Generalized Wannier Functions and Effective Hamiltonians*

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An effective Hamiltonian for an electron in a periodic lattice in a uniform magnetic field can be formulated rigorously in terms of an orthonormal set of basis functions. These functions are obtained from one another by application of magnetic translation operators. The Wannier functions turn out to be a special case of this more general set, applicable in the absence of magnetic fields. Not only are these functions not uniquely defined, but the form of the effective Hamiltonian will depend on their manner of selection, with the exception that at zero field the effective Hamiltonian is unique. A multiband effective Hamiltonian suitable for breakdown calculations is described.

1. INTRODUCTION

THE effective Hamiltonian for electrons in periodic potentials is conveniently formulated in terms of Wannier functions.[1–4] These functions, which we denote by $a(\mathbf{r}-\mathbf{R}_n)$, form an orthonormal set of basis functions which spans the space of a single energy band. This fact is not sufficient to define the functions uniquely since this property is obtained by defining $a(\mathbf{r})$ according to the relation

$$a(\mathbf{r})=g^{-1/2}\sum_{\mathbf{k}} e^{i\phi(\mathbf{k})}b_{\mathbf{k}}(\mathbf{r}), \tag{1}$$

where $\phi(\mathbf{k})$ is any real function of $\mathbf{k}$, and $b_{\mathbf{k}}(\mathbf{r})$ are Bloch functions. The sum is over the g states in a Brillouin zone. (One obtains an integral in the limit of an infinite crystal.) The phases $\phi(\mathbf{k})$ are usually chosen so as to localize $a(\mathbf{r})$ about the origin.[4–7] The effective Hamiltonian is obtained by using the Wannier functions as a basis for a one-band representation, namely

$$\phi(\mathbf{r})=\sum_n \psi(\mathbf{R}_n)a(\mathbf{r}-\mathbf{R}_n). \tag{2}$$

It then follows from the time-independent Schrödinger equation that ψ satisfies the relation

$$E(\mathbf{P})\psi(\mathbf{r})=E\psi(\mathbf{r}), \tag{3}$$

where $E(\mathbf{P})$ is the operator obtained by replacing $\mathbf{k}$ by the momentum operator $\mathbf{P}$ in the energy function $E(\mathbf{k})$. (We choose units in which $\hbar=1$.) The solutions of Eq. (3) are plane waves, $e^{i\mathbf{k}\cdot\mathbf{r}}$, with corresponding eigenvalues $E(\mathbf{k})$. If one deals with a potential $V(\mathbf{r})$ perturbing the system, which is sufficiently slowly varying that interband coupling can be neglected, such that

$$\langle a(\mathbf{r}-\mathbf{R}_n)\,|\,V\,|\,a(\mathbf{r}-\mathbf{R}_m)\rangle\approx V(\mathbf{R}_n)\delta_{n,m}, \tag{4}$$

then the equation for ψ becomes

$$E(\mathbf{P})\psi(\mathbf{r})+V(\mathbf{r})\psi(\mathbf{r})=E\psi(\mathbf{r}). \tag{5}$$

This is the one-band effective Hamiltonian formulation, which has the virtue that all information having to do with the periodic lattice potential is contained in $E(\mathbf{p})$. This formulation is suitable for potential perturbations such as that which results from an external electric field. However, we cannot deal with magnetic fields without modifying the formulation somewhat. The complete one-electron Hamiltonian is modified, in the presence of magnetic fields, by replacing the momentum operator $\mathbf{p}$ by the kinetic momentum $\boldsymbol{\pi}=\mathbf{p}+e\mathbf{A}/c$, where $\mathbf{A}$ is the vector potential. It is thus natural to attempt a formulation of the effective Hamiltonian in which $E(\mathbf{p})$ is replaced by $E(\boldsymbol{\pi})$.[8] This simple result, which seems to fit observations, is not so simply derived. Its validity was first established by Kohn[9] in the limit of weak magnetic fields. He was able to establish an operator $H(\boldsymbol{\pi})$ in the form of a power series in the field B,

$$H(\boldsymbol{\pi})=\sum_n B^n f_n(\boldsymbol{\pi}), \tag{6}$$

in which the term $f_0(\boldsymbol{\pi})$ is the energy-band function $E(\boldsymbol{\pi})$. Subsequently Blount[10] and Roth[11] were able to simplify Kohn's derivation. The question of the convergence of the series has not been answered to the author's knowledge. These derivations justify the use of an effective Hamiltonian asymptotically as B approaches zero.

In a previous paper[12] the author was able to establish the validity of an effective Hamiltonian, not restricted to weak fields. The approach made use of the invariance properties of the Hamiltonian for a uniform magnetic field. The transformation properties of the eigenfunctions were found by means of group theory and from these it was possible to construct a set of orthonormal functions analogous to Wannier functions. However, the particular effective Hamiltonian obtained was not simply related to $E(\mathbf{k})$, even for small fields, and in fact did not even have the same symmetry properties. The trouble stems from the fact, noted earlier by Kohn,[9] that the form of the effective Hamiltonian is not unique.

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As will be shown presently there are a variety of ways to form generalized Wannier functions. In contrast to the unperturbed zero-field case, the form of $H(\pi)$ depends sensitively on the choice of basis functions. It is desirable to be able to choose them in such a way that the effective Hamiltonian reduces to $E(\pi)$ in the limit of zero field. In this way one can establish the validity of an effective Hamiltonian for finite fields, the form of which should be given correctly by the asymptotic expressions referred to previously.[9–11] It should be noted that it is only the form of the effective Hamiltonian which is under consideration here. The validity of an effective Hamiltonian is established for arbitrary magnetic fields.

2. GENERALIZED WANNIER FUNCTIONS

We recapitulate briefly the group-theoretical results established in I for *rational* magnetic fields. In this case the magnetic field is along a lattice vector and the flux through a two-dimensional cell is $l/N(hc/e)$, a rational multiple of a flux quantum.[13] The restriction to rational fields is for convenience only and has negligible effect on the consequences. The energy eigenfunctions, which are N-fold degenerate, serve as basis functions for ray representations of the translation group. These representations are characterized by a wave vector $\mathbf{q}$ whose domain is smaller than a Brillouin zone by a factor N in each of the directions normal to the field. The density of points in $\mathbf{q}$ space is the same as that of points in $\mathbf{k}$ space, determined by the volume of the crystal. The energy is a continuous function of $\mathbf{q}$, lying in narrow bands whose spacing depends on l as well as N. Typical values of N are usually in excess of 10^4 for presently available fields. We can think of the states of a single energy band as decomposing into N such magnetic sub-bands. The over-all density of states is only slightly altered by the magnetic field.

A generalized Wannier function can be obtained as a linear combination of states from these N sub-bands. However, it is more instructive to generate functions with the orthogonality properties of Wannier functions without reference to eigenfunctions. We define a function $\phi_{ml}{}^{n,\mathbf{q}}(\mathbf{r})$ which serves as the lth partner function of a representation denoted by $\mathbf{q}$. The pair of labels n, m are additional indices, which could designate the mth magnetic sub-band within the nth band, for example. In what follows the n label will not be explicitly included. It should be noted that only a portion of Hilbert space is under consideration. The full Hilbert space can be obtained by making use of functions corresponding to different n labels. We assume the functions so defined are orthonormal. This is automatically satisfied for functions belonging to different representations, or to functions which differ in l. These functions transform under the magnetic translation operators, defined in I, according to the relation

$$T(\mathbf{R})\phi_{ml}{}^{\mathbf{q}}=\sum_{l'}\phi_{ml'}{}^{\mathbf{q}}D_{ll'}{}^{\mathbf{q}}(\mathbf{R}). \tag{7}$$

We assume only that the matrices $\mathbf{D}^{\mathbf{q}}(\mathbf{R})$ are equivalent (differing by a unitary transformation) to the matrices $\mathbf{D}^{\mathbf{q}}(\mathbf{R})$ defined in I. We will refer to the latter as the standard representations.

We are now in a position to define a generalized Wannier function $A(\mathbf{r})$ by the relation

$$A(\mathbf{r})=(N/g)^{1/2}\sum_{l,m,\mathbf{q}}D_{lm}{}^{\mathbf{q}}(E)\phi_{ml}{}^{\mathbf{q}}(\mathbf{r}), \tag{8}$$

where g is the order of the group, and E is the identity operation corresponding to $\mathbf{R}=0$. The sum over m as well as l is from 1 to N. The matrix corresponding to E is the unit matrix with elements $D_{lm}{}^{\mathbf{q}}(E)=\delta_{l,m}$ so that Eq. (8) can be written as

$$A(\mathbf{r})=(N/g)^{1/2}\sum_{m,\mathbf{q}}\phi_{mm}{}^{\mathbf{q}}(\mathbf{r}). \tag{9}$$

Under magnetic translation, Eq. (8) becomes

$$T(\mathbf{R})A(\mathbf{r})=(N/g)^{1/2}\sum_{l,m,\mathbf{q}}D_{lm}{}^{\mathbf{q}}(\mathbf{R})\phi_{ml}{}^{\mathbf{q}}(\mathbf{r}), \tag{10}$$

where we have made use of Eq. (7) and the fact that the matrices $\mathbf{D}$ are isomorphic to magnetic translations. Denoting the translated function by $A(\mathbf{R};\mathbf{r})$, or more compactly as $A(\mathbf{R})$, we find for the scalar product of two such functions

$$\begin{aligned}\langle A(\mathbf{R}')\,|\,A(\mathbf{R})\rangle&=(N/g)\sum_{l,l',m,m',\mathbf{q},\mathbf{q}'}D_{l'm'}{}^{*\mathbf{q}'}(\mathbf{R}')\\&\quad\times D_{lm}{}^{\mathbf{q}}(\mathbf{R})\langle\phi_{m'l'}{}^{\mathbf{q}'}\,|\,\phi_{ml}{}^{\mathbf{q}}\rangle\\&=(N/g)\sum_{l,m,\mathbf{q}}D_{lm}{}^{*\mathbf{q}}(\mathbf{R}')D_{lm}{}^{\mathbf{q}}(\mathbf{R})\\&=\delta_{\mathbf{R},\mathbf{R}'},\end{aligned} \tag{11}$$

where the last step follows by virtue of the orthogonality relations for irreducible representations. If we want the functions $A(\mathbf{R})$ to span the states of N magnetic sub-bands it is sufficient to choose the functions $\phi_{ml}{}^{\mathbf{q}}$ as eigenfunctions in the mth sub-band. However, a more general form of $A(\mathbf{r})$ is obtained by letting $\phi_{ml}{}^{\mathbf{q}}$ be a linear combination of eigenfunctions $\psi_{ml}{}^{\mathbf{q}}$ according to the unitary transformation

$$\phi_{ml}{}^{\mathbf{q}}=\sum_{m'}W_{mm'}{}^{\mathbf{q}}\psi_{m'l}{}^{\mathbf{q}}. \tag{12}$$

The orthonormal set of eigenfunctions ψ are basis functions for the same representations as the set ϕ. The eigenfunctions which serve as basis functions for the standard representations are denoted by $\Psi_{ml}{}^{\mathbf{q}}$. These differ from the set $\psi_{ml}{}^{\mathbf{q}}$ by a second unitary transformation

$$\psi_{ml}=\sum_{l'}\Psi_{ml'}{}^{\mathbf{q}}V_{l'l}{}^{\mathbf{q}}. \tag{13}$$

From Eqs. (9), (12), and (13) we obtain

$$A(\mathbf{r})=(N/g)^{1/2}\sum_{l,m,\mathbf{q}}U_{lm}{}^{\mathbf{q}}\Psi_{ml}{}^{\mathbf{q}}, \tag{14}$$

where

$$\mathbf{U}^{\mathbf{q}}=\mathbf{V}^{\mathbf{q}}\mathbf{W}^{\mathbf{q}}. \tag{15}$$

If we regard $\Psi_{ml}{}^{\mathbf{q}}$ as the (m,l) element of a matrix we

[13] The quantum of flux used here is twice the value of the superconducting flux quantum.

can write Eq. (14) in compact form in terms of the trace:

$$A(\mathbf{r})=\mathrm{Tr}[(N/g)^{1/2}\textstyle\sum_{\mathbf{q}}\mathbf{U}^{\mathbf{q}}\boldsymbol{\Psi}^{\mathbf{q}}]. \tag{16}$$

This is the generalized Wannier function expressed in terms of standard eigenfunctions and an arbitrary unitary $N\times N$ matrix $\mathbf{U}$.

In the special case of zero magnetic field, Eq. (16) reduces to the definition of the conventional Wannier function given in Eq. (1). In that case the representations are one dimensional so that the sum over $\mathbf{q}$ is taken over an ordinary Brillouin zone. The eigenfunctions $\Psi^{\mathbf{q}}$ are the Bloch functions, and the unitary one-dimensional matrices $\mathbf{U}^{\mathbf{q}}$ are merely phase factors $e^{i\phi(\mathbf{q})}$. When dealing with 1×1 matrices the concept of trace is superfluous. This result does not necessarily imply that it is always possible to define a generalized Wannier function for small magnetic field which approaches the conventional one in the limit of vanishing field.

3. EFFECTIVE HAMILTONIAN

Because of the arbitrary unitary matrix $\mathbf{U}$ in the definition of the generalized Wannier function, we will find a corresponding lack of uniqueness in the single-band effective Hamiltonian based on these functions. This arbitrariness is investigated here. We seek a form which approaches $E(\boldsymbol{\pi})$ in the limit of weak magnetic fields.

As shown in I the effective Hamiltonian can be written in the form

$$H(\boldsymbol{\pi})=\textstyle\sum_{\mathbf{R}}\epsilon(\mathbf{R})\exp(-i\mathbf{R}\cdot\boldsymbol{\pi}), \tag{17}$$

where $\epsilon(\mathbf{R})$ is defined as

$$\epsilon(\mathbf{R})=\langle A(\mathbf{R})|H|A(0)\rangle. \tag{18}$$

From Eq. (10) we find

$$\begin{aligned}\epsilon(\mathbf{R})&=N/g\textstyle\sum_{l,l',m,m',\mathbf{q},\mathbf{q}'}D_{lm}{}^{*\mathbf{q}}(\mathbf{R})\\&\quad\times D_{l'm'}{}^{\mathbf{q}'}(0)\langle\phi_{ml}{}^{\mathbf{q}}|H|\phi_{m'l'}{}^{\mathbf{q}'}\rangle\\&=N/g\textstyle\sum_{l,m,\mathbf{q}}D_{lm}{}^{*\mathbf{q}}(\mathbf{R})H_{ml}{}^{\mathbf{q}}\\&=\mathrm{Tr}[N/g\textstyle\sum_{\mathbf{q}}\mathbf{D}^{*\mathbf{q}}(\mathbf{R})\mathbf{H}^{\mathbf{q}}],\end{aligned} \tag{19}$$

where $H_{ml}{}^{\mathbf{q}}=\langle\phi_{mn}{}^{\mathbf{q}}|H|\phi_{ln}{}^{\mathbf{q}}\rangle$, and is independent of n. We recall that the matrix $\mathbf{H}^{\mathbf{q}}$ can be brought to diagonal form $\mathbf{H}_d{}^{\mathbf{q}}$, by means of the unitary transformation $\mathbf{W}^{\mathbf{q}}$, and that the representative matrices $\mathbf{D}^{\mathbf{q}}(\mathbf{R})$ can be brought to the standard form $\mathbf{D}^{\mathbf{q}}(\mathbf{R})$, by means of the unitary transformation $\mathbf{V}^{\mathbf{q}}$. Making use of the facts that the trace is invariant to cyclic permutations, and that $\mathbf{U}^{\mathbf{q}}=\mathbf{V}^{\mathbf{q}}\mathbf{W}^{\mathbf{q}}$, it is a straightforward matter to obtain the following relations

$$\begin{aligned}\epsilon^*(\mathbf{R})&=\mathrm{Tr}[N/g\textstyle\sum_{\mathbf{q}}\mathbf{U}^{\dagger}\mathbf{D}^{\mathbf{q}}(\mathbf{R})\mathbf{U}\mathbf{H}_d{}^{*\mathbf{q}}]\\&=\mathrm{Tr}[N/g\textstyle\sum_{\mathbf{q}}\mathbf{D}^{\mathbf{q}}(\mathbf{R})\mathbf{U}\mathbf{H}_d{}^{*\mathbf{q}}\mathbf{U}^{\dagger}].\end{aligned} \tag{20}$$

Thus the most general effective Hamiltonian can be obtained by use of Eq. (19) with either $\mathbf{H}^{\mathbf{q}}$ in diagonal form and some arbitrary choice of representation, or equivalently by using standard representations, with $\mathbf{H}^{\mathbf{q}}$ in arbitrary form.

The asymptotic expansions[9–11] mentioned earlier yield an effective Hamiltonian which approaches the zero-field form as the magnetic field approaches zero. We may thus hope to find an appropriate choice of $\mathbf{U}^{\mathbf{q}}$ for which $A(\mathbf{r})$ closely approximates $a(\mathbf{r})$ in weak magnetic fields. Luttinger[14] derived an approximate one-band effective Hamiltonian, making use of the set of functions obtained from $a(\mathbf{r})$ by magnetic translations. We recall that, in the symmetric gauge, a magnetic translation consists of a pure translation combined with the gauge transformation $\exp[\frac{1}{2}i(\boldsymbol{\beta}\times\mathbf{R})\cdot\mathbf{r}]$, where $\boldsymbol{\beta}=e\mathbf{B}/\hbar c$. The basis functions $a(\mathbf{R};\mathbf{r})$ are thus of the form

$$a(\mathbf{R};\mathbf{r})=a(\mathbf{r}+\mathbf{R})\exp[\tfrac{1}{2}i(\boldsymbol{\beta}\times\mathbf{R})\cdot\mathbf{r}]. \tag{21}$$

The functions are not orthonormal because of the presence of the plane-wave term. However, the matrix element $\langle a(\mathbf{r})|a(\mathbf{R};\mathbf{r})\rangle$ can be expected to be very small in general, since the wave vector of the plane wave is of the order 0.2×10^{-9} $(\mathbf{B}\times\mathbf{R})$ atomic units, with $\mathbf{B}$ in gauss and $\mathbf{R}$ in atomic units. The problem of forming a set of orthonormal functions from the set $a(\mathbf{R};\mathbf{r})$ is analogous to the problem, in the absence of a field, of forming orthonormal functions from a set of orbitals $\phi(\mathbf{r}-\mathbf{R})$. In the latter case one forms Bloch sums of orbitals, which are then normalized. The resulting Bloch functions are added, as in Eq. (1), to form the orthonormal functions. In the present problem, instead of Bloch sums we make use of the group projection operators[12] (of which the Bloch sum is a special case) to form functions with the symmetry properties of the eigenfunctions. If we make use of the standard representations, the projection operators are equivalent to a Bloch sum in the lattice planes defined by $\mathbf{a}_1$ and $\mathbf{a}_3$, while in the $\mathbf{a}_2$ direction the sum only couples planes separated by $N\mathbf{a}_2$. A particular partner function for a given representation will appear N times, each associated with a different set of planes. These N functions can be orthonormalized, by the Schmidt procedure, for example. In this way each function associated with a given set of planes is modified by a slight admixture of the other functions. If it were not for this mixing, application of Eq. (9) would yield the result $A(\mathbf{r})=a(\mathbf{r})$. Thus the actual function obtained deviates from $a(\mathbf{r})$ by a small admixture of the other basis functions. For commonly available fields, the deviation is expected to be extremely small.

The Schmidt process for orthonormalizing a set of functions is not the most satisfactory method for the functions under consideration. In this method the different functions are not on an equal footing, since one function is retained unmodified except for a scale factor. A second one is then chosen, combined linearly with the

[14] J. M. Luttinger, Phys. Rev. 84, 814 (1951).

first so that the resulting function is orthogonal to it, and normalized. A third function is mixed with these two, and so on. Thus certain functions undergo more modification than others.

A more symmetric procedure is obtained by "rotating" each of the normalized functions (regarded as vectors) simultaneously. The rotation of the vector $\mathbf{X}_n$ transforms it to $\mathbf{X}_n'$, where

$$\mathbf{X}_n' = \eta[\mathbf{X}_n - \tfrac{1}{2}\textstyle\sum_{i\neq n}(\mathbf{X}_n\cdot\mathbf{X}_i)\mathbf{X}_i], \tag{22}$$

and η is a normalizing factor. The primed vectors are not fully orthogonal, but their scalar products are of order ϵ^2 if the original ones are of order ϵ. This procedure can be repeated to any order, and a corresponding one-band effective Hamiltonian can be obtained that is sufficient for problems involving isolated bands.

The previous formulation ignores interband effects. In most physical applications it is sufficient to neglect these except when dealing with nearly touching or overlapping bands. We will thus not concern ourselves with the general case, but rather deal with a formulation involving only a few bands. In principle, we could use a direct generalization of our previous method. The procedure would be to start with conventional Wannier functions $a^n(\mathbf{r})$ from each band n, and use group projection operators on these. Orthonormalization of these functions would involve some interband mixing. From the resulting functions we could form the sets of generalized Wannier functions $A^n(\mathbf{R})$, which have the property

$$\langle A^n(\mathbf{R})\,|\,A^m(\mathbf{R}')\rangle = \delta_{n,m}\delta_{\mathbf{R},\mathbf{R}'}. \tag{23}$$

The multiband effective Hamiltonian $\mathbf{H}(\boldsymbol{\pi})$ is then a matrix operator. In this representation the Schrödinger equation becomes

$$\textstyle\sum_n H_{mn}(\boldsymbol{\pi})f_n(\mathbf{r}) = Ef_m(\mathbf{r}), \tag{24}$$

where

$$H_{mn}(\boldsymbol{\pi}) = \textstyle\sum_{\mathbf{R}}\epsilon_{mn}(\mathbf{R})e^{-i\mathbf{R}\cdot\boldsymbol{\pi}} \tag{25}$$

and

$$\epsilon_{mn}(\mathbf{R}) = \langle A^m(\mathbf{R})\,|\,H\,|\,A^n(0)\rangle. \tag{26}$$

It should be noted again that the functions $f_m(\mathbf{r})$ are to be evaluated at lattice points only.

The formulation just given yields a conceptual framework on which to base approximation methods, when interband effects become important. However, it is inconvenient to apply directly in the form given, since the orthonormalization procedure can be carried out in a variety of ways, and is generally cumbersome. The size of the off-diagonal elements in the effective Hamiltonian does not necessarily give a true indication of the interband mixing caused by the magnetic field, since the functions $A^n(\mathbf{R})$ do not refer to the original bands. As already noted, the orthogonalization procedure used in forming these functions can be carried out in such a way that there is a large amount of admixture of other bands. In zero field this would correspond to mixing Bloch functions from different bands in forming the Wannier functions.

We wish to establish a useful approximation procedure, based on the ideas presented, which does not depend sensitively on the details of the form of the effective Hamiltonian. We consider first the matrix $\mathbf{H}(\mathbf{k})$ obtained by replacing the operator $\boldsymbol{\pi}$ by the vector $\mathbf{k}$ in the effective Hamiltonian. If we diagonalize this matrix, in the absence of fields, the diagonal elements are the original energy-band functions $E^n(\mathbf{k})$, no matter how much interband mixing one used in the original choice of Wannier functions. The corresponding result does not hold in the presence of a magnetic field. In that case the diagonal terms depend on the original choices of $A^n(\mathbf{R})$. However, it is usually a sufficient approximation to neglect this fact and assume that the multiband effective Hamiltonian can be obtained by writing the zero-field effective Hamiltonian in some nondiagonal form, and replacing $\mathbf{p}$ by $\boldsymbol{\pi}$. Recently, Hardy[15] has shown that there exists a particular form for which this result is rigorous. However, it is not clear that one can find this form simply. It turns out, however, that the results are not too sensitive to the particular form chosen, and that one can go a long way in the analysis merely from a knowledge of $E^n(\mathbf{k})$. Some of these remarks will be illustrated in an accompanying paper[16] in which calculations using model effective Hamiltonians are carried out.

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