Exact k-q solution for a Bloch electron in a constant electric field

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In a series of recent papers, a new method for exactly solving the Schrödinger equation for a single electron in a crystal subjected to a constant, external, electric field (Wannier-Stark problem) has been presented. In the present report, the k-q representation of J. Zak [Phys. Rev. **168**, 686 (1968)] is shown to give exactly these same results.

The k-q representation was introduced by Zak[1] who claimed that it is a natural method for exploiting the crystal symmetries of translation in real and reciprocal wave-vector space such as to reduce the complexity of the equations governing the motion of a crystal electron subjected to external fields. This method does not seem to have been applied to very many problems in solid-state physics—probably because the method is unfamiliar and also because the problems to which it has been applied have been mired in controversy. In particular the question of the existence or nonexistence of the so-called Wannier-Stark ladder states[2] and the question of Bloch oscillations have heretofore not been convincingly answered within the k-q representation approach. Emin and I have recently shown[3] that exact solutions to the time-dependent and time-independent Schrödinger equations for the electric field problem may be found in terms of electric-field-dependent (EFD) Bloch functions as suggested earlier by Wannier,[2] Kittel,[4] and others. Crucial to the derivation of these exact results is the realization that the position operator may be decomposed into two terms: one which is periodic with the periodicity of the lattice (this may be visualized as a sawtooth function) and a second term which is not periodic (a staircase function). The periodic component may be interpreted as physically no more than a polarization effect within a unit cell and as such should not induce interband transitions. This term is therefore to be included in the crystal periodic potential. We then solve the resulting Bloch equations which include this EFD term (electric field times sawtooth function) and use these EFD Bloch functions as a complete orthonormal basis in which to expand the exact solutions. The other component of the position operator is then shown to couple only k states within the *same* EFD band. The reader is referred to our papers[2,5] for further discussion.

This decomposition of the position operator into two terms is quite explicit in the k-q representation, yet a solution analogous to ours has not been previously presented. In fact, in reading discussions of the k-q representation, one gets the erroneous impression that such a solution would be incorrect. I now briefly present the essential features of the k-q representation and then derive the exact EFD Bloch solutions using the k-q method. For clarity the derivation is in one dimension; the extension to three dimensions is straightforward.

The k-q representation is a quantum-mechanical representation which uses the basis functions

$$\psi_{kq}(x)=f(kq)e^{ikx}\sum_{l=-\infty}^{\infty}e^{i2\pi l(x-q)/a}\ . \tag{1}$$

These are eigenstates of the translation operators in real and reciprocal space:

$$\begin{aligned} &T(a)\psi_{kq}(x)\equiv e^{ipa}\psi_{kq}(x)=e^{ika}\psi_{kq}(x)\ , \\ &\tau\left[\frac{2\pi}{a}\right]\psi_{kq}(x)\equiv e^{i2\pi x/a}\psi_{kq}(x) \\ &\qquad\qquad =e^{i2\pi q/a}\psi_{kq}(x)\ , \end{aligned} \tag{2}$$

where a is the lattice spacing, Na is the total length of the crystal, $\hbar=1$, and the k values are restricted to $k=2\pi j/Na$, $j=0,1,\ldots,N-1$. The $f(kq)$ are arbitrary phase factors. It is important to also note that q is restricted to $0\le q<a$. In other words q takes values in a unit cell while k takes values in the first Brillouin zone. The sum over l in Eq. (1) is a periodic representation of $\delta(x-q)$ for $0\le q<a$. It is easily shown that the $\psi_{kq}(x)$ are complete and may be chosen orthonormal;[1] namely, upon replacing $k\to 2\pi j/Na$ and henceforth using j as a label

$$\sum_{j=0}^{N-1}\int_0^a dq\,\psi_{jq}^*(x)\psi_{jq}(x')=\delta(x-x') \tag{3}$$

and

$$\int_0^{Na}dx\ \psi_{j'q'}^*(x)\psi_{jq}(x)=\delta_{j'j}\delta(q'-q)\ . \tag{4}$$

Equations (3) and (4) are actually phase dependent, depending on one's choice of $f(jq)$; however, this phase dependence is easily taken into account when deriving operator representations in the j-q representation. If we make Zak's phase choice $f(jq)=\sqrt{a/2\pi}\,e^{-i2\pi jq/Na}$ we find that, in the j-q representation, the operators p and x are represented as

$$p=-i\frac{\partial}{\partial q}\ , \tag{5}$$

$$x=\frac{iNa}{2\pi}\frac{\partial}{\partial j}+q\ . \tag{6}$$

I address the question of what the operation $\partial/\partial j$ means below.

The problem with which we are concerned, namely, finding the eigenstates and eigenvalues of a single electron in a periodic crystal potential subjected to a constant, homogeneous, external electric field, is the problem of finding solutions to Schrödinger's equation in the x representation:

$$\left[\frac{p^2}{2m}+V(x)+eEx\right]\psi_\alpha(x)=E_\alpha\psi_\alpha(x)\ . \tag{7}$$

If we expand $\psi_\alpha(x)$ in terms of the $\psi_{jq}(x)$ as

$$\psi_\alpha(x)=\sum_{j=0}^{N-1}\int_0^a dq\ C^\alpha(jq)\psi_{jq}(x) \tag{8}$$

then Schrödinger's equation is, in the j-q representation,

$$\left[\frac{1}{2m}\left[-i\frac{\partial}{\partial q}\right]^2+V(q)+eE\left[\frac{iNa}{2\pi}\frac{\partial}{\partial j}+q\right]\right]C^\alpha(jq) =E_\alpha C^\alpha(jq)\ . \tag{9}$$

That V is a function of q only is easily shown.[1] I have attempted to be quite careful and specific in discussing which values of $k=2\pi j/Na$ and q are relevant. Equation (9) is to be solved for $j=0,1,\ldots,N-1$ and $0\le q<a$; however, we may, if we wish, extend the definitions of all j- and q-dependent terms in any manner so long as consistency is maintained. Such an extension is equivalent to a phase choice for $f(jq)$. With Zak's choice of phase we have

$$\begin{aligned} &C^\alpha(j+N,q)=C^\alpha(j,q)\ ,\\ &C^\alpha(j,q+a)=e^{i2\pi j/N}C^\alpha(j,q)\ . \end{aligned} \tag{10}$$

These may be interpreted as boundary conditions for the allowed solutions of Eq. (9). Finally, since j is an integer we must determine what is to be meant by the operation $\partial/\partial j$ in the j-q representation of x. I addressed this same question in a recent Letter[5] in which I proved that one may use $\partial/\partial j$ in formal proofs so long as it ultimately operates on a function of j written in a Wannier-type representation

$$F(j)=\sum_{s=0}^{N-1}e^{i2\pi js/N}F(s) \tag{11}$$

and s is always interpreted as s mod$N$.

Since $C^\alpha(jq)$ are periodic in $j\to j+N$, the $C^\alpha(jq)$ do, in fact, have such a Wannier representation and the proof in Ref. 5 is directly applicable to the present j-q derivations.

As mentioned previously, we see that the virtue of the j-q representation (with this choice of phase) is that it explicitly decouples x into two terms: q which is periodic, and $(iNa/2\pi)(\partial/\partial j)$ which, as I shown below, does not change the EFD band indices. To proceed, first solve the following equation, where $\lambda=eE$:

$$\left[-\frac{1}{2m}\frac{\partial^2}{\partial q^2}+V(q)+\lambda q\right]F^\beta(\lambda\mid jq)=\epsilon_\beta^\lambda F^\beta(\lambda\mid jq) \tag{12}$$

subject to

$$\begin{aligned} &F^\beta(\lambda\mid j+N,q)=F^\beta(\lambda\mid j,q)\ ,\\ &F^\beta(\lambda\mid j,a)=e^{i2\pi j/N}F^\beta(\lambda\mid j,0)\ ,\\ &\frac{\partial}{\partial q}F^\beta(\lambda\mid j,a)=e^{i2\pi j/N}\frac{\partial}{\partial q}F^\beta(\lambda\mid j,0)\ . \end{aligned} \tag{13}$$

It is clear that the solutions to Eq. (12) with boundary conditions (13) are EFD Bloch functions

$$F^\beta(\lambda\mid jq)=F_n(\lambda\mid jq)\equiv e^{i2\pi jq/Na}u_n(\lambda\mid jq)\ , \tag{14}$$

where the quantum index β may now be identified with the crystal momentum j and EFD band index n. Here $u_n(\lambda\mid j,q+a)=u_n(\lambda\mid j,q)$. Since $F_n(\lambda\mid j+N,q)=F_n(\lambda\mid j,q)$ we have the Wannier representation in terms of EFD Wannier functions

$$F_n(\lambda\mid jq)=\sum_{s=0}^{N-1}e^{i2\pi js/N}w_n(\lambda\mid q-sa)\ . \tag{15}$$

We may also write

$$\epsilon_\beta^\lambda=\epsilon_n(\lambda\mid j)=\sum_{s=0}^{N-1}e^{i2\pi js/N}\epsilon_n(\lambda\mid s)$$

to derive

$$\left[-\frac{1}{2m}\frac{\partial^2}{\partial q^2}+V(q)+\lambda q\right]w_n(\lambda\mid q-sa) =\sum_{s=0}^{N-1}\epsilon_n(\lambda\mid s-s')w_n(\lambda\mid q-s'a)\ . \tag{16}$$

To solve Eq. (9) use the ansatz

$$C^\alpha(jq)=A_n^\alpha(\lambda\mid j)F_n(\lambda\mid jq)\ ,$$

where

$$A_n^\alpha(\lambda\mid j)=\sum_{s=0}^{N-1}e^{i2\pi js/N}A_n^\alpha(\lambda\mid s)\ . \tag{17}$$

This gives

$$\left[-\frac{1}{2m}\frac{\partial^2}{\partial q^2}+V(q)+\lambda q+\frac{i\lambda Na}{2\pi}\frac{\partial}{\partial j}\right]A_n^\alpha(\lambda\mid j)F_n(\lambda\mid jq) =E_\alpha A_n^\alpha(\lambda\mid j)F_n(\lambda\mid jq)\ . \tag{18}$$

Rewrite using the above Wannier representations and then sum both sides with $\sum_{j=0}^{N-1}e^{-i2\pi jl/N}$ to arrive at

$$\sum_{s=0}^{N-1}A_n^\alpha(\lambda\mid l-s)\sum_{s'=0}^{N-1}\epsilon_n(\lambda\mid s-s')w_n(\lambda\mid q-s'a)-\lambda al\sum_{s'=0}^{N-1}A_n^\alpha(\lambda\mid l-s')w_n(\lambda\mid q-s'a) =E_\alpha\sum_{s'=0}^{N-1}A_n^\alpha(\lambda\mid l-s')w_n(\lambda\mid q-s'a)\ . \tag{19}$$

Next, using the orthonormality of the Wannier functions, we have that Eq. (19) gives

$$N\delta_{nn'}\left[\sum_{s=0}^{N-1} A_n^{\alpha}(\lambda \mid l-s)\epsilon_n(\lambda \mid s-l')-\lambda a l A_n^{\alpha}(\lambda \mid l-l')\right]=N\delta_{nn'}E_{\alpha}A_n^{\alpha}(\lambda \mid l-l') \ . \tag{20}$$

It is clear from Eq. (20) that we may associate the eigenstate index α with the band index n and another index β: $\alpha \rightarrow (n',\beta)$,

$$E_{\alpha} \rightarrow E_{n'\beta}(\lambda) \ ,$$

$$A_n^{\alpha}(\lambda \mid s) \rightarrow A_n^{n'\beta}(\lambda \mid s) \ ,$$

such that $A_n^{n'\beta}=0$ unless $n'=n$ and therefore $A_n^{n\beta} \rightarrow A_n^{\beta}$. We next use the fact that $A_n^{\beta}(\lambda \mid s)$ only depends on s with values from 0 to $N-1$ (and is extended periodically modulo N) to set $l'=0$ with l with values from 0 to $N-1$. We then have that if $A_n^{\beta}(\lambda \mid s)$ and $E_{n\beta}(\lambda)$ solve

$$\sum_{s=0}^{N-1} A_n^{\beta}(\lambda \mid s)\epsilon_n(\lambda \mid l-s)=[E_{n\beta}(\lambda)+\lambda l a]A_n^{\beta}(\lambda \mid l) \tag{21}$$

that $C_n^{\beta}(\lambda \mid jq)=A_n^{\beta}(\lambda \mid j)F_n(\lambda \mid jq)$ solves Eq. (9) and therefore that

$$\psi_n^{\beta}(\lambda \mid x) \equiv \sum_{j=0}^{N-1} \int_0^a dq \ A_n^{\beta}(\lambda \mid j)F_n(\lambda \mid jq)e^{-i2\pi jq/Na}\psi_{jq}(x) \tag{22}$$

exactly solves the original Schrödinger equation, (7), with eigenvalues $E_{n\beta}(\lambda)$ given by the Nth-order secular equation (21). Equation (21) is the same equation which I had previously derived in Ref. 5 using a different approach [this is easily shown by converting Eq. (17) in Ref. 5 to Wannier representation]. Finally, using the δ-function property of $\psi_{jq}(x)$ as a function of q, Eq. (22) reduces to

$$\psi_n^{\beta}(\lambda \mid x)=\sum_{j=0}^{N-1} A_n^{\beta}(\lambda \mid j)e^{i2\pi jx/Na}u_n(\lambda \mid jx)$$

for β with values of 0 to $N-1$, which is just the form of the solution presented previously in Refs. 3 and 5. I have therefore shown that the j-q representation gives the same exact results as derived previously using different methods.

Though the preceding j-q derivation is fairly simple, I personally believe that the representation of the position operator given in Ref. 5 is more useful. In particular the j-q basis functions seem to be, in some sense, an overcomplete set. This may be seen in Eq. (20) where we have more indices than are needed for the solution. In the representation of Ref. 5 we write

$$\begin{aligned} x\psi_{nj}(x) &= x\sum_{s=0}^{N-1} e^{i2\pi js/N}w_n(x-sa) \\ &= \sum_{s=0}^{N-1}(x-sa)e^{i2\pi js/N}w_n(x-sa)+\sum_{s=0}^{N-1} sae^{i2\pi js/N}w_n(x-sa) \\ &= \sum_{s=0}^{N-1}(x-sa)e^{i2\pi js/N}w_n(x-sa)-\frac{iNa}{2\pi}\frac{\partial}{\partial j}\psi_{nj}(x) \ , \end{aligned}$$

where $\partial/\partial j$ again must be defined in terms of its effect on a Wannier representation. The first term may be rewritten using

$$\psi_{nj}(x)=e^{i2\pi jx/Na}u_{nj}(x)$$

so

$$\begin{aligned} u_{nj}(x) &= e^{-i2\pi jx/Na}\psi_{nj}(x) \\ &= e^{-i2\pi jx/Na}\sum_{s=0}^{N-1} e^{i2\pi js/N}w_n(x-sa) \\ &= \sum_{s=0}^{N-1} e^{-i2\pi j(x-sa)/Na}w_n(x-sa) \ . \end{aligned}$$

Hence

$$\sum_{s=0}^{N-1}(x-sa)e^{i2\pi js/N}w_n(x-sa)=e^{i2\pi jx/Na}\frac{iNa}{2\pi}\frac{\partial}{\partial j}u_{nj}(x) \ .$$

This looks much like the standard crystal momentum representation for x. There are, however, two differences: (1) We now understand that $\partial/\partial j$ is valid only when operating on Wannier representations (this gives rise to secular determinants, not differential equations) and (2) in our earlier papers we showed that the appropriate Bloch functions to use are the EFD Bloch functions, not the usual zero-electric-field Bloch functions.

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