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Effective-Hamiltonian theory for electrons in deformed crystals: III. Wavepacket dynamics in externally applied magnetic fields

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Abstract. A formalism for an effective-Hamiltonian description of electron dynamics in inhomogeneously distorted crystal lattices which was recently developed by Brown in 1983 and Brown and Oldfield in 1988 is extended to include the effects of an externally applied magnetic field with slow spatial variation. Spatially averaged distortion-modified operators for velocity and acceleration are derived for wavepackets constructed from suitably defined Wannier functions and simplified expressions appropriate to the small-wavevector approximation are presented for these operators. The formalism is well suited to applications concerning the effects of lattice defects on magnetic orbits and magnetotransport properties.

1. Introduction

Effective-Hamiltonian techniques were initially developed to describe conduction electron dynamics in perfect crystals. These methods allow a shift of attention from rapidly oscillating total wavefunctions to the slowly varying envelope or 'modulating function' (MF). Through the use of effective-mass parameters, they allow a free-electron-type description of electron dynamics in a crystal subject to external fields. Such a description is valid provided that the width of the wavepacket being studied is much larger than the lattice constant (Ashcroft and Mermin 1976) and provided that the fields are sensibly constant across the packet.

It has been shown (Brown 1983, Brown and Oldfield 1988, hereafter referred to as I and II, respectively) that effective-Hamiltonian methods can be applied to distorted crystals by expressing electron wavepackets as linear combinations of Wannier functions matching the local distortion. Extension of this formalism to include externally applied electromagnetic fields is desirable, thereby permitting application to galvanomagnetic, thermodynamic and transport phenomena in deformed crystals.

The case of an electric field is straightforward (simply add its potential to the deformation potential of I and II) and will not be further discussed. Several workers (see, e.g., Peierls 1933, Adams 1952, Luttinger and Kohn 1955, Wannier 1962, Kohn 1959, Blount 1962a, b, Roth 1962, 1966, Wannier and Fredkin 1962, Zak 1968, 1969, 1972) have developed effective-Hamiltonian formalisms which incorporate magnetic fields. None of these can be applied to inhomogeneously strained crystals, as is readily seen by comparing their zero-field limit with the strain-dependent effective Hamiltonian of I and II or of Bardeen and Shockley (1950). Although the methods used by the above researchers in studying magnetic fields are rather complex, they all confirm the basic correctness of the analysis of Luttinger (1951), at least for magnetic fields which vary sufficiently slowly in space. It is the aim of this paper to include magnetic field effects in the strained crystal formulation of I and II. We follow Luttinger (1951) and assume, as in II, that the distortions and their gradients are small, so that only linear terms in the distortion tensor $\boldsymbol{\beta}$ and its first derivative $\boldsymbol{\beta}'$ need to be retained. We show in § 2 that, as might be expected, the effective Hamiltonian in the presence of a magnetic field is obtained by replacing occurrences of the momentum operator $\boldsymbol{p} = -\mathrm{i}\hbar\boldsymbol{\nabla}$ by an operator $\boldsymbol{P} = \boldsymbol{p} - q\boldsymbol{A}$ containing the vector potential $\boldsymbol{A}$ of the magnetic field. In § 3, we consider the form of the effective Hamiltonian and other dynamical operators in the small-wavevector approximation. The results are summarised and discussed in § 4.

2. The effective Hamiltonian in the presence of a magnetic field

The results of this section rely heavily on those of II, to which frequent reference will be made. The notation used in II will be adopted here without further comment. Changes in the effective Hamiltonian for a charge q result from the inclusion in the one-electron Hamiltonian

$$H = (1/2m)[-\mathrm{i}\hbar\boldsymbol{\nabla} - q\boldsymbol{A}(\boldsymbol{r})]^2 + V(\boldsymbol{r}) \tag{2.1}$$

of the vector potential $\boldsymbol{A}(\boldsymbol{r})$ of the magnetic field. Operators which do not contain the one-electron Hamiltonian are clearly unchanged by magnetic field terms. Thus $D^{\mathrm{op}}_{n'n}$ (II, (2.41)) and $\zeta_{n'n}$ (II, (2.30)) and the parameters $W_{n'nq}$, $W_{n'niq}$ and $Y_{n'ni}$ (II, (2.31)–(2.33)) remain as defined in II. Furthermore, the formal definitions of $\eta_{n'n}$ (II, (2.47)) and $\tilde{H}_{n'n}$ (II, (2.58)) can be retained, if the one-electron Hamiltonian implicit in the definitions is modified as indicated by (2.1).

Evaluating the operator (cf II, (2.58))

$$\tilde{H}_{n'n} = \sum_{mm'} \sum_{t^0} (D^{-1/2})^{\mathrm{op}}_{nm'} H_{m'm} (D^{+1/2})^{\mathrm{op}}_{mn} \tag{2.2}$$

one encounters products of the type $\eta_{nm'}(\boldsymbol{R}'', \boldsymbol{t}_{R''R})\zeta_{m'n'}(\boldsymbol{R}', \boldsymbol{t}_{R'R''})$ where $\boldsymbol{R}$, $\boldsymbol{R}'$ and $\boldsymbol{R}''$ are atomic site vectors of the distorted lattice, and $\boldsymbol{t}_{R''R}$ is the distance between atomic sites in the distorted lattice, i.e. $\boldsymbol{t}_{R''R} = \boldsymbol{R} - \boldsymbol{R}''$. Here, as in II, we use the short-hand notation $\boldsymbol{t} = \boldsymbol{t}_{R'R}$. Since $\zeta_{m'n'}(\boldsymbol{R}', \boldsymbol{t}_{R'R''})$ is proportional to the distortion gradients, it is necessary to consider only the zeroth-order terms of $\eta_{nm'}(\boldsymbol{R}'', \boldsymbol{t}_{R''R})$ in such products, i.e. to first order,

$$\eta_{nm'}(\boldsymbol{R}'', \boldsymbol{t}_{R''R})\zeta_{m'n'}(\boldsymbol{R}', \boldsymbol{t}_{R'R''}) = \left(\int a^{0*}_n(\boldsymbol{r} - \boldsymbol{R}'')H^{\mathrm{hom}}(0)a^0_{m'}(\boldsymbol{r} - \boldsymbol{R})\,\mathrm{d}^3r\right)\zeta_{m'n'}(\boldsymbol{R}', \boldsymbol{t}_{R'R''}) \tag{2.3}$$

where $a^0_n(\boldsymbol{r} - \boldsymbol{R})$ is a Wannier function of the nth band of the undistorted lattice, centred at atomic site R and $H^{\mathrm{hom}}(\boldsymbol{e}_R)$ is the one-electron Hamiltonian (2.1) for a lattice which has homogeneous distortion $\boldsymbol{e}_R$ and has the same orientation as that unit cell in the inhomogeneously distorted lattice which contains $\boldsymbol{R}$.

If an externally applied magnetic field varies sufficiently slowly that it can be considered constant over the range R_0 of the Wannier functions (R_0 is of the order of the lattice constant, as discussed in II) and has a magnitude small compared with $\hbar/eR_0^2$

(Teichler 1974) (note that our R_0 corresponds to Teichler's d) then, for arbitrary $M_n(\boldsymbol{R}')$ (Luttinger 1951),

$$\sum_{t^0} H^{\text{hom}}(\boldsymbol{e}_{R'})a_n(\boldsymbol{r}-\boldsymbol{R}';\boldsymbol{e}_{R'})M_n(\boldsymbol{R}') = \sum_{t^0} a_n(\boldsymbol{r}-\boldsymbol{R}';\boldsymbol{e}_{R'})E_n(\boldsymbol{P}_{R'}/\hbar;\boldsymbol{e}_{R'})M_n(\boldsymbol{R}') \tag{2.4}$$

where we have defined operators (operating on the MFs)

$$\boldsymbol{p}_{R'} = -\mathrm{i}\hbar\boldsymbol{\nabla}_{R'} \tag{2.5}$$

$$\boldsymbol{P}_{R'} = \boldsymbol{p}_{R'} - q\boldsymbol{A}(\boldsymbol{R}') \tag{2.6}$$

and $E_n(\boldsymbol{k};\boldsymbol{e}_{R'})$ is the nth band dispersion relation for the lattice with homogeneous distortion $\boldsymbol{e}_{R'}$. The summation in (2.4) is, alternatively, over all lattice site vectors $\boldsymbol{R}'$ of the homogeneously deformed crystal since, for a fixed reference atom at $\boldsymbol{R}$, there is one-to-one correspondence between the $\boldsymbol{t}^0$ and the $\boldsymbol{R}'$. Using (2.4) in (2.3) and invoking the orthogonality of the Wannier functions allows us to write

$$\sum_{t^0_{R''R}}\sum_{t^0_{R'R''}}\sum_{m'} \eta_{nm'}(\boldsymbol{R}'',\boldsymbol{t}_{R''R})\zeta_{m'n'}(\boldsymbol{R}',\boldsymbol{t}_{R'R''}) = \sum_{t^0_{R'R}} E^0_n\left(\frac{\boldsymbol{P}_{R'}}{\hbar}\right)\zeta_{nn'}(\boldsymbol{R}',\boldsymbol{t}_{R'R}). \tag{2.7}$$

As a result, (2.2) can be written to first order (cf II, (2.59)) as

$$\tilde{H}_{n'n} = \tfrac{1}{2}\sum_{t^0}[\eta_{n'n}(\boldsymbol{R}',\boldsymbol{t}^0) + \eta^*_{nn'}(\boldsymbol{R},-\boldsymbol{t}^0)] - \tfrac{1}{4}[E^0_n(\boldsymbol{P}_{R'}/\hbar;\boldsymbol{e}_{R'})$$

$$+ E^0_{n'}(\boldsymbol{P}_{R'}/\hbar;\boldsymbol{e}_{R'})]\sum_{t^0}[\zeta_{n'n}(\boldsymbol{R}',\boldsymbol{t}^0) + \zeta^*_{nn'}(\boldsymbol{R},-\boldsymbol{t}^0)]. \tag{2.8}$$

The matrix elements of the one-electron Hamiltonian between Wannier functions of a homogeneously deformed crystal are

$$\xi_n[\boldsymbol{T}(\boldsymbol{t}^0,\boldsymbol{\beta}_{R'}),\boldsymbol{e}_{R'}] = \int a^*_n(\boldsymbol{r}-\boldsymbol{R}';\boldsymbol{e}_{R'})H^{\text{hom}}(\boldsymbol{e}_{R'})a_n(\boldsymbol{r}-\boldsymbol{R};\boldsymbol{e}_{R'})\,\mathrm{d}^3r \tag{2.9}$$

where $\boldsymbol{T} = \boldsymbol{R} - \boldsymbol{R}'$ is a lattice vector of the homogeneously deformed lattice. If (2.9) is multiplied by $\exp(-\mathrm{i}\boldsymbol{T}\cdot\boldsymbol{k})$, where $\boldsymbol{k}$ is any wavevector and summed over $\boldsymbol{R}$ (or, equivalently, $\boldsymbol{t}^0$) an analysis similar to that of Luttinger (1951) leads to the equation

$$\sum_{t^0}\xi_n[\boldsymbol{T}(\boldsymbol{t}^0,\boldsymbol{\beta}_{R'});\boldsymbol{e}_{R'}]\exp(-\mathrm{i}\boldsymbol{T}\cdot\boldsymbol{k}) = E_n\left(\boldsymbol{k}-\frac{q}{\hbar}\boldsymbol{A}(\boldsymbol{R}');\boldsymbol{e}_{R'}\right). \tag{2.10}$$

The complex conjugate of the Fourier transform of (2.10) is

$$\xi^*_n[\boldsymbol{T}(-\boldsymbol{t}^0,\boldsymbol{\beta}_{R'});\boldsymbol{e}_{R'}] = \frac{\Omega}{8\pi^3}\int \mathrm{d}^3k\, E_n\left(\boldsymbol{k}-\frac{q}{\hbar}\boldsymbol{A}(\boldsymbol{R}');\boldsymbol{e}_{R'}\right)\exp(-\mathrm{i}\boldsymbol{T}\cdot\boldsymbol{k}) \tag{2.11}$$

where the integration is over the Brillouin zone of the homogeneously deformed crystal. The validity of (2.11) allows the analysis in Appendix 3 in II to be repeated, merely replacing $E_n(\boldsymbol{k};\boldsymbol{e}_{R'})$ by $E_n(\boldsymbol{k}-(q/\hbar)\boldsymbol{A}(\boldsymbol{R}');\boldsymbol{e}_{R'})$ throughout.

Following II, we define the normalisation factor

$$\mathcal{D}(\boldsymbol{R}') = 1/[1+\Theta(\boldsymbol{R}')] \tag{2.12}$$

where $\Theta(\boldsymbol{R}')$ is the dilation at $\boldsymbol{R}'$. We define a new operator

$$\hat{H}_{n'n} = \mathcal{D}^{1/2}\tilde{H}_{n'n}\mathcal{D}^{-1/2} \tag{2.13}$$

which operates on normalised modulating functions

$$\hat{M}_n = \mathcal{D}^{1/2}\tilde{M}_n. \tag{2.14}$$

Finally, by making the replacement $-\mathrm{i}\boldsymbol{\nabla}_{R'} = \boldsymbol{k}$, we can write the effective Hamiltonian in the presence of a magnetic field in an equivalent form to that presented in II (cf II, (4.12)–(4.15))

$$\hat{H}_{n'n} = \delta_{n'n}\hat{H}_n(-\mathrm{i}\nabla/\hbar) + \hat{h}_{n'n}(-\mathrm{i}\nabla/\hbar, \boldsymbol{A}) \tag{2.15}$$

with

$$H_n(\boldsymbol{p}) = \mathscr{D}^{1/2}\{E_n(\boldsymbol{P}/\hbar; e(\boldsymbol{r})) + (\mathrm{i}/2)\beta_{ij,j}[\partial E_n^0(\boldsymbol{P}/\hbar)/\partial k_i] - (\mathrm{i}/2)\varepsilon_{\alpha,j}(\partial/\partial k_q)[\partial E_n(\boldsymbol{P}/\hbar; e)/\partial \varepsilon_\alpha]_{e=0}\}\mathscr{D}^{-1/2} \tag{2.16}$$

and

$$\hat{h}_{n'n}(\boldsymbol{p}, \boldsymbol{A}) = \tfrac{1}{2}\sum_{t^0}[Q_{n'n}(\boldsymbol{r}, \boldsymbol{t}^0) + Q^*_{nn'}(\boldsymbol{r}, -\boldsymbol{t}^0)] \tag{2.17}$$

where we have used

$$\begin{aligned} Q_{n'n}(\boldsymbol{r}, \boldsymbol{t}^0) = [\![& -\tfrac{1}{2}\beta_{qj,1}(\boldsymbol{r})t_j^0 t_1^0\{V_{n'nq}(\boldsymbol{r}, \boldsymbol{t}^0) - \tfrac{1}{2}W_{n'nq}(\boldsymbol{t}^0)[E_n^0(\boldsymbol{P}/\hbar) + E_{n'}^0(\boldsymbol{P}/\hbar)]\} \\ & - t_p^0\varepsilon_{jiq}\omega_{j,p}(\boldsymbol{r})\{V_{n'niq}(\boldsymbol{r}, \boldsymbol{t}^0) - \tfrac{1}{2}W_{n'nq}(\boldsymbol{t}^0)[E_n^0(\boldsymbol{P}/\hbar) + E_{n'}^0(\boldsymbol{P}/\hbar)]\} \\ & + t_p^0\varepsilon_{i,p}(\boldsymbol{r})\{U_{n'ni}(\boldsymbol{r}, \boldsymbol{t}^0) - \tfrac{1}{2}Y_{n'nq}(\boldsymbol{t}^0)[E_n^0(\boldsymbol{P}/\hbar) + E_{n'}^0(\boldsymbol{P}/\hbar)]\} \\ & + \beta_{kl,m}(\boldsymbol{r})I_{n'n}^{klm}(\boldsymbol{t}^0)]\!]\exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{t}^0). \end{aligned} \tag{2.18}$$

In (2.15)–(2.18) we have replaced $\boldsymbol{R}'$ by $\boldsymbol{r}$, since the MFs are now to be treated as continuous functions. The parameters $V_{n'nq}$, $V_{n'niq}$ and $U_{n'ni}$ have an explicit spatial dependence when a magnetic field is present. It will be seen that, except in the exponential term in $\hat{h}_{n'n}$, the effective Hamiltonian in the presence of a magnetic field is obtained by replacing all occurrences of $\boldsymbol{p}$ in the zero-field Hamiltonian by $\boldsymbol{P}$.

3. Effective Hamiltonian and dynamical operators in the small-wavevector approximation

As was done in I and II, the form of the effective Hamiltonian and the corresponding dynamical oprators will now be presented in the simplified form appropriate to the small-wavevector dispersion relation (cf Hunter and Nabarro 1953):

$$E_n(\boldsymbol{p}, \boldsymbol{e}) = C_n\Theta + (1/2m_n)K_{ij}^{(n)}p_ip_j \tag{3.1}$$

with

$$K_{ij}^{(n)} = \alpha^{(n)}e_{ij} + \delta_{ij}(1 + \gamma^{(n)}\Theta + \mu^{(n)}e_{(ii)}) \tag{3.2}$$

where there is no summation over the parenthetical indices.

In the calculations which follow, the explicit form of operator elements containing derivatives of the distortion will be largely ignored. Although in principle they may be calculated, their expression is complicated, conveying little physical insight. They are of little importance compared with terms in the distortion tensor itself.

Since $K_{ij}^{(n)} = K_{ji}^{(n)}$, no further symmetrisation due to the non-commutation of $\boldsymbol{p}$ and $\boldsymbol{A}$ is necessary when evaluating expressions of the type (2.16), etc, using (3.1). The dispersion relation in the presence of a magnetic field is thus

$$E_n(\boldsymbol{P}/\hbar) = C_n\Theta + (1/2m_n)K_{ij}^{(n)}P_iP_j \tag{3.3}$$

with $K_{ij}^{(n)}$ as given in (3.2). After substitution of this expression into (2.16), it is not difficult to show that

$$\hat{H}_{n'n} = \delta_{n'n}[C_n\Theta(\boldsymbol{r}) + (1/2m_n)P_iK_{ij}^{(n)}P_j] + \hat{h}_{n'n}(\boldsymbol{p}, \boldsymbol{A}) \tag{3.4}$$

with $\hat{h}_{n'n}$ as in (2.17).

Using the expressions presented in II for the spatially averaged position (II, (4.21)) and for the time derivative of an operator (II, (4.11)), the velocity operator corresponding to the effective Hamiltonian (3.4) is

$$(\hat{v}_p)_{n'n} = \delta_{n'n}(1/2m_n)(P_q K_{qp}^{(n)} + K_{qp}^{(n)} P_q) + \partial \hat{h}_{n'n}/\partial p_p. \qquad (3.5)$$

Before discussing the probability current density and the acceleration operator, we remark briefly on Hamilton's equations in relation to the effective Hamiltonian. By defining a canonical momentum operator $\boldsymbol{p}_{n'n}$ as in II (II, (4.37)) it is easy to show that Hamilton's equations (cf II, (4.36) and (4.38)) are satisfied by the effective Hamiltonian (3.4). It should be noted that in the presence of a magnetic field there are contributions to both of Hamilton's equations from terms off diagonal in the band indices, as these terms are not independent of position if $\boldsymbol{A}(\boldsymbol{r}) \neq 0$.

At this point, we introduce a notation for that part of the velocity operator which is strictly diagonal in the band indices:

$$V_p^{(n)} = (1/2m_n)(P_q K_{qp}^{(n)} + K_{qp}^{(n)} P_q). \qquad (3.6)$$

In II, we showed that a spatially averaged probability current density satisfying the usual continuity relation (cf II, (4.24)) exists for a general effective Hamiltonian. In the interests of brevity, we omit from the expressions presented here the part of the current density which is non-diagonal in the band indices. Then it is easy to show that

$$\bar{J}_p = \tfrac{1}{2}\sum_n M_n^* V_p^{(n)} M_n + \mathrm{cc} + \mathrm{O}(\beta') \qquad (3.7)$$

which, on using (3.6), becomes

$$\bar{J}_p = \sum_n \frac{1}{4m_n} M_n^* (p_q K_{qp}^{(n)} + K_{qp}^{(n)} p_q) M_n + \mathrm{cc} + \sum_n \frac{q}{m_n} A_q K_{pq}^{(n)} M_n^* M_n. \qquad (3.8)$$

In the case of zero distortion, (3.8) reduces to the usual distortion-free expression for probability current density in a magnetic field (see e.g. Landau and Lifshitz 1958).

The acceleration, given by the commutator of the effective Hamiltonian (3.4) and the velocity (3.5), is, to first order in distortions and distortion gradients,

$$\begin{aligned}(\hat{a}_q)_{n'n} = \delta_{n'n}[-(C_n/m_n)\Theta_{,i} &+ (1/m_n^2)(K_{qi,m}^{(n)} - \tfrac{1}{2}K_{im,q}^{(n)})P_i P_m + (q/2m)\varepsilon_{jmi} \\ &\times (B_j K_{qi}^{(n)} V_m^{(n)} + V_m^{(n)} K_{qi}^{(n)} B_j)] + (1/2\mathrm{i}\hbar m_n)[(\partial h_{n'n}/\partial p_q)P_i P_i \\ &- 2h_{n'n}P_q] - (1/2\mathrm{i}\hbar m_{n'})[P_i P_i(\partial h_{n'n}/\partial p_q) - 2P_q h_{n'n}]. \end{aligned} \qquad (3.9)$$

To obtain (3.9), we have used the definition of the vector potential

$$\boldsymbol{B} = \boldsymbol{\nabla} \times \boldsymbol{A} \qquad (3.10)$$

to write the commutator between the components of $\boldsymbol{P}$ as

$$[P_i, P_j] = \mathrm{i}\hbar q \varepsilon_{ijk} B_k \qquad (3.11)$$

where ε_{ijk} is the completely anti-symmetric unit tensor of third order. If distortion gradients are sufficiently small, the third term in (3.9) will dominate, as it is proportional to the distortions themselves. In the case of homogeneous distortion the acceleration is given by

$$(\hat{a}_q)_{n'n} = \delta_{n'n}(q/2m)\varepsilon_{jmi}(B_j K_{qi}^{(n)} V_m^{(n)} + V_m^{(n)} K_{qi}^{(n)} B_j) \qquad (3.12)$$

which reduces further, for zero distortion, to the form obtained using conventional effective-Hamiltonian theory applied to perfect crystals,

$$(\hat{a}_q)_{n'n} = \delta_{n'n}(q/2m_n)(\boldsymbol{B} \times \boldsymbol{V}_0^{(n)} - \boldsymbol{V}_0^{(n)} \times \boldsymbol{B}) \quad \text{where} \quad \boldsymbol{V}_0^{(n)} = (1/2m_n)(\boldsymbol{p} - q\boldsymbol{A}). \qquad (3.13)$$

4. Summary and conclusion

We have shown in § § 2 and 3 how the effective-Hamiltonian formalism developed in I and II can be extended to include the effects of an externally applied magnetic field. The modified effective Hamiltonian (2.15)–(2.18) controls the evolution of modulating functions (2.14) through a Schrödinger-like equation of type II, (4.7).

Incorporation of the effects of magnetic fields into the effective-Hamiltonian description of inhomogeneously distorted crystals opens the way to several applications. Of particular interest is the failure of the magnetoresistance of simple metals to saturate at high magnetic fields. It follows from the present formalism (Brown 1988) that dislocations, even in crystals with closed Fermi surfaces, produce real-space orbits which are not closed. Such orbits lead to a non-saturation of high-field magnetoresistance (Ashcroft and Mermin 1976, pp 236–239) and the formalism presented here provides a means of investigating this phenomenon.

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