

Effective Hamiltonians and Wavefunctions for Electrons in Deformed Crystals

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Abstract

An effective Hamiltonian for electrons in inhomogeneously deformed crystals is derived by expanding the wavefunction in terms of Wannier functions of the homogeneously deformed crystal. The physical interpretation of the modulating functions which determine the amplitude of each Wannier function in the expansion, and which are governed by the effective Hamiltonian, is investigated. This leads to strain-dependent expressions for the probability density and current, averaged over the fluctuations within each unit cell. The operators which represent, in the Hilbert space of the modulating functions, similarly averaged physical observables are introduced and explicit strain-dependent expressions for the velocity and momentum operators are obtained. Applications of the theory are foreshadowed and its relationship to previous deformation-potential theories is examined.

1. Introduction

Effective Hamiltonian (EH) methods such as those developed by Peckar (1946), Slater (1949) and Luttinger and Kohn (1955), and reviewed by Weinreich (1965) and Slater (1967), simplify the study of electron motion in crystals subjected to slowly varying potential fields arising from external sources or from certain crystal defects. The simplification is achieved by focussing attention on a slowly varying envelope function which modulates the amplitude of a fine-structured cellular component of the total wavefunction. In this way the details of the lattice potential, and of the wavefunction fluctuations within each unit cell, are effectively removed from the problem, and enter only through the band-structure parameters (effective masses) that appear in the EH, which determines the modulating function (MF).

Bardeen and Shockley (1950) and Harrison (1958) extended the EH method to describe electrons in statically deformed crystals. Its principal applications have been to the study of electron scattering by static crystal defects, notably dislocations (see Hunter and Nabarro 1953, and references therein) and, via the adiabatic principle, to the study of electron-phonon interactions (Bardeen and Shockley 1950; Sham and Ziman 1963). The book by Ziman (1960) discusses much of this work, including the associated screening effects in metals. These early papers and related work by Blount (1959), Whitfield (1961) and others will be discussed in Section 5.

The present paper considers the physical interpretation of the modulating function M which is defined by equation (3) and satisfies the effective mass equation (13) (see Section 2). Although one could conceivably regard M purely as a mathematical aid

to constructing the total wavefunction Ψ , and therefore not bother too much about its physical meaning, practically the whole point of the EH method would be lost if this view was taken. The reduction in complexity, both conceptual and mathematical, which is promised by the EH formalism, can only be realized in practice if the boundary conditions applying to (13) and the physical interpretation of its solutions can be expressed directly in terms of the MFs. For example, in applications to transport problems the relationship between the group velocity (averaged over the fluctuations within each unit cell) of a wavepacket and the MF which represents that wavepacket must be understood. This matter is not trivial since the relationship in question [see equation (38); also (24) and (31)] differs from the conventional one. This and related differences have their origin in the forms (14) and (30) of the EH, which differ from the familiar form $V - \hbar^2 \nabla^2 / 2m$ (hereafter called the 'standard form') of complete Hamiltonians. The situation is similar to the well-known modifications to the current expression etc., which accompany the introduction of a magnetic vector potential into the Hamiltonian (Landau and Lifshitz 1965, Sections 19 and 114).

In Section 2 we begin by deriving an EH for inhomogeneously deformed crystals, using a representation based on Wannier functions which are defined for the homogeneously strained crystal. This may be regarded as an extension of the method developed by Slater (1949) for undeformed crystals. It improves on the approach due to Teichler (1981), who employed the Wannier functions of the undeformed crystal, and on those due to Gutzwiller and Wells (1966), Kawamura (1978) and Brown (1979), who used atomic orbitals. Our approach is more or less equivalent to the Bloch representation adopted by Bardeen and Shockley (1950) but has certain advantages, as discussed in Section 5.

The physical interpretation of the MFs is considered in Section 3 and operators representing spatially averaged dynamical variables are introduced. In particular, strain-dependent velocity and current operators, suitable for the study of transport properties in deformed crystals, are obtained. The formulae of Section 3 are shown to reduce to familiar results for the case of uniform strain. Their application to inhomogeneous deformations is then illustrated for the case of a screw dislocation.

Following Teichler (1981) we consider in Section 4 the role of gauge transformations. We show that, except for special cases, it is impossible to reduce the EH to the standard form and hence to remove the strain dependence from the expressions for the spatially averaged current etc.

The relationship of the present work to previous theories is discussed in Section 5. Our results are summarized and possible applications of the theory, and its extension to include time-dependent deformations, are briefly discussed in Section 6.

2. Effective-mass Equation for Deformed Crystals

Let $b_n(\mathbf{k}, \mathbf{r}, \mathbf{e})$ be a Bloch function of band n and wavevector $\mathbf{k}$ in a crystal which is obtained by homogeneously straining (with strain tensor $\mathbf{e} = e_{ij}$) the original stress-free crystal of N unit cells. We define the Wannier functions

$$a_n(\mathbf{r} - \mathbf{R}, \mathbf{e}) = N^{-\frac{1}{2}} \sum_{\mathbf{k}} \exp(-i \mathbf{k} \cdot \mathbf{R}) b_n(\mathbf{k}, \mathbf{r}, \mathbf{e}), \quad (1)$$

where the sum is over the allowed wavevectors in the first Brillouin zone of the homogeneously strained crystal. The functions a_n , defined for each lattice point $\mathbf{R}$ of the homogeneously strained crystal, are mutually orthogonal and are normalized

to unity if this is so for the b_n . The a_n form a complete set suitable for the expansion of an arbitrary single-electron wavefunction of the crystal for which they are defined. Each Wannier function is more or less localized near the point $\mathbf{r} = \mathbf{R}$, the degree of localization depending on the choice of phases of the Bloch functions. The above properties are discussed by Weinreich (1965) and Callaway (1974).

The theory which follows uses the basis functions (1) defined for different homogeneous strains. In order that the Wannier functions vary continuously with strain, and hence that the wavefunction (see equation 3) varies continuously with position, it is necessary that the phases of the Bloch functions appearing in (1) should vary continuously with strain. This can be ensured by following the procedure of Weinreich (1965, Section 8.6), which specifies the phases by reference to the unit cell of the reciprocal lattice, the morphology of which changes continuously with strain. We can therefore complete the definition (1) and at the same time ensure an optimum degree of localization by choosing the Bloch phases according to Weinreich's equation (8.47). The remaining additive constant in the phase can be disposed of by requiring, say, that $b_n(0, 0, 0)$ be real and positive. We thereby obtain functions b_n , and hence a_n , which are uniquely* defined functions of the coordinates x_i and X_i of $\mathbf{r}$ and $\mathbf{R}$ respectively once the directions of the coordinate axes are specified, provided that we also specify that only pure strain, i.e. zero (rigid) rotation, is involved in passing from the unstrained state to that of uniform strain. In all that follows the coordinate axes are regarded as fixed in space; for definiteness we may imagine them chosen to lie along those directions of the unstrained crystal which are conventionally used to define the elastic moduli.

The rigorous completeness of the functions (1) allows an arbitrary wavefunction of the *homogeneously* strained crystal to be expanded as

$$\Psi^h(\mathbf{r}, t) = \Omega_0^{\frac{1}{2}} \sum_{n\mathbf{R}} M_n^h(\mathbf{R}, t) a_n(\mathbf{r} - \mathbf{R}, \mathbf{e}), \quad (2)$$

where the sum is over all bands and lattice points of the homogeneously strained crystal and we have introduced the unit-cell volume Ω_0 of the unstrained crystal. The localization of the Wannier functions implies that only those terms for which $|\mathbf{r} - \mathbf{R}|$ is less than some finite radius R_0 need be retained in the sum. This suggests that locally satisfactory basis functions for the *inhomogeneously* deformed crystal can be obtained by using the functions (1), but defined for the homogeneous strain $\mathbf{e}$ equal to the local strain $\mathbf{e}(\mathbf{r})$, and expressed as functions of coordinates obtained from those of $\mathbf{r} - \mathbf{R}$ by rotating the crystal such that the orientation of its unit cell at $\mathbf{r}$ is brought into coincidence with that of the homogeneously deformed crystal discussed above. Denoting this latter operation which ensures the correct orientation of the basis functions by the subscript 'rot', we therefore expand an arbitrary wavefunction of the arbitrarily deformed crystal as

$$\Psi(\mathbf{r}, t) = \Omega_0^{\frac{1}{2}} \sum_{n\mathbf{R}} M_n(\mathbf{R}, t) a_n\{(\mathbf{r} - \mathbf{R})_{\text{rot}}, \mathbf{e}(\mathbf{r})\}, \quad (3)$$

where the sum is now over the atomic sites of the inhomogeneously deformed crystal. The expansion of Ψ in terms of tightly bound atomic s orbitals (Gutzwiller and Wells

* We assume that any ambiguities due to degeneracies can be removed along with the degeneracies by applying an infinitesimal perturbation.

1966; Kawamura 1978; Brown 1979) is a special case of (3) for which the orientation operation is not necessary.

The basis functions employed in (3) are intuitively the best choice available for the present application. They presumably depart from strict completeness due to the nonzero gradients of strain and rotation, but if these are sufficiently small we can adopt (3) with confidence.† Using this wavefunction in the Schrödinger equation

$$H\Psi = i\hbar\partial\Psi/\partial t, \quad (4)$$

where H is the one-electron Hamiltonian of the deformed crystal, we obtain

$$i\hbar\sum_{nR}\Delta_{mn}(\mathbf{R}',\mathbf{R})\partial M_n(\mathbf{R},t)/\partial t = \sum_{nR}H_{mn}(\mathbf{R}',\mathbf{R})M_n(\mathbf{R},t), \quad (5)$$

where

$$\Delta_{mn}(\mathbf{R}',\mathbf{R}) = \int_V a_m^*\{(r-\mathbf{R}')_{\text{rot}}, \mathbf{e}(\mathbf{r})\} a_n\{(r-\mathbf{R})_{\text{rot}}, \mathbf{e}(\mathbf{r})\} d^3r, \quad (6)$$

$$H_{mn}(\mathbf{R}',\mathbf{R}) = \int_V a_m^*\{(r-\mathbf{R}')_{\text{rot}}, \mathbf{e}(\mathbf{r})\} H a_n\{(r-\mathbf{R})_{\text{rot}}, \mathbf{e}(\mathbf{r})\} d^3r. \quad (7)$$

The integrals are over the volume V of the deformed crystal. The orthonormality of the Wannier functions for homogeneous strains implies that (6) differs from $\delta_{mn}\delta_{\mathbf{R}'\mathbf{R}}$ only by terms which are negligible, provided that the relative change in deformation over the distance R_0 is small. Further, since the Wannier functions are localized near their respective atomic sites, we may neglect those H_{mn} for which $|\mathbf{R}-\mathbf{R}'|$ exceeds some fixed radius $R'_0 \approx R_0$, and then for slowly varying strains we can replace $\mathbf{e}(\mathbf{r})$ by $\mathbf{e}(\mathbf{R}')$ in (7). Finally, if we neglect corrections proportional to the gradients of the strains and rotations, we observe that not only must the lattice potential at points $\mathbf{r}$ in the neighbourhood of $\mathbf{R}'$ be identical to that in the homogeneously strained lattice of strain $\mathbf{e}(\mathbf{R}')$, but also that the orientation of the Wannier functions (as specified by the 'rot' operation) near $\mathbf{r} = \mathbf{R}'$ is also that appropriate to the homogeneously strained lattice. It follows that the integral (7) is simply the Wannier matrix element $\delta_{mn}\xi_n^h\{\mathbf{R}'-\mathbf{R}, \mathbf{e}(\mathbf{R}')\}$ of the Hamiltonian of the homogeneously strained lattice and (5) becomes

$$i\hbar\partial M_m(\mathbf{R}',t)/\partial t = \sum_{|\mathbf{R}|<R'_0}\xi_m^h\{\mathbf{R}, \mathbf{e}(\mathbf{R}')\} M_m(\mathbf{R}'-\mathbf{R},t), \quad (8)$$

where the sum is over the lattice vectors of the homogeneously strained lattice of strain $\mathbf{e}(\mathbf{R}')$. We note that the band diagonalization was not assumed but arose naturally, for slowly varying strains, from the properties of the Wannier matrix elements (Callaway 1974, equation 5.1.36).

† Following previous work (see e.g. Bardeen and Shockley 1950; Hunter and Nabarro 1953), we will subsequently neglect terms involving the gradients of both strains and rotations which contribute to the EH (14) arising from (3). This approximation is valid provided that the relative changes in strain and rotation over a distance of one wavelength of the MF are small compared with unity. This condition will normally be more critical than the possible incompleteness of the basis functions, for which the characteristic length over which the change in deformation must be small is of the order of the localization radius R_0 .

Further reduction of (8) follows if we suppose that the fractional change of M over a distance of one lattice constant is small. Then M can be regarded as a function of a continuous variable and (Slater 1967, equation A1-19)

$$\exp(-\mathbf{R} \cdot \nabla_{\mathbf{R}'}) M(\mathbf{R}', t) \equiv M(\mathbf{R}' - \mathbf{R}, t), \quad (9)$$

so that (8) becomes the differential equation

$$i\hbar \partial M_m(\mathbf{r}, t) / \partial t = E_m^h \{ -i \nabla, \mathbf{e}(\mathbf{r}) \} M_m(\mathbf{r}, t), \quad (10)$$

where we have written (Callaway 1974, equation 5.1.38)

$$\sum_{|\mathbf{R}| < R_0} \xi_m^h \{ \mathbf{R}, \mathbf{e}(\mathbf{R}') \} \exp(-i \mathbf{k} \cdot \mathbf{R}) = E_m^h \{ \mathbf{k}, \mathbf{e}(\mathbf{R}') \}, \quad (11)$$

the dispersion relation for the crystal of homogeneous strain $\mathbf{e}(\mathbf{R}')$. Note that by incorporating the elastic rotations into the arguments of the Wannier functions of (3) we arrive at MFs which, by equation (10), depend only on the (symmetric) strain tensor.

Equation (10) which governs the evolution of the MFs is the main result of this section. To see its implications we consider an unstrained crystal of cubic symmetry and write (Hunter and Nabarro 1953) for a given band

$$\begin{aligned} E^h(\mathbf{k}, \mathbf{e}) = E_1 \Theta + \frac{\hbar^2 k^2}{2m_1} \left\{ 1 + \Theta \left(\frac{m_1}{m_2} - \frac{m_1}{3m_3} \right) \right\} \\ + \frac{\hbar^2}{2m_3} e_{ij} k_i k_j + \frac{\hbar^2}{2m_4} (e_{11} k_1^2 + e_{22} k_2^2 + e_{33} k_3^2), \end{aligned} \quad (12)$$

where the parameters E_1 and m_x depend on the band structure, and energy is measured from the band minimum, assumed to be at $\mathbf{k} = 0$. Here, and elsewhere unless otherwise stated, summation over the values 1, 2, 3 of repeated indices is implied and $\Theta = e_{ii}$ is the dilatation. On using equation (12) in (10) we get

$$i\hbar \partial M(\mathbf{r}, t) / \partial t = H_e M(\mathbf{r}, t), \quad (13)$$

where

$$H_e = E_1 \Theta(\mathbf{r}) - \frac{\hbar^2}{2m_1} K_{ij}(\mathbf{r}) \frac{\partial^2}{\partial x_i \partial x_j} \quad (14)$$

is the EH and

$$K_{ij} = K_{ji} = \frac{m_1}{m_3} e_{ij} + \delta_{ij} \left\{ 1 + \left(\frac{m_1}{m_2} - \frac{m_1}{3m_3} \right) \Theta + \frac{m_1}{m_4} e_{(ii)} \right\}. \quad (15)$$

The parentheses around the subscript indices in (15) indicate that summation is not implied. Since strain gradients have been largely ignored in our derivation the order of the various factors in the terms of (12) and hence in (14) is not important. However, in the next section it will be convenient to order them so as to make H_e hermitian. We observe that the form (14), with the K_{ij} being linear functions of the strains, is

not restricted to cubic symmetry but arises generally by expanding $E^h(\mathbf{k}, \mathbf{e})$ for small $\mathbf{k}$ and $\mathbf{e}$ and using the inversion symmetry of the homogeneously strained lattice.

The EH (14) is identical to that derived by Bardeen and Shockley (1950) using a Bloch representation. It reduces to the tight-binding result of Gutzwiller and Wells (1966), Kawamura (1978) and Brown (1979) in the special case

$$m_4 = \infty, \quad 3m_1 = 2m_2 = 6m_3. \quad (16)$$

3. Physical Interpretation

The probability of finding the electron in the volume element ΔV , assumed to contain many atomic sites of the deformed crystal, is

$$P_{\Delta V} = \int_{\Delta V} |\Psi(\mathbf{r}, t)|^2 d^3r. \quad (17)$$

Because of the absence of interband mixing implied by (8) it is sufficient to consider only those wavefunctions Ψ which are made up of states (1) arising from a single band. Then substituting (3) in equation (17) yields

$$P_{\Delta V} = \Omega_0 \sum_{\Delta V} |M(\mathbf{R}, t)|^2, \quad (18)$$

where the sum is over those atomic sites of the deformed crystal which are contained in ΔV . In arriving at (18) the approximate orthonormality of the Wannier functions, for slowly varying deformations, has been used, and it is assumed that the linear dimensions of ΔV considerably exceed the 'range' R_0 of the Wannier functions, introduced following equation (2).

Since the number of atoms in ΔV is $\Delta V/\Omega_0(1 + \Theta)$ we obtain from (18) an *average probability density*

$$\bar{\rho}(\mathbf{r}, t) \equiv (1/\Delta V)P_{\Delta V} = |M(\mathbf{r}, t)|^2 D(\mathbf{r}), \quad (19)$$

where

$$D(\mathbf{r}) \equiv \{1 + \Theta(\mathbf{r})\}^{-1}. \quad (20)$$

Hence the normalization to be imposed on the solutions of (13) is

$$\int_V |M(\mathbf{r}, t)|^2 D(\mathbf{r}) d^3r = 1, \quad (21)$$

where we emphasize that the integral is over the volume V of the *deformed* crystal. Although minor simplifications of (21) and subsequent formulae of this section accrue by introducing the function $N \equiv D^{\frac{1}{2}}M$, we will continue to work with the MF defined by (3), taking the view that the appearance of the quantity D in the formulae, some of which would otherwise take on 'conventional' forms, is a useful reminder that the MFs are not (total) wavefunctions.

In correspondence to (19) a similarly averaged probability flux density $\bar{\mathbf{j}}$ could be obtained, at least in principle, by integrating the flux

$$\mathbf{j}(\mathbf{r}, t) \equiv (\hbar/2im)(\Psi^* \nabla \Psi - \Psi \nabla \Psi^*) \quad (22)$$

over the surface of the volume ΔV . This approach turns out to be intractable, principally because the Wannier functions do not vary slowly with position and so

cannot usefully be expanded (nor *a fortiori* can their gradients) in terms of elastic strains. However, the continuity requirement

$$\partial \bar{\rho} / \partial t + \operatorname{div} \bar{\mathbf{j}} = 0 \quad (23)$$

implies, together with (13) and (14), that

$$\bar{\mathbf{j}}_p = (\hbar/2i m_1) DK_{pq}(M^* M_{,q} - M M_{,q}^*), \quad (24)$$

provided we continue to ignore terms in the strain gradients. The subscript commas in (24) denote differentiation with respect to x_q . Since only the divergence of the current enters (23) this equation would still be satisfied if the curl of an arbitrary vector field were added to (24). Such terms, which can only involve the elastic displacement or rotation fields, can be ruled out by considering the special cases of pure translation and rigid rotation. The completeness of (24) is verified by the observation that the coordinate transformation $\mathbf{r} \rightarrow \mathbf{r} + \mathbf{u}(\mathbf{r})$, which in the special case (16) transforms ∇^2 to the differential form in the EH (14), also transforms the standard expression (22) for the current to the form (24). Here $\mathbf{u}(\mathbf{r})$ is the elastic displacement

$$e_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}). \quad (25)$$

For further discussion of the role of coordinate and gauge transformations see Section 4.

We now derive some further results pertaining to MFs and to operators defined on their Hilbert space, thereby enabling a dynamical theory based only on the spatially averaged values of physical observables to be established.

The identity (again neglecting strain gradients)

$$\operatorname{div}\{DK_{ij}(M_\alpha^* M_{\beta,j} - M_\beta M_{\alpha,j}^*)\} \equiv DK_{ij}(M_\alpha^* M_{\beta,ij} - M_\beta M_{\alpha,ij}^*), \quad (26)$$

for any two MFs M_α and M_β , follows from the symmetry of (15). Using it, we readily find that two nondegenerate normalizable eigenstates of the EH (14) are orthogonal, i.e. if

$$H_e M_\alpha = E_\alpha M_\alpha, \quad H_e M_\beta = E_\beta M_\beta, \quad (27a, b)$$

then

$$\int_V M_\alpha^*(\mathbf{r}, t) M_\beta(\mathbf{r}, t) D(\mathbf{r}) d^3 r = \delta_{\alpha\beta}, \quad (27c)$$

provided $E_\alpha \neq E_\beta$. As usual, linear combinations of degenerate eigenstates can be found such that equations (27) apply to them also. For continuously distributed eigenvalues, $\delta_{\alpha\beta}$ must be replaced by $\delta(E_\alpha - E_\beta)$. In proving the result (27) it is convenient to require either that the MFs vanish at the surface of the deformed crystal or to impose periodic boundary conditions across the volume V , which should then be chosen to be of suitable shape. As is the case with the total wavefunction, the precise form of the boundary conditions need not concern us, so long as our interest is directed at bulk properties.

Following (27c) and (21) we define the inner product of two MFs as

$$\langle M_\alpha | M_\beta \rangle \equiv \int_V M_\alpha^*(\mathbf{r}, t) M_\beta(\mathbf{r}, t) D(\mathbf{r}) d^3 r. \quad (28)$$

Any linear operator A in the Hilbert space of the MFs, which represents the value of a (spatially averaged) physical quantity, must have real expectation values $\langle M | AM \rangle$ for all MFs. This implies (Messiah 1961, Section 5.3) that for any M_α and M_β

$$\langle M_\alpha | AM_\beta \rangle = \langle M_\beta | AM_\alpha \rangle^*. \quad (29)$$

The hermiticity property (29) is readily verified for the EH upon integrating by parts, after writing

$$H_e = E_1 \Theta - \frac{\hbar^2}{2m_1} D^{-\frac{1}{2}} \frac{\partial}{\partial x_i} K_{ij} \frac{\partial}{\partial x_j} D^{\frac{1}{2}}. \quad (30)$$

This symmetric form differs from (14) only by terms involving strain gradients and terms of second and higher order in the strains. The hermiticity of (30) is exact and it is tempting to speculate that it correctly includes the deformation gradient and higher order terms which were previously omitted from (14) and which cannot easily be included in the analysis. The corresponding probability flux, which *exactly* satisfies the continuity condition (23) when (30) is used, is

$$\dot{j}_p = \frac{\hbar}{2im_1} \left(D^{\frac{1}{2}} M^* K_{pq} \frac{\partial}{\partial x_q} (D^{\frac{1}{2}} M) - \text{complex conjugate} \right). \quad (31)$$

On changing to the Heisenberg picture (Schiff 1968, p. 170) we find that the operators vary with time according to

$$dA/dt = \partial A / \partial t + (i/\hbar)(H_e A - A H_e). \quad (32)$$

Upon using (30) in (32) we find that the operator which represents the velocity of the modulating envelope is

$$\dot{x}_p = \frac{\hbar}{2im_1} D^{-\frac{1}{2}} \left(\frac{\partial}{\partial x_q} K_{qp} + K_{pq} \frac{\partial}{\partial x_q} \right) D^{\frac{1}{2}}, \quad (33)$$

whose (exact) hermiticity may be readily verified. Its expectation value is related to the spatially averaged probability flux by

$$\langle M | \dot{x}_p | M \rangle = \int_V \dot{j}_p d^3r, \quad (34)$$

as expected.

On introducing the operator

$$P_j \equiv -i\hbar \partial / \partial x_j, \quad (35)$$

we can write equation (30) as

$$H_e = E_1 \Theta + D^{-\frac{1}{2}} P_i (K_{ij} / 2m_1) P_j D^{\frac{1}{2}}, \quad (36)$$

and then (32) yields

$$\dot{x}_i = \partial H_e / \partial P_i, \quad \dot{P}_i = -\partial H_e / \partial x_i, \quad (37a, b)$$

so that P_i represents the (spatially averaged) conjugate momentum. The relationship between kinetic and conjugate momenta is, from (33) and (35),

$$m_1 \dot{x}_i = \frac{1}{2} D^{-\frac{1}{2}} (K_{ij} P_j + P_j K_{ji}) D^{\frac{1}{2}}. \quad (38)$$

When the MF takes the form of a wavepacket which, at a given time, is large only in the neighbourhood of some point $\mathbf{r}$, only this region will contribute to the expectation values of the above operators. They can then be taken to represent the *local* values of velocity, conjugate momentum, energy etc., averaged over the unit cell at $\mathbf{r}$. This interpretation is useful in studying the semiclassical trajectories of electrons in deformed crystals.

When applied to homogeneously strained crystals the above formulae reduce to familiar results. One readily verifies that in these cases the stationary solutions of (13) normalized according to (21) are

$$M_n(\mathbf{r}, t) = V_0^{-\frac{1}{2}} \delta_{nm} \exp\{i \mathbf{k} \cdot \mathbf{r} - i E_m^h(\mathbf{k}, \mathbf{e})t/\hbar\}, \quad (39)$$

where V_0 is the volume of the undeformed crystal. Using (39) in (3) and carrying out a trivial inversion of (1) shows that the total wavefunction Ψ corresponding to (39) is simply the Bloch function of wavevector $\mathbf{k}$ of the homogeneously strained crystal. If some arbitrary degree of rigid rotation is included in the 'deformation', the solution (39) leads to a Bloch function whose wavevector $\mathbf{k}'$ is obtained from $\mathbf{k}$ by the same rigid rotation. The expectation value of (spatially averaged) velocity appropriate to (39) may be calculated using (33):

$$\mathbf{v}_m(\mathbf{k}) = (1/\hbar) \nabla_{\mathbf{k}} E_m^h(\mathbf{k}, \mathbf{e}), \quad (40)$$

as expected. The spatially averaged probability current density corresponding to (39) is given by (24) or (31) as

$$\mathbf{j}_i = (\hbar/m_1 V) K_{ij} k_j, \quad (41)$$

where $V = V_0(1 + \Theta)$. It may readily be verified that the strain-dependent terms of (15) are required on the right of (41) to ensure that (34) reduces to (40).

A nontrivial illustration of the use of the present formalism is provided by the case of a screw dislocation of Burgers vector b parallel to the x_3 axis of an elastically isotropic solid. In cylindrical polar coordinates the only nonvanishing (cartesian) strain components are (Nabarro 1967)

$$e_{13} = e_{31} = -(b/4\pi r) \sin \theta, \quad e_{23} = e_{32} = (b/4\pi r) \cos \theta. \quad (42a, b)$$

Seeking the stationary solutions of (13) we write

$$M(\mathbf{r}, t) \exp(i Et/\hbar) \equiv \psi(\mathbf{r}) \equiv \xi(r, \theta) \exp(i k_3 x_3). \quad (43)$$

On substituting this together with (42) into (13) and using (30) for H_e , we get

$$\left\{ \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \left(\frac{\partial}{\partial \theta} + i \alpha \right)^2 + \kappa^2 \right\} \xi(r, \theta) = 0, \quad (44)$$

where

$$\alpha = m_1 b k_3 / 4\pi m_3, \quad \kappa^2 = 2m_1 E/\hbar^2 - k_3^2. \quad (45a, b)$$

We have omitted all nonlinear and strain-gradient terms from (30), except for the term α^2/r^2 which was retained in (44) to reproduce the equation studied by Aharonov and Bohm (1959) in a well-known paper concerned with the effects on electrons of a magnetic vector potential $\mathbf{A} = -\alpha \hbar \hat{\theta}/er$ in a region with an excluded cylindrical core. The relevance of this problem to that of a dislocated crystal was pointed out

by Kawamura (1978) and has been further pursued in a number of papers (see Kawamura *et al.* 1982, and references therein). In view of the analogy with this magnetic problem we might expect the x_1 and x_2 components of (24) to take the form (Landau and Lifshitz 1965, p. 486)

$$\bar{j}_\beta = (\hbar/2i m_1)(M^* M_{,\beta} - M M_{,\beta}^*) + e A_\beta |M|^2 / m_1 c, \quad (46)$$

where $\beta = 1, 2$. This is readily verified to be the case. It should be emphasized that the close correspondence between dislocation and magnetic properties only applies to solutions of the type (43).

Pursuing the above analogy further, one might perhaps expect the component $\bar{j}_3$ to also take the form (46), with $A_3 = 0$, but this is not the case. Further, it is natural to enquire whether the scattering amplitude calculated by Aharonov and Bohm (1959) might also describe the scattering of electrons by a screw dislocation. Certainly the proportionality of the Aharonov–Bohm scattering amplitude to $\sin \frac{1}{2} b k_3$ accurately reflects the scattering expected from the phase mismatch (Kawamura 1978, Section 1) due to the dislocation, both near $k_3 = 0$ and $k_3 = n\pi/b$, but, as explained below, its angular dependence is not generally correct.

Just as for conventional potential-scattering problems, it seems that the only practical means of obtaining scattering cross sections etc. for isolated crystal defects is to apply the first Born approximation to (14) or (36). It is therefore important to understand the apparent failure (Corinaldesi and Rafelli 1978) of the Born approximation when applied to the Aharonov–Bohm problem. Similar difficulties have been encountered by Yosida and Kawamura (1979) and Kawamura *et al.* (1982). A rather lengthy analysis, the details of which will be published elsewhere, confirms that the trouble is due to two conflicting limiting processes. The Aharonov–Bohm equation (44) strictly applies only outside a core radius r_0 ; it was obtained for all space only by considering the limiting case where $r_0 \rightarrow 0$ and the enclosed magnetic flux (proportional to α) was kept fixed. This is clearly at odds with the limit $\alpha \rightarrow 0$ which is implied in applying the (first) Born approximation. Further, the Aharonov–Bohm boundary condition $\xi(0, \theta) = 0$ is at odds with the ‘small’ change in the wavefunction assumed when arriving at the Born approximation. By studying the problem with r_0 and α both nonzero one can identify two regimes, according to whether $2|\alpha| \ln(2/\kappa r_0)$ is $\gg 1$ or $\ll 1$. In the former regime the Aharonov–Bohm scattering amplitude is found to apply, while in the latter the Born amplitude applies. For dislocations, a natural core radius is provided by the lattice constant and, with α given by (45a), it follows that for spherical Fermi surfaces the Born approximation applies everywhere outside two small caps centred on the poles (defined by the dislocation axis). Within these polar regions, which account for about 1% of the total Fermi surface area, the Aharonov–Bohm result prevails.

4. Role of Gauge Transformations

The mapping

$$\mathbf{r}' \rightarrow \mathbf{r} = \mathbf{r}' + \mathbf{U}(\mathbf{r}) \quad (47)$$

applied to the kinetic energy operator $-(\hbar \nabla')^2 / 2m_1$ and its plane-wave eigenfunctions constitutes a gauge transformation (Teichler 1981) which transforms the operator to

$$\mathcal{H}_K = -\frac{\hbar^2}{2m_1} \left(\nabla^2 + 2E_{ij} \frac{\partial^2}{\partial x_i \partial x_j} + (\nabla^2 \mathbf{U}) \cdot \nabla \right). \quad (48)$$

We have dropped terms of second order in $U_{i,j}$ and first order in $U_{i,jk}$ and introduced

$$E_{ij} = \frac{1}{2}(U_{i,j} + U_{j,i}). \quad (49)$$

Since (48) is similar in form to the kinetic part of (14) it is natural to ask whether it may be possible to reduce the latter to standard form and obtain a corresponding simplification of the formulae of Section 3, simply by changing the independent variable. The question reduces to one of the existence of differentiable (and hence continuous) functions $U_i(\mathbf{r})$ such that

$$2E_{ij} = K_{ij} - \delta_{ij} = \frac{m_1}{m_3} e_{ij} + \delta_{ij} \left(\left(\frac{m_1}{m_2} - \frac{m_1}{3m_3} \right) \Theta + \frac{m_1}{m_4} e_{(ii)} \right). \quad (50)$$

The existence of such functions requires (Sokolnikoff 1956, Section 10)

$$E_{11,23} = -E_{23,11} + E_{31,21} + E_{12,31}. \quad (51)$$

On using (50) in (51) we find the condition

$$(2m_3/m_1)E_{11,23} = -e_{23,11} + e_{31,21} + e_{12,31} = e_{11,23}, \quad (52)$$

where the last equality follows from a compatibility equation, of the same form as (51), satisfied by the elastic strains e_{ij} . Substituting (52) into (50) yields the condition

$$(1/m_4)e_{11,23} = \{(1/3m_3) - (1/m_2)\}\Theta_{,23}. \quad (53)$$

Similar constraints follow from the remaining five compatibility requirements (Sokolnikoff 1956). These are all satisfied (trivially) for all strain fields in the special case of the dispersion law (16). In this case the choice $\mathbf{U} \equiv \mathbf{u}$, the elastic displacement, in the transformation (47) produces a kinetic energy operator (48) which is identical to (14), and the same transformation* changes the current expression from the form (22) to (24). Hence the inverse transformation applied to (14) and (24) reduces these expressions to standard forms. But in general equation (53) and the other similar constraints severely restrict the strain fields for which (14) and *a fortiori* (30) can be reduced to standard form. For example, integration of (53) and the two equations obtained from it by cyclic permutation of indices shows that Θ must be of the form $f_1(x_2, x_3) + f_2(x_3, x_1) + f_3(x_1, x_2)$ for arbitrary functions f_i .

The lesser aim of removing only the mixed derivative terms from (14) can always be achieved by choosing $\mathbf{U} = (m_1/2m_3)\mathbf{u}$. However, in the important case of dislocated crystals, the elastic displacement $\mathbf{u}(\mathbf{r})$ is a multivalued function (Nabarro 1967) and it can further be shown that no single-valued function $\mathbf{U}(\mathbf{r})$ can achieve the desired reduction. Therefore a *multivalued* solution of the transformed equation must be sought in order that the final $M(\mathbf{r}, t)$ is single valued.† Such a procedure may sometimes be convenient (Kawamura *et al.* 1982), but usually it is simpler to seek single-valued solutions of the more complicated equation, especially for scattering solutions where the Born approximation may be used.

* One must take account of the effect of the transformation on the dimensions and orientations of area elements.

† Tassie and Peshkin (1961), Merzbacher (1962) and Kretschmar (1965) have emphasized that even in multiply connected bodies the total wavefunction (and hence its MF) must be single valued if physically simple boundary conditions are to apply.

The relationship between these considerations and those of Teichler (1981) is explored in the next section.

5. Comparison with Previous Theories

No other authors appear to have considered the expression for the spatially averaged current in terms of the MFs, nor the forms of the linear operators which represent spatially averaged physical observables. The discussion in this section is therefore restricted to earlier derivations of EHs similar to (14) or (30).

Early applications of the effective-mass method by Peckar (1946) who used a Bloch representation, and Slater (1949) who used Wannier functions, were aimed at the study of electron motion in slowly varying potentials (due, for example, to substitutional impurities) superposed on a periodic crystal potential.

The extension of Slater's (1949) formulation to include deformed crystals is the subject of Section 2 of the present paper. The extension of Peckar's approach to the case of deformed crystals was made by Bardeen and Shockley (1950, referred to in this section as BS). Their treatment was designed to deal with electron-phonon interactions, and difficulties arise when one seeks to apply it to more general (slowly varying static) deformations. For example, it is clear from the appearance of the elastic displacement function as an argument in BS (equation A.4) that the wavefunction depends, in general, on elastic rotations as well as strains. Yet rotation dependence is omitted from the basis functions introduced by BS (A.13). It is then clear that any basis function ψ_h of BS (A.13), which closely approximates the wavefunction of the deformed crystal in some localized region, rapidly gets out of step with the lattice as one moves from such a region to a neighbouring one whose rotation angles are different. This leads to additional correction terms involving rotations in BS (A.14). Examination of these shows that for small rotations the conclusions of BS are unchanged, but large rotations (including rigid rotations, although these can be dealt with by a trivial reformulation of the theory) introduce large corrections which effectively invalidate the theory. On the other hand, the Wannier formulation of the present paper includes rotations of arbitrary magnitude, provided their spatial variation is sufficiently slow. It is also clear, either from the form of the correction terms in BS (A.14) or by considering the increasing mismatch between the Bloch functions and the lattice as one moves away from the origin of coordinates, that the BS formulation does not extend, for example, to the case of tensile strains which continue to increase with distance over many unit cells. Yet, in this case of large interatomic separations, the Wannier functions simply reduce to atomic orbitals and the theory of Section 2 still applies.

If one tries to overcome these difficulties of the BS formulation by redefining the origin and orientation of each Bloch function for each unit cell, one encounters continuity problems of the type discussed by Harrison (1958, referred to as H). Although the H cellular method leads to an effective Hamiltonian (25) of H similar to our equation (30), the complete wavefunction (3) of H is defined only within ellipsoidal cells which do not exactly cover the crystal space. While the treatment of H may be acceptable for the estimation of energy eigenvalues, this incompleteness in the definition of the wavefunction, and the associated lack of continuity, would appear to rule out estimates of the particle current and velocity, even their averages over several unit cells. The localization of the Wannier basis functions, which enables the above problems to be avoided, constitutes a clear advantage.

A further advantage of the Wannier formulation of Section 2 is found in the diagonalization of (6) with respect to the band index, which emerges more simply and clearly from the properties of the Wannier functions than it does in the approaches of H or BS. Finally, we point out that both H and BS rely on a small wavevector expansion at an early stage in the development of their respective theories, whereas we adopt this approximation only after arriving at the general result (12), which may alternatively be expanded about $k \neq 0$.

The special case of screw-dislocated crystals was examined by Gutzwiller and Wells (1966) using a tight-binding representation. Their EH may be obtained as a special case of (14) by adopting the effective masses (16). Their results were rediscovered and extended by Kawamura (1978, 1980), still within the tight-binding approximation. This work was recently extended further by Teichler (1981, referred to as T) who employed the Wannier functions of the undeformed crystal as basis functions. If we follow T and introduce the vectors T_γ from the atom at R to its neighbours in the deformed crystal, then on writing the matrix element $H(R, R+T_\gamma)$ of (7) as $H'(R, T_\gamma)$ we can use (9) to write (8) as

$$i \partial M(R, t) / \partial t = \sum_{\gamma} H'(R, T_{\gamma}) \exp(i T_{\gamma} \cdot p) M(R, t), \quad (54)$$

where for simplicity we have dropped the band index. Following T, we have set $p = -i \nabla_R$ and have changed to units in which $\hbar = 1$. If the vector $T_\gamma = T_\gamma(R)$ maps into T_γ^0 in the undeformed crystal then for slowly varying strains we have $T_\gamma^0 = T_\gamma \cdot \{1 - \beta(R)\}$, where the distortion tensor β has elements $\beta_{ij} = u_{j,i}$. One readily shows that $T_\gamma \cdot p = T_\gamma^0 \cdot \pi$, where

$$\pi = p + a; \quad a = \{1 - \beta(R)\}^{-1} \cdot \beta(R) \cdot p. \quad (55a, b)$$

Then (54) can be rewritten as

$$i \partial M(R, t) / \partial t = \mathcal{H}(R, \pi) M(R, t), \quad (56)$$

where

$$\mathcal{H}(R, \pi) = \sum_{\gamma} H'(R, T_{\gamma}) \exp(i T_{\gamma}^0 \cdot \pi). \quad (57)$$

Equations (56) and (57) are identical to (5) and (6) of T respectively, *except* that our matrix elements are those of the Wannier functions defined for the homogeneously strained crystal of strain $e(R)$; we observe that the band diagonalization of (7) employed in arriving at (56) holds rigorously (to the neglect of the gradients $u_{i,jk}$ of the distortion tensor) for these basis functions, but not if those of the undeformed crystal are used.*

In T it is emphasized that (56) is invariant under the gauge transformation

$$M(R, t) \rightarrow M'(R, t) = \exp\{i U(R) \cdot p\} M(R, t), \quad (58a)$$

$$\pi \rightarrow \pi' = \pi - \{1 - \beta(R)\}^{-1} \cdot E(R) \cdot p, \quad (58b)$$

$$E_{ij} = U_{j,i}, \quad (58c)$$

* Although, for the sufficiently localized tight-binding functions implicit in Teichler's (1981) paper, band diagonalization applies trivially.

so that the distortion term in (55) can be eliminated by the transformation (58) with $U \equiv \mathbf{u}$. However, this merely reduces (57) to

$$\mathcal{H}(\mathbf{R}, \mathbf{p}) = \sum_{\gamma} H'(\mathbf{R}, \mathbf{T}_{\gamma}) \exp(i \mathbf{T}_{\gamma}^0 \cdot \mathbf{p}), \quad (59)$$

where H' still depends on the strain, both through strain-dependent corrections to the potential energy and through the dependence of the Wannier functions (1) on the strain. The strain dependence persists, even if the Wannier functions of the undeformed crystal are used, due both to the strain corrections in the potential energy and to the strain dependence of the vectors $\mathbf{T}_{\gamma}(\mathbf{R})$. We conclude that only in the special case where the $H'(\mathbf{R}, \mathbf{T}_{\gamma})$ do not depend on the deformation, as assumed by Gutzwiller and Wells (1966), Kawamura (1978) and Brown (1979), can the strain dependence of the EH (59) be removed by a coordinate transformation. This case, which for small wavevectors is equivalent to the dispersion law (12) with the effective masses (16), was discussed in Section 4.

Taking another point of view we can use the small strain expansion (12) of $\mathbf{T}$ to write (59) in the form

$$\mathcal{H}(\mathbf{R}, \mathbf{p}) = \mathcal{H}_0(\mathbf{p}) + e_{ij} P_{ij}(\mathbf{p}). \quad (60)$$

Changing from $\mathbf{p}$ to $\boldsymbol{\pi}$ using the transformation (58) adds several terms to the first term on the right of (60) which are linear in the E_{ij} , and which we may suppose are of the same order as the strains e_{ij} . The remaining terms on the right of (60) are unchanged, to this order. The elimination of strains from $\mathcal{H}$ therefore rests on choosing $U(\mathbf{R})$ such that the terms generated from $\mathcal{H}_0$ are equal and opposite to $e_{ij} P_{ij}$. The impossibility of this, in general, was demonstrated in Section 4.

The approach of Hunter and Nabarro (1953, referred to as HN) is quite different from that of the present paper and those already discussed. These authors adopted a trial solution for the complete time-independent wavefunction of the form

$$\psi(\mathbf{r}) = \exp\{i W(\mathbf{r})\} U \{\nabla W, \mathbf{r} - \mathbf{u}, \boldsymbol{\alpha}(\mathbf{r})\}, \quad (61)$$

where $\mathbf{u}$ is the elastic displacement and $\boldsymbol{\alpha}$ is the distortion tensor previously denoted $\boldsymbol{\beta}$ in (55). The functions W and U satisfy (21) and (23) of HN respectively. The latter equation, although it contains an operator superficially similar to (14), differs from it in several ways, not least of which is the absence of effective-mass parameters. Nevertheless, HN finally emerged with a scattering amplitude, based on their equation (25), which is identical to that obtained from our (14). However, their analysis is unsatisfactory for dislocated crystals since, if (as is implied) a single-valued solution $U(\mathbf{k}, \mathbf{r}', \boldsymbol{\alpha})$ of their (23) is sought, then setting $\mathbf{r}' = \mathbf{r} - \mathbf{u}$ will generate the multivalued solution (61). Actually their (slowly varying) solution (22) for W , which applies for a screw dislocation, is also multivalued but cannot compensate for the multivaluedness of U since this is a much more complicated function which varies significantly throughout a single unit cell. The complicated nature of U also rules out, at least from a practical point of view, the possibility of seeking an appropriately multivalued solution of (23) of HN in order that U in (61) should become single valued. We conclude that the approach of HN cannot be applied to dislocated crystals without substantial modification. Similar remarks apply to the dislocation

studies of Dubrovsky *et al.* (1969) who used methods similar to those developed by Blount (1959) and Whitfield (1961) for the electron-phonon problem. None of these are effective-mass methods. All employed a transformation of the type (47) and can only be used to advantage if the displacement function is single valued.

6. Discussion

The aim of this paper has been to establish a sound basis for the study of electron propagation in deformed crystals using EH methods. In Section 2 the EH (14), due originally to Bardeen and Shockley (1950), was rederived using a Wannier representation. It governs the evolution of the MFs, which determine the contributions to the total crystal wavefunction of Wannier functions centred on each atomic site.

The physical interpretation of the MFs and the operators defined on their Hilbert space was considered in Section 3. It was shown that these operators, which represent the values of physical observables averaged over the volume of a unit cell of the deformed crystal, take forms which differ from the conventional ones, but which reduce to the latter in cases of zero or uniform strain. In Section 4 it was demonstrated that the strain dependence of these 'deformation operators', including the EH itself, cannot generally be transformed away by a change of coordinates. Hence the formulae presented here provide the simplest formulation of the theory attainable.

The results of the present theory can be applied to a wide range of problems of electron propagation in deformed crystals. In contemplating applications, the following points should be kept in mind:

(1) If the strains are sufficiently localized the methods of atomic scattering theory may be applied to the EH and it will frequently be sufficient to use the first Born approximation. This extends to scattering by isolated dislocations provided the restrictions discussed at the end of Section 3 are observed.

(2) For non-localized deformations, which may be due to a distribution of crystal defects or to externally applied macroscopic forces, the EH can provide the basis of a semiclassical discussion of electron trajectories. In this way it should be possible to extend to microscopic heterogeneities the study of current-distortion effects (see Chambers 1968, p. 319) previously carried out only for macroscopic imperfections, as reviewed by Fletcher (1982). We observe that electric and magnetic fields may readily be incorporated into the EH, leading to a theory of transport properties in deformed crystals (see also point 4 below).

(3) In applying the theory to metals the problems posed by non-infinitesimal Fermi wavevectors are no more severe than those appearing in previous applications of 'deformation potential' theory (see e.g. Hunter and Nabarro 1953, and references therein). The study of Fermi surfaces more complicated than those allowed by (12) or (14) can be achieved by expanding the dispersion relation about points other than $\mathbf{k} = 0$ (Luttinger and Kohn 1955). For example, Kawamura (1980) has studied regions of the Fermi surface near Brillouin zone boundaries. For the dispersion relation (12), the requirement of charge neutrality can be shown to lead to the condition

$$E_1 = \frac{2}{3}\zeta_0(1 - 3m_1/2m_2 - m_1/2m_4), \quad (62)$$

where ζ_0 is the Fermi energy of the undeformed crystal. This result and the accompanying one that $\delta\zeta = 0$, i.e. the absolute position of the Fermi level is not shifted

by an arbitrary strain, provided (12) applies, are in complete agreement with the (more general) considerations of Ziman (1960, Section 5.6).

(4) It is readily demonstrated that those terms of the velocity operator (33) of first order in the strains may make important contributions to the transport coefficients, contributions which are omitted if the conventional operator $\mathbf{v} = -(\hbar/m)\nabla$ is adopted. For scattering by crystal defects the additional effects are particularly important if the relaxation rate is dominated by processes, such as electron-phonon interactions, which are independent of the strain fields of the static defects. The additional terms then contribute significantly to the deviations from Matthiessen's rule.

Detailed applications of the theory will be presented in subsequent publications.

The extension of the method of Section 2 to deal with time-dependent deformations involves the addition of the term

$$\Delta_m(\mathbf{R}') = i\hbar\Omega_0^{\frac{1}{2}}\dot{e}_{ij}(\mathbf{R}', t) \sum_{n\mathbf{R}} P_{ij}^{mn}\{\mathbf{R}', \mathbf{R}, \mathbf{e}(\mathbf{R}', t)\} M_n(\mathbf{R}, t) \quad (63)$$

to the left of (5), where

$$P_{ij}^{mn}(\mathbf{R}', \mathbf{R}, \mathbf{e}) = \int_V a_m^*\{(\mathbf{r}-\mathbf{R}')_{\text{rot}}, \mathbf{e}\} \partial a_n\{(\mathbf{r}-\mathbf{R})_{\text{rot}}, \mathbf{e}\} / \partial e_{ij} d^3r. \quad (64)$$

We readily find that (64) implies

$$P_{ij}^{mn}(\mathbf{R}', \mathbf{R}, \mathbf{e}) = P_{ij}^{mn}(\mathbf{R}' - \mathbf{R}, 0, \mathbf{e}) \equiv P_{ij}^{mn}(\mathbf{R}' - \mathbf{R}, \mathbf{e}), \quad (65)$$

and, defining

$$\tilde{P}_{ij}^{mn}(\mathbf{k}, \mathbf{e}) = \sum_{\mathbf{R}} P_{ij}^{mn}(\mathbf{R}, \mathbf{e}) \exp(-i\mathbf{R} \cdot \mathbf{k}), \quad (66)$$

equation (63) takes the form

$$\Delta_m(\mathbf{R}') = i\hbar\Omega_0^{\frac{1}{2}}\dot{e}_{ij}(\mathbf{R}', t) \sum_n \tilde{P}_{ij}^{mn}\{-i\nabla_{\mathbf{R}'}, \mathbf{e}(\mathbf{R}', t)\} M_n(\mathbf{R}', t), \quad (67)$$

where M_n is now regarded as a (slowly varying) function of a continuous variable $\mathbf{R}'$. It follows from (66), (64) and (1) that

$$\tilde{P}_{ij}^{mn}(\mathbf{k}, \mathbf{e}) = \int_{\text{crystal}} b_m^*(\mathbf{k}, \mathbf{r}, \mathbf{e}) \partial b_n(\mathbf{k}, \mathbf{r}, \mathbf{e}) / \partial e_{ij} d^3r \quad (68a)$$

$$\equiv N \int_{\text{cell}} U_m^*(\mathbf{k}, \mathbf{r}, \mathbf{e}) \partial U_n(\mathbf{k}, \mathbf{r}, \mathbf{e}) / \partial e_{ij} d^3r, \quad (68b)$$

where the integrals (68a) and (68b) are over the entire crystal of *uniform* strain $\mathbf{e}$ and its unit cell respectively, and U_n is the periodic part of the Bloch function. If (67) is required only to first order in the strains, the strain derivatives of (68) can be evaluated at $\mathbf{e} = 0$ and the integrals evaluated over the undeformed crystal. A full investigation of the effects of time dependence requires evaluation of the parameters (68). This study, which promises to bridge the gap (Ziman 1960, Section 5.12) between the adiabatic and relaxation regimes, will be completed in a future publication.

References

- Aharonov, Y., and Bohm, D. (1959). *Phys. Rev.* **115**, 485.
- Bardeen, J., and Shockley, W. (1950). *Phys. Rev.* **80**, 72.
- Blount, E. I. (1959). *Phys. Rev.* **114**, 418.
- Brown, R. A. (1979). *J. Phys.* F **9**, L241.
- Callaway, J. (1974). 'Quantum Theory of the Solid State', Parts A and B (Academic: New York).
- Chambers, R. G. (1968). 'Electrons in Metals', Simon Fraser Lectures on Solid State Physics, Vol. 1 (Eds J. F. Cochran and R. R. Haering), p. 283 (Gordon and Breach: New York).
- Corinaldesi, E., and Rafelli, F. (1978). *Am. J. Phys.* **46**, 1185.
- Dubrovsky, I. M., Molodkin, V. M., Tikhonov, L. V., and Tikhonova, Ye. A. (1969). *Fiz. Metal. Metalloved.* **27**, 21.
- Fletcher, R. (1982). *Can. J. Phys.* **60**, 679.
- Gutzwiller, M. C., and Wells, R. O. (1966). *J. Phys. Chem. Solids* **27**, 349.
- Harrison, W. A. (1958). *Phys. Rev.* **110**, 14.
- Hunter, S. C., and Nabarro, F. R. N. (1953). *Proc. R. Soc. London A* **220**, 542.
- Kawamura, K. (1978). *Z. Phys.* B **29**, 101.
- Kawamura, K. (1980). *Prog. Theor. Phys. (Kyoto)* Suppl. No. 69, 258.
- Kawamura, K., Zempo, Y., and Irie, Y. (1982). *Prog. Theor. Phys. (Kyoto)* **67**, 1263.
- Kretzschmar, M. (1965). *Z. Phys.* **185**, 73.
- Landau, L. D., and Lifshitz, E. M. (1965). 'Quantum Mechanics' (Pergamon: London).
- Luttinger, J. M., and Kohn, W. (1955). *Phys. Rev.* **97**, 869.
- Merzbacher, E. (1962). *Am. J. Phys.* **30**, 237.
- Messiah, A. (1961). 'Quantum Mechanics', Vols 1 and 2 (North-Holland: Amsterdam).
- Nabarro, F. R. N. (1967). 'Theory of Crystal Dislocations' (Clarendon: Oxford).
- Peckar, S. (1946). *J. Phys. (Moscow)* **10**, 431.
- Schiff, L. I. (1968). 'Quantum Mechanics' (McGraw-Hill: New York).
- Sham, L. J., and Ziman, J. M. (1963). In 'Solid State Physics, Advances in Research and Applications', Vol. 15 (Eds F. Seitz and D. Turnbull), p. 221 (Academic: New York).
- Slater, J. C. (1949). *Phys. Rev.* **76**, 1952.
- Slater, J. C. (1967). 'Quantum Theory of Molecules and Solids', Vol. 3 (McGraw-Hill: New York).
- Sokolnikoff, I. S. (1956). 'Mathematical Theory of Elasticity' (McGraw-Hill: New York).
- Tassie, L. J., and Peshkin, M. (1961). *Ann. Phys. (New York)* **16**, 177.
- Teichler, H. (1981). *Phys. Lett. A* **87**, 113.
- Weinreich, G. (1965). 'Solids: Elementary Theory for Advanced Students' (Wiley: New York).
- Whitfield, G. D. (1961). *Phys. Rev.* **121**, 720.
- Yosida, Y., and Kawamura, K. (1979). *Z. Phys.* B **32**, 355.
- Ziman, J. M. (1960). 'Electrons and Phonons' (Clarendon: Oxford).

