

Existence of Wannier-Stark localization

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The eigenstates of an electron in an arbitrarily long periodic chain under the influence of an applied electric field are determined. The interaction of the electron with the electric field is divided into two components. The first component has the lattice periodicity and is incorporated into the system's periodic potential. It describes the electric-field-induced alteration of each of the periodic potential wells. The second component, a nonperiodic steplike function, is shown to have vanishing interband matrix elements. Indeed, it produces Wannier-Stark localization with its eigenvalues yielding Wannier-Stark ladders. Thus it is shown that the Wannier-Stark localization survives consideration of multiple electronic energy bands.

I. INTRODUCTION

In a periodic system each electronic state of each local potential well is degenerate with each corresponding state of every other local potential well. As a result of this degeneracy, the electronic eigenstates of a periodic system form bands of delocalized states which extend over the entire solid. The application of an electric field generally lifts the degeneracy between the local electronic levels. As a result, the electronic states may become localized. This localization phenomenon may be described in terms of the electric field driving an electron through a range of wave-vector values only to have it reflected at the edge of a Brillouin zone.¹

Wannier-Stark localization has been studied in a single-band tight-binding model of a one-dimensional periodic chain.² In the absence of the electric field, the electronic eigenstates and eigenvalues of the n th electronic energy band of a chain of N potential wells are

$$|n, k\rangle = N^{-1} \sum_l \exp(-ikal) |n, l\rangle \quad (1)$$

and

$$E(n, k) = E_n - 2b_n \cos(ka) . \quad (2)$$

Here k is the electronic wave vector, $-\pi/a \leq k \leq \pi/a$, a is the intersite separation, $|n, l\rangle$ is the Wannier state and E_n is the energy of the n th electronic state of the l th potential well, and $4b_n$ is the electronic bandwidth of the n th electronic energy band. The imposition of an electric field E along the direction of the chain lifts the energetic degeneracy between equivalent electronic states of different potential wells. With the neglect of interband matrix elements of the electric field perturbation to the energy of an electron of charge e , $-eEx$, the tight-binding eigenstates and eigenvalues of the infinite chain are found to be²

$$|n, m\rangle = \sum_l J_{l-m}(2b_n/eEa) |n, l\rangle \quad (3)$$

and

$$E(n, m) = E_n - (eEa)m . \quad (4)$$

Here m is an integer which serves as a site index, and $J_{l-m}(z)$ is the Bessel function of order $l-m$ and argument z . The eigenstate $|n, m\rangle$, termed a Wannier-Stark state, is a localized electronic state composed of a superposition of the Wannier states of the n th level of the system's potential wells. It is centered about the m th site with a spatial extent $\simeq 4b_n/eE$ and has the energy $E(n, m)$. The eigenvalue spectrum is a series of levels separated by the energy eEa . This energy spectrum of equally spaced electronic energy levels is termed a Wannier-Stark ladder.

Since the introduction of the concept of Wannier-Stark states, there has been concern about the significance of neglecting the matrix elements of the electric field's energy eEx between different electronic energy bands.³⁻¹² Namely, will the inclusion of interband matrix elements lift the constraint of localization? In other words, will Wannier-Stark ladders survive with the inclusion of interband matrix elements?

Here, the problem of Wannier-Stark localization is approached from a different point of view. Namely, as illustrated in Fig. 1, the fact that the application of an electric field produces two distinct effects is exploited. First, the imposition of the electric field alters the shape of each potential well in an equivalent manner. Second, the electric field shifts the energy of each equivalent potential well relative to one another by an integral multiple of eEa . These two effects have different characters. The first effect preserves the system's periodicity while the second effect does not. As such, it is only the second effect which can lead to electronic localization. Taking cognizance of this difference, the electric-field-dependent portion of the electron's potential energy is divided into the two components illustrated in Fig. 2. The saw-toothed portion maintains the system's periodicity, while the steplike portion does not.

Since the saw-toothed portion of the field-dependent

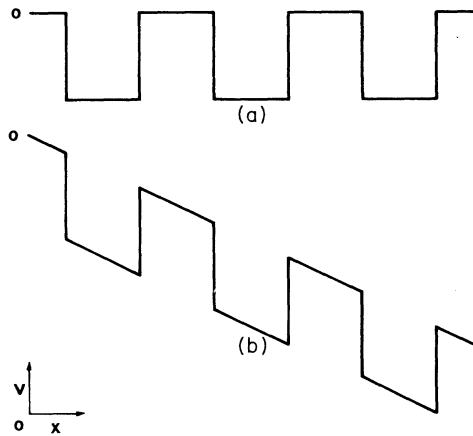


FIG. 1. A portion of a periodic (square-well) potential is shown (a) before and (b) after the application of a spatially constant electric field.

potential is periodic, it is incorporated into the system's periodic potential. The *electric-field-dependent* Bloch-like eigenstates of this periodic potential are then utilized as the basis functions for an expansion upon which the eigenfunction of the complete Hamiltonian is based. This procedure has conceptual and computational virtues. This is because this method separates the two effects of the electric field. Namely, by adopting the electric-field-dependent Bloch-like states as the basis functions, the field-dependent alteration of each of the wells of the periodic potential is exactly taken into account. Indeed, with the field-free Bloch states as the basis states, the electric-field-induced alteration of the

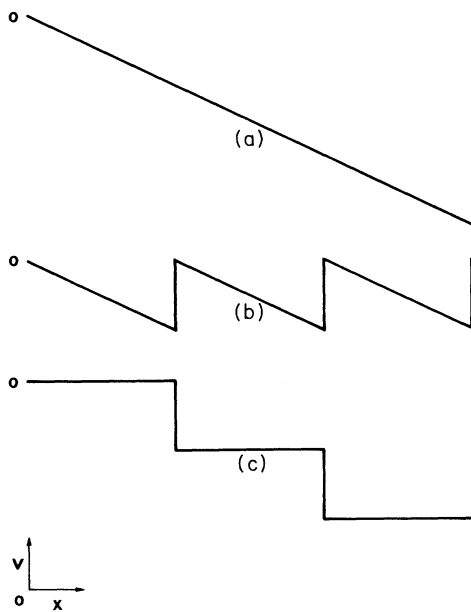


FIG. 2. The electric field potential energy $-eEx$ is plotted against x in (a), and is decomposed into periodic and non-periodic components which are shown in (b) and (c), respectively.

potential wells requires a mixing of all of the system's bands. In addition, in the present approach, the remaining portion of the electric-field-dependent term, the step-like potential, has the sole effect of providing a non-periodic potential which can localize the system's eigenfunctions.

The calculation of the system's electronic eigenfunctions and eigenvalues is presented in Sec. II. It is found that the system's eigenstates are Wannier-Stark states and the energy eigenvalues form a Wannier-Stark ladder. Furthermore, there are no matrix elements of the Hamiltonian between the electric-field-dependent Bloch states. This implies that matrix elements of $-eEx$ between field-free Bloch states arise solely from representing the polarized electronic states as a superposition of the eigenstates of the field-free potential. The paper concludes with a brief summary in Sec. III.

II. EIGENFUNCTIONS AND EIGENVALUES

Consider an electron, with charge e , placed in a one-dimensional potential of N sites under the influence of a spatially and temporally constant electric field E . The Hamiltonian for this system is

$$H = \hat{p}^2/2m + \sum_{m=1}^N V(x - ma) - eEx, \quad (5)$$

where \hat{p} is the momentum operator of the electron, m is the electron's mass, $V(x - ma)$ is that portion of the periodic potential arising from the m th potential well, and a is the separation between potential wells. The total length of the chain of N potential wells is Na .

The electric-field-dependent term of Eq. (5) may be decomposed, as illustrated in Fig. 2, into a periodic portion and a steplike component. The Hamiltonian of the system may then be reexpressed as

$$H = \hat{p}^2/2m + \sum_{m=1}^N V_E(x - ma) - (eEa) \sum_{m=1}^N S(x/a - m). \quad (6)$$

Here, $V_E(x - ma)$, the local potential, is the sum of the field-free local potential, $V(x - ma)$, and that portion of the saw-toothed component of the electric-field potential energy which is contained in the region of the m th potential well. $S(x)$ is the step function:

$$S(x) = 0 \quad \text{for } x < 1, \quad (7)$$

and

$$S(x) = 1 \quad \text{for } x \geq 1. \quad (8)$$

The periodic portion of the system's potential energy is now utilized as the periodic potential which generates electric-field-dependent Bloch-like eigenfunctions. Specifically, we adopt the first two terms of the Hamiltonian of Eq. (6) as H_E :

$$H_E = \hat{p}^2/2m + \sum_{m=1}^N V_E(x - ma). \quad (9)$$

The electric-field-dependent Bloch function associated with the n th level of the potential well, $|E;n,k\rangle$, is a solution of the eigenvalue equation

$$H_E |E;n,k\rangle = \varepsilon(E;n,k) |E;n,k\rangle. \quad (10)$$

where $\varepsilon(E;n,k)$ is the field-dependent electronic energy associated with wave vector k of the n th electronic energy band.

The eigenfunction of the total Hamiltonian, Eq. (6), belonging to the m th eigenvalue ε_m is then expressed as a superposition of the electric-field-dependent Bloch

functions:

$$\psi_m(E;x) = \sum_{n',k'} A_m(E;n',k') |E;n',k'\rangle. \quad (11)$$

With the inclusion of all energy bands, this expansion is in terms of a complete set of states which span the space defined by the solid. As such, the expansion provides an appropriate representation of the electronic states of an electron in the solid. Introducing Eq. (11) into Eq. (8) and "multiplying" through by $\langle E;n,k|$, we obtain an equation for the expansion coefficients, the $A_m(E;n,k)$'s:

$$[\varepsilon(E;n,k) - \varepsilon_m] A_m(E;n,k) = (eEa) \sum_{n',k'} \left\langle E;n,k \left| \sum_{m=1}^N S(x/a - m) \right| E;n',k' \right\rangle A_m(E;n',k'). \quad (12)$$

Proceeding to evaluate the matrix elements on the right-hand side of Eq. (12), the field-dependent Bloch functions are expressed as a product of functions:

$$|E;n',k'\rangle = \exp(ik'x) u_{E;n',k'}(x), \quad (13)$$

where the $u_{E;n',k'}(x)$'s are periodic in x :

$$u_{E;n',k'}(x + ha) = u_{E;n',k'}(x), \quad (14)$$

with h being an integer. The matrix elements are then given by the relation

$$\begin{aligned} \left\langle E;n,k \left| \sum_{m=1}^N S(x/a - m) \right| E;n',k' \right\rangle &= \int_0^{Na} dx \exp[i(k'-k)x] u_{E;n,k}^*(x) u_{E;n',k'}(x) \sum_{m=1}^N S(x/a - m) \\ &= \sum_{m=1}^{N-1} \int_{ma}^{Na} dx \exp[i(k'-k)x] u_{E;n,k}^*(x) u_{E;n',k'}(x), \end{aligned} \quad (15)$$

where the properties of the step function have been utilized in obtaining the second equality.

Now the periodicity properties of the $u_{E;n',k'}(x)$'s, expressed in Eq. (14), are exploited in writing the matrix elements of Eq. (15) in terms of an integral over a single unit cell. Explicitly, one has

$$\begin{aligned} \left\langle E;n,k \left| \sum_{m=1}^N S(x/a - m) \right| E;n',k' \right\rangle &= \sum_{m=1}^{N-1} \sum_{p=m}^{N-1} \int_{pa}^{(p+1)a} dx \exp[i(k'-k)x] u_{E;n,k}^*(x) u_{E;n',k'}(x) \\ &= \sum_{m=1}^{N-1} \sum_{p=m}^{N-1} \exp[i(k'-k)pa] \int_0^a dx \exp[i(k'-k)x] u_{E;n,k}^*(x) u_{E;n',k'}(x) \\ &= I(n,k;n',k') \sum_{m=1}^{N-1} \sum_{p=m}^{N-1} \exp[i(k'-k)pa]. \end{aligned} \quad (16)$$

In obtaining this result, each of the integrals over x in Eq. (15) first is expressed as a summation of integrals over individual unit cells. Then, x is replaced successively by $x - pa$ in each integral of the p summation. Because of the periodicity relationships given in Eq. (14), each of the remaining integrals has a common value equal to

$$\begin{aligned} I(n,k;n',k') &= \int_0^a dx \exp[i(k'-k)x] \\ &\quad \times u_{E;n,k}^*(x) u_{E;n',k'}(x). \end{aligned} \quad (17)$$

Finally, it has been noted that, since this integral is independent of the cell number (i.e., the indices m and p), it can be extracted from the summations over the unit

cells.

The terms within the double summation in the final equality of Eq. (16) may be rearranged so as to yield the relationship

$$\sum_{m=1}^{N-1} \sum_{p=m}^{N-1} \exp[i(k'-k)pa] = \sum_{m=0}^{N-1} m \exp[i(k'-k)ma]. \quad (18)$$

We evaluate this m summation by expressing it as the derivative with respect to k' of a different m summation which is then evaluated using the sum rule for the quasi-momenta, the k 's. Explicitly, we have

$$\begin{aligned} \sum_{m=0}^{N-1} m \exp[i(k'-k)ma] &= \frac{1}{ia} \frac{\partial}{\partial k'} \sum_{m=0}^{N-1} \exp[i(k'-k)ma] \\ &= \frac{N}{ia} \frac{\partial}{\partial k'} \delta_{k,k'}, \end{aligned} \quad (19)$$

where $\delta_{k,k'}=0$ for $k \neq k'$ and $\delta_{k,k'}=1$ for $k=k'$. With the incorporation of Eqs. (18) and (19) into Eq. (16), we have

$$\begin{aligned} \left\langle E;n,k \left| \sum_{m=1}^N S(x/a-m) \right| E;n',k' \right\rangle \\ = I(n,k;n',k') \frac{N}{ia} \frac{\partial}{\partial k'} \delta_{k,k'}. \end{aligned} \quad (20)$$

The expansion coefficients, the $A_m(E;n,k)$'s, may now be found. In particular, we substitute Eq. (20) into Eq. (12), reexpress the derivative of the delta function, and use the relations derived in the Appendix,

$$\delta_{k,k'} NI(n,k;n',k) = \delta_{n,n'} \delta_{k,k'}$$

and

$$\delta_{k,k'} \frac{\partial}{\partial k'} I(n,k;n',k') = 0,$$

to obtain

$$\begin{aligned} [\varepsilon(E;n,k) - \varepsilon_m] A_m(E;n,k) &= -ieEN \sum_{n',k'} I(n,k;n',k') \frac{\partial}{\partial k'} (\delta_{k,k'}) A_m(E;n',k') \\ &= ieEN \sum_{n',k'} \delta_{k,k'} \frac{\partial}{\partial k'} [A_m(E;n',k') I(n,k;n',k')] \\ &= ieE \frac{\partial}{\partial k} A_m(E;n,k). \end{aligned} \quad (21)$$

We see that the expansion coefficients associated with different energy bands are independent of one another. Thus the expansion coefficients are found by integrating this differential equation:

$$A_m(E;n,k) = \exp \left[-i \int_0^k dk' [\varepsilon(E;n,k') - \varepsilon_m] / eE \right], \quad (22)$$

with $A_m(E;n',k)=0$ for $n' \neq n$. Indeed, it has previously been argued that the interband matrix elements of a steplike potential vanish.¹³

The energy eigenvalues are found by requiring that the wave function, and hence these expansion coefficients, be single valued with respect to a shift of the wave vector by a reciprocal-lattice vector to an identical point;¹⁴ $A_m(E;n,k+2\pi/a)$ must equal $A_m(E;n,k)$. Utilizing Eq. (22), this periodicity requirement is expressed as

$$\int_0^{2\pi/a} dk' [\varepsilon(E;n,k') - \varepsilon_m] / eE = 2\pi M, \quad (23)$$

where M is an integer. The energy eigenvalue then must satisfy the condition

$$\varepsilon_m = (eEa)M + (a/2\pi) \int_0^{2\pi/a} dk' \varepsilon(E;n,k'). \quad (24)$$

Thus different eigenvalues, characterized by different values of m , correspond to different values of the integer M and energy-band index n . The Wannier-Stark ladder is evident: Different energy eigenvalues associated with a given energy band are separated by integral multiples of the field-related portion of the energy, eEa . These separate Stark ladders form an interpenetrating system of eigenvalues which essentially form a quasicontinuum in the energy eigenvalue spectrum. This agrees with other studies of the eigenvalue spectrum for this prob-

lem.¹⁵

The eigenfunctions associated with the expansion coefficients of Eq. (22) are localized. These Wannier-Stark localized states have the properties which characterize the specific example cited in Eq. (3) of the Introduction of this paper. To observe that these states are indeed localized, one may insert Eq. (22) into Eq. (11) and represent the Bloch states as a superposition of localized Wannier states, as given by Eq. (A6). Aside from spatial oscillations, the wave function associated with a particular value of M falls off as the distance of site p from the eigenfunction's center at Ma , $|p-M|a$, becomes sufficiently large that the predominant k dependence within the k summation of Eq. (11) is provided by $\exp[ika(p-M)]$. Then, when $|p-M|a \gg \varepsilon(E;n,k)/eE$ for all k ($\approx b_n/eE$), the spatial decay is caused by the canceling contributions to the k summations from essentially all values of k .

III. SUMMARY AND CONCLUSIONS

The application of an electric field to a periodic chain produces two distinct effects. The imposition of the field alters the shape of each of the potential wells. In addition, it shifts the potential energy of each well relative to one another. The first effect preserves the system's periodicity while the second does not. The Wannier-Stark localization, therefore, only arises from the second effect.

As illustrated in Fig. 2, both effects are included when the total electric-field-related energy $-eEx$ is treated as a perturbation on the field-free bands. However, treating the first effect, the electronic polarization resulting from the electric-field-induced deformations of the potential wells, in such a scheme is extremely difficult.

Namely, the electronic polarization resulting from deforming each of the system's potential wells from its field-free form mixes *all* of the system's field-free electronic energy bands. Thus it is cumbersome, if not impossible, to adequately represent the electronic eigenstates in the presence of an electric field in terms of the field-free electronic energy bands.

Here, an alternative procedure is adopted. Namely, from the outset, the periodic portion of the electric field portion of the electronic energy is incorporated into the electron's periodic potential. This produces an electric-field-dependent electronic band structure. The electronic eigenstates which result upon inclusion of the nonperiodic, steplike, portion of the electron's potential energy are then represented as a superposition of the Bloch-like electric-field-dependent electronic states. In this scheme there is no mixing between different bands of the electric-field-dependent electronic states. As a result, the calculation is readily performed. It is found that the electronic eigenvalues are interpenetrating Wannier-Stark ladders. Put another way, Wannier-Stark localization survives when multiple electronic energy bands are considered.

Thus the incorporation of the electric-field-induced deformation of the potential wells into the periodic potential of the zeroth-order Hamiltonian, Eq. (9), eliminates the interband matrix elements. Physically, this means that the interband matrix elements of $-eEx$ which occur in the usual formulation *only* arise as a means of representing the electronic polarization due to the deformation of every potential well in terms of a superposition of the field-free Bloch states. In other words, the usual interband terms are simply due to the field-dependent alteration of the *shapes* of the potential wells. They are not related to the existence of Wannier-Stark localization.

It should be noted that simple Wannier-Stark localization will only exist if the length of the sample in the direction of the applied electric field is very much longer than the spatial extent of a Wannier-Stark state. If this

is not the case, the boundary conditions provide a significant perturbation for a large fraction of the system's electronic states. This size effect can destroy a Wannier-Stark ladder.⁶ The spatial extent of a Wannier-Stark state is $\simeq W/eE$, where W is the electronic bandwidth of the relevant electronic energy band. Thus the existence of a Wannier-Stark ladder requires that the relevant length (Na for our periodic chain) greatly exceed W/eE . With an electronic bandwidth of 2 eV and an electric field strength of 10^6 V/cm, this restricts the Wannier-Stark ladder to structures of *much* greater width than 200 Å.

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APPENDIX: PROPERTIES OF $I(n, k; n', k')$

In this appendix we investigate the properties of the overlap function defined in Eq. (17):

$$I(n, k; n', k') = \int_0^a dx \exp[i(k' - k)x] \times u_{E; n, k}^*(x) u_{E; n', k'}(x). \quad (\text{A1})$$

We proceed by expressing matrix elements involving the Bloch functions $|E; n, k\rangle$ in terms of matrix elements evaluated within only the single unit cell defined by x lying within 0 and a .

We begin by writing the orthonormality condition between Bloch functions,

$$\langle E; n, k | E; n', k' \rangle = \delta_{n, n'} \delta_{k, k'},$$

in terms of $I(n, k; n', k')$:

$$\begin{aligned} \langle E; n, k | E; n', k' \rangle &= \int_0^{Na} dx \exp[i(k' - k)x] u_{E; n, k}^*(x) u_{E; n', k'}(x) \\ &= \sum_{p=0}^{N-1} \int_{pa}^{(p+1)a} dx \exp[i(k' - k)x] u_{E; n, k}^*(x) u_{E; n', k'}(x) \\ &= \sum_{p=0}^{N-1} \exp[i(k' - k)pa] \int_0^a dx \exp[i(k' - k)x] u_{E; n, k}^*(x) u_{E; n', k'}(x) \\ &= N \delta_{k, k'} I(n, k; n', k'). \end{aligned} \quad (\text{A2})$$

In obtaining this relation: (1) the x integration over the interval from 0 to Na is written as a sum of N intervals of length a ; (2) the periodicity of the $u_{E; n, k}(x)$'s with respect to a translation of x by multiples of a is exploited; (3) the vanishing of the p summation when $k \neq k'$ is noted; and (4) the definition of $I(n, k; n', k')$ contained in (A1) is adopted. We now combine Eq. (A2) with the orthonormality condition for Bloch functions to obtain

$$\delta_{k, k'} N I(n, k; n', k') = \delta_{k, k'} \delta_{n, n'}. \quad (\text{A3})$$

Hence, $I(n, k; n', k')$ vanishes when $k = k'$ and $n \neq n'$. Equation (A3) is the first of the two equations cited in the text above Eq. (21).

To obtain the second relation cited in the text above Eq. (21), we differentiate $I(n, k; n', k')$, as defined in (A1), with respect to k' to obtain the relation

$$N\delta_{k,k'}\frac{\partial}{\partial k'}I(n,k;n',k')=N\delta_{k,k'}\left[i\int_0^a dx xu_{E;n,k}^*(x)u_{E;n',k}(x)+\int_0^a dx u_{E;n,k}^*(x)\frac{\partial}{\partial k}u_{E;n',k}(x)\right]. \quad (\text{A4})$$

The first term of the right-hand side (rhs) of Eq. (A4) is clearly associated with electronic polarization within a unit cell. The second term of the rhs of Eq. (A4) is just the so-called polarization term which occurs in the standard expression for the matrix element of x with Bloch states^{16,17}

$$\langle E;n,k|x|E;n',k'\rangle=-i\frac{\partial}{\partial k'}(\delta_{k,k'}\delta_{n,n'})+iN\delta_{k,k'}\int_0^a dx u_{E;n,k}^*(x)\frac{\partial}{\partial k}u_{E;n',k}(x). \quad (\text{A5})$$

We now compare these two ‘‘polarization’’ terms.

The matrix element of x between Bloch states of the same value of the wave vector is now obtained by two methods. First, we express the Bloch function associated with band index n and wave vector k in terms of a superposition of Wannier functions centered about site p , $w_{E;n}(x-pa)$:

$$|E;n,k\rangle=N^{-1/2}\sum_{p=0}^{N-1}\exp(ikpa)w_{E;n}(x-pa). \quad (\text{A6})$$

This enables us to express the first term on the rhs of Eq. (A5) within a spatial representation for $k=k'$:

$$\begin{aligned} & -i\frac{\partial}{\partial k'}(\delta_{k,k'}\delta_{n,n'})|_{k=k'} \\ & =-i\delta_{k,k'}\delta_{n,n'}N^{-1}\sum_{p=0}^{N-1}\sum_{p'=0}^{N-1}(ip'a)\exp[ia(k'p'-kp)]\int_0^{Na} dx w_{E;n}^*(x-pa)w_{E;n}(x-p'a) \\ & =a\delta_{k,k'}\delta_{n,n'}N^{-1}\sum_{p=0}^{N-1}\sum_{p'=0}^{N-1}p'\delta_{p,p'} \\ & =a\delta_{k,k'}\delta_{n,n'}N^{-1}\sum_{p=0}^{N-1}p \\ & =\delta_{k,k'}\delta_{n,n'}a(N-1)/2. \end{aligned} \quad (\text{A7})$$

Here we have used the orthonormality of Wannier states of the same energy band with respect to the site indices p and p' .

Combining Eqs. (A5) and (A7), we have

$$\langle E;n,k|x|E;n',k\rangle=\delta_{n,n'}a(N-1)/2+iN\int_0^a dx u_{E;n,k}^*(x)\frac{\partial}{\partial k}u_{E;n',k}(x). \quad (\text{A8})$$

We may also obtain the matrix element of x between Bloch states of the same k by expressing the integral over the entire range of x as the sum of N integrals which each extend over a single unit cell. In particular,

$$\begin{aligned} \langle E;n,k|x|E;n',k\rangle & =\int_0^{Na} dx xu_{E;n,k}^*(x)u_{E;n',k}(x) \\ & =\sum_{p=0}^{N-1}\int_{pa}^{(p+1)a} dx xu_{E;n,k}^*(x)u_{E;n',k}(x) \\ & =\sum_{p=0}^{N-1}\int_0^a dy(y+pa)u_{E;n,k}^*(y)u_{E;n',k}(y) \\ & =\sum_{p=0}^{N-1}\int_0^a dy yu_{E;n,k}^*(y)u_{E;n',k}(y)+a\sum_{p=0}^{N-1}p\int_0^a dy u_{E;n,k}^*(y)u_{E;n',k}(y) \\ & =N\int_0^a dy yu_{E;n,k}^*(y)u_{E;n',k}(y)+a\sum_{p=0}^{N-1}p(\delta_{n,n'}/N) \\ & =N\int_0^a dy yu_{E;n,k}^*(y)u_{E;n',k}(y)+\delta_{n,n'}a(N-1)/2. \end{aligned} \quad (\text{A9})$$

In carrying out the above computation, we have (1) made the change of variable $y=x-pa$ in each integration of the p summation, (2) utilized the orthogonality condition for the Bloch states of the same wave vector with respect to the band indices n and n' , (3) evaluated two elementary summations.

Combining Eqs. (A8) and (A9) yields

$$i \int_0^a dx x u_{E;n,k}^*(x) u_{E;n',k}(x) = - \int_0^a dx u_{E;n,k}^*(x) \frac{\partial}{\partial k} u_{E;n',k}(x) . \quad (\text{A10})$$

That is, the two polarization terms in Eq. (A4) are equal in magnitude but opposite in sign. Inserting Eq. (A10) in Eq. (A4) gives the condition presented in the text above Eq. (21):

$$\delta_{k,k'} \frac{\partial}{\partial k'} I(n,k;n',k') = 0 . \quad (\text{A11})$$

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