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Wannier-Slater theorem for solids with nonuniform band structure

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The Wannier-Slater theorem for the Hamiltonian of a solid in an external field of force is generalized for solids with a nonuniform band structure, such as graded-gap mixed semiconductors. Our formulation is related to that of Gora and Williams, and their effective-mass equation is obtained if a $\vec{k}$-space Taylor expansion is permissible. This paper extends a too-restricted, earlier discussion by us in connection with transport in position-dependent band structures. The concept of a graded effective mass $\overleftrightarrow{M}$ and position-dependent band bottom E_c is derived from this treatment. It is pointed out, however, that the concept of a position-dependent effective mass has no strict quantum-mechanical validity. In the correspondence limit, Hamilton's equations lead to an acceleration which contains the effect of an external field $\overleftrightarrow{M}^{-1}\cdot\vec{F}$, plus a dissipative term which stems from the deviation in periodicity of the crystal potential.

I. INTRODUCTION

Transport in solids with a nonuniform composition is important in various types of devices, such as graded mixed semiconductors, graded heterojunctions, and others. In these cases the band structure is nonuniform, which means that the band contours such as the bottom of the conduction band or the top of the valence band depend on position, even in the absence of external fields of force. This is expressed by writing the band energies as $\mathscr{E}(\vec{k},\vec{r})$, where $\vec{k}$ denotes the crystal momentum in the Brillouin zone and $\vec{r}$ is the position. In the presence of external fields of force with potential energy $\Psi(\vec{r})$, the total energy is denoted as $E(\vec{k},\vec{r}) = \mathscr{E}(\vec{k},\vec{r}) + \Psi(\vec{r})$. The validity of the concept of position-dependent band structure needs further elucidation, however, since clearly the solution of Schrödinger's equation involves position-independent energies. This matter can be best handled with the Wannier-Slater theorem, which provides an effective Hamiltonian operator H_W for an electron in such a band structure. The total energy $E(\vec{k},\vec{r})$ then follows from H_W by the correspondence rule. Needless to say, $E(\vec{k},\vec{r})$ is a semiclassical concept, the band contours providing the classical turning points for electrons in the band; these turning points occur where the quantum-mechanical wave function damps out.

The expansion, up to orders k^2, of $\mathscr{E}(\vec{k},\vec{r})$ about the extrema of the band provides a position-dependent effective mass $m^*(\vec{r})$. This concept is, however, not without difficulty since, usually, no wave packets can be constructed from particles with variable effective mass. Clearly, the Hamiltonian operator must remain Hermitian.

The problem has been considered by a number of investigators, in particular in two basic papers by Gora and Williams.[1,2] Their papers, however, cast the problem directly in the less general effective-mass approximation. Leibler[3] provided an explicit proof of their results, but unfortunately this paper follows a very terse method, involving many details which obscure the result, and an experimental verification will scarcely yield the parameters which enter this theory. Therefore, we believe it to be useful to provide a simple proof using the method of Slater's original paper[4] for Wannier's theorem.[5] This proof also improves an earlier too-restricted computation in one of our papers on transport theory for which this problem arose[6] (see, in particular, Appendix A of Ref. 6). Other papers involving graded band structures deal with conductivity[7] and intraband magnetoabsorption.[8] Transport effects in nonuniform band structures involve terms described by "quasifields"; see our papers[6,9] and the references therein.

II. DERIVATION OF THE THEOREM

We consider band electrons in the virtual-crystal approximation; in this view the crystal potential is equal to the macroscopic weighted average of the potentials of the contributing chemical constituents. We denote the Hamiltonian due to this potential by $H_0(\lambda)+\mathscr{L}(\vec{r})H_1(\vec{r},\lambda)$; here $H_0(\lambda)$ involves the crystal potential due to the composition λ prevailing at some lattice site $\vec{l}$. In a hypothetical sample in which the composition $\lambda(\vec{l}\,)$ were periodically extended through all space, the crystal potential would everywhere be that of $H_0(\lambda)$. In the actual sample, the deviation from this potential is given by $\mathscr{L}(\vec{r})H_1(\vec{r},\lambda)$. Here $\mathscr{L}(\vec{r})$ is a slowly varying grading function, while $H_1(\vec{r},\lambda)$ is the difference in crystal potential at a point $\vec{r}$, caused by the fact that the composition varies with respect to the composition λ. As an example, consider a linearly graded mixture of two constituents A and B with crystal potentials V_A and V_B, respectively. Then, letting λ be the composition at $x=0$ where we have 100% constituent A, while at $x=d$ we have 100% constituent B, we find

$$\mathscr{L}(\vec{r})H_1(\vec{r},\lambda)=(x/d)(V_B-V_A)\ ,$$

while

$$H_0(\lambda)=V_A-(\hbar^2/2m)\nabla^2\ .$$

In special cases, e.g., that of strain or nonuniform temperature, the kinetic-energy operator must also be graded.[6]

We assume that the band electrons are also subject to potential energy due to external forces, denoted as $\Psi(\vec{r})$. Then quite generally we have

$$H=H_0(\lambda)+\mathscr{L}(\vec{r})H_1(\vec{r},\lambda)+\Psi(\vec{r})\ . \tag{2.1}$$

For the hypothetical homogeneous sample of composition λ the Bloch functions will be denoted as $\phi_{\vec{k},\beta}(\vec{r},\lambda)$, where $\vec{k}$ is the crystal momentum quantized in the first Brillouin zone, and β is the band index. For our present purpose the Bloch functions which extend throughout the crystal are not an appropriate representation. Thus we also introduce the localized Wannier functions $W_\beta(\vec{r}-\vec{l},\lambda)$; these functions peak near $\vec{r}\approx\vec{l}$, where $\vec{l}$ is a lattice vector. The Wannier functions for variable $\vec{l}$ form a complete orthogonal basis, related to the Bloch functions by[5,6]

$$\phi_{\vec{k},\beta}(\vec{r},\lambda)=N^{-1/2}\sum_{\vec{l}}e^{i\vec{k}\cdot\vec{l}}\,W_\beta(\vec{r}-\vec{l},\lambda)\ , \tag{2.2}$$

$$W_\beta(\vec{r}-\vec{l},\lambda)=N^{-1/2}\sum_{\vec{k}}e^{-i\vec{k}\cdot\vec{l}}\,\phi_{\vec{k},\beta}(\vec{r},\lambda)\ , \tag{2.3}$$

where N is the number of unit cells in the sample. Following Slater,[4] we expand the electron wave function ψ for the actual sample in the Wannier functions $W(\vec{r}-\vec{l},\lambda)$,

$$\psi(\vec{r})=\sum_{\vec{l}\,',\beta'}F_{\beta'}(\vec{l}\,')W_{\beta'}(\vec{r}-\vec{l}\,',\lambda)\ . \tag{2.4}$$

Substitution into the Schrödinger equation $H\psi=E\psi$, where E is the total energy eigenvalue, gives

$$\sum_{\vec{l}\,',\beta'}F_{\beta'}(\vec{l}\,')HW_{\beta'}(\vec{r}-\vec{l}\,',\lambda)=E\sum_{\vec{l}\,',\beta'}F_{\beta'}(\vec{l}\,')W_{\beta'}(\vec{r}-\vec{l}\,',\lambda)\ . \tag{2.5}$$

This is multiplied by $W_\beta^*(\vec{r}-\vec{l},\lambda)$ and integrated over all space. We then obtain, using the orthogonality of the Wannier functions,

$$\sum_{\vec{l}\,',\beta'}F_{\beta'}(\vec{l}\,')\int W_\beta^*(\vec{r}-\vec{l},\lambda)HW_{\beta'}(\vec{r}-\vec{l}\,',\lambda)d^3r=EF_\beta(\vec{l}\,)\ . \tag{2.6}$$

The left-hand side contains three terms, obtained by substituting (2.1). For the first term of (2.6) we find, using (2.3),

$$\begin{aligned}\sum_{\vec{l}\,',\beta'}F_{\beta'}(\vec{l}\,')\int W_\beta^*(\vec{r}-\vec{l},\lambda)H_0(\lambda)W_{\beta'}(\vec{r}-\vec{l}\,',\lambda)d^3r&=N^{-1}\sum_{\vec{l}\,',\beta'}F_{\beta'}(\vec{l}\,')\\&\quad\times\sum_{\vec{k},\vec{k}\,'}e^{i(\vec{k}\cdot\vec{l}-\vec{k}\,'\cdot\vec{l}\,')}\int\phi^*_{\vec{k},\beta}H_0(\lambda)\phi_{\vec{k}\,',\beta'}d^3r\\&=N^{-1}\sum_{\vec{L},\vec{k}}e^{i\vec{k}\cdot\vec{L}}\,\mathscr{E}_{\beta0}(\vec{k},\lambda)F_\beta(\vec{l}-\vec{L})\ ,\end{aligned} \tag{2.7}$$

where we set $\vec{L}=\vec{l}-\vec{l}\,'$; $\mathscr{E}_{\beta0}(\vec{k},\lambda)$ is the band energy in a sample of homogeneous composition λ.

For the second term of (2.6) we must evaluate

$$\sum_{\vec{l}\,',\beta'} F_{\beta'}(\vec{l}\,')\int W^*_\beta(\vec{r}-\vec{l},\lambda)\mathscr{L}(\vec{r})H_1(\vec{r},\lambda)W_{\beta'}(\vec{r}-\vec{l}\,',\lambda)d^3r \ . \tag{2.8}$$

Since $\mathscr{L}(\vec{r})$ is a slowly varying function, and $W_\beta(\vec{r}-\vec{l})$ is only appreciable for $\vec{r}$ close to $\vec{l}$, we write, with Gora and Williams,[2]

$$\begin{aligned}\int W^*_\beta(\vec{r}-\vec{l},\lambda)\mathscr{L}(\vec{r})H_1(\vec{r},\lambda)W_{\beta'}(\vec{r}-\vec{l}\,',\lambda)d^3r & \\ &\approx \tfrac{1}{2}[\mathscr{L}(\vec{l})+\mathscr{L}(\vec{l}\,')]\int W^*_\beta(\vec{r}-\vec{l},\lambda)H_1(\vec{r},\lambda)W_{\beta'}(\vec{r}-\vec{l}\,',\lambda)d^3r \\ &= \tfrac{1}{2}N^{-1}[\mathscr{L}(\vec{l})+\mathscr{L}(\vec{l}\,')]\sum_{\vec{k},\vec{k}\,'} e^{i(\vec{k}\cdot\vec{l}-\vec{k}\,'\cdot\vec{l}\,')}\int \phi^*_{\vec{k},\beta}H_1(\vec{r},\lambda)\phi_{\vec{k}\,',\beta'}d^3r \ .\end{aligned} \tag{2.9}$$

Since H_1 is similar to the crystal Hamiltonian $H_0(\lambda)$, we may, to a first approximation, assume that states of different $\vec{k}$ values are not mixed; likewise, we assume that no band mixing occurs (the latter can be easily included, however; see Ref. 1). We then write

$$\int \phi^*_{\vec{k},\beta}H_1(\vec{r},\lambda)\phi_{\vec{k}\,',\beta'}d^3r \approx S_\beta(\vec{k},\lambda)\delta_{\vec{k}\vec{k}\,'}\delta_{\beta\beta'} \ . \tag{2.10}$$

With (2.9) and (2.10) we obtain, for the second term of (2.6),

$$\tfrac{1}{2}N^{-1}\sum_{\vec{L},\vec{k}} e^{i\vec{k}\cdot\vec{L}}S_\beta(\vec{k},\lambda)F_\beta(\vec{l}-\vec{L})[\mathscr{L}(\vec{l})+\mathscr{L}(\vec{l}-\vec{L})] \ . \tag{2.11}$$

The third term is treated as in Ref. 6. We assume that Ψ induces no band-band transitions (Zener effect), and so $\beta'=\beta$; also, Ψ must vary slowly over a unit cell. We then have

$$\begin{aligned}\Psi_{\beta\beta'}(\vec{l},\vec{l}\,') &\equiv \int W^*_\beta(\vec{r}-\vec{l})\Psi(\vec{r})W_{\beta'}(\vec{r}-\vec{l}\,')d^3r \\ &\approx \tfrac{1}{2}[\Psi(\vec{l})+\Psi(\vec{l}\,')]\int W^*_\beta(\vec{r}-\vec{l})W_{\beta'}(\vec{r}-\vec{l}\,')d^3r = \Psi(\vec{l})\delta_{\vec{l}\vec{l}\,'}\delta_{\beta\beta'} \ .\end{aligned} \tag{2.12}$$

Hence the third contribution becomes $\Psi(\vec{l})F_\beta(\vec{l})$.

Finally, we collect terms and we assume that there is a continuous function $F_\beta(\vec{r})$ which at the lattice sites $\vec{l}$ takes the values $F_\beta(\vec{l})$. This is not unreasonable since in the absence of H_1 and Ψ expansion of a Bloch function yields $F_\beta(\vec{l})\propto\exp(i\vec{k}\cdot\vec{l})$; see (2.2) and (2.4). These are the lattice projections of plane waves, $F_\beta(\vec{r})\propto\exp(i\vec{k}\cdot\vec{r})$. We thus obtain

$$\begin{aligned}N^{-1}\sum_{\vec{L},\vec{k}} e^{i\vec{k}\cdot\vec{L}}\mathscr{E}_{\beta 0}(\vec{k},\lambda)F_\beta(\vec{r}-\vec{L})+\tfrac{1}{2}N^{-1}\sum_{\vec{L},\vec{k}} e^{i\vec{k}\cdot\vec{L}}S_\beta(\vec{k},\lambda)F_\beta(\vec{r}-\vec{L})[\mathscr{L}(\vec{r})+\mathscr{L}(\vec{r}-\vec{L})] & \\ +\Psi(\vec{r})F_\beta(\vec{r})=E_\beta F_\beta(\vec{r}). &\end{aligned} \tag{2.13}$$

The final reduction goes as in Slater's paper.[4] Since $\mathscr{E}_{\beta 0}(\vec{k},\lambda)$ is periodic in reciprocal-lattice space, it permits a Fourier series on the direct lattice. Thus, for the first term in (2.13) we have

$$N^{-1}\sum_{\vec{L},\vec{L}\,',\vec{k}} e^{i\vec{k}\cdot(\vec{L}+\vec{L}\,')}A_\beta(\vec{L}\,')F(\vec{r}-\vec{L})=\sum_{\vec{L}\,'}A_\beta(\vec{L}\,')e^{i\vec{L}\,'\cdot(-i\vec{\nabla})}F_\beta(\vec{r})=\mathscr{E}_{\beta 0}(-i\vec{\nabla},\lambda)F_\beta(\vec{r}) \ . \tag{2.14}$$

The second term is similarly treated. Expanding $S_\beta(\vec{k},\lambda)$ into a Fourier series on the direct lattice, we obtain, for the second term of (2.13),

$$\tfrac{1}{2}[\mathscr{L}(\vec{r})S_\beta(-i\vec{\nabla},\lambda)+S_\beta(-i\vec{\nabla},\lambda)\mathscr{L}(\vec{r})]F_\beta(\vec{r}) \ . \tag{2.15}$$

Note that the operator $S_\beta(-i\vec{\nabla},\lambda)$ works on everything to its right.

The full result for (2.13) now becomes

$$\{\mathscr{E}_{\beta 0}(-i\vec{\nabla},\lambda)+\tfrac{1}{2}[\mathscr{L}(\vec{r})S_\beta(-i\vec{\nabla},\lambda)+S_\beta(-i\vec{\nabla},\lambda)\mathscr{L}(\vec{r})]+\Psi(\vec{r})\}F_\beta(\vec{r})=E_\beta F_\beta(\vec{r}) \ . \tag{2.16}$$

This is the generalized Wannier-Slater theorem. The factor in curly brackets is the new Wannier Hamiltonian,

$$H_{W\beta}=\mathscr{E}_{\beta 0}(-i\vec{\nabla},\lambda)+\tfrac{1}{2}[\mathscr{L}(\vec{r})S_\beta(-i\vec{\nabla},\lambda)+S_\beta(-i\vec{\nabla},\lambda)\mathscr{L}(\vec{r})]+\Psi(\vec{r}) \ . \tag{2.17}$$

III. DISCUSSION

The Wannier Hamilton operator must remain Hermitian. That this is so is most easily seen from the Fourier series for $S_\beta(\vec{k},\lambda)$. Expanding the exponentials in powers of $\vec{k}$, we notice that the operator in the square brackets in (2.17) contains terms of the form

$$\Omega_n = \mathscr{L}(\vec{r})(i\vec{\nabla})^n + (i\vec{\nabla})^n \mathscr{L}(\vec{r}) \; . \tag{3.1}$$

These operators are Hermitian; they are also self-adjoint if the proper periodic boundary conditions are used on the boundary of the sample.[2] Thus the eigenvalues of (2.17) are real.

In the effective-mass approximation we write, expanding about the extrema $\vec{k}_m$ in the Brillouin zone,

$$\begin{aligned} \mathscr{E}_{\beta 0}(\vec{k},\lambda) = {} & \mathscr{E}_{\beta 0}(\vec{k}_m,\lambda) \\ & \pm \tfrac{1}{2}\hbar^2(\vec{k}-\vec{k}_m)(\vec{k}-\vec{k}_m) : \overleftrightarrow{M}_{\beta 0}^{-1} \; . \end{aligned} \tag{3.2}$$

Here $\mathscr{E}_{\beta 0}(\vec{k}_m,\lambda)$ is the band energy of a hypothetical homogeneous sample evaluated at the extrema of the band; $\overleftrightarrow{M}_{\beta 0}$ is the effective-mass tensor of such a sample. The plus sign holds near the bottom of a band (electrons) and the minus sign holds near the top of a band (holes). Further, we write

$$S_\beta(\vec{k},\lambda) = \alpha_\beta \pm \tfrac{1}{2}(\vec{k}-\vec{k}_m)(\vec{k}-\vec{k}_m) : \overleftrightarrow{\gamma}_\beta \; , \tag{3.3}$$

where for simplicity we assume that the curvature of the S function is similar to that of $\mathscr{E}_{\beta 0}(\vec{k},\lambda)$. We now find for the Wannier Hamiltonian the effective-mass form, placing the origin of $\vec{k}$ space at $\vec{k}_m$,

$$\begin{aligned} H_{W\beta} = {} & \mathscr{E}_{\beta 0}(0,\lambda) + \mathscr{L}(\vec{r})\alpha_\beta + \Psi(\vec{r}) \mp \tfrac{1}{2}\hbar^2 \overleftrightarrow{M}_{\beta 0}^{-1} : \vec{\nabla}\vec{\nabla} \\ & \mp \tfrac{1}{4}\overleftrightarrow{\gamma}_\beta : [\mathscr{L}(\vec{r})\vec{\nabla}\vec{\nabla} + \vec{\nabla}\vec{\nabla}\mathscr{L}(r)] \; . \end{aligned} \tag{3.4}$$

This is basically the same as in Eq. (7) of the paper by Gora and Williams.[2] The first two terms define a position-dependent band bottom or top,

$$\mathscr{E}_{\beta\,\text{contour}}(\vec{r}) = \mathscr{E}_{\beta 0}(0,\lambda) + \mathscr{L}(\vec{r})\alpha_\beta \; . \tag{3.5}$$

The last two terms define a position-dependent effective-mass tensor,

$$\overleftrightarrow{M}_\beta^{-1}(\vec{r}) = \overleftrightarrow{M}_{\beta 0}^{-1} + \hbar^{-2}\overleftrightarrow{\gamma}_\beta \mathscr{L}(\vec{r}) \; . \tag{3.6}$$

This effective-mass tensor has only classical significance, however (see below); in the quantum-mechanical treatment appropriate symmetrizing, not evident from (3.6) by itself, must occur.

From (3.3), (2.10), and (2.2), we also notice that

$$\begin{aligned} \alpha_\beta = S_\beta(0,\lambda) & = \int \phi_{0\beta}^{*} H_1(\vec{r},\lambda)\phi_{0\beta} d^3 r \\ & = N^{-1} \sum_{\vec{l},\vec{l}\,'} W_\beta^{*}(\vec{r}-\vec{l},\lambda) H_1(\vec{r},\lambda) W_\beta(\vec{r}-\vec{l}\,') \\ & \approx H_{1\beta} \; , \end{aligned} \tag{3.7}$$

where $H_{1\beta}$ is a matrix element between Wannier functions. Thus in (3.5) the spatial dependence of the band minimum becomes $\mathscr{L}(\vec{r})H_{1\beta}$. This is the same as in Ref. 6 [our $H_{1\beta}$ of Eq. (A18) there corresponds with our present $\mathscr{L}(\vec{r})H_{1\beta}$]. We note, however, that the spatial effective-mass dependence was missing in Ref. 6. The result (3.7) was used in Ref. 6 to compute the deformation potential for the case of elastic strain.[10,11]

We finally consider the classical or correspondence limit. We then can introduce the classical equivalent Hamiltonian by replacing in (2.17) $-i\vec{\nabla}$ by $\vec{k} = \vec{p}/\hbar$. Then we find

$$H_{\text{eq},\beta}(\vec{k},\vec{r}) = \mathscr{E}_{\beta 0}(\vec{k},\lambda) + \mathscr{L}(\vec{r}) S_\beta(\vec{k},\lambda) + \Psi(\vec{r}) \; . \tag{3.8}$$

The symmetrizing in the second term on the right-hand side has now disappeared. In (3.8), $\mathscr{E}_{\beta 0}(\vec{k},\lambda)$ is still the band energy of the hypothetical homogeneous sample of composition λ. It is now appropriate to introduce the position-dependent band energy $\mathscr{E}_\beta(\vec{k},\vec{r})$ by

$$\mathscr{E}_\beta(\vec{k},\vec{r}) = \mathscr{E}_{\beta 0}(\vec{k},\lambda) + \mathscr{L}(\vec{r}) S_\beta(\vec{k},\lambda) \; . \tag{3.9}$$

We note that this is independent of the arbitrarily chosen composition parameter λ. The total electron energy is denoted, as in our previous papers, by $E_\beta(\vec{k},\vec{r})$:

$$\begin{aligned} E_\beta(\vec{k},\vec{r}) & = \mathscr{E}_\beta(\vec{k},\vec{r}) + \Psi(r) \\ & = H_{\text{eq},\beta}(\vec{k},\vec{r}) \; . \end{aligned} \tag{3.10}$$

Let $E_\beta(\vec{k}_m,\vec{r})$ refer to the minimum $E_c(\vec{r})$ for the conduction band or maximum $E_v(\vec{r})$ for the valence band. Then noting that the remainder of the energy is kinetic energy, we have

$$E(\vec{k},\vec{r}) = E_c(\vec{r}) + W(\vec{k},\vec{r}) \tag{3.11}$$

for the conduction band, and

$$E(\vec{k},\vec{r}) = E_v(\vec{r}) - W_h(\vec{k},\vec{r}) \tag{3.12}$$

for the valence band, where W_h is the hole kinetic energy ($W_h \ge 0$). These equations, containing position-dependent kinetic energy for electrons or holes, were our starting point for the solution of the Boltzmann transport equation in Ref. 6. These results have therefore been fully justified by the present quantum-mechanical treatment.

In the correspondence limit, the motion of wave packets centered about some $\vec{\mathrm{k}}_0$ satisfies Hamilton's equations; thus we have, from (3.10),

$$\frac{d\vec{\mathrm{r}}}{dt}=\vec{\mathrm{v}}_\beta=\frac{\partial H_\beta}{\partial\vec{\mathrm{p}}}=\frac{1}{\hbar}\vec{\nabla}_{\vec{\mathrm{k}}}\mathscr{E}_\beta\ , \tag{3.13}$$

$$\vec{\mathrm{F}}_\beta=\frac{-\partial H_\beta}{\partial\vec{\mathrm{r}}}=\hbar\frac{d\vec{\mathrm{k}}}{dt}=-\vec{\nabla}E_\beta\ . \tag{3.14}$$

In view of (3.11) and (3.12), we also have

$$\vec{\mathrm{F}}_n=-\vec{\nabla}E_c-\vec{\nabla}W\ , \tag{3.15}$$

$$\vec{\mathrm{F}}_p=+\vec{\nabla}E_v-\vec{\nabla}W_h\ , \tag{3.16}$$

for the conduction band and valence band, respectively. These equations give the total external force acting on the electrons or holes. Since the Bloch velocity is now a function of position,

$$\begin{aligned}&\vec{\mathrm{v}}_\beta=\vec{\mathrm{v}}_\beta(\vec{\mathrm{k}},\vec{\mathrm{r}})\ ,\\ &\vec{\mathrm{a}}_\beta=\frac{d\vec{\mathrm{v}}_\beta}{dt}=(\vec{\nabla}\vec{\mathrm{v}}_\beta)\cdot\vec{\mathrm{v}}_\beta+\frac{1}{\hbar^2}\vec{\nabla}_{\vec{\mathrm{k}}}\vec{\nabla}_{\vec{\mathrm{k}}}\mathscr{E}_\beta\cdot\vec{\mathrm{F}}_\beta\\ &\qquad=-\overleftrightarrow{T}_\beta^{-1}\cdot\vec{\mathrm{v}}_\beta\pm\overleftrightarrow{M}_\beta^{-1}\cdot\vec{\mathrm{F}}_\beta\ ,\end{aligned} \tag{3.17}$$

where $\overleftrightarrow{M}_\beta^{-1}=\pm\vec{\nabla}_{\vec{\mathrm{k}}}\vec{\nabla}_{\vec{\mathrm{k}}}\mathscr{E}_\beta/\hbar^2$ is the position-dependent effective mass and where $\overleftrightarrow{T}_\beta^{-1}=-\vec{\nabla}\vec{\mathrm{v}}_\beta$ is a position-dependent relaxation-time tensor. We note the extra term $\overleftrightarrow{T}_\beta^{-1}\cdot\vec{\mathrm{v}}_\beta$ over the result for the position-independent band structure. This extra term indicates that the acceleration does not stem solely from the external field, but also from the deviation in periodicity of the crystal potential, experienced by the electrons or holes. This term provides a dissipative force, characterized by the relaxation-time tensor $\overleftrightarrow{T}$.

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