Time evolution of a Bloch electron in a constant electric field

C. F. Hart
Department of Physics, Southern Illinois University, Carbondale, Illinois 62901-4401

David Emin
Sandia National Laboratories, Albuquerque, New Mexico 87185-5800

(Received 16 November 1987)

We describe the time evolution of a Bloch electron in a constant electric field in terms of electric-field-dependent Bloch functions. These basis functions take into account the equivalent (periodic) electric-field-induced alteration of each of the electronic potential wells of the crystal. In this scheme, all interband matrix elements vanish. As a result, we obtain a relatively simple expression for the time evolution of an electron in a periodic potential under the influence of a constant electric field.

I. INTRODUCTION

There has been a long-standing interest in understanding the properties of an electron in the periodic potential of a crystal under the influence of a spatially and temporally constant electric field. In this note, we discuss the time evolution of a Bloch electron in such an electric field.

The application of an electric field has two distinct effects on the electronic potential for an electron in a crystal. These two effects are illustrated in Fig. 1. First, the shape of each of the crystal's electronic potential wells is altered in an equivalent way by the electric field. Second, the application of the electric field shifts the energy of each of the crystal's electronic potential wells. The first effect maintains the periodicity of the electronic potential while the second effect does not.

Focusing attention on the second of these effects, Wannier argued that, with the neglect of interband matrix elements, the electronic eigenstates of an electron in a periodic potential become localized in the presence of an electric field.[1] The resulting (localized) single-band eigenstates are now termed Wannier-Stark states. Recently, we have shown that when the electronic states are described in terms of electric-field-dependent Bloch states (which account for the equivalent electric-field-induced alteration of each of the wells of the periodic potential), all interband matrix elements vanish.[2] Thus, we have a general proof of Wannier-Stark localization.

In Sec. II of this paper we extend our previous work by examining the time evolution of an electron in a periodic potential under the influence of a constant electric field. In our treatment, the Hamiltonian for the Bloch states which serve as the basis states for our description includes the equivalent electric-field-dependent alteration of the shape of each of the crystal's potential wells. As a result, in this scheme the interband matrix elements vanish. Thus, an electron prepared with a given wave vector within a given electric-field-dependent energy band always remains within that energy band. This provides us with a relatively simple description of the electron's motion. The equations of motion derived in Sec. II are explicitly solved in Sec. III.

Recently, Krieger and Iafrate[3] considered the time evolution of a Bloch electron in a constant electric field within a scheme in which the electron's wave vector is an explicit function of time. Their development is complicated by their taking the basis states to be the zero-

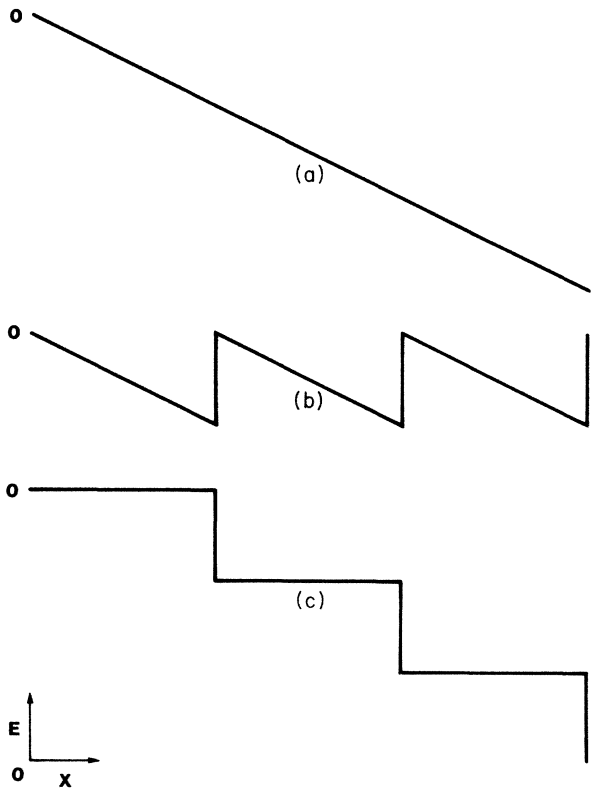

FIG. 1. The potential energy due to the electric field, $-eEx$, is plotted against x in (a). This potential energy may be decomposed into periodic and nonperiodic components in the manner shown in (b) and (c), respectively.

electric-field Bloch states. In Sec. IV of this paper, we modify their approach so that the electronic eigenstates used as basis states include the effect of the electric-field-induced alteration of the shape of each potential well. Again, we find that the interband matrix elements vanish. The equations of motion within this scheme then become extremely simple. This section concludes with our showing that the equations of motion within the Krieger-Iafrate scheme are equivalent to those obtained in Sec. II.

The paper concludes with a brief summary and discussion. We regard this work as providing further confirmation of the ideas originally advanced by Wannier.[1]

II. EQUATIONS OF MOTION FOR A BLOCH ELECTRON IN A CONSTANT ELECTRIC FIELD

For simplicity, we consider an electron in a one-dimensional periodic solid of N units of length a under the influence of a spatially and temporally constant electric field E directed along the crystal, i.e., in the x direction. As in Ref. 2, we restrict ourselves to the case of an arbitrarily long chain $N \rightarrow \infty$.

Following other treatments of this problem,[3,4] we write the Hamiltonian for this situation within the Coulomb gauge. That is, the vector potential in the x direction is written as $A = -cEt$, where c is the velocity of light and t is the time, while the scalar potential vanishes. The time-dependent Schrödinger equation for this situation is then

$$[(\hat{p} - eA/c)^2/2m + V(x)]\Psi(x,t) = i\hbar\partial\Psi(x,t)/\partial t \ , \tag{1}$$

where $\hat{p}$ is the operator for the electron's momentum in the x direction, e and m are, respectively, the electron's charge and mass, and $V(x)$ is the periodic potential for the electron provided by the crystal.

To solve Eq. (1), we find it useful to represent $\Psi(x,t)$ as a superposition of eigenfunctions, $\phi_j(x,t)$, of index j:

$$\Psi(x,t) = \sum_j B_j(t)\phi_j(x,t) \ , \tag{2}$$

where the $B_j(t)$ are the expansion coefficients associated with the eigenstate of index j. In particular, as in the work of Krieger and Iafrate,[3] the stationary states we choose are the eigenstates of an "*instantaneous*" periodic Hamiltonian. Our "instantaneous" Hamiltonian is characterized by the periodic potential $U(x,E)$ and the "time" t:

$$[(\hat{p} - eA/c)^2/2m + U(x,E)]\phi_j(x,t) = \varepsilon_j(E)\phi_j(x,t) \ . \tag{3}$$

In this formulation of the problem, t is regarded as just a parameter which enters into Eq. (3) through the t dependence of A. As a result, the "*stationary*" eigenfunctions and eigenvalues of this Hamiltonian depend explicitly on t. The expansion of Eq. (2) is possible because these eigenstates comprise a complete and orthonormal set of basis functions.

Our Hamiltonian, Eq. (3), differs from the standard zero-electric-field Hamiltonian (and that of Krieger and Iafrate) in that the periodic potential we choose is an explicit function of the electric field. Thus, $U(x,E)$ is *not* generally equal to $V(x)$ of Eq. (1). Rather, we take $U(x)$ to be the sum of the field-free periodic potential, $V(x)$, and the (saw-toothed) electric-field-dependent *periodic* potential associated with the electric field's equivalently altering the shape of the potential of each cell of the crystal [cf. Fig. 1(b)].

The eigenfunction associated with a given i and t may be written as[3]

$$\phi_j(x,t) = \exp[i(eA/\hbar c)x]\chi_j(x)$$

$$= \exp[-i(eEt/\hbar)x]\chi_j(x) \ , \tag{4}$$

where we have incorporated the relation $A = -cEt$ and $\chi_j(x)$ satisfies the stationary second-order differential equation:

$$[\hat{p}^2/2m + U(x,E)]\chi_j(x) = \varepsilon_j(E)\chi_j(x) \ . \tag{5}$$

Since the potential energy of Eqs. (3) and (5), $u(x,E)$, is periodic in x, the "stationary" basis functions are of the Bloch form. Thus, the "stationary" eigenfunctions may be characterized by a band index n and a wave vector k:

$$\phi_j(x,t) = \phi_{n,k}(x,t) = \exp[i(k - eEt/\hbar)x]u_{n,k}(x,E) \ . \tag{6}$$

Thus, the wave functions, $\phi_j(x,t)$, and the eigenvalues, $\varepsilon_j(E)$, that we utilize are different from the customary zero-field Bloch states and energies is that they depend explicitly on the electric field E.

Within the standard treatment of Bloch electrons, in which n and k are simply numbers, the t dependence of $\phi_{n,k}(x,t)$ is explicit. Thus, we have

$$i\hbar\partial\phi_{n,k}(x,t)/\partial t = (eEx)\phi_{n,k}(x,t) \ . \tag{7}$$

We can now determine the time evolution of a Bloch electron in a periodic solid in the presence of a constant electric field. In particular, following the standard projection procedure, we obtain

$$[\varepsilon_{n',k'}(E) - i\hbar\partial/\partial t]B_{n',k'}(t) = \sum_{n,k} B_{n,k}(t)\int_0^{Na} dx\ \phi^*_{n',k'}(x,t)[U(x,E) - V(x) + (eEx)]\phi_{n,k}(x,t) \ , \tag{8}$$

where we have utilized Eqs. (1)–(3) and (7).

In our scheme, as shown in Fig. 1, the electronic potential energy associated with the applied electric field, $-eEx$, is written as a sum of a periodic portion, $U(x,E) - V(x)$, and a steplike portion, $-(eEa)\sum_{m=1}^{N} S(x/a - m)$:

$$-eEx = [U(x,E) - V(x)] - (eEa)\sum_{m=1}^{N} S(x/a - m) \ , \tag{9}$$

where our one-dimensional periodic solid is composed of N equivalent units of length a. In Eq. (9), $S(x)$ is a step function: $S(x) = 0$ for $x < 0$ and $S(x) = 1$ for $x \geq 0$. Inserting Eq. (9) into Eq. (8), we have

$$[\varepsilon_{n',k'}(E)-i\hbar\partial/\partial t]B_{n',k'}(t)=(eEa)\sum_{n,k}B_{n,k}(t)\int_0^{Na}dx\,\phi^*_{n',k'}(x,t)\left[\sum_{m=1}^{N}S(x/a-m)\right]\phi_{n,k}(x,t)\ . \tag{10}$$

At this point, we note that the right-hand side of Eq. (10) is identical in form to the right-hand side of Eq. (12) of Ref. 2. Thus, we simply incorporate the manipulations of Ref. 2 into our present work to reexpress Eq. (10) as [cf. Eq. (21) of Ref. 2]

$$[\varepsilon_{n,k}(E)-i\hbar\partial/\partial t]B_{n,k}(t)=ieE\,\partial B_{n,k}(t)/\partial k\ , \tag{11}$$

where, for simplicity of notation, we have relabeled the indices n' and k' as n and k. We note that the equations of motion, Eq. (11), do not couple states of different energy-band index. Furthermore, presuming the time dependence of $B_{n,k}(t)$ to be $\exp(-i\varepsilon t/\hbar)$, one regains (as one must) the time-independent eigenvalue expression given by Eq. (21) of Ref. 2.

III. SOLUTION OF THE EQUATIONS OF MOTION

At this point, we proceed to solve the equations of motion, Eq. (11). To begin, we write the expansion coefficients as

$$B_{n,k}(t)=b_{n,k}(t)\exp[i\theta_{n,k}(t)]\ ,$$

where $b_{n,k}(t)$ and $\theta_{n,k}(t)$ are real. Substituting this definition into Eq. (11) and separating the imaginary and real portions of the resulting complex differential equation, we find

$$\hbar\partial b_{n,k}(t)/\partial t+eE\,\partial b_{n,k}(t)/\partial k=0 \tag{12a}$$

and

$$\varepsilon(k,E)+\hbar\partial\theta_{n,k}(t)/\partial t+eE\,\partial\theta_{n,k}(t)/\partial k=0\ , \tag{12b}$$

respectively. From Eq. (12a) one observes that the k and t dependencies of $b_{n,k}(t)$ are such that b is a function of the single parameter, $k-eEt/\hbar$. That is,

$$b_{n,k}(t)=b_{n,\,k-eEt/\hbar}\ ,$$

where k may be regarded as a function of t such that $\hbar\partial k/\partial t=eE$. Furthermore, from Eq. (12b) one has that

$$\theta_{n,k}(t)=-\int_{k_0}^{k(t)}dk'\varepsilon(k',E)/eE\ ,$$

where we have taken the electron to be prepared in state k_0 at $t=0$. In addition, with this initial condition,

$$b_{n,\,k-eEt/\hbar}=\delta_{k_0,\,k-eEt/\hbar}\ .$$

Thus, with our initial conditions, the expansion coefficients become

$$B_{n,k}(t)=\delta_{k_0,\,k-eEt/\hbar}\exp\left[-i\int_{k_0}^{k_0+eEt/\hbar}dk'\varepsilon(k',E)/eE\right]\ . \tag{13}$$

Then, inserting the expansion coefficients, Eq. (13), into Eq. (2), we find the time evolution of an electron prepared in an electric-field-dependent Bloch state:

$$\begin{aligned}\Psi(x,t)&=\phi_{n,\,k_0+eEt/\hbar}(x,t)\exp\left[-i\int_{k_0}^{k_0+eEt/\hbar}dk'\varepsilon(k',E)/eE\right]\\&=\exp(ik_0x)u_{n,\,k_0+eEt/\hbar}(x)\exp\left[i\int_{k_0}^{k_0+eEt/\hbar}dk'\varepsilon(k',E)/eE\right]\ .\end{aligned} \tag{14}$$

In accord with the prior exposition of this paper, this wave function is written in the Coulomb gauge. Converting to the customary gauge, in which the electric field is written in terms of only a scalar potential, results in multiplying the wave function of Eq. (14) by the phase factor $\exp[i(eEt/\hbar)x]$. The wave function in this standard gauge is then

$$\underline{\Psi}(x,t)=\chi_{n,\,k_0+eEt/\hbar}(x,E)\exp\left[-i\int_{k_0}^{k_0+eEt/\hbar}dk'\varepsilon(k',E)/eE\right]\ , \tag{15}$$

where $\chi_{n,k}(x,E)$ is the electric-field-dependent Bloch function. This exact expression has the same form as the Houston function derived when matrix elements between different electric-field-free Bloch states are neglected.[5] In the present work, by formulating the problem in terms of electric-field-dependent Bloch states, the interband matrix elements actually vanish. The actual motion, described by Eq. (15), is thus seen to be periodic in time with the period h/eEa.

IV. EQUATIONS OF MOTION WITHIN A MODIFIED KRIEGER-IAFRATE SCHEME

Krieger and Iafrate employ a different approach to determining the time evolution of a Bloch electron in a constant electric field.[3] In particular, they note that t is just a parameter in the "stationary" solutions, Eq. (6). As such, they *define* a t-dependent fiducial point for k such that

$$(k-eEt/\hbar)=K, \quad -\pi/a<K\leq\pi/a \ . \tag{16}$$

In this scheme k is an explicit function of time such that $\partial k/\partial t=eE/\hbar$ and $k-eEt/\hbar$ is independent of time. Thus, in this formulation, we see from Eq. (6) that

$$\partial\phi_{n,k}(x,t)/\partial t=(eE/\hbar)\exp[i(k-eEt/\hbar)x] \times\partial u_{n,k}(x,E)/\partial k \ . \tag{17}$$

We now can determine the time evolution of an electron prepared in a Bloch state when an electric field is applied. To obtain the electron's equations of motion within the above-described scheme, we again follow the standard projection procedure. Namely, we (a) insert Eq. (2) into Eq. (1), (b) employ Eq. (3), (c) multiply each term by $\phi^*_{n',k'}(x,t)$, and (d) integrate all terms over x to obtain

$$[\varepsilon_{n',k'}(E)-i\hbar\partial/\partial t]B_{n',k'}(t)=\sum_{n,k}B_{n,k}(t)\int_0^{Na}dx\ \phi^*_{n',k'}(x,t)[U(x,E)-V(x)+i\hbar\partial/\partial t]\phi_{n,k}(x,t) \ . \tag{18}$$

Incorporating Eqs. (6) and (17) in Eq. (18), we find

$$[\varepsilon_{n',k'}(E)-i\hbar\partial/\partial t]B_{n',k'}(t)=\sum_{n,k}B_{n,k}(t)\int_0^{Na}dx\ \exp[i(k-k')x]u^*_{n',k'}(x,t)[U(x,E)-V(x)+(ieE)\partial/\partial k]u_{n,k}(x,t) \ . \tag{19}$$

We now break up the x integration into a series of N integrations over each of the N unit cells. Exploiting the periodicity of the functions appearing within these x integrations, we obtain

$$\begin{aligned}
&[\varepsilon_{n',k'}(E)-i\hbar\partial/\partial t]B_{n',k'}(t) \\
&\quad=\sum_{n,k}B_{n,k}(t)\sum_{m=0}^{N-1}\exp[i(k-k')ma] \\
&\qquad\qquad\times\int_0^a dx\ \exp[i(k-k')x]u^*_{n',k'}(x,t)[U(x,E)-V(x)+(ieE)\partial/\partial k]u_{n,k}(x,t) \\
&\quad=N\sum_n B_{n,k'}\int_0^a dx\ u^*_{n',k'}(x,t)[U(x,E)-V(x)+(ieE)\partial/\partial k']u_{n,k'}(x,t) \\
&\quad=(eE)\sum_n B_{n,k'}\int_0^a dx\ u^*_{n',k'}(x,t)(-x+i\partial/\partial k')u_{n,k'}(x,t) \ .
\end{aligned} \tag{20}$$

In passing from the first to second equality of Eq. (20), we have noted that

$$\sum_{m=0}^{N-1}\exp[i(k-k')ma]=N$$

when $k=k'$ and vanishes otherwise. In obtaining the third equality of Eq. (20) from its second equality, we have noted that $U(x,E)-V(x)=-eEx$ in the first unit cell (cf. Fig. 1). Finally, we recall from Ref. 2 [cf. Eq. (A10) of Ref. 2] that the integral which appears in the last equality of Eq. (20) vanishes:

$$\int_0^a dx\ u^*_{n',k'}(x,t)(-x+i\partial/\partial k)u_{n,k'}(x,t)=0 \ . \tag{21}$$

Thus, using Eq. (21) in Eq. (20), we find the equations of motion in the scheme in which (1) k varies linearly with time, and (2) the electric-field-dependent alteration of the potential wells of the solid is incorporated into the Bloch states. Specifically, the equations of motion are

$$[\varepsilon_{n,k(t)}(E)-i\hbar\partial/\partial t]B_{n,k(t)}(t)=0 \ , \tag{22}$$

where for ease of notation n' and k' have been replaced by n and k. In addition, k has been written as $k(t)$ in the subscripts of Eq. (22) to emphasize that k is an explicit function of time within this approach.

To compare the equations of motion within the two schemes [Eqs. (22) and (11)], we rewrite the t differentiation of Eq. (22) to obtain

$$[\varepsilon_{n,k(t)}(E)-i\hbar\partial B_{n,k(t)}(t)/\partial t]\,|_k=ieE\partial B_{n,k(t)}(t)/\partial k\,|_t \ , \tag{23}$$

where we have noted that $\partial k/\partial t=eE/\hbar$ in the formulation in which k varies linearly with t. Thus, Eqs. (11) and (22) are equivalent to one another. That is, Eq. (22) emerges in a formulation in which k varies linearly with time, while Eq. (11) describes the motion when k is regarded as independent of time.

V. SUMMARY AND CONCLUSIONS

In this work we have considered the evolution in time of an electron in a periodic one-dimensional chain under the influence of a constant electric field. The potential energy associated with the application of the electric field to the electron is decomposed into a portion which has the periodicity of the lattice and one that does not. The periodic portion of the electric field potential energy is included within the periodic potential which is used in obtaining the system's *electric-field-dependent* Bloch states. We find that the remaining component does not produce matrix elements between these electric-field-dependent

energy bands. The absence of interband matrix elements greatly simplifies the equations of motion for the electron. In fact, the resulting equations of motion are solved exactly in Sec. III to yield a relatively simple expression for the time evolution of an electron which is initially prepared in an electric-field-dependent Bloch state.

We have obtained the equations of motion in two different schemes. The first formulation, presented in Sec. II, uses a conventional representation for the electron's quasimomenta. Namely, the quasimomenta which enumerate the Bloch states are constants. The second approach, presented in Sec. IV, is a modified version of a procedure developed by Krieger and Iafrate,[3] in which the quasimomenta are defined as being linear functions of time. Both methods yield equivalent results.

The physical picture which emerges from our work is that an electron in an arbitrarily large lattice is localized by the application of an electric field. Thus, in the absence of scattering, an electron prepared in an electric-field-dependent Bloch state exercises a periodic motion with a period of h/eEa. This Wannier-Stark localization occurs because the energetic degeneracy between adjacent sites, which characterizes quasifree motion, is lifted by the application of an electric field.

Finally, we stress that the standardly occurring interband matrix elements arise only as a result of representing the effect of altering the shape of each of the equivalent potential wells of the lattice in terms of a mixing of the electric-field-free Bloch eigenstates. We, however, include the effect of the electric-field-dependent alteration of the shape of each of the potential wells of a solid in the electric-field-dependent Bloch states which serve as a basis for our representation. Thus, interband matrix elements vanish in our approach. As a result, our procedure yields a greatly simplified description of the time development of an electron in a periodic system under the influence of a constant electric field.

ACKNOWLEDGMENTS

One of us (D.E.) performed his portion of this work with the support of the U.S. Department of Energy under Contract No. DE-AC04-76DP00789.

[1]G. H. Wannier, *Elements of Solid State Theory* (Cambridge University Press, London, 1959), pp. 190–193.
[2]D. Emin and C. F. Hart, Phys. Rev. B **36**, 7353 (1987).
[3]J. B. Krieger and G. J. Iafrate, Phys. Rev. B **33**, 5494 (1986).
[4]C. Kittel, *Quantum Theory of Solids* (Wiley, New York, 1963), pp. 190 and 191.
[5]J. Callaway, *Quantum Theory of the Solid State* (Academic, New York, 1974), Eq. (6.1.41).