}$ when one employs a time-independent gauge with $\phi=-e\mathscr{E}\cdot\mathbf{r}$ is eliminated here from the outset.[20] Then substituting

$$\psi(\mathbf{r},t)=\sum_i a_i(t)\phi_i'(\mathbf{r},t) \tag{10}$$

into Eq. (1) and multiplying both sides of the resultant equation by $\exp(-ie\mathbf{A}\cdot\mathbf{r}/\hbar c)\phi^*_{n'\mathbf{k}'}$ and integrating over the volume of the crystal at time t yields

$$\varepsilon_n(\mathbf{k}(t))a_{n\mathbf{k}(t)}=i\hbar\frac{\partial a_{n\mathbf{k}(t)}}{\partial t}+F\sum_{n'}X_{nn'}(\mathbf{k}(t))a_{n'\mathbf{k}(t)}\ , \tag{11}$$

where we have specialized to the case $\mathscr{E}=\mathscr{E}(t)\hat{i}$ and have employed the orthonormality of the Bloch functions, the fact that $e\mathbf{A}/\hbar c+\mathbf{k}$ is time independent according to Eq. (8) and

$$\frac{\partial}{\partial t}U_{n\mathbf{k}(t)}=\frac{\partial}{\partial k_x}U_{n\mathbf{k}}\cdot\frac{dk_x}{dt}=\frac{F}{\hbar}\frac{\partial}{\partial k_x}U_{n\mathbf{k}}\ .$$

Here $U_{n\mathbf{k}}$ is the periodic part of the Bloch function and

$$X_{nn'}(\mathbf{k})\equiv\frac{1}{i}\int U^*_{n\mathbf{k}}\frac{\partial}{\partial k_x}U_{n'\mathbf{k}}d\tau\ . \tag{12}$$

It follows from Eq. (11) that the coefficients $a_{n\mathbf{k}(t)}$ are coupled only to the $a_{n'\mathbf{k}(t)}$, i.e., coupled only to the same $\mathbf{k}$. Therefore for a given $\mathbf{k}$, letting

$$a_{n\mathbf{k}(t)}=\alpha_n(t)\exp\left[-\frac{i}{\hbar}\int_0^t\varepsilon_n(\mathbf{k}(t'))dt'\right] \tag{13}$$

in Eq. (11) yields

$$\dot{\alpha}_n(t)=\frac{F(t)}{i\hbar}\sum_{n'}\alpha_{n'}(t)X_{nn'}(\mathbf{k}(t))\exp\left[\frac{i}{\hbar}\int_0^t[\varepsilon_n(\mathbf{k}(t'))-\varepsilon_{n'}(\mathbf{k}(t'))]dt'\right]\ , \tag{14}$$

which is equivalent to Houston's result which he derived employing a scalar potential to represent the effect of the electric field. However, unlike Houston's method we have not employed an expansion which is periodic on the boundaries to find the solution corresponding to a nonperiodic Hamiltonian nor have we required the CMR of the operator x as required in the usual time-dependent perturbation theory formalism. In the Appendix we show the equivalence of the Houston expansion and that given by Eq. (10) by employing a gauge transformation.

If initially, before the field is turned on, the electron state can be described by a Bloch wave in band n with $\mathbf{k}=\mathbf{k}(t=0)$, then at $t=0$

$$\alpha_{n'}=\delta_{nn'}\ , \tag{15}$$

and for sufficiently short times for which $\alpha_{n'}\ll 1$, $n'\neq n$, we can substitute Eq. (15) into Eq. (14) to obtain

$$\alpha_{n'}(t)=\int_0^t\frac{F(t')}{i\hbar}X_{n'n}(\mathbf{k}(t'))\exp\left[\frac{i}{\hbar}\int_0^{t'}[\varepsilon_{n'}(\mathbf{k}(t''))-\varepsilon_n(\mathbf{k}(t''))]dt''\right]dt'\ . \tag{16}$$

Specializing to the case $F=\text{const}$ for $t>0$ for a field in the direction of a reciprocal-lattice vector $\mathbf{G}$ and evaluating the integral for N traversals of a BZ by employing the periodicity of $X_{n'n}(\mathbf{k})$ and $\varepsilon_n(\mathbf{k})$, we obtain

$$|\alpha_{n'}(NT)|^2=\frac{\sin^2(\beta N/2)}{\sin^2(\beta/2)}\left|\int_{-G/2}^{G/2}X_{n'n}(\mathbf{k})\exp\left[\frac{i}{F}\int_0^{k_x}[\varepsilon_{n'}(k_x',\mathbf{k}_\perp)-\varepsilon_n(k_x',\mathbf{k}_\perp)]dk_x'\right]dk_x\right|^2\ , \tag{17}$$

where

$$\beta\equiv\frac{1}{F}\int_{-G/2}^{G/2}[\varepsilon_{n'}(\mathbf{k})-\varepsilon_n(\mathbf{k})]dk_x \tag{18}$$

and T is the period for one traversal (i.e., one Bloch oscillation) of the BZ given by

$$T=\frac{\hbar G}{F}\ . \tag{19}$$

For large N, $|\alpha_{n'}|^2$ will increase provided $\beta\to 2\pi(M+\delta)$ with M an integer and $\delta\ll 1$ in which case

$$\sin^2(\beta N/2)/\sin^2(\beta/2)\to N^2$$

with a width $\sim 1/N$. Argyres[5] has shown using a similar expression, that the corresponding transmission coefficient, i.e., the transmission probability per period T arising from Eq. (17) is

$$P_{nn'}=\left|\int_{-G/2}^{G/2}X_{n'n}(\mathbf{k})\exp\left[\frac{i}{F}\int_0^{k_x}[\varepsilon_{n'}(k_x',\mathbf{k}_\perp)-\varepsilon_n(k_x',\mathbf{k}_\perp)]dk_x'\right]dk_x\right|^2\ , \tag{20}$$

which is equivalent to Kane's result.[4] Using the expression for $P_{nn'}$ obtained by Kane in a two-band model, the tunneling probability is $<10^{-17}$ for typical band parameters[7] for $\mathscr{E} \lesssim 10^6$ V/cm which leads to the conclusion that if scattering is neglected the wave function given by Eq. (7) is a good approximation to the exact wave function for many Bloch oscillations provided $NP_{nn'} \ll 1$. In addition, it is easy to show that the condition $\beta = 2\pi M$ is equivalent to the requirement in the Kane-Argyres theory that elastic tunneling takes place only between Wannier-Stark quantized energy states. This follows from the fact that in the latter theory the Stark energy levels, $E_{n\nu}$, are given by

$$\frac{1}{F}\int_{-G/2}^{G/2}[E_{n\nu}-\varepsilon_n(\mathbf{k})]dk_x = 2\pi\nu ,$$

where ν is an integer. Therefore

$$\frac{1}{F}\int_{-G/2}^{G/2}\{[E_{n\nu}-\varepsilon_n(\mathbf{k})] - [E_{n'\nu}-\varepsilon_{n'}(\mathbf{k})]\}dk_x = 2\pi(\nu-\nu') .$$

Thus, if $E_{n\nu}=E_{n'\nu}$ to allow elastic tunneling,

$$\beta \equiv \frac{1}{F}\int_{-G/2}^{G/2}[\varepsilon_{n'}(\mathbf{k})-\varepsilon_n(\mathbf{k})]dk_x = 2\pi(\nu-\nu') = 2\pi M ,$$

therefore, although we have not had to determine whether the system has discrete Stark-like levels, our calculation automatically gives rise to a selection rule which is equivalent to that which would be obtained by requiring conservation of energy for tunneling between Stark levels in different bands.

Furthermore, if we wish to consider optical absorption while representing the effect of the homogeneous electric field by a vector potential as done above we must add to this vector potential a vector potential $\mathbf{A}_{\mathrm{RF}}$ representing the incident radiation field. If we treat the resulting $\mathbf{p}\cdot\mathbf{A}_{\mathrm{RF}}$ term in the Hamiltonian as a perturbation and neglect the terms in $|\mathbf{A}_{\mathrm{RF}}|^2$ and $X_{nn'}$ as small, we can calculate the $|\alpha_{n'}(t)|^2$ as performed above. The result analogous to Eq. (16) for the perturbation would then be

$$\alpha_{n'}(t) \sim \int_0^t p_{n'n}(\mathbf{k}(t'))\exp\left[\frac{i}{\hbar}\int_0^{t'}[\varepsilon_{n'}(\mathbf{k}(t''))-\varepsilon_n(\mathbf{k}(t''))\pm\hbar\omega]dt''\right]dt' , \tag{21}$$

where we have, as usual, neglected the wave vector of the photon. Then, making the same change of variables that led to Eq. (17), and evaluating the integral as a sum corresponding to N traversals of the BZ, we would obtain the result analogous to Eq. (17), i.e.,

$$|\alpha_{n'}(NT)|^2 \sim \frac{\sin^2(\beta' N/2)}{\sin^2(\beta'/2)}\left|\int_{-G/2}^{G/2}p_{n'n}(\mathbf{k})\exp\left[\frac{i}{F}\int_0^{k_x}[\varepsilon_{n'}(\mathbf{k}')-\varepsilon_n(\mathbf{k}')\pm\hbar\omega]dk_x'\right]dk_x\right|^2 , \tag{22}$$

where

$$\beta' \equiv \frac{1}{F}\int_{-G/2}^{G/2}[\varepsilon_{n'}(\mathbf{k})-\varepsilon_n(\mathbf{k})\pm\hbar\omega]dk_x . \tag{23}$$

As in the tunneling case, $|\alpha_{n'}|^2$ continues to grow if $\beta' = 2\pi M'$ where M' is an integer. It then follows from Eq. (23) that if $M' \to M'+1$, $\omega \to \omega + \Delta\omega$, where

$$\frac{1}{F}\hbar\Delta\omega G = 2\pi$$

or

$$\hbar\Delta\omega = \frac{2\pi F}{G} , \tag{24}$$

which is exactly the energy spacing between Wannier-Stark levels. Thus the increase in optical absorption experimentally obtained by Koss and Lambert[17] can also be derived without requiring the assumption of Stark quantized energy levels,[18] the enhanced absorption at these values of ω arising purely from a selection rule involving the Houston functions.

In summary, in this section we have considered the dynamics of a Bloch electron in a homogeneous electric field using a time-dependent formalism in which the electric field is represented by a time-dependent vector potential that is independent of position. The Hamiltonian then has the same spatial periodicity as the crystal potential. It is then possible to employ periodic boundary conditions for a finite crystal to enumerate the (time-dependent) eigenfunctions of the instantaneous Hamiltonian. These eigenfunctions are the Houston states multiplied by a phase factor that is dependent on the vector potential. The time-dependent wave vectors $\mathbf{k}(t)$ then change continuously with time and are allowed to take on all values in a periodic zone scheme. The electron dynamics are completely described by the energy-band functions and Bloch states of the unperturbed crystal.

This method avoids any discussion of the energy eigenvalues of the time-independent Hamiltonian that would be obtained if the effect of the electric field were represented by a scalar potential. It also avoids the need to impose boundary conditions on a nontranslationally invariant Hamiltonian.

Moreover, by employing a vector potential, the $F \to 0$ limit can be taken without regard to whether L is finite or infinite and the solutions reduce to the unperturbed Bloch states for $F \to 0$.

The results for the tunneling probability are the same as those obtained using Stark-Wannier quantized energy levels, and for typical semiconductors they justify the use of Houston functions to describe the electron dynamics for many cycles of the BZ for electric fields $\lesssim 10^6$ V/cm. The "ladder" in the optical absorption originally predicted on the basis of assuming the existence of Wannier-Stark

quantized energy levels is also obtained as a result of a selection rule using Houston functions without any assumed energy quantization.

Finally, we note that both the present treatment of optical absorption and that of Callaway[18] completely neglects the effect of electron scattering. In either case, this approximation is valid provided the relaxation time for scattering is long compared to the Bloch period. However, Muller *et al.*[24] have observed that this condition is not satisfied in the experiment performed by Koss and Lambert so that a proper comparison between theory and their results would require a description of electron dynamics and optical absorption which includes the effects of electron scattering.

III. ANALYSIS OF PREVIOUS OBJECTIONS TO BLOCH OSCILLATIONS

Zak[10] has shown that if the time-independent field is represented by a scalar potential the dropping of the interband coupling terms, as done by Kane,[4] leads to quantized energy levels, whereas an exact treatment of the Schrödinger equation results in a continuum with $-\infty < E < \infty$. Rabinovitch and Zak[15] have adopted this argument, and claim that, although the neglect of the interband coupling leads to the Houston functions,[3] the inclusion of these terms leads to the result that the Houston functions cannot be a valid approximation to the wave function for times as long as or longer than the period of one Bloch oscillation. They essentially base their argument on the fact that the Houston function does not give the same time development as the exact solution, in the kq representation, of an initial state which, at $t=0$, is an energy eigenfunction of the Hamiltonian including the electric field.

This is not a valid criticism for the following reason. The time-independent Schrödinger equation including the field in one dimension is

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi + v(x)\psi - Fx\psi = E\psi(x) \; . \tag{25}$$

As Rabinovitch and Zak[14] have pointed out elsewhere, there is only one solution of this equation for a given E, the other exponentially increasing as $x \to \infty$. Thus, unlike the case when $F=0$, we cannot take linear combinations of two degenerate states to form two other states that carry current. Consequently, unlike Bloch states, the solutions of Eq. (25) separately do not carry current. The solution of the time-dependent Schrödinger equation corresponding to this initial state is

$$\Psi(x,t) = e^{-iEt/\hbar}\psi(x) \tag{26}$$

and is definitely not a Houston function.

The reason for this is that Eq. (26) gives the time development of a state which is an eigenfunction of H, while the Houston functions give the time development of a state (subject to the same H) which at $t=0$ is in a given Bloch state. If $\psi(x)$ were expanded in terms of Bloch states, we would necessarily have all Bloch states in the sum with nonzero coefficients. If one waited a long time after turning on the field, a state which is originally described by a single Bloch function would first evolve as a Houston function, and if the time is sufficiently long, this state would then tunnel into all the other bands and would require a many-band description. The argument by Rabinovitch and Zak that the Houston function does not represent the correct time development of an eigenstate of the field-dependent Hamiltonian is therefore correct but irrelevant—it is supposed to represent the time development of an eigenfunction of the field-free Hamiltonian after the field has been turned on, and is a valid description of such a state for times sufficiently short so that tunneling to other bands is negligible, which, in practice, is satisfied for many periods of the Bloch oscillation.

It is interesting to note that Koss and Lambert[17] employed a field strength $\mathscr{E} \approx 10^5$ V/cm for GaAs, which yields a tunneling probability per oscillation, Pcv, of $O(10^{-100})$ and a Bloch oscillation period, $T \approx 10^{-12}$ sec. Thus even after 3×10^7 sec ≈ 1 year, the probability that an electron initially in a given Bloch state tunnels out of the valence band is infinitesimal, so the use of Houston functions to calculate the absorption rate is completely justified.

Similarly, the criticisms of Churchill and Holmstrom are irrelevant to the existence of Bloch oscillations within a band. By taking linear combinations of the solutions given by Eq. (25), they construct Bloch-like solutions, with time-dependent $k(t)$, of the time-dependent Schrödinger equation. However, their solutions do not correspond to an electron in a given Bloch state at a time before the field is turned on and moreover, as they note, their solutions do not even reduce to the usual field-free Bloch states as $F \to 0$. A more detailed analysis of their results has been given elsewhere.[25]

We therefore conclude that the objections of Rabinovitch and Zak, and of Churchill and Holmstrom, to the existence of Bloch oscillations are not valid and that the conventional diagrams showing $\mathbf{k}(t)$ moving along $\varepsilon(\mathbf{k})$ curves and propagating in a periodic zone scheme (or undergoing an umklapp process back into the first BZ) are justified, provided the time is sufficiently short that tunneling into other bands is negligible. As we have seen in the case of experiments performed on GaAs by Koss and Lambert, these times can be astronomically large even for relatively high fields.

Our conclusions are hardly surprising if one makes similar considerations concerning the effect of turning on a weak electric field on an electron initially in the ground state of a hydrogen atom. Here, as in the crystalline case, the energy spectrum, including the field described by a scalar potential, is continuous, although the system without the field has discrete levels separated by energy gaps. The electron state is then not well described by an eigenfunction of the field-dependent Hamiltonian (as Rabinovitch and Zak use) or by some equally weighted linear combination of these extended states summed over an infinite set of discrete energy levels (as done by Churchill and Holmstrom). A more useful description is one in which the eigenfunctions of the instantaneous Hamiltonian (in which the effects of the electric field are treated in terms of a vector potential) are employed to describe the system. Then, unlike the case in which a scalar potential

is employed to represent the effect of the field, the field-dependent terms are continuous functions of time, and thus permit the eigenfunctions of the unperturbed Hamiltonian also to be the eigenfunctions of the perturbed Hamiltonian at the instant the field is turned on. It is then straightforward to obtain the time development of the system for times small compared to the inverse ionization (i.e., tunneling) rate by employing a linear combination of the eigenfunctions of the instantaneous Hamiltonian to represent the state of the system. In the crystalline case, as we have shown, this leads naturally to the use of Houston functions to describe the electron dynamics, including the coupling to other bands, which leads to a calculation of the tunneling rate.

APPENDIX: DERIVATION OF HOUSTON'S EQUATIONS BY APPLICATION OF A GAUGE TRANSFORMATION

It is well known[26] that if

$$H\psi = i\hbar\dot{\psi} \tag{A1}$$

with

$$H = \frac{[\mathbf{p}-(e/c)\mathbf{A}]^2}{2m} + e\phi + v(\mathbf{r}) , \tag{A2}$$

then under the gauge transformation

$$\mathbf{A}' = \mathbf{A} + \nabla\chi, \quad \phi' = \phi - \frac{1}{c}\frac{\partial\chi}{\partial t} , \tag{A3}$$

the solution of

$$H'\psi' = i\hbar\dot{\psi}' , \tag{A4}$$

where

$$H' = \frac{[\mathbf{p}-(e/c)\mathbf{A}']^2}{2m} + e\phi' + v(\mathbf{r}) \tag{A5}$$

is

$$\psi' = e^{ie\chi/\hbar c}\psi . \tag{A6}$$

Letting

$$\chi \equiv c\int_0^t \mathscr{E}(t')dt'\cdot\mathbf{r} , \tag{A7}$$

we have from Eqs. (2) and (A3)

$$\mathbf{A}' = 0, \quad \phi' = -\mathscr{E}(t)\cdot\mathbf{r} . \tag{A8}$$

Thus if ψ is a solution of Eq. (1) with $\mathbf{A}$ given by Eq. (2), the corresponding solution of

$$\left[\frac{p^2}{2m} + v(\mathbf{r}) - e\mathscr{E}(t)\cdot\mathbf{r}\right]\psi' = i\hbar\dot{\psi}' \tag{A9}$$

is

$$\psi' = e^{-ie\mathbf{A}\cdot\mathbf{r}/\hbar c}\psi . \tag{A10}$$

With use of Eq. (10) this may be written

$$\psi'(\mathbf{r},t) = \sum_{n,\mathbf{k}(t)} a_{n\mathbf{k}(t)}\phi_{n\mathbf{k}(t)}(\mathbf{r}) , \tag{A11}$$

where the $a_{n\mathbf{k}}$ satisfy Eq. (11) and the $\mathbf{k}(t)$ are given by Eq. (8).

Thus the assumption made by Houston that the expansion given by Eq. (A11) can be employed to obtain the solution of Eq. (A9) is justified precisely because the $\mathbf{k}(t)$ change as a function of time according to Eq. (8). However, unlike Houston's method, the present work does not assume an expansion of periodic functions is a solution of a nonperiodic Hamiltonian. In addition, the equation satisfied by the $a_{n\mathbf{k}(t)}$, i.e., Eq. (11), is here derived without requiring the CMR of the operator x.

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