Spin-orbit coupling in superlattices

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We derive the spin-orbit coupling Hamiltonian of standard superlattices in the crystal momentum representation and discuss the effect of zone folding on spin-orbit interactions. We show that the dominant part of the spin-orbit coupling comes from the electronic motion across superlattice interfaces.

In a recent paper,[1] the author developed a band theory of superlattices, based on the crystal momentum representation. This theory did not take into account the spin-orbit interaction. In the present paper we derive the spin-orbit coupling Hamiltonian of standard superlattices in the crystal momentum representation and discuss the effect of the folding of the homogeneous crystal Brillouin zone into the superlattice Brillouin zone on spin-orbit interactions. We show that the dominant part of the spin-orbit coupling in superlattices comes from the electronic motion across interfaces.

Consider the geometry illustrated in Fig. 1, in which layers of crystals A and B alternate. Assume that the lattices of A and B match. As in Ref. 1, we begin with a finite number $\mathcal{N}$ of quantum wells in a sample of length $\mathcal{L}_z$; then, at a later stage in the calculation, we let $\mathcal{N}\rightarrow\infty$ and $\mathcal{L}_z\rightarrow\infty$, while keeping constant the density of the wells per unit length, $\rho=\mathcal{N}/\mathcal{L}_z$.

The crystal potential in a superlattice is modulated along the superlattice axis by a shape function [for odd $\mathcal{N}$; Fig. 1(a)]

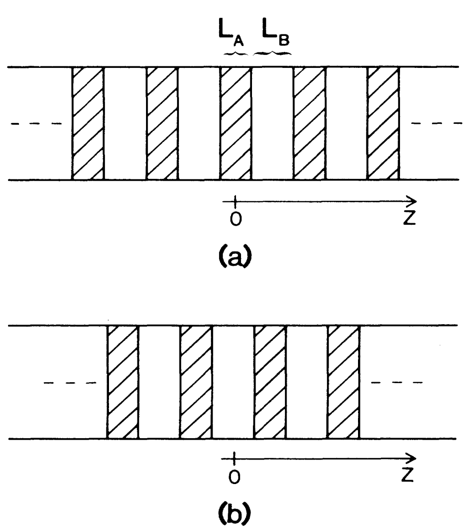

FIG. 1. Origin of the coordinates for (a) odd and (b) even $\mathcal{N}$.

$$S(z)=\sum_{n=-(\mathcal{N}-1)/2}^{(\mathcal{N}-1)/2}[\Theta(z-nL+L_A/2)-\Theta(z-nL-L_A/2)]\ , \tag{1}$$

where Θ is the step function and $L=L_A+L_B$ is the superlattice period. Since the spin-orbit coupling involves a derivative of the crystal potential, $S(z)$ leads to singular terms in the configuration space. Such singular terms are entirely appropriate under the assumption of conservation of electron current, which is equivalent to taking the electronic velocity $\mathbf{v}$ and momentum $\mathbf{p}$ ($\mathbf{p}=m\mathbf{v}$) as continuous quantities.

One can obtain the quantum-mechanical spin-orbit Hamiltonian from the classical spin-orbit coupling Hamiltonian

$$H_{\rm SO}=-e\hbar\boldsymbol{\sigma}\cdot\mathbf{B}/(2mc)\ , \tag{2}$$

where $\hbar\boldsymbol{\sigma}/2$ is spin and $\mathbf{B}$ is the magnetic field seen by the moving electron in its rest frame. $\mathbf{B}$ transforms into an electric field $\mathbf{E}$ in the crystal frame:

$$\mathbf{B}=-\mathbf{E}\times(\mathbf{v}/c)=-\mathbf{E}\times\mathbf{p}/(mc)\ . \tag{3}$$

The Thomas precession contributes a factor $\frac{1}{2}$; therefore,

$$H_{\rm SO}=-\hbar^2\sigma(e\mathbf{E}\times\mathbf{p})/(4m^2c^2)\ . \tag{4}$$

Here the superlattice electric field is determined by

$$e\mathbf{E}=-\nabla[V_B+(V_A-V_B)S]\ . \tag{5}$$

$V_{A,B}$ are the homogeneous crystal potentials. Thus, the total superlattice Hamiltonian, including the spin-orbit coupling, is given by

$$H=H_B+H_{AW}+H_{S1}+H_{S2}\ , \tag{6a}$$

where

$$H_B=\frac{\mathbf{p}^2}{2m}+V_B+\frac{\hbar}{4m^2c^2}\boldsymbol{\sigma}\cdot(\nabla V_B\times\mathbf{p})\ , \tag{6b}$$

$$H_{AW}=(V_A-V_B)S\ , \tag{6c}$$

$$H_{S1}=\frac{\hbar}{4m^2c^2}(V_A-V_B)\boldsymbol{\sigma}\cdot(\nabla S\times\mathbf{p})\ , \tag{6d}$$

and

$$H_{S2}=\frac{\hbar}{4m^2c^2}S\sigma\cdot[\nabla(V_A-V_B)\times\mathbf{p}] . \quad (6e)$$

H_{AW} is discussed in Ref. 1. H_{S1} arises from the pulse of the magnetic field that an electron senses as it crosses an interface. H_{S2} is the difference between the spin-orbit coupling Hamiltonians of the homogeneous crystals, modulated by the shape function. The magnetic field which it corresponds to has essentially the same periodicity as the homogeneous crystals.

To find the matrix elements of H in the crystal momentum representation determined by one of the homogeneous crystals, say B, we write the ordinary Bloch functions in terms of the momentum Bloch functions:

$$\psi_{n\mathbf{k}\mu}(\mathbf{x})=\frac{1}{\mathscr{V}^{1/2}}\sum_{\mathbf{G}}\phi_{n\mu}(\mathbf{k}-\mathbf{G})e^{i(\mathbf{k}-\mathbf{G})\cdot\mathbf{x}} . \quad (7)$$

Here n is the band index; μ is the spinor index ($\mu=1,2$); $\mathbf{k}$ is the electronic momentum confined to the homogeneous crystal Brillouin zone; $\mathbf{G}$ is the reciprocal lattice vector; $\phi_{n\mu}$ is the momentum Bloch function spinor component; and $\mathscr{V}$ is the crystal volume. $\phi_{n\mu}$'s obey the normalization and completeness relations[2]

$$\sum_{\mathbf{G},\mu}\phi^*_{n\mu}(\mathbf{k}-\mathbf{G})\phi_{n'\mu}(\mathbf{k}-\mathbf{G})=\delta_{nn'} , \quad (8a)$$

$$\sum_{n}\phi^*_{n\mu}(\mathbf{k}-\mathbf{G})\phi_{n\mu'}(\mathbf{k}-\mathbf{G}')=\delta_{\mu\mu'}\delta_{\mathbf{G}\mathbf{G}'} . \quad (8b)$$

Similarly,

$$\sum_{\mu}\int_{\text{cryst}}d\mathbf{x}\psi^*_{n\mathbf{k}\mu}(\mathbf{x})\psi_{n'\mathbf{k}'\mu}(\mathbf{x})=\delta_{nn'}\delta(\mathbf{k},\mathbf{k}') , \quad (9a)$$

$$\sum_{n,\mathbf{k}}\psi^*_{n\mathbf{k}\mu}(\mathbf{x})\psi_{n\mathbf{k}\mu'}(\mathbf{x}')=\delta_{\mu\mu'}\delta(\mathbf{x}-\mathbf{x}') . \quad (9b)$$

Our notation is such that, for continuous $\mathbf{k}$'s, $\delta(\mathbf{k},\mathbf{k}')=(2\pi)^3\mathscr{V}^{-1}\delta(\mathbf{k}-\mathbf{k}')$. For discrete $\mathbf{k}$'s, $\delta(\mathbf{k},\mathbf{k}')$ is the kronecker delta.

Let the spinor $\psi_\mu(\mathbf{x})$ be a solution of H with the eigenvalue ε:

$$\sum_{\mu'}H_{\mu\mu'}\psi_{\mu'}=\varepsilon\psi_\mu . \quad (10)$$

Since the set $\{\psi_{n\mathbf{k}\mu}\}$ is complete, ψ_μ can be expanded as

$$\psi_\mu(\mathbf{x})=\sum_{n,\mathbf{k}}a_n(\mathbf{k})\psi^B_{n\mathbf{k}\mu}(\mathbf{x}) . \quad (11)$$

Substituting (11) into (10), multiplying with $\psi^B_{n'\mathbf{k}'\mu}$, integrating over the crystal volume, and summing over μ, one finds the stationary Schrödinger equation in the unfolded crystal momentum representation:

$$\sum_{n',\mathbf{k}'}H_{n\mathbf{k};n'\mathbf{k}'}a_{n'}(\mathbf{k}')=\varepsilon a_n(\mathbf{k}) , \quad (12a)$$

where

$$H_{n\mathbf{k};n'\mathbf{k}'}=\sum_{\mu,\mu'}\int_{\text{cryst}}d\mathbf{x}\psi^{B*}_{n\mathbf{k}\mu}(\mathbf{x})H_{\mu\mu'}\psi^B_{n'\mathbf{k}'\mu'}(\mathbf{x}) . \quad (12b)$$

The space integrals in (12b) can be evaluated by expanding the crystal potentials:

$$V_{A,B}(\mathbf{x})=\sum_{\mathbf{G}}\mathscr{V}^{A,B}_{\mathbf{G}}e^{i\mathbf{G}\cdot\mathbf{x}} . \quad (13)$$

A typical space integral in (12b) is then of the form

$$\frac{1}{\mathscr{V}}\int_{\text{cryst}}d\mathbf{x}e^{i(\mathbf{k}-\mathbf{G}-\mathbf{k}'+\mathbf{G}')\cdot\mathbf{x}}=\delta(\mathbf{k},\mathbf{k}')\delta_{\mathbf{G}\mathbf{G}'} . \quad (14)$$

The factorization on the right-hand side of (14) is due to the fact $\mathbf{k}$ is confined to the Brillouin zone of the homogeneous crystals.

Using (6)–(9), (13), and (14), one finds

$$(H_B)_{n\mathbf{k};n'\mathbf{k}'}=\delta_{nn'}\delta(\mathbf{k},\mathbf{k}')E^B_n(\mathbf{k}) , \quad (15a)$$

$$(H_{AW})_{n\mathbf{k};n'\mathbf{k}'}=\frac{2}{\mathscr{L}_z}\sum_{\mathbf{G},\mathbf{G}',\mathbf{G}'',\mu}\delta_\perp(\mathbf{k}-\mathbf{G},\mathbf{k}'-\mathbf{G}'+\mathbf{G}'')W(\mathbf{G}'')\phi^{B*}_{n\mu}(\mathbf{k}-\mathbf{G})\phi^B_{n'\mu}(\mathbf{k}'-\mathbf{G}')$$
$$\times\frac{\sin[L_A(k_z-k_z'-G_z+G_z'-G_z'')/2]}{(k_z-k_z'-G_z+G_z'-G_z'')}\frac{\sin[\mathscr{N}L(k_z-k_z')/2]}{\sin[L(k_z-k_z')/2]} , \quad (15b)$$

$$(H_{S1})_{n\mathbf{k};n'\mathbf{k}'}=\frac{i\hbar^2}{2m^2c^2\mathscr{L}_z}\sum_{\mathbf{G},\mathbf{G}',\mathbf{G}'',\mu,\mu'}\delta_\perp(\mathbf{k}-\mathbf{G},\mathbf{k}'-\mathbf{G}'+\mathbf{G}'')W(\mathbf{G}'')\phi^{B*}_{n\mu}(\mathbf{k}-\mathbf{G})\{\sigma\cdot[\hat{\mathbf{z}}\times(\mathbf{k}'-\mathbf{G}')]\}_{\mu\mu'}\phi^B_{n'\mu'}(\mathbf{k}'-\mathbf{G}')$$
$$\times\sin[L_A(k_z-k_z'-G_z+G_z'-G_z'')/2]\frac{\sin[\mathscr{N}L(k_z-k_z')/2]}{\sin[L(k_z-k_z')/2]} , \quad (15c)$$

and

$$(H_{S2})_{n\mathbf{k};n'\mathbf{k}'}=\frac{i\hbar^2\pi}{2m^2c^2\mathscr{L}_z}\sum_{\mathbf{G},\mathbf{G}',\mathbf{G}'',\mu,\mu'}\delta_\perp(\mathbf{k}-\mathbf{G},\mathbf{k}'-\mathbf{G}'+\mathbf{G}'')W(\mathbf{G}'')\frac{\sin[\mathscr{N}L(k_z-k_z')/2]}{\sin[L(k_z-k_z')/2]}$$
$$\times\frac{\sin[L_A(k_z-k_z'-G_z+G_z'-G_z'')/2]}{(k_z-k_z'-G_z+G_z'-G_z'')}\phi^{B*}_{n\mu}(\mathbf{k}-\mathbf{G})\{\sigma\cdot[(\mathbf{k}'-\mathbf{G}')\times\mathbf{G}'']\}_{\mu\mu'}\phi^B_{n'\mu'}(\mathbf{k}'-\mathbf{G}') . \quad (15d)$$

Here, $E^B_n(\mathbf{k})$ is the band energy of the homogeneous crystal B, $\delta_\perp$ restricts only the transverse components, and

$$W(\mathbf{G})=\mathscr{V}^A_{\mathbf{G}}-\mathscr{V}^B_{\mathbf{G}} . \tag{15e}$$

In the superlattice limit, one has[1]

$$\lim_{\substack{\mathscr{N},\mathscr{L}_z\to\infty \\ \mathscr{N}/\mathscr{L}_z\to\rho}} \frac{1}{\mathscr{L}_z}\frac{\sin[\mathscr{N}L(k_z-k_z')/2]}{\sin[L(k_z-k_z')/2]}\delta_\perp(\mathbf{k}-\mathbf{G},\mathbf{k}'-\mathbf{G}'+\mathbf{G}'')=\rho\delta_\perp(\mathbf{G},\mathbf{G}'-\mathbf{G}'')\sum_l \delta\left[\mathbf{k},\mathbf{k}'+\frac{2\pi l\hat{\mathbf{z}}}{L}\right] , \tag{16}$$

where l varies over integers. According to (16), $\mathbf{k}$ and $\mathbf{k}'$ are equal modulo $(2\pi l\hat{\mathbf{z}}/L)$. This fact leads to the folding of the Brillouin zone of the homogeneous crystals into the superlattice Brillouin zone. Assume a cubic lattice for the homogeneous crystals, with one of the crystal axes along the $\hat{\mathbf{z}}$ direction. As in Ref. 1, define

$$\mathbf{k}=\boldsymbol{\kappa}+\frac{2\pi l}{L}\hat{\mathbf{z}} , \tag{17a}$$

where

$$k_x=\kappa_x , \tag{17b}$$

$$k_y=\kappa_y , \tag{17c}$$

$$-\frac{\pi}{L}<\kappa_z<\frac{\pi}{L} , \tag{17d}$$

$$l=0,\pm1,\pm2,\ldots,\pm(l_0-1) , \tag{17e}$$

$$l_0=L/a . \tag{17f}$$

a is the fundamental lattice constant of the homogeneous crystals along the $\hat{\mathbf{z}}$ axis. Define also

$$a_{nl}(\boldsymbol{\kappa})=a_n\left[\boldsymbol{\kappa}+\frac{2\pi l\hat{\mathbf{z}}}{L}\right] , \tag{18a}$$

$$E^B_{nl}(\boldsymbol{\kappa})=E^B_n\left[\boldsymbol{\kappa}+\frac{2\pi l\hat{\mathbf{z}}}{L}\right] . \tag{18b}$$

The Schrödinger equation (12a) becomes

$$\sum_{n',l'}\mathscr{H}_{nl;n'l'}(\boldsymbol{\kappa})a_{n'l'}(\boldsymbol{\kappa})=\varepsilon a_{nl}(\boldsymbol{\kappa}) , \tag{19a}$$

where

$$\mathscr{H}_{nl;n'l'}(\boldsymbol{\kappa})=\delta_{nn'}\delta_{ll'}E^B_{nl}(\boldsymbol{\kappa})+\mathscr{H}^{AW}_{nl;n'l'}(\boldsymbol{\kappa})+\mathscr{H}^{S1}_{nl;n'l'}(\boldsymbol{\kappa})+\mathscr{H}^{S2}_{nl;n'l'}(\boldsymbol{\kappa}) , \tag{19b}$$

$$\mathscr{H}^{AW}_{nl;n'l'}(\boldsymbol{\kappa})=\frac{\rho L}{\pi}\sum_{\mathbf{G},\mathbf{G}',M}W\left[\mathbf{G}'-\mathbf{G}+\frac{2\pi M\hat{\mathbf{z}}}{a}\right](-1)^{l_AM}\frac{\sin[\pi l_A(l-l')/l_0]}{(l-l'-l_0M)}$$
$$\times\sum_\mu \phi^{B*}_{n\mu}\left[\boldsymbol{\kappa}+\frac{2\pi l\hat{\mathbf{z}}}{L}-\mathbf{G}\right]\phi^B_{n'\mu}\left[\mathbf{k}+\frac{2\pi l'\hat{\mathbf{z}}}{L}-\mathbf{G}'\right] , \tag{19c}$$

$$\mathscr{H}^{S1}_{nl;n'l'}(\boldsymbol{\kappa})=\frac{i\hbar^2\rho}{2m^2c^2}\sum_{\mathbf{G},\mathbf{G}',M}W\left[\mathbf{G}'-\mathbf{G}+\frac{2\pi M\hat{\mathbf{z}}}{a}\right](-1)^{l_AM}\sin[\pi l_A(l-l')/l_0]$$
$$\times\sum_{\mu,\mu'}\phi^{B*}_{n\mu}\left[\boldsymbol{\kappa}+\frac{2\pi l\hat{\mathbf{z}}}{L}-\mathbf{G}\right]\{\boldsymbol{\sigma}\cdot[\hat{\mathbf{z}}\times(\boldsymbol{\kappa}-\mathbf{G}')]\}_{\mu\mu'}\phi^B_{n'\mu'}\left[\boldsymbol{\kappa}-\mathbf{G}'+\frac{2\pi l'\hat{\mathbf{z}}}{L}\right] , \tag{19d}$$

and

$$\mathscr{H}^{S2}_{nl;n'l'}(\boldsymbol{\kappa})=\frac{i\hbar^2\rho L}{4m^2c^2}\sum_{\mathbf{G},\mathbf{G}',M}W\left[\mathbf{G}'-\mathbf{G}+\frac{2\pi M\hat{\mathbf{z}}}{a}\right](-1)^{l_AM}\frac{\sin[\pi l_A(l-l')/l_0]}{(l-l'-l_0M)}$$
$$\times\sum_{\mu,\mu'}\phi^{B*}_{n\mu}\left[\boldsymbol{\kappa}+\frac{2\pi l\hat{\mathbf{z}}}{L}-\mathbf{G}\right]\left\{\boldsymbol{\sigma}\cdot\left[\left[\mathbf{G}-\mathbf{G}'-\frac{2\pi M\hat{\mathbf{z}}}{a}\right]\times\left[\boldsymbol{\kappa}-\mathbf{G}'+\frac{2\pi l'\hat{\mathbf{z}}}{L}\right]\right]\right\}_{\mu\mu'}$$
$$\times\phi^B_{n'\mu'}\left[\boldsymbol{\kappa}-\mathbf{G}'+\frac{2\pi l'\hat{\mathbf{z}}}{L}\right] . \tag{19e}$$

In the expressions above, M varies over all integers and $l_A = L_A/a$. Clearly, the eigenvalues of (19a) can be designated by $\varepsilon_{nl}(\boldsymbol{\kappa})$. The corresponding solution can be written as

$$\psi_{nl\mu}(\mathbf{x}) = \sum_{n',l'} a_{n'l'}^{(nl)}(\boldsymbol{\kappa}) \psi^B_{n',\boldsymbol{\kappa}+(2\pi l'\hat{\mathbf{z}}/L),\mu}(\mathbf{x}) . \tag{20}$$

Thus each superlattice subband is represented by a spinor wave function which generally does not have purely spin-up or spin-down character.

There are several interesting features of the Hamiltonian given in (19). From (19d) and (19e), one sees that the spin-orbit self-coupling of a subband occurs only through $\mathcal{H}^{S2}$, since

$$\mathcal{H}^{S1}_{nl;n'l}(\boldsymbol{\kappa}) = 0 , \tag{21a}$$

and

$$\mathcal{H}^{S2}_{nl;n'l}(\boldsymbol{\kappa}) = \frac{i\hbar^2 \pi \rho L_A}{4m^2c^2} \sum_{\mathbf{G},\mathbf{G}'} W(\mathbf{G}'-\mathbf{G}) \sum_{\mu,\mu'} \phi^{B*}_{n\mu}\left[\boldsymbol{\kappa} + \frac{2\pi l\hat{\mathbf{z}}}{L} - \mathbf{G}\right] \times \left\{\boldsymbol{\sigma}\cdot\left[(\mathbf{G}-\mathbf{G}')\times\left[\boldsymbol{\kappa}-\mathbf{G}'+\frac{2\pi l\hat{\mathbf{z}}}{L}\right]\right]\right\}_{\mu\mu'} \phi^B_{n'\mu'}\left[\boldsymbol{\kappa}-\mathbf{G}'+\frac{2\pi l\hat{\mathbf{z}}}{L}\right] . \tag{21b}$$

$\mathcal{H}^{S2}$ arises from the zone folding of the difference of the spin-orbit interactions of the homogeneous crystals A and B. The lowest-order contribution of this zone folding to the spin-orbit energy shift of a subband is given by

$$\delta\varepsilon^{S0}_{nl}(\boldsymbol{\kappa}) = \mathcal{H}^{S2}_{nl;nl}(\boldsymbol{\kappa}) . \tag{21c}$$

For $l \neq l'$, the effect of the zone folding on the spin-orbit coupling of subbands (for both $\mathcal{H}^{S1}$ and $\mathcal{H}^{S2}$) depends on the fraction l_A/l_0. Because of our assumption that the superlattice interfaces, as well as the crystal layers, are reproduced perfectly throughout the crystal, l_A/l_0 is a fixed ratio of two integers. Let int(x) designate the integer nearest to x. Two subbands l and l' are strongly coupled by the spin-orbit interactions, if

$$\text{int}[2l_A(l-l')/l_0] = 2r+1 , \tag{22a}$$

where r is an integer. l and l' are weakly coupled, or not coupled at all, if

$$\text{int}[2l_A(l-l')/l_0] = 2r . \tag{22b}$$

For example, if $2l_A = l_0$ (that is, $L_A = L_B$), l and l' are strongly coupled by the spin-orbit interactions for $l-l' = \pm1, \pm3, \pm5, \ldots$, while they are not coupled at all for $l-l' = 0, \pm2, \pm4, \ldots$. Intermediate coupling occurs for l and l' such that

$$l - l' \approx r\frac{l_0}{l_A} + \frac{l_0}{4l_A} . \tag{22c}$$

The most significant feature of the superlattice Hamiltonian is the appearance of a spin-orbit coupling due to the presence of interfaces, namely $\mathcal{H}^{S1}$. When an electron crosses an interface, it experiences a pulse of magnetic field in its rest frame. $\mathcal{H}^{S1}$ describes the coupling of this magnetic field to the electronic spin. We expect $\mathcal{H}^{S1}$ to be an order of magnitude larger than $\mathcal{H}^{S2}$, and thus to dominate the spin-orbit interactions in a superlattice. This can be seen from the fact that $W(\mathbf{G})$ obtains its largest value for $\mathbf{G}=\mathbf{0}$ and that $W(0)$ is generally an order of magnitude larger than the nearest W for finite $\mathbf{G}$.[3] Thus, if we set $M=0$ and $\mathbf{G}=\mathbf{G}'$ in (19), we find

$$\mathcal{H}^{S1}_{nl;n'l'}(\boldsymbol{\kappa}) \cong \frac{i\hbar^2 \rho W(0)}{2m^2c^2} \sin[\pi l_A(l-l')/l_0] \sum_{\mathbf{G},\mu,\mu'} \phi^{B*}_{n\mu}\left[\boldsymbol{\kappa}+\frac{2\pi l\hat{\mathbf{z}}}{L}\right] \{\boldsymbol{\sigma}\cdot[\hat{\mathbf{z}}\times(\boldsymbol{\kappa}-\mathbf{G})]\}_{\mu\mu'} \phi^B_{n'\mu'}\left[\boldsymbol{\kappa}-\mathbf{G}+\frac{2\pi l'\hat{\mathbf{z}}}{L}\right] , \tag{23a}$$

and

$$\mathcal{H}^{S2}_{nl;n'l'}(\boldsymbol{\kappa}) \cong 0 . \tag{23b}$$

$\mathcal{H}^{S1}$ can be written in terms of quantities that are related to the position and momentum operators of the electron in the homogeneous crystals. To obtain the spinor representation of the position operator, one can use

$$\sum_n \phi^*_{n\mu'}(\mathbf{k}-\mathbf{G}) \psi_{n\mathbf{k}\mu}(\mathbf{x}) = \delta_{\mu\mu'} e^{i(\mathbf{k}-\mathbf{G})\cdot\mathbf{x}} , \tag{24a}$$

which follows from the completeness relations. For fixed μ,

$$e^{i(\mathbf{k}-\mathbf{G})\cdot\mathbf{x}} = \sum_n \phi^*_{n\mu}(\mathbf{k}-\mathbf{G}) \psi_{n\mathbf{k}\mu}(\mathbf{x}) . \tag{24b}$$

The operation of $\mathbf{x}$ on $\psi_{n\mathbf{k}\mu}$ can be written as

$$\mathbf{x}\psi_{n\mathbf{k}\mu}(\mathbf{x}) = \sum_{n',\mathbf{k}',\mu'} \psi_{n'\mathbf{k}'\mu'}(\mathbf{x}) (\mathbf{x})_{n'\mathbf{k}'\mu';n\mathbf{k}\mu} . \tag{25a}$$

The left-hand side is given by

$$\mathbf{x}\psi_{n\mathbf{k}\mu}=\sum_{\mathbf{G}}\phi_{n\mu}(\mathbf{k}-\mathbf{G})\left[-i\frac{\partial}{\partial\mathbf{k}}\right]e^{i(\mathbf{k}-\mathbf{G})\cdot\mathbf{x}}$$

$$=\sum_{n',\mathbf{G}\psi_{n'\mathbf{k}\mu}}(\mathbf{x})\phi_{n\mu}(\mathbf{k}-\mathbf{G})\left[-i\frac{\partial}{\partial\mathbf{k}}\phi^{*}_{n'\mu}(\mathbf{k}-\mathbf{G})\right]. \tag{25b}$$

Thus,

$$(\mathbf{x})_{n\mathbf{k}\mu;n'\mathbf{k}'\mu'}=-i\delta_{nn'}\delta_{\mu\mu'}\frac{\partial}{\partial\mathbf{k}}\delta(\mathbf{k},\mathbf{k}')+\delta(\mathbf{k},\mathbf{k}')\mathbf{X}_{n\mu;n'\mu'}(\mathbf{k}), \tag{26a}$$

where $\mathbf{X}$ is the interband component of the position operator:

$$\mathbf{X}_{n\mu;n'\mu'}(\mathbf{k})=\delta_{\mu\mu'}\sum_{\mathbf{G}}\phi^{*}_{n\mu}(\mathbf{k}-\mathbf{G})i\frac{\partial}{\partial\mathbf{k}}\phi_{n'\mu}(\mathbf{k}-\mathbf{G}). \tag{26b}$$

Note that $\mathbf{X}$ given by (26b) is diagonal in the spinor space. This is in contrast to the discussion of Ref. 4, where it is assumed that $\mathbf{X}$ has nonvanishing matrix elements for $\mu\neq\mu'$. The representation of the momentum operator is obtained in a similar fashion:

$$\mathbf{p}\psi_{n\mathbf{k}\mu}(\mathbf{x})=\sum_{n',\mathbf{k}',\mu'}\psi_{n'\mathbf{k}'\mu'}(\mathbf{x})(\mathbf{p})_{n'\mathbf{k}'\mu';n\mathbf{k}\mu}, \tag{27a}$$

$$(\mathbf{p})_{n\mathbf{k}\mu;n'\mathbf{k}'\mu'}=\delta_{\mu\mu'}\delta(\mathbf{k},\mathbf{k}')\hbar\times\sum_{\mathbf{G}}(\mathbf{k}-\mathbf{G})\phi_{n\mu}(\mathbf{k}-\mathbf{G})\phi^{*}_{n'\mu}(\mathbf{k}-\mathbf{G}). \tag{27b}$$

It is also diagonal in the spinor space.

The interband component of the position operator can be converted into an equation for the momentum Bloch functions in the $\mathbf{k}$ space. Multiplying $\mathbf{X}_{n'\mu';n\mu}$ by $\phi_{n'\mu'}$ and using (8b), one finds

$$i\frac{\partial}{\partial\mathbf{k}}\phi_{n\mu}(\mathbf{k}-\mathbf{G})=\sum_{n',\mu'}\phi_{n'\mu'}(\mathbf{k}-\mathbf{G})\mathbf{X}_{n'\mu';n\mu}(\mathbf{k}). \tag{28}$$

This equation can be used for an approximate integration of the momentum Bloch functions. If l_0 is sufficiently large, which is almost always the case in practice, the continuous operator X_z can be replaced by a constant operator with respect to k_z in the slices of the Brillouin zone corresponding to different l's. As in Ref. 1, define

$$[\mathscr{D}^{\pm|l|}(\mathbf{k})]_{n\mu;n'\mu'}=\left[\prod_{j=0}^{|l|-1}e^{\mp i(2\pi/L)X_z(\mathbf{k}+2\pi j\hat{\mathbf{z}}/L)}\right]_{n\mu;n'\mu'}. \tag{29a}$$

Then,

$$\phi_{n\mu}\left[\mathbf{k}-\mathbf{G}+\frac{2\pi l}{L}\hat{\mathbf{z}}\right]=\sum_{n',\mu'}\phi_{n'\mu'}(\boldsymbol{\kappa}-\mathbf{G})[\mathscr{D}^{l}(\boldsymbol{\kappa})]_{n'\mu';n\mu}. \tag{29b}$$

$\mathscr{D}^{l}$ is actually diagonal in the spinor indices, because X_z is.

Finally, let us define the operator

$$\boldsymbol{\Pi}_{n\mu;n'\mu'}(\mathbf{k})=\hbar\sum_{\mathbf{G}}(\mathbf{k}-\mathbf{G})\phi^{*}_{n\mu}(\mathbf{k}-\mathbf{G})\phi_{n'\mu'}(\mathbf{k}-\mathbf{G}). \tag{30a}$$

Although not identical, $\boldsymbol{\Pi}$ is related to $\mathbf{p}$:

$$(\mathbf{p})_{n\mathbf{k}\mu;n'\mathbf{k}'\mu'}=\delta_{\mu\mu'}\delta(\mathbf{k},\mathbf{k}')\boldsymbol{\Pi}_{n\mu;n'\mu}(\mathbf{k}). \tag{30b}$$

Utilizing the results above, $\mathscr{H}^{S1}$ can be written as

$$\mathscr{H}^{S1}_{nl;n'l'}(\boldsymbol{\kappa})=\frac{i\hbar pW(0)}{2m^2c^2}\sin[\pi l_A(l-l')/l_0]\sum_{n'',n''',\mu,\mu'}[\mathscr{D}^{l\dagger}_{B}(\boldsymbol{\kappa})]_{n\mu;n''\mu}\{\boldsymbol{\sigma}_{\mu\mu'}\cdot[\hat{\mathbf{z}}\times\boldsymbol{\Pi}^{B}_{n''\mu;n'''\mu'}(\boldsymbol{\kappa})]\}[\mathscr{D}^{l'}_{B}(\boldsymbol{\kappa})]_{n'''\mu';n'\mu'}. \tag{31}$$

$\mathscr{D}^{l}_{B}$'s are related to directly measurable quantities such as the momentum matrix elements and the energy band gaps of the homogeneous crystal B. However, $\boldsymbol{\sigma}\cdot(\hat{\mathbf{z}}\times\boldsymbol{\Pi}^{B})$ is nonzero only for the matrix elements which are off-diagonal in the spinor space. This fact prohibits further simplification of the Hamiltonian into an expression involving only the momentum matrix elements. The f-sum rule[5] does not appear to be usable, since it involves sums over spinor indices, mixing the diagonal and off-diagonal spinor matrix elements.

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