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Wannier functions for lattices in a magnetic field

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Abstract. This paper considers the definition and properties of Wannier functions for Bloch electrons in a magnetic field. When the quantized Hall conductance of a band is non-zero, conventional Wannier functions with good localization properties cannot be constructed. The difficulty can be overcome by slightly broadening the definition of the Wannier function: the generalized Wannier functions are a good basis set, and well localized. They are generated by applying magnetic translations to a set of $|N|$ fundamental Wannier states: if the number of flux quanta per unit cell is q/p (a rational number), and the Hall conductance integer is M, then N satisfies $Mq + Np = 1$.

Unlike conventional Wannier functions, the definition of these Wannier states depends upon the choice of the basis vectors for lattice translations. The paper gives the transformation properties of the Wannier functions induced by reassignment of the primitive-lattice basis vectors.

1. Introduction

The use of localized basis states for representation of a wavefunction often has significant analytical and conceptual advantages. A well known example is the Wannier function basis, which is a set of localized states constructed from a Bloch band for an electron in a periodic potential. A fundamental Wannier state $|\phi\rangle$ is constructed by integrating the Bloch states $|B(\boldsymbol{k})\rangle$ with respect to the wavevector $\boldsymbol{k}$, over the Brillouin zone BZ:

$$|\phi\rangle = \int_{\mathrm{BZ}} \mathrm{d}\boldsymbol{k}\ |B(\boldsymbol{k})\rangle. \tag{1.1}$$

If the Bloch states are an analytic function of $\boldsymbol{k}$, and periodic on the Brillouin zone, this state is well localized. An orthonormal set of Wannier functions spanning the states which comprise the Bloch band is generated by translating the fundamental Wannier state through a set of lattice translations $\boldsymbol{R}$:

$$|\phi(\boldsymbol{R})\rangle = \hat{T}(\boldsymbol{R})|\phi\rangle \tag{1.2}$$

where in the absence of a magnetic field the translation operator is $\hat{T}(\boldsymbol{R}) = \exp[-\mathrm{i}\hat{\boldsymbol{p}}\cdot\boldsymbol{R}/\hbar]$, with $\hat{\boldsymbol{p}} = -\mathrm{i}\hbar\boldsymbol{\nabla}$. The Wannier function basis is particularly convenient when the electrons in the band are also subject to localized interactions, either with impurities or with other charged particles (such as electron–hole attraction leading to the formation of Wannier excitons) [1]. Wannier function bases have also proved very useful for analysing quasiperiodic potentials [2], and quantized charge transport [3, 4]. Their properties are discussed clearly in [5].

When there is a magnetic field present in addition to the periodic potential, the use of Wannier function bases becomes problematic. The difficulty arises because the Bloch functions are not, in general, a periodic and analytic function of the Bloch wavevector: the phase of the wavefunction increases by $2\pi M$ (where M takes integer values) upon traversing the boundary of the Brillouin zone (the precise meaning of this statement is explained in references [4] and [6]). The Bloch states can only be made periodic and analytic when $M = 0$. It has been proved that M is the quantized Hall conductance integer of the Bloch band [6]. When M is non-zero, conventional Wannier functions are not well localized [7–9].

A simple modification of the definition of the Wannier functions can be proposed, in which the Bloch states are multiplied by an analytic function $f(\boldsymbol{k})$ with zeros with total index $-M$. These states are unsatisfactory because they do not form a complete set, in the sense that the Bloch states for which $\boldsymbol{k}$ is a zero of $f(\boldsymbol{k})$ cannot be expanded in these localized states [8, 9].

This paper will discuss the case where the electron is confined to a two-dimensional plane, with cartesian coordinates (x, y) perpendicular to the magnetic field: the results also apply directly to the three-dimensional cases where the motion along the direction of the magnetic field is separable from the other degrees of freedom. Bloch bands exist when the magnetic flux passing through a unit cell and the flux quantum h/e are rationally related, with ratio p/q. When the magnetic field strength is not rational, the spectrum has a Cantor set structure [10, 11]. The definition of satisfactory Wannier functions can be extended to the case of non-rational fields [2], but this will not be considered in the present paper.

This paper describes the construction of sets of generalized Wannier functions which overcome the difficulties discussed in [7–9]. The generalized Wannier functions are well localized, and form a complete basis. A form of the generalized Wannier functions was introduced in [2], for the phase-space lattice Hamiltonian, which is a realistic model for Bloch electrons in a magnetic field. In this paper I will describe two different types of generalized Wannier function, one of which (the type II functions) correspond to those introduced in [2]. The derivation will be much more direct, and also has the advantage of using only a minimal set of algebraic properties of the Bloch states, rather than being tied to a specific representation. Another advantage is that it is applicable for an arbitrary lattice, whereas the calculation in [2] only considers the case of a square lattice, aligned with the coordinate system, in a limiting case where the problem can be modelled by a one-dimensional effective Hamiltonian.

Unlike conventional Wannier functions, the definition of these Wannier states depends upon the choice of the basis vectors for lattice translations. The paper gives the transformation properties of the Wannier functions induced by a reassignment of the primitive-lattice basis vectors. Also, in common with conventional Wannier functions, the functions are not invariant under transformations of the Bloch states of the form

$$|B(\boldsymbol{k})\rangle \to |B'(\boldsymbol{k})\rangle = \exp[\mathrm{i}\theta(\boldsymbol{k})]|B(\boldsymbol{k})\rangle \tag{1.3}$$

where $\theta(\boldsymbol{k})$ is periodic on the Brillouin zone of a lattice: these will be referred to as *gauge transformations*. The corresponding transformations of both types of Wannier function will be discussed in a subsequent paper, together with operations representing the effect of continuous translations on the Wannier functions.

2. Bloch states for rational magnetic fields

The basis vectors of the primitive lattice are denoted by $\boldsymbol{A}_1$ and $\boldsymbol{A}_2$, and the reciprocal-lattice vectors by $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$; these satisfy

$$\boldsymbol{A}_i \cdot \boldsymbol{a}_j = 2\pi\delta_{ij}. \tag{2.1}$$

The Hamiltonian $\hat{H}$ commutes with a set of translation operators $\hat{T}(\boldsymbol{A}_i)$:

$$[\hat{H}, \hat{T}(\boldsymbol{A}_i)] = 0. \tag{2.2}$$

These translations are termed magnetic translation operators: they were introduced by Brown [12] and Zak [13] for the special case of the symmetric gauge. Appendix A gives a simple discussion of the form of the magnetic translation operators for a general linear gauge, and also considers why linear gauges are preferred.

When the translation operator $\hat{T}(\boldsymbol{A}_i)$ acts on an eigenfunction, the result is an eigenfunction with the same energy (either a phase factor times the same eigenfunction, or a linear combination of degenerate eigenfunctions). For translations through lattice vectors, the magnetic translation operators satisfy

$$\hat{T}(\boldsymbol{A}_1)\hat{T}(\boldsymbol{A}_2) = \exp[2\pi \mathrm{i} q/p]\hat{T}(\boldsymbol{A}_2)\hat{T}(\boldsymbol{A}_1) \tag{2.3}$$

where q/p is the number of flux quanta per unit cell; throughout this paper I will assume that p and q are integers with no common divisor (p will be taken to be positive). For general translations, the magnetic translations satisfy:

$$\hat{T}(\boldsymbol{R}_1)\hat{T}(\boldsymbol{R}_2) = \exp\left[\frac{2\pi \mathrm{i} q}{p}\frac{(\boldsymbol{R}_1 \times \boldsymbol{R}_2)}{(\boldsymbol{A}_1 \times \boldsymbol{A}_2)}\right]\hat{T}(\boldsymbol{R}_2)\hat{T}(\boldsymbol{R}_1). \tag{2.4}$$

The magnetic translation operators form a 'projective' or 'ray' group [12, 13]: they satisfy

$$\hat{T}(\boldsymbol{R}_1 + \boldsymbol{R}_2) = \exp[\mathrm{i}\theta(\boldsymbol{R}_1, \boldsymbol{R}_2)]\hat{T}(\boldsymbol{R}_1)\hat{T}(\boldsymbol{R}_2). \tag{2.5}$$

The phase factor implies that the closure property of the group is lost, and many of the results of group theory cease to be applicable. The translation operators still satisfy the relations (2.3), (2.4) if they are multiplied by arbitrary phase factors; in the remainder of this paper it will be assumed that these phases are chosen such that

$$\hat{T}(\boldsymbol{R}_1 + \boldsymbol{R}_2) = \exp\left[\frac{\pi \mathrm{i} q}{p}\frac{(\boldsymbol{R}_1 \times \boldsymbol{R}_2)}{(\boldsymbol{A}_1 \times \boldsymbol{A}_2)}\right]\hat{T}(\boldsymbol{R}_2)\hat{T}(\boldsymbol{R}_1). \tag{2.6}$$

Equation (2.3) implies that

$$[\hat{T}(p\boldsymbol{A}_1), \hat{T}(\boldsymbol{A}_2)] = 0 \tag{2.7}$$

so Bloch's theorem [5] applies on a superlattice spanned by $p\boldsymbol{A}_1$ and $\boldsymbol{A}_2$, where the $\boldsymbol{A}_i$ are any choice of lattice vectors. Eigenfunctions can therefore be found which satisfy

$$\hat{T}(p\boldsymbol{A}_1)|B(\boldsymbol{k})\rangle = \exp[\mathrm{i}p\boldsymbol{k}\cdot\boldsymbol{A}_1]|B(\boldsymbol{k})\rangle \tag{2.8}$$

$$\hat{T}(\boldsymbol{A}_2)|B(\boldsymbol{k})\rangle = \exp[\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{A}_2]|B(\boldsymbol{k})\rangle. \tag{2.9}$$

The Bloch eigenfunctions $|B(\boldsymbol{k})\rangle$ have p-fold degeneracy (since $\hat{T}(\boldsymbol{A}_1)|B(\boldsymbol{k})\rangle$ is also an eigenfunction). Using (2.3),

$$\hat{T}(\boldsymbol{A}_2)\hat{T}(\boldsymbol{A}_1)|B(\boldsymbol{k})\rangle = \exp[\mathrm{i}(\boldsymbol{k} - q\boldsymbol{a}_2/p)\cdot\boldsymbol{A}_2]\hat{T}(\boldsymbol{A}_1)|B(\boldsymbol{k})\rangle \tag{2.10}$$

implying that the eigenfunction $\hat{T}(\boldsymbol{A}_1)|B(\boldsymbol{k})\rangle$ satisfies (2.8) with $\boldsymbol{k}$ replaced by $\boldsymbol{k} - q\boldsymbol{a}_2/p$. It also satisfies (2.8), implying that the Bloch states can be defined such that

$$\hat{T}(\boldsymbol{A}_1)|B(\boldsymbol{k})\rangle = \exp[\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{A}_1]|B(\boldsymbol{k} - q\boldsymbol{a}_2/p)\rangle \tag{2.11}$$

which defines a gauge relation on Bloch states separated by $q\boldsymbol{a}_2/p$.

The following periodicity conditions can be imposed on the Bloch states:

$$|B(\boldsymbol{k} + \boldsymbol{a}_2)\rangle = |B(\boldsymbol{k})\rangle \tag{2.12}$$

$$|B(\boldsymbol{k} + \boldsymbol{a}_1/p)\rangle = \exp[\mathrm{i}M\boldsymbol{k}\cdot\boldsymbol{A}_2]|B(\boldsymbol{k})\rangle \tag{2.13}$$

where M is a topological index called the Chern integer, which corresponds to the quantized Hall conductance integer of the Bloch band [6]. Throughout the remainder of this paper it will be assumed that the Bloch states are gauged so that these conditions are satisfied. Another integer N will play an important role; this index is related to M by a diophantine equation

$$qM + pN = 1. \tag{2.14}$$

Applying (2.12) M times, this leads to an alternative form which is sometimes useful:

$$|B(\boldsymbol{k} - \boldsymbol{a}_2/p)\rangle = \exp[-\mathrm{i}M\boldsymbol{k}\cdot\boldsymbol{A}_1]\hat{T}(M\boldsymbol{A}_1)|B(\boldsymbol{k})\rangle. \tag{2.15}$$

Equations (2.9), (2.11), (2.12) and (2.13) define the essential properties of the Bloch states: they represent a constraint on the gauge of the Bloch states, and also a constraint on the way that the wavevector $\boldsymbol{k}$ is used to label the p-fold-degenerate states. Bloch states satisfying these equations will be termed *canonical* with respect to the set of basis vectors $\boldsymbol{A}_1$ and $\boldsymbol{A}_2$. The gauge of the Bloch states is not uniquely specified by these four equations: the states remain canonically gauged after applying the transformation (1.3) if the phase $\theta(\boldsymbol{k})$ satisfies

$$\theta(\boldsymbol{k} + \boldsymbol{a}_1/p) = \theta(\boldsymbol{k}) = \theta(\boldsymbol{k} + \boldsymbol{a}_2/p). \tag{2.16}$$

3. Wannier functions

Two types of Wannier function will be defined, termed types I and II.

3.1. Type I Wannier functions

Consider the set of states

$$|C(\boldsymbol{k})\rangle = \hat{T}\left(-\frac{pM}{2\pi}(\boldsymbol{k}\cdot\boldsymbol{A}_1)\boldsymbol{A}_2\right)|B(\boldsymbol{k})\rangle. \tag{3.1}$$

These are periodic on the Brillouin zone reciprocal to the superlattice

$$|C(\boldsymbol{k} + \boldsymbol{a}_1/p)\rangle = |C(\boldsymbol{k})\rangle \tag{3.2}$$
$$|C(\boldsymbol{k} + \boldsymbol{a}_2)\rangle = |C(\boldsymbol{k})\rangle. \tag{3.3}$$

Provided that the potential is smooth and the bands are non-degenerate, these states can be gauged so that they are an analytic function of $\boldsymbol{k}$. Well-localized states can be formed by integrating over $\boldsymbol{k}$; using the usual construction for Wannier functions gives the following pair of reciprocal relations:

$$\begin{aligned} |C(\boldsymbol{k})\rangle &= \sum_{\boldsymbol{R}} \exp[-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}]|\chi(\boldsymbol{R})\rangle \\ |\chi(\boldsymbol{R})\rangle &= \frac{p}{4\pi^2}\int_{\mathrm{BZ}[\boldsymbol{a}_1/p,\boldsymbol{a}_2]} \mathrm{d}\boldsymbol{k}\ \exp[\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}]|C(\boldsymbol{k})\rangle \end{aligned} \tag{3.4}$$

where the Brillouin zone BZ is spanned by the vectors $\boldsymbol{a}_1/p$, $\boldsymbol{a}_2$, and the $\boldsymbol{R}$ are points of a superlattice $\boldsymbol{R} = n_1 p\boldsymbol{A}_1 + n_2\boldsymbol{A}_2$. The state $|\chi(\boldsymbol{R})\rangle$is localized about the lattice point $\boldsymbol{R}$. The Wannier states $|\chi(\boldsymbol{R})\rangle$ form an orthonormal set: $\langle\chi(\boldsymbol{R})|\chi(\boldsymbol{R}')\rangle = \delta_{\boldsymbol{R},\boldsymbol{R}'}$.

The states $|\chi(\boldsymbol{R})\rangle$ are not all images of each other under translations: consider the effect of applying a general lattice translation to $|\chi(\boldsymbol{R})\rangle$. For lattice vectors $n_1\boldsymbol{A}_1 + n_2\boldsymbol{A}_2$,

$$\hat{T}(n_2\boldsymbol{A}_2)\hat{T}(n_1\boldsymbol{A}_1)|C(\boldsymbol{k})\rangle = \exp\left[\mathrm{i}\left(pN(\boldsymbol{k}\cdot\boldsymbol{A}_1)n_1 + (\boldsymbol{k}\cdot\boldsymbol{A}_2)n_2 - \frac{2\pi\mathrm{i}qn_1n_2}{p}\right)\right]|C(\boldsymbol{k} - n_1q\boldsymbol{a}_2/p)\rangle. \tag{3.5}$$

It follows that, if $\boldsymbol{R} = pm_1\boldsymbol{A}_1 + m_2\boldsymbol{A}_2$,

$$\hat{T}(n_2\boldsymbol{A}_2)\hat{T}(n_1\boldsymbol{A}_1)|\chi(\boldsymbol{R})\rangle = \exp\left[\frac{2\pi\mathrm{i}qm_2n_1}{p}\right]|\chi(\boldsymbol{R} + pNn_1\boldsymbol{A}_1 + n_2\boldsymbol{A}_2)\rangle. \tag{3.6}$$

Applying lattice translations does not therefore generate the full set of states $|\chi(\boldsymbol{R})\rangle$. The full set of Wannier functions can be generated by applying lattice translations $\hat{T}(\boldsymbol{R})$, $\boldsymbol{R} = pn_1\boldsymbol{A}_1 + n_2\boldsymbol{A}_2$, to a set of fundamental Wannier functions

$$|\chi_\mu\rangle = |\chi(\mu p\boldsymbol{A}_1)\rangle \qquad \mu = 0, \ldots, |N| - 1. \tag{3.7}$$

In particular, the Wannier function associated with a general lattice site is

$$|\chi\big(p(Nn_1 + \mu)\boldsymbol{A}_1 + n_2\boldsymbol{A}_2\big)\rangle = \hat{T}(n_2\boldsymbol{A}_2)\hat{T}(n_1\boldsymbol{A}_1)|\chi_\mu\rangle. \tag{3.8}$$

It is useful to be able to invert the relationship defining the $|\chi_\mu\rangle$, and express the Bloch states in terms of the Wannier functions: from (3.1) and (3.2),

$$|B(\boldsymbol{k})\rangle = \sum_{\boldsymbol{R}=p(Nn_1+\mu)\boldsymbol{A}_1+n_2\boldsymbol{A}_2} \exp[-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}]\hat{T}\left(\frac{pM}{2\pi}(\boldsymbol{k}\cdot\boldsymbol{A}_1)\boldsymbol{A}_2\right)|\chi(\boldsymbol{R})\rangle. \tag{3.9}$$

Using (3.8), $|B(\boldsymbol{k})\rangle$ can be written as a sum over a primitive lattice:

$$|B(\boldsymbol{k})\rangle = \sum_{\boldsymbol{R}=n_1\boldsymbol{A}_1+n_2\boldsymbol{A}_2} \exp[-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}]\hat{T}(n_2\boldsymbol{A}_2)\hat{T}(n_1\boldsymbol{A}_1)\hat{T}\left(\frac{pM}{2\pi}(\boldsymbol{k}\cdot\boldsymbol{A}_1)\boldsymbol{A}_2\right) \times \sum_\mu \exp[-\mathrm{i}p\mu(\boldsymbol{k}\cdot\boldsymbol{A}_1)]|\chi_\mu\rangle. \tag{3.10}$$

3.2. Type II Wannier functions

The expression (3.10) is satisfying in that the sum runs over sites of the primitive lattice, but it is has the unsatisfactory feature that the final summation over μ depends upon $\boldsymbol{k}$. This undesirable feature can be removed by considering a different set of fundamental Wannier states $|\phi_\mu\rangle$, defined in terms of the $|\chi_\mu\rangle$ states by

$$|\phi_\mu\rangle = \frac{1}{N}\sum_{\mu'=0}^{|N|-1} \exp[-2\pi\mathrm{i}\mu\mu'/N]\hat{T}(-\mu'\boldsymbol{A}_1/N)|\chi_{\mu'}\rangle. \tag{3.11}$$

The inverse relationship is

$$|\chi_\mu\rangle = \sum_{\mu'=0}^{|N|-1} \exp[2\pi\mathrm{i}\mu\mu'/N]\hat{T}(\mu\boldsymbol{A}_1/N)|\phi_{\mu'}\rangle. \tag{3.12}$$

Using (3.10), and noting that the sum over μ can be absorbed into a sum over $n_1' = Nn_1 + \mu$, the Bloch states can be expressed in terms of the functions $|\phi_\mu\rangle$ as follows:

$$|B(\boldsymbol{k})\rangle = \sum_{\boldsymbol{R}=n_1\boldsymbol{A}_1/N+n_2\boldsymbol{A}_2} \sum_{\mu=0}^{|N|-1} \exp[-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}]\exp[2\pi\mathrm{i}n_1\mu/N] \times \hat{T}(n_2\boldsymbol{A}_2)\hat{T}(n_1\boldsymbol{A}_1/N)\hat{T}\left(\frac{pM}{2\pi}(\boldsymbol{k}\cdot\boldsymbol{A}_1)\boldsymbol{A}_2\right)|\phi_\mu\rangle. \tag{3.13}$$

In this expression the $\boldsymbol{k}$-dependence of the Wannier functions has been removed, at the expense of making the lattice sum run over a lattice which is $|N|$ times denser than the primitive lattice. This equation is analogous to equation (3.15) of reference [2]. The derivation given here has several advantages: it is more direct, it uses (as far as appears possible) only algebraic properties rather than a specific representation, and it is formulated for a general lattice.

4. Transformations of Bloch states

4.1. Motivation

When the Chern integer M is non-zero, the canonical Bloch states defined in section 2 depend upon the basis vectors of the primitive lattice, $\boldsymbol{A}_1$ and $\boldsymbol{A}_2$. The choice of basis vectors for the lattice is arbitrary. It is therefore desirable to understand how the Bloch states and Wannier states are transformed under a change of the basis vectors.

The possible changes of basis are of the form

$$\begin{pmatrix} \boldsymbol{A}'_1 \\ \boldsymbol{A}'_2 \end{pmatrix} = \begin{pmatrix} N_{11} & N_{12} \\ N_{21} & N_{22} \end{pmatrix} \begin{pmatrix} \boldsymbol{A}_1 \\ \boldsymbol{A}_2 \end{pmatrix} = \tilde{N} \begin{pmatrix} \boldsymbol{A}_1 \\ \boldsymbol{A}_2 \end{pmatrix} \tag{4.1}$$

with $\det(\tilde{N}) = 1$, with all of the elements N_{ij} being integer valued. The objective is to define, for every such matrix $\tilde{N}$, the corresponding transformation of the Bloch and Wannier states. This task is simplified by noting that every transformation $\tilde{N}$ can be written as a product of elementary operations, parametrized by three integers n_1, n_2, n_3:

$$\tilde{N}(n_1, n_2, n_3) = \tilde{S}(n_1)\tilde{R}\tilde{S}(n_2)\tilde{R}\tilde{S}(n_3) \tag{4.2}$$

where

$$\tilde{S}(n) = \begin{pmatrix} 1 & n \\ 0 & 1 \end{pmatrix} = [\tilde{S}(1)]^n \qquad \tilde{R} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{4.3}$$

The matrix $\tilde{R}$ represents an exchange of identity of the basis vectors, combined with an inversion of one of them; note that in a square lattice, $\tilde{R}$ would represent a $\pi/2$ rotation, and for this reason this operation will be referred to as the elementary rotation. The matrix $\tilde{S}(n)$ represents a shear transformation; the general shear transformation is itself composed of a product of $\tilde{S}(1)$. The effect of a general transformation on the Bloch or Wannier states is determined by taking a composition of the images of elementary transformations acting on the Bloch or Wannier states. In this section, the transformations of canonical Bloch states corresponding to elementary rotations and shears will be obtained. The corresponding transformations for Wannier states are obtained in section 5.

4.2. General approach

It will be convenient to collect together the relations defining the canonical gauge of the Bloch states:

$$\hat{T}(\boldsymbol{A}_1)|B(\boldsymbol{k})\rangle = \exp[\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{A}_1]|B(\boldsymbol{k} - q\boldsymbol{a}_2/p)\rangle \tag{4.4a}$$

$$\hat{T}(\boldsymbol{A}_2)|B(\boldsymbol{k})\rangle = \exp[\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{A}_2]|B(\boldsymbol{k})\rangle \tag{4.4b}$$

$$|B(\boldsymbol{k} + \boldsymbol{a}_1/p)\rangle = \exp[\mathrm{i}M\boldsymbol{k}\cdot\boldsymbol{A}_2]|B(\boldsymbol{k})\rangle \tag{4.4c}$$

$$|B(\boldsymbol{k} + \boldsymbol{a}_2)\rangle = |B(\boldsymbol{k})\rangle. \tag{4.4d}$$

The requirement is to find a transformation of the Bloch states such that these four equations are satisfied with the original vectors $\boldsymbol{A}_i$, $\boldsymbol{a}_i$ replaced by the transformed vectors $\boldsymbol{A}'_i$ and

$\boldsymbol{a}_i'$. The transformed Bloch states must be a linear combination of degenerate Bloch states: using (2.11), this can be achieved by applying translations through multiples of $\boldsymbol{A}_1$, of the form

$$|B'(\boldsymbol{k})\rangle = \sum_{\lambda=0}^{p-1} \alpha_\lambda(\boldsymbol{k}) \hat{T}(\lambda \boldsymbol{A}_1)|B(\boldsymbol{k})\rangle. \tag{4.5}$$

It may also be necessary to apply a gauge transformation to the translation operators, of the form

$$\hat{T}'(\boldsymbol{R}) = \exp[\mathrm{i}\boldsymbol{c} \cdot \boldsymbol{R}]\hat{T}(\boldsymbol{R}) \tag{4.6}$$

so in (4.4), $\hat{T}(\boldsymbol{A}_i)$ would be replaced by $\hat{T}'(\boldsymbol{A}_i')$. The transformed translation operators still satisfy all of the relations (2.3) to (2.7). The motivation for including this gauge transformation is that, if it were not included, equation (2.8) might not be satisfied by the transformed states.

The normalization of the Bloch states has not been discussed, and the transformation will not necessarily preserve normalization.

4.3. *Rotation of Bloch states*

The elementary rotation has the following action on both the direct and the reciprocal lattice:

$$\begin{aligned} \boldsymbol{A}_1' &= \boldsymbol{A}_2 \qquad & \boldsymbol{A}_2' &= -\boldsymbol{A}_1 \\ \boldsymbol{a}_1' &= \boldsymbol{a}_2 \qquad & \boldsymbol{a}_2' &= -\boldsymbol{a}_1. \end{aligned} \tag{4.7}$$

The objective is to find a set of Bloch states satisfying (4.4*a*)–(4.4*d*) with the rotated vectors $\boldsymbol{A}_i'$ and $\boldsymbol{a}_i'$ replacing the original ones. This may involve taking linear combinations of degenerate Bloch states. Consider the properties of the state

$$|S(\boldsymbol{k})\rangle = \sum_{\lambda=0}^{p-1} |B(\boldsymbol{k} + q\lambda \boldsymbol{a}_2/p)\rangle. \tag{4.8}$$

Systematic application of (4.4) shows that this satisfies the following conditions:

$$\hat{T}(\boldsymbol{A}_1)|S(\boldsymbol{k})\rangle = \exp[\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{A}_1]|S(\boldsymbol{k})\rangle \tag{4.9a}$$

$$\hat{T}(\boldsymbol{A}_2)|S(\boldsymbol{k})\rangle = \exp[\mathrm{i}pN\boldsymbol{k} \cdot \boldsymbol{A}_2]|S(\boldsymbol{k} + q\boldsymbol{a}_1/p)\rangle \tag{4.9b}$$

$$|S(\boldsymbol{k} + \boldsymbol{a}_2/p)\rangle = |S(\boldsymbol{k})\rangle \tag{4.9c}$$

$$|S(\boldsymbol{k} + \boldsymbol{a}_1)\rangle = \exp[\mathrm{i}pM\boldsymbol{k} \cdot \boldsymbol{A}_2]|S(\boldsymbol{k})\rangle. \tag{4.9d}$$

These are sufficiently similar to the required relations that the transformed Bloch states can be obtained by making a gauge transformation of the $|S(\boldsymbol{k})\rangle$:

$$|B'(\boldsymbol{k})\rangle = \exp[\mathrm{i}\theta(\boldsymbol{k})]|S(\boldsymbol{k})\rangle. \tag{4.10}$$

Requiring that the $|B'(\boldsymbol{k})\rangle$ satisfy (4.4) with the rotated vectors, these relations imply the following conditions on the gauge function $\theta(\boldsymbol{k})$:

$$\theta(\boldsymbol{k} + q\boldsymbol{a}_1/p) = \theta(\boldsymbol{k}) - Mq\boldsymbol{k} \cdot \boldsymbol{A}_2 \tag{4.11a}$$

$$\theta(\boldsymbol{k} + \boldsymbol{a}_2/p) = \theta(\boldsymbol{k}) - M\boldsymbol{k} \cdot \boldsymbol{A}_1 \tag{4.11c}$$

$$\theta(\boldsymbol{k} - \boldsymbol{a}_1) = \theta(\boldsymbol{k}) + pM\boldsymbol{k} \cdot \boldsymbol{A}_2 \tag{4.11d}$$

(note that there is no condition on $\theta(\boldsymbol{k})$ from (4.4*b*), and that in this case $\boldsymbol{c} = \boldsymbol{0}$ in (4.6)). Equations (4.11) are solved by writing $\theta = \alpha k_1 k_2$, where $k_i = \boldsymbol{k} \cdot \boldsymbol{A}_i$: on substitution, it is found that $\alpha = -Mp/2\pi$. The transformed Bloch state is therefore

$$|B'(\boldsymbol{k})\rangle = \exp\left[-\mathrm{i}\frac{pM}{2\pi}(\boldsymbol{k}\cdot\boldsymbol{A}_1)(\boldsymbol{k}\cdot\boldsymbol{A}_2)\right]\sum_{\lambda=0}^{p-1}|B(\boldsymbol{k}+\lambda q\boldsymbol{a}_2/p)\rangle$$
$$= \exp\left[-\mathrm{i}\frac{pM}{2\pi}k_1k_2\right]\sum_{\lambda=0}^{p-1}\exp[\mathrm{i}\lambda k_1]\hat{T}(-\lambda\boldsymbol{A}_1)|B(\boldsymbol{k})\rangle. \tag{4.12}$$

4.4. Shearing transformation of Bloch states

The action of the shearing transformation on the basis vectors of the primitive lattice and their reciprocal lattice is

$$\begin{aligned} \boldsymbol{A}'_1 &= \boldsymbol{A}_1 + n\boldsymbol{A}_2 \qquad & \boldsymbol{A}'_2 &= \boldsymbol{A}_2 \\ \boldsymbol{a}'_1 &= \boldsymbol{a}_1 & \boldsymbol{a}'_2 &= \boldsymbol{a}_2 - n\boldsymbol{a}_1. \end{aligned} \tag{4.13}$$

In this case, no mixing of Bloch states is required: a gauge transformation

$$|B'(\boldsymbol{k})\rangle = \exp[\mathrm{i}\theta(\boldsymbol{k})]|B(\boldsymbol{k})\rangle \tag{4.14}$$

is sufficient, but the translation operators must be gauge transformed. The transformed Bloch states (4.14) satisfy

$$\begin{aligned} \hat{T}(p\boldsymbol{A}'_1)|B'(\boldsymbol{k})\rangle &= (-1)^{pqn}\exp[\mathrm{i}p\boldsymbol{k}\cdot\boldsymbol{A}'_1]|B'(\boldsymbol{k})\rangle \\ \hat{T}(\boldsymbol{A}'_2)|B'(\boldsymbol{k})\rangle &= \exp[\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{A}'_2]|B'(\boldsymbol{k})\rangle. \end{aligned} \tag{4.15}$$

The factor $(-1)^{pqn}$ is removed by setting $\boldsymbol{c} = \frac{1}{2}qn\boldsymbol{a}_1$ in (4.6), so

$$\hat{T}'(\boldsymbol{A}'_1) = (-1)^{qn}\exp[-\mathrm{i}\pi qn/p]\hat{T}(\boldsymbol{A}_1)\hat{T}(n\boldsymbol{A}_2) \qquad \hat{T}'(\boldsymbol{A}'_2) = \hat{T}(\boldsymbol{A}_2). \tag{4.16}$$

It is found that (4.4*b*) is satisfied immediately in the primed variables. The relations (4.4*a*), (4.4*c*) and (4.4*d*) lead to the following relations for the gauge function $\theta(\boldsymbol{k})$:

$$\theta(\boldsymbol{k} - q\boldsymbol{a}'_2/p) = \theta(\boldsymbol{k}) + \frac{\pi qn}{p}\big(p - 1 + 2qM\big) - qMn(\boldsymbol{k}\cdot\boldsymbol{A}_2) + 2\pi L_1 \tag{4.17a}$$
$$\theta(\boldsymbol{k} + \boldsymbol{a}_1/p) = \theta(\boldsymbol{k}) + 2\pi L_2 \tag{4.17c}$$
$$\theta(\boldsymbol{k} + \boldsymbol{a}'_2) = \theta(\boldsymbol{k}) + npM(\boldsymbol{k}\cdot\boldsymbol{A}_2) + 2\pi L_3 \tag{4.17d}$$

where the terms $2\pi L_i$, with L_i integers, are included because the phase differences are only determined to within multiples of 2π. It is anticipated that a solution can be found of the form

$$\theta(k_1, k_2) = \alpha k_2^2 + \beta k_2 \tag{4.18}$$

with $L_2 = 0$. Upon substitution, it is found that $\alpha = npM/4\pi$, and that (4.17*a*) and (4.17*d*) lead to the following equations for β:

$$\frac{\pi Mnq^2}{p} - \frac{2\pi q}{p}\beta = \frac{\pi qn}{p}\big(p - 1 + 2qM\big) + 2\pi L_1 \tag{4.19a}$$
$$\pi pMn + 2\pi\beta = 2\pi L_3. \tag{4.19d}$$

Eliminating β from these equations leads to the following equation for the integers L_1 and L_3:

$$pL_1 + qL_3 = \mathcal{N}n \qquad \mathcal{N} = \tfrac{1}{2}pq(N + M - 1). \tag{4.20}$$

Comparison with (2.14) shows that the solutions are

$$L_1 = \mathcal{N} N n \qquad L_3 = \mathcal{N} M n. \tag{4.21}$$

It must be verified that these are integer values: this is established by showing that $\mathcal{N}$ is integer valued. To verify this, note that in the case where both p and q are odd, $pN + qM$ is even when N and M have the same parity. This latter condition contradicts (2.14), implying that for p, q both odd, $N + M - 1$ is even.

The value of the coefficient β in (4.18) is now determined by (4.19d) and (4.21). The Bloch states are therefore transformed as follows:

$$|B'(\boldsymbol{k})\rangle = \exp\left[\mathrm{i}\left(\frac{npM}{4\pi}(\boldsymbol{k}\cdot\boldsymbol{A}_2)^2 + nM(\mathcal{N} - \tfrac{1}{2}p)(\boldsymbol{k}\cdot\boldsymbol{A}_2)\right)\right]|B(\boldsymbol{k})\rangle \tag{4.22}$$

where $\mathcal{N}$ is given by (4.20).

5. Transformations of Wannier functions

5.1. General considerations

In the preceding section, rules were given for transformation of a set of canonical Bloch states when the basis vectors of the lattice are changed from $\boldsymbol{A}_1$, $\boldsymbol{A}_2$ to $\boldsymbol{A}'_1$, $\boldsymbol{A}'_2$. Now the corresponding transformations of the Wannier functions will be calculated.

The fundamental Wannier functions for the transformed basis vectors are

$$|\chi'_\mu\rangle = |\chi'(\mu p\boldsymbol{A}'_1)\rangle \qquad \mu = 0, \ldots, |N| - 1 \tag{5.1}$$

where, using (3.1) and (3.4),

$$|\chi'(\boldsymbol{R})\rangle = \frac{p}{4\pi^2}\int_{\mathrm{BZ}'} \mathrm{d}\boldsymbol{k}\ \exp[\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}]\hat{T}'\left(-\frac{pM}{2\pi}(\boldsymbol{k}\cdot\boldsymbol{A}'_1)\boldsymbol{A}'_2\right)|B'(\boldsymbol{k})\rangle \tag{5.2}$$

and where BZ$'$ is the Brillouin zone for the transformed superlattice, spanned by the vectors $\boldsymbol{a}'_1/p$ and $\boldsymbol{a}'_2$. Here $|B'(\boldsymbol{k})\rangle$ is the transformed Bloch state, which is in general a linear combination of p degenerate Bloch states; using (2.15) this may be written in the form (4.5). Using (3.7) to (3.9), the transformed Wannier functions are then of the form

$$\begin{aligned}|\chi'_\mu\rangle = \frac{p}{4\pi^2}\int_{\mathrm{BZ}'} \mathrm{d}\boldsymbol{k}\ &\exp[\mathrm{i}p(\mu k'_1 - \mu' k_1)]\hat{T}'\left(-\frac{pM}{2\pi}k'_1\boldsymbol{A}'_2\right)\sum_{\lambda=0}^{p-1}\alpha_\lambda(\boldsymbol{k})\hat{T}(\lambda\boldsymbol{A}_1)\\ &\times\ \hat{T}\left(\frac{pM}{2\pi}k_1\boldsymbol{A}_2\right)\sum_{\mu'=0}^{|N|-1}\ \sum_{\boldsymbol{R}=pNn_1\boldsymbol{A}_1+n_2\boldsymbol{A}_2}\exp\big[-\mathrm{i}\big(\boldsymbol{k}\cdot\boldsymbol{R}\big)\big]\\ &\times\ \hat{T}(n_2\boldsymbol{A}_2)\hat{T}(n_1\boldsymbol{A}_1)|\chi_{\mu'}\rangle\end{aligned} \tag{5.3}$$

where $k_i = \boldsymbol{k}\cdot\boldsymbol{A}_i$ and $k'_i = \boldsymbol{k}\cdot\boldsymbol{A}'_i$. This expression may be written in the form

$$|\chi'_\mu\rangle = \sum_{\mu'=0}^{|N|-1}\int_{\mathrm{BZ}'} \mathrm{d}\boldsymbol{k}\ \hat{Q}_{\mu\mu'}(\boldsymbol{k})\hat{B}(\boldsymbol{k})|\chi_{\mu'}\rangle = \sum_{\mu'=0}^{|N|-1}\hat{M}_{\mu\mu'}|\chi_{\mu'}\rangle \tag{5.4}$$

where

$$\begin{aligned}\hat{Q}_{\mu\mu'}(\boldsymbol{k}) = \frac{p}{4\pi^2}\sum_{\lambda_1=0}^{p-1}\sum_{\lambda_2=0}^{p-1}&\exp\big[\mathrm{i}p\big(\mu k'_1 - \mu' k_1\big)\big]\exp\big[-\mathrm{i}\lambda_2 k_2\big]\alpha_\lambda(\boldsymbol{k})\\ &\times\ \hat{T}'\left(\frac{pM}{2\pi}k'_1\boldsymbol{A}'_2\right)\hat{T}(\lambda_1\boldsymbol{A}_1)\hat{T}\left(\frac{pM}{2\pi}k_1\boldsymbol{A}_2\right)\hat{T}(\lambda_2\boldsymbol{A}_2)\end{aligned} \tag{5.5}$$

and

$$\hat{B}(\boldsymbol{k}) = \sum_{n_1=-\infty}^{\infty}\sum_{n_2=-\infty}^{\infty} \exp\big[-\mathrm{i}p\big(Nn_1\boldsymbol{A}_1 + n_2\boldsymbol{A}_2\big)\cdot\boldsymbol{k}\big]\hat{T}(pn_2\boldsymbol{A}_2)\hat{T}(n_1\boldsymbol{A}_1)$$
$$= \sum_{\boldsymbol{R}=p(n_1N\boldsymbol{A}_1+n_2\boldsymbol{A}_2)} \exp[-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}]\hat{T}\left(\frac{(\boldsymbol{R}\cdot\boldsymbol{a}_2)}{2\pi}\boldsymbol{A}_2\right)\hat{T}\left(\frac{(\boldsymbol{R}\cdot\boldsymbol{a}_1)}{2\pi pN}\boldsymbol{A}_1\right). \tag{5.6}$$

The operator $\hat{B}(\boldsymbol{k})$ is periodic on a subset of the Brillouin zones BZ and BZ$'$:

$$\hat{B}(\boldsymbol{k}+\boldsymbol{a}_1/p) = \hat{B}(\boldsymbol{k}+\boldsymbol{a}_2/p) = \hat{B}(\boldsymbol{k}). \tag{5.7}$$

The product $\hat{Q}_{\mu\mu'}(\boldsymbol{k})\hat{B}(\boldsymbol{k})$ must be periodic on the Brillouin zone BZ$'$. The operator $\hat{Q}_{\mu\mu'}(\boldsymbol{k})$ satisfies

$$\begin{aligned} &\hat{Q}_{\mu\mu'}(\boldsymbol{k}+\boldsymbol{K}_i) = \hat{Q}_{\mu\mu'}(\boldsymbol{k})\hat{X}_i(\boldsymbol{k}) \\ &\boldsymbol{K}_1 = \boldsymbol{a}_1'/p \qquad \boldsymbol{K}_2 = \boldsymbol{a}_2' \end{aligned} \tag{5.8}$$

where the operators $\hat{X}_i(\boldsymbol{k})$ satisfy $\hat{X}_i(\boldsymbol{k})\hat{B}(\boldsymbol{k}) = \hat{B}(\boldsymbol{k})$. This equation is satisfied by combining translation operators and complex exponentials, and the operators $\hat{Q}_{\mu\mu'}(\boldsymbol{k})$ satisfy

$$\hat{Q}_{\mu\mu'}(\boldsymbol{k}+\boldsymbol{K}_i) = \exp\big[-\mathrm{i}\big(\boldsymbol{k}\cdot\boldsymbol{R}_i\big)\big]\hat{Q}_{\mu\mu'}(\boldsymbol{k})\hat{T}\left(\frac{(\boldsymbol{R}_i\cdot\boldsymbol{a}_2)}{2\pi}\boldsymbol{A}_2\right)\hat{T}\left(\frac{(\boldsymbol{R}_i\cdot\boldsymbol{a}_1)}{2\pi pN}\boldsymbol{A}_1\right) \tag{5.9}$$

where the vectors $\boldsymbol{R}_i$ are vectors drawn from the lattice sum in the second equation of (5.6), of the of the form $\boldsymbol{R}_i = p(J_{i1}N\boldsymbol{A}_1 + J_{i2}\boldsymbol{A}_2)$, with J_{ij} integers.

Provided that $\boldsymbol{R}_1$ and $\boldsymbol{R}_2$ are not linearly dependent, the sum over superlattice vectors $\boldsymbol{R}$ in (5.3) may be written in the form

$$\sum_{\boldsymbol{R}} = \sum_{m_1\boldsymbol{R}_1+m_2\boldsymbol{R}_2}\sum_{\boldsymbol{r}} \tag{5.10}$$

where in the first summation m_1 and m_2 run from $-\infty$ to ∞, and the second summation runs over a finite set of lattice vectors; the number of vectors $\boldsymbol{r}$ is $|\boldsymbol{R}_1\times\boldsymbol{R}_2|/(|\boldsymbol{A}_1\times\boldsymbol{A}_2|pN)$.

Using (5.9) and (5.10), and noting that the lattice translations $\hat{T}(\boldsymbol{R})$ in the second form of (5.6) commute, equation (5.4) can be simplified as follows:

$$\begin{aligned} |\chi_\mu'\rangle &= \sum_{\mu'=0}^{|N|-1}\int_{\mathrm{BZ}'}\mathrm{d}\boldsymbol{k}\ \hat{Q}_{\mu\mu'}(\boldsymbol{k}) \sum_{\boldsymbol{R}=m_1\boldsymbol{R}_1+m_2\boldsymbol{R}_2} \exp[-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}]\hat{T}\left(\frac{(\boldsymbol{R}\cdot\boldsymbol{a}_2)}{2\pi}\boldsymbol{A}_2\right)\hat{T}\left(\frac{(\boldsymbol{R}\cdot\boldsymbol{a}_1)}{2\pi pN}\boldsymbol{A}_1\right) \\ &\quad\times\sum_{\boldsymbol{r}}\exp[-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}]\hat{T}\left(\frac{(\boldsymbol{r}\cdot\boldsymbol{a}_2)}{2\pi}\boldsymbol{A}_2\right)\hat{T}\left(\frac{(\boldsymbol{r}\cdot\boldsymbol{a}_1)}{2\pi pN}\boldsymbol{A}_1\right)|\chi_{\mu'}\rangle \\ &= \sum_{\mu'=0}^{|N|-1}\sum_{\boldsymbol{K}=m_1\boldsymbol{a}_1'/p+m_2\boldsymbol{a}_2'}\int_{\mathrm{BZ}'}\mathrm{d}\boldsymbol{k}\ \hat{Q}_{\mu\mu'}(\boldsymbol{k}+\boldsymbol{K}) \\ &\quad\times\sum_{\boldsymbol{r}}\exp[-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}]\hat{T}\left(\frac{(\boldsymbol{r}\cdot\boldsymbol{a}_2)}{2\pi}\boldsymbol{A}_2\right)\hat{T}\left(\frac{(\boldsymbol{r}\cdot\boldsymbol{a}_1)}{2\pi pN}\boldsymbol{A}_1\right)|\chi_{\mu'}\rangle \\ &= \sum_{\mu'=0}^{|N|-1}\int\mathrm{d}\boldsymbol{k}\ \hat{Q}_{\mu\mu'}(\boldsymbol{k})\sum_{\boldsymbol{r}}\exp[-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}]\hat{T}\left(\frac{(\boldsymbol{r}\cdot\boldsymbol{a}_2)}{2\pi}\boldsymbol{A}_2\right)\hat{T}\left(\frac{(\boldsymbol{r}\cdot\boldsymbol{a}_1)}{2\pi pN}\boldsymbol{A}_1\right)|\chi_{\mu'}\rangle. \end{aligned} \tag{5.11}$$

In the final expression the integral is over the full range of $\boldsymbol{k}$, which is more convenient to evaluate, and the infinite sum appearing in (5.3) has been replaced by a finite one.

The operators $\hat{Q}_{\mu\mu'}(\boldsymbol{k})$ are linear combinations of translation operators, with arguments which are linear in $\boldsymbol{k}$, combined together with weights which are phase factors which are quadratic functions of the components of $\boldsymbol{k}$. The transformation of the Wannier functions is therefore constructed from operators of the following form:

$$\hat{S}(\tilde{\alpha}) = \int \mathrm{d}\boldsymbol{x}\ \exp\left[\frac{\mathrm{i}}{2\overline{h}}\left(\boldsymbol{x}^{\mathrm{T}}\tilde{\alpha}\boldsymbol{x}\right)\right]\hat{T}(\boldsymbol{x}) \tag{5.12}$$

where $\tilde{\alpha}$ is a symmetric 2×2 matrix, and $\overline{h}$ is a constant defined by the relation

$$\hat{T}(\boldsymbol{x})\hat{T}(\boldsymbol{x}') = \exp\left[\frac{\mathrm{i}}{2\overline{h}}\left(\boldsymbol{x}\times\boldsymbol{x}'\right)\right]\hat{T}(\boldsymbol{x}+\boldsymbol{x}'). \tag{5.13}$$

Comparison with (2.6) shows that $\overline{h}$ is shorthand for $(p/2\pi q)|\boldsymbol{A}_1\times\boldsymbol{A}_2|$: the symbol $\overline{h}$ was used because (5.13) is the algebra of the Weyl–Heisenberg operators in quantum mechanics. The transformation from the old Wannier states $|\chi_\mu\rangle$ to the new states $|\chi'_\mu\rangle$ is a linear combination of operators of the form $\hat{S}(\tilde{\alpha})$ and translation operators; it is therefore important to interpret the action of the $\hat{S}(\tilde{\alpha})$. The operator (5.12) is characterized in appendix B, where it is shown that it effects a transformation of the argument of a translation operator

$$\hat{T}(\boldsymbol{R}') = \exp\left[\frac{\mathrm{i}}{2\overline{h}}\left(\boldsymbol{R}^{\mathrm{T}}\tilde{K}\boldsymbol{R}\right)\right]\hat{S}^{-1}(\tilde{\alpha})\hat{T}(\boldsymbol{R})\hat{S}(\tilde{\alpha}) \tag{5.14}$$

where $\tilde{K}$ is a 2×2 matrix discussed in appendix B, and $\boldsymbol{R}$ is obtained by a linear transformation of $\boldsymbol{R}'$:

$$\boldsymbol{R}' = \tilde{M}(\tilde{\alpha})\boldsymbol{R} \qquad \det(\tilde{M}) = 1. \tag{5.15}$$

The operator (5.12) can therefore be interpreted as effecting a linear, area-preserving transformation. The transformation matrix $\tilde{M}$ is

$$\tilde{M} = (2\tilde{\alpha}-\tilde{J})^{-1}(2\tilde{\alpha}+\tilde{J}) \qquad \tilde{J} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}. \tag{5.16}$$

It is difficult to carry the calculation any further for a general transformation $\tilde{N}$. Instead, the transformation of Wannier functions for the cases of the generalized rotation $\tilde{R}$ and the shear transformation $\tilde{S}(n)$ will be considered separately. The general transformation can be found by using (4.2) to compose the results of these elementary transformations.

5.2. *Rotation of type I Wannier functions*

In this case (4.12) shows that the coefficients in (4.5) are

$$\alpha_\lambda(\boldsymbol{k}) = \exp\left[-\mathrm{i}\frac{pM}{2\pi}k_1k_2\right]\exp[-\mathrm{i}\lambda k_1]. \tag{5.17}$$

and the operators $\hat{Q}_{\mu\mu'}(\boldsymbol{k})$ are therefore

$$\begin{aligned} Q_{\mu\mu'}(\boldsymbol{k}) = \frac{p}{4\pi^2}\exp[\mathrm{i}p(\mu k_2-\mu' k_1)]\sum_{\lambda_1=0}^{p-1}\sum_{\lambda_2=0}^{p-1}\exp[-\mathrm{i}(\lambda_1k_1+\lambda_2k_2)]\exp\left[-\mathrm{i}\frac{pM}{2\pi}k_1k_2\right] \\ \times\ \hat{T}\left(\left(\frac{pM}{2\pi}k_2+\lambda_1\right)\boldsymbol{A}_1\right)\hat{T}\left(\left(\frac{pM}{2\pi}k_1+\lambda_2\right)\boldsymbol{A}_2\right) \end{aligned} \tag{5.18}$$

where $\hat{B}(\boldsymbol{k})$ is defined by (5.6); this satisfies the relations (5.8), (5.10) in the form

$$\begin{aligned} \hat{Q}_{\mu\mu'}(k_1, k_2+2\pi/p) &= \exp[-\mathrm{i}pMNk_1]\hat{Q}_{\mu\mu'}(k_1,k_2)\hat{T}(M\boldsymbol{A}_1) \\ \hat{Q}_{\mu\mu'}(k_1-2\pi, k_2) &= \exp[\mathrm{i}pMk_2]\hat{Q}_{\mu\mu'}(k_1,k_2)\hat{T}(-pM\boldsymbol{A}_2) \end{aligned} \tag{5.19}$$

implying that the vectors $\boldsymbol{R}_i$ are

$$\boldsymbol{R}_1 = pNM\boldsymbol{A}_1 \qquad \boldsymbol{R}_2 = -pM\boldsymbol{A}_2. \tag{5.20}$$

The form of (5.11) in this case is then

$$\begin{aligned}
|\chi'_\mu\rangle &= \frac{p}{4\pi^2}\sum_{\mu'=0}^{|N|-1}\sum_{l_1=0}^{|M|-1}\sum_{l_2=0}^{|M|-1}\int \mathrm{d}\boldsymbol{k}\ \exp[-\mathrm{i}p(Nk_1l_1+k_2l_2)]\hat{Q}_{\mu\mu'}(\boldsymbol{k})\hat{T}(pl_2\boldsymbol{A}_2)\hat{T}(l_1\boldsymbol{A}_1)|\chi_{\mu'}\rangle \\
&= \frac{p}{4\pi^2}\sum_{\mu'=0}^{|N|-1}\sum_{l_1=0}^{|M|-1}\sum_{l_2=0}^{|M|-1}\sum_{\lambda_1=0}^{p-1}\sum_{\lambda_2=0}^{p-1}\int_{-\infty}^{\infty}\mathrm{d}k_1\int_{-\infty}^{\infty}\mathrm{d}k_2\ \exp[\mathrm{i}p(\mu k_2-\mu' k_1)] \\
&\quad\times \exp[-\mathrm{i}(\lambda_2k_2+\lambda_1k_1)]\exp[-\mathrm{i}p(Nl_1k_1+l_2k_2)]\exp\left[-\mathrm{i}\frac{pM}{2\pi}k_1k_2\right] \\
&\quad\times \hat{T}\left(\left(\frac{pM}{2\pi}k_2+\lambda_1\right)\boldsymbol{A}_1\right)\hat{T}\left(\left(\frac{pM}{2\pi}k_1+\lambda_2\right)\boldsymbol{A}_2\right)\hat{T}(pl_2\boldsymbol{A}_2)\hat{T}(l_1\boldsymbol{A}_1)|\chi_{\mu'}\rangle \\
&= \frac{p}{4\pi^2}\sum_{\mu'=0}^{|N|-1}\sum_{l_1=0}^{|M|-1}\sum_{l_2=0}^{|M|-1}\sum_{\lambda_1=0}^{p-1}\sum_{\lambda_2=0}^{p-1}\int_{-\infty}^{\infty}\mathrm{d}k_1\int_{-\infty}^{\infty}\mathrm{d}k_2\ \exp[-2\pi\mathrm{i}ql_1\lambda_2/p] \\
&\quad\times \exp[-\mathrm{i}(p\mu'+\lambda_1+l_1)k_1]\exp[-\mathrm{i}(-p\mu+\lambda_2+pl_2)k_2]\exp\left[-\frac{\mathrm{i}pM}{2\pi}k_1k_2\right] \\
&\quad\times \hat{T}\left(\left(\frac{pM}{2\pi}k_2+\lambda_1+l_1\right)\boldsymbol{A}_1\right)\hat{T}\left(\left(\frac{pM}{2\pi}k_1+\lambda_2+pl_2\right)\boldsymbol{A}_2\right)|\chi_{\mu'}\rangle.
\end{aligned} \tag{5.21}$$

After making a change of variables, equation (5.21) can be rearranged to write the operator $\hat{M}_{\mu\mu'}$ in the form

$$\begin{aligned}
\hat{M}_{\mu\mu'} &= \frac{1}{pM^2}\sum_{l_1=0}^{|M|-1}\sum_{l_2=0}^{|M|-1}\sum_{\lambda_1=0}^{p-1}\sum_{\lambda_2=0}^{p-1}\exp\left[\frac{2\pi\mathrm{i}}{pM}\big(-p\mu(l_1+\lambda_1)\right. \\
&\quad\left. +\ (l_1+\lambda_1+p\mu')(pl_2+\lambda_2)-qMl_1\lambda_2\big)\right]\hat{O}_{\mu\mu'}
\end{aligned} \tag{5.22}$$

where

$$\hat{O}_{\mu\mu'} = \int_{-\infty}^{\infty}\mathrm{d}x_1\int_{-\infty}^{\infty}\mathrm{d}x_2\ \exp\left[\frac{2\pi\mathrm{i}}{M}(\mu x_1-\mu' x_2)\right]\exp\left[-\frac{2\pi\mathrm{i}}{pM}x_1x_2\right]\hat{T}(x_1\boldsymbol{A}_1)\hat{T}(x_2\boldsymbol{A}_2). \tag{5.23}$$

The summations in (5.22) can all be performed, giving the simple result

$$\hat{M}_{\mu\mu'} = \exp\left[\frac{2\pi\mathrm{i}p}{M}\mu\mu'\right]\hat{O}_{\mu\mu'}. \tag{5.24}$$

This expression can be interpreted by expressing $\hat{O}_{\mu\mu'}$ in terms of the operator introduced in equation (5.12). Using the substitutions $\hbar = p(\boldsymbol{A}_1\times\boldsymbol{A}_2)/2\pi q$, the operator $\hat{O}_{\mu\mu'}$ can be related to the operators $\hat{S}(\tilde{\alpha},\boldsymbol{b})$ which are discussed in appendix B:

$$\hat{O}_{\mu\mu'} = \hat{S}(\tilde{\alpha},\boldsymbol{b}) \qquad \tilde{\alpha} = \frac{\frac{1}{2}qM-1}{qM}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} \qquad \boldsymbol{b} = \frac{p}{qM}(\mu,-\mu'). \tag{5.25}$$

This can be related to the operator $\hat{S}(\alpha)$ using (B.13). The matrices $\tilde{\beta}$, $\tilde{K}'$ appearing in (B.13), and the symplectic transformation $\tilde{M}$ characterizing the action of $\hat{S}(\tilde{\alpha})$ are

$$\tilde{\beta} = \frac{qM}{pN}\begin{pmatrix} 0 & 1 \\ pN & 0 \end{pmatrix} \qquad \tilde{K}' = \frac{(\frac{1}{2}qM-1)qM}{pN}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + 2\tilde{\beta}$$
$$\tilde{M} = \begin{pmatrix} (pN)^{-1} & 0 \\ 0 & pN \end{pmatrix}. \tag{5.26}$$

which gives

$$\hat{S}(\tilde{\alpha}, \boldsymbol{b}) = \exp\left[-\frac{\pi\mathrm{i}(1+pN)}{NM}\mu\mu'\right]\hat{S}(\alpha)\hat{T}(-\mu'\boldsymbol{A}_1/N + p\mu\boldsymbol{A}_2). \tag{5.27}$$

Substituting these results into (5.24), and using (2.6) to partition the translation operator gives

$$\hat{M}_{\mu\mu'} = \exp\left[-\frac{2\pi\mathrm{i}q\mu\mu'}{N}\right]\hat{S}(\tilde{\alpha})\hat{T}\big(\mu p\boldsymbol{A}_2\big)\hat{T}\big(-\mu'\boldsymbol{A}_1/N\big). \tag{5.28}$$

A more symmetric form is obtained by using (B.4) to commute one of the translation operators through $\hat{S}(\tilde{\alpha})$. The matrix $\tilde{K}$ which defines the phase Φ through (B.10) evaluates to

$$\tilde{K} = \frac{(\frac{1}{2}qM-1)qM}{pN}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & -pN \\ (pN)^{-1} & 0 \end{pmatrix}. \tag{5.29}$$

Because this matrix has no diagonal components, the phase Φ in (B.4) evaluates to zero, and so

$$\hat{M}_{\mu\mu'} = \exp\left[-\frac{2\pi\mathrm{i}q\mu\mu'}{N}\right]\hat{T}(\mu\boldsymbol{A}_2/N)\hat{S}(\tilde{\alpha})\hat{T}(-\mu'\boldsymbol{A}_1/N). \tag{5.30}$$

5.3. Shearing transformation of type I Wannier functions

The case of the shearing transformation, specified by (4.13), must be treated differently; this is because the vectors $\boldsymbol{R}_1$ and $\boldsymbol{R}_2$ introduced in (5.9) are not linearly independent, implying that (5.10) cannot be used. This case is therefore treated from first principles.

The transformation of the Bloch states is a simple gauge transformation, $|B(\boldsymbol{k})\rangle = \exp[\mathrm{i}\theta(k_2)]|B(\boldsymbol{k})\rangle$, with the phase $\theta(k_2)$ given by (4.22). Using equation (5.3), the transformed Wannier states are therefore

$$|\chi'_\mu\rangle = \frac{p}{4\pi^2}\sum_{\mu'=0}^{|N|-1}\int_0^{2\pi/p}\mathrm{d}k'_1\int_0^{2\pi}\mathrm{d}k'_2\ \exp\big[\mathrm{i}p\big(\mu k'_1 - \mu'(k'_1 - nk'_2)\big)\big]$$
$$\times\ \hat{T}'\left(-\frac{pM}{2\pi}k'_1\boldsymbol{A}_2\right)\exp[\mathrm{i}\theta(k_2)]\hat{T}\left(\frac{pM}{2\pi}(k'_1 - nk'_2)\boldsymbol{A}_2\right)$$
$$\times\sum_{n_1=-\infty}^{\infty}\sum_{n_2=-\infty}^{\infty}\exp[-\mathrm{i}(pNn_1(k'_1 - nk'_2) + n_2k'_2)]\hat{T}(n_2\boldsymbol{A}_2)\hat{T}(n_1\boldsymbol{A}_1)|\chi_{\mu'}\rangle. \tag{5.31}$$

The integration over k'_1 can be carried out immediately, giving

$$|\chi'_\mu\rangle = \frac{1}{2\pi}\int_0^{2\pi}\mathrm{d}k\ \exp[\mathrm{i}pn\mu k]\exp[\mathrm{i}\theta(k)]\sum_{m=-\infty}^{\infty}\exp[-\mathrm{i}mk]\hat{T}\left(\left(-\frac{pMn}{2\pi}k + m\right)\boldsymbol{A}_2\right)|\chi_\mu\rangle$$
$$\equiv\sum_{m=-\infty}^{\infty}\int_0^{2\pi}\mathrm{d}k\ \exp[-\mathrm{i}mk]\hat{Q}_\mu(k)\hat{T}(m\boldsymbol{A}_2)|\chi_\mu\rangle \equiv \hat{M}_\mu|\chi_\mu\rangle \tag{5.32}$$

where the last two equalities define the operators $\hat{Q}_\mu(k)$ and $\hat{M}_\mu$; note that only the term $\mu' = \mu$ contributes. The operator $\hat{Q}_\mu(k)$ satisfies

$$\hat{Q}_\mu(k+2\pi) = \exp[\mathrm{i}pMnk]\hat{Q}_\mu(k)\hat{T}(-pMn\boldsymbol{A}_2). \tag{5.33}$$

The operator $\hat{M}_\mu$, which effects the transformation of the Wannier functions, can therefore be written as

$$\begin{aligned}\hat{M}_\mu &= \sum_{\lambda=0}^{|pMn|-1}\sum_{m=-\infty}^{\infty}\int_0^{2\pi}\mathrm{d}k\ \exp[-\mathrm{i}\lambda k]\exp[-\mathrm{i}pMnmk]\hat{Q}_\mu(k)\hat{T}(pMnm\boldsymbol{A}_2)\hat{T}(\lambda\boldsymbol{A}_2)\\ &= \sum_{\lambda=0}^{|pMn|-1}\int_{-\infty}^{\infty}\mathrm{d}k\ \exp[-\mathrm{i}\lambda k]\hat{Q}_\mu(k)\hat{T}(\lambda\boldsymbol{A}_2)\\ &= \frac{1}{2\pi}\sum_{\lambda=0}^{|pMn|-1}\int_{-\infty}^{\infty}\mathrm{d}k\ \exp\left[\mathrm{i}\frac{pMn}{4\pi}k^2\right]\exp\left[\mathrm{i}\left(pn\mu-\lambda+Mn(\mathcal{N}-\tfrac{1}{2}p)\right)k\right]\\ &\quad\times\hat{T}\left(\left(-\frac{pMn}{2\pi}k+\lambda\right)\boldsymbol{A}_2\right)\end{aligned} \tag{5.34}$$

where the final equality used (4.22). Making the successive changes of variables, $\lambda' = \lambda - pn\mu - Mn(\mathcal{N} - \frac{1}{2}p)$ and $x = -pMnk/2\pi + \lambda'$, this can be written in the form

$$\begin{aligned}\hat{M}_\mu &= \frac{1}{2\pi}\sum_{\lambda=0}^{|pMn|-1}\int_{-\infty}^{\infty}\mathrm{d}k\ \exp\left[\frac{\mathrm{i}pMnk^2}{4\pi}\right]\exp[-\mathrm{i}\lambda' k]\hat{T}\left(\left(-\frac{pMn}{2\pi}k+\lambda'\right)\boldsymbol{A}_2\right)\\ &\quad\times\hat{T}(pn\mu\boldsymbol{A}_2)\hat{T}(Mn(\mathcal{N}-\tfrac{1}{2}p)\boldsymbol{A}_2)\\ &= \frac{1}{pMn}\sum_{\lambda=0}^{|pMn|-1}\exp\left[\frac{-\pi\mathrm{i}}{pMn}\left(\lambda-pn\mu-Mn(\mathcal{N}-\tfrac{1}{2})\right)^2\right]\\ &\quad\times\hat{s}(\alpha)\hat{T}(pn\mu\boldsymbol{A}_2)\hat{T}\left(Mn(\mathcal{N}-\tfrac{1}{2}p)\boldsymbol{A}_2\right)\end{aligned} \tag{5.35}$$

where $\hat{s}(\alpha)$ is an operator defined in appendix B, equation (B.15), with $\alpha = 1/qMn$. It is convenient to define the sum

$$S(N,n) = \frac{1}{N}\sum_{\lambda=0}^{|N|-1}\exp\left[\frac{-\pi\mathrm{i}(\lambda-n+\frac{1}{2}N)^2}{N}\right]. \tag{5.36}$$

It is easily seen that this is independent of n, so the argument n can be dropped, and the sum can also be evaluated explicitly:

$$S(N,n) = S(N,n+1) \equiv S(N) = \exp[-\mathrm{i}\pi/4]/\sqrt{N}. \tag{5.37}$$

Because the sum is independent of μ, it is just a numerical factor determining the normalization of the transformed states; since the normalization has not been specified, this factor can be dropped, and the operator transforming the Wannier states will be written as

$$\hat{M}_\mu = \hat{s}(\alpha)\hat{T}(pn\mu\boldsymbol{A}_2)\hat{T}\left(Mn(\mathcal{N}-\tfrac{1}{2}p)\boldsymbol{A}_2\right). \tag{5.38}$$

In appendix B, it is shown that the operator $\hat{s}(\alpha)$ has the effect of a shearing transformation: for $\overline{h} = p/2\pi q$ and $\alpha = 1/qMn$,

$$\hat{s}(\alpha)\hat{T}(\boldsymbol{R}) = \hat{T}(\boldsymbol{R}')\hat{s}(\alpha) \tag{5.39}$$

where the relationship between $\boldsymbol{R}'$ and $\boldsymbol{R}$ is

$$\boldsymbol{R}' = \tilde{M}\boldsymbol{R} \qquad \tilde{M} = \begin{pmatrix}1 & 0\\ qMn & 1\end{pmatrix}. \tag{5.40}$$

5.4. Transformation for type II Wannier functions

Equations (5.30) and (5.38) give the transformations for the type I Wannier functions under elementary rotations and shear transformations respectively. The corresponding transformations for the type II Wannier functions are obtained using (3.11) and (3.12).

The transformed type II Wannier function is given by (3.11), with the translation operator replaced by a translation through the transformed lattice vector $\boldsymbol{A}_1'$:

$$|\phi_\mu'\rangle = \sum_{\mu'=0}^{|N|-1} \exp\left[-\frac{2\pi \mathrm{i}\mu\mu'}{N}\right]\hat{T}'(-\mu'\boldsymbol{A}_1'/N)|\chi_{\mu'}'\rangle. \tag{5.41}$$

The prime on the translation operator indicates that it may have to include the gauge factor (4.6).

In the case of the elementary rotation, the transformation for the type II Wannier functions is easily determined from (5.30): using the facts that in this case $\boldsymbol{A}_1' = \boldsymbol{A}_2$ and $\hat{T}'(\boldsymbol{R}) = \hat{T}(\boldsymbol{R})$,

$$\begin{aligned}|\phi_\mu'\rangle &= \frac{1}{N\sqrt{p}}\sum_{\lambda=0}^{|N|-1}\sum_{\lambda'=0}^{|N|-1} \exp\left[\frac{2\pi\mathrm{i}}{N}(\lambda q-\mu)\lambda\right]\hat{S}(\tilde{\alpha})\hat{T}(\lambda'\boldsymbol{A}_1/N)|\chi_{\lambda'}\rangle \\ &= \frac{1}{N\sqrt{p}}\sum_{\lambda=0}^{|N|-1}\sum_{\lambda'=0}^{|N|-1}\sum_{\mu'=0}^{|N|-1} \exp\left[\frac{2\pi\mathrm{i}}{N}\big(q\lambda\lambda'-\lambda\mu+\lambda'\mu'\big)\right]\hat{S}(\tilde{\alpha})|\phi_{\mu'}\rangle.\end{aligned} \tag{5.42}$$

The sum over λ' vanishes unless $q\lambda+\mu' = 0 \bmod N$; this condition can also be written as $\lambda = -M\mu'$. The required transformation of type II Wannier functions corresponding to an elementary rotation of the lattice basis vectors is therefore

$$|\phi_\mu'\rangle = \frac{1}{\sqrt{p}}\sum_{\mu'=0}^{|N|-1} \exp\left[-\frac{2\pi\mathrm{i}M\mu\mu'}{N}\right]\hat{S}(\tilde{\alpha})|\phi_{\mu'}\rangle. \tag{5.43}$$

Next consider the case of the elementary shear transformation, where $\boldsymbol{A}_1' = \boldsymbol{A}_1 + n\boldsymbol{A}_2$, and $\hat{T}'(\boldsymbol{R}) = \exp[\frac{1}{2}\mathrm{i}qn\boldsymbol{a}_1\cdot\boldsymbol{R}]\hat{T}(\boldsymbol{R})$. Using (5.38), the transformation of the type II Wannier functions is therefore

$$\begin{aligned}|\phi_\mu'\rangle &= \frac{1}{N}\sum_{\mu'=0}^{|N|-1}\sum_{\lambda=0}^{|N|-1} \exp\left[\frac{2\pi\mathrm{i}}{N}\big(\mu'-\mu-\tfrac{1}{2}qn)\lambda\big)\right]\hat{T}\big(-\lambda(\boldsymbol{A}_1+n\boldsymbol{A}_2)/N\big) \\ &\quad\times \hat{s}(\alpha)\hat{T}(pn\lambda\boldsymbol{A}_2)\hat{T}\big(Mn(\mathcal{N}-\tfrac{1}{2}p)\boldsymbol{A}_2\big)\hat{T}(\lambda\boldsymbol{A}_1/N)|\phi_{\mu'}\rangle \\ &= \frac{1}{N}\sum_{\mu'=0}^{|N|-1}\sum_{\lambda=0}^{|N|-1} \exp\left[\frac{2\pi\mathrm{i}}{N}\big(\mu'-\mu-\tfrac{1}{2}qn(pN-pNM+qNM)\big)\lambda-\tfrac{1}{2}qn\lambda^2\right] \\ &\quad\times \hat{T}\big(-\lambda(\boldsymbol{A}_1+n\boldsymbol{A}_2)/N\big)\hat{s}(\alpha)\hat{T}(\lambda\boldsymbol{A}_1/N+pn\lambda\boldsymbol{A}_2) \\ &\quad\times \hat{T}\big(Mn(\mathcal{N}-\tfrac{1}{2}p)\boldsymbol{A}_2\big)|\phi_{\mu'}\rangle\end{aligned} \tag{5.44}$$

where (2.14) and (4.20) have been used to simplify the exponents. Using (5.39), the translation operators which depend upon λ are eliminated. After further use of equations (2.14) and (4.20),

$$|\phi_\mu'\rangle = \sum_{\mu'=0}^{|N|-1} K(\mu-\mu')\hat{s}(\alpha)\hat{T}\big(Mn(\mathcal{N}-\tfrac{1}{2}p)\boldsymbol{A}_2\big)|\phi_{\mu'}\rangle \tag{5.45}$$

where the coefficients $K(\mu - \mu')$ are obtained from

$$K(\nu) = \frac{1}{N} \sum_{\lambda=0}^{|N|-1} \exp\left[-\frac{2\pi \mathrm{i}}{N}\left(\tfrac{1}{2}qn\lambda^2 + \nu\lambda - \tfrac{1}{2}qnN\lambda\right)\right]. \tag{5.46}$$

The coefficients satisfy the relations

$$K(\nu + N) = K(\nu) \qquad K(-\nu) = K^*(\nu) \qquad K(0) = 0.$$

6. Summary

The purpose of this section is to highlight the most significant results, and to discuss the definitions upon which they are based.

When conventional Wannier functions are defined, it is assumed that the Bloch states are periodic functions of the Bloch wavevector $\boldsymbol{k}$, as well as being eigenfunctions of the lattice translation operators $\hat{T}(\boldsymbol{A}_i)$, with eigenvalues $\exp[\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{A}_i]$. In the case where a rational magnetic field (with q/p flux quanta per unit cell) is applied, in general both of these conditions need to be modified. The Bloch states are p-fold degenerate, and their phase increases by $2\pi M$ on traversing the boundary of the unit cell. Throughout this paper it has been assumed that the Bloch states are chosen to satisfy the following eigenvalue and periodicity conditions discussed in section 2:

$$\hat{T}(\boldsymbol{A}_1)|B(\boldsymbol{k})\rangle = \exp[\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{A}_1]|B(\boldsymbol{k} - q\boldsymbol{a}_2/p)\rangle \tag{6.1a}$$

$$\hat{T}(\boldsymbol{A}_2)|B(\boldsymbol{k})\rangle = \exp[\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{A}_2]|B(\boldsymbol{k})\rangle \tag{6.1b}$$

$$|B(\boldsymbol{k} + \boldsymbol{a}_1/p)\rangle = \exp[\mathrm{i}M\boldsymbol{k} \cdot \boldsymbol{A}_2]|B(\boldsymbol{k})\rangle \tag{6.1c}$$

$$|B(\boldsymbol{k} + \boldsymbol{a}_2)\rangle = |B(\boldsymbol{k})\rangle. \tag{6.1d}$$

Except when $p = 1$ and $M = 0$, these conditions depend upon the choice of lattice basis vectors $\boldsymbol{A}_i$.

The method for constructing the Wannier functions was discussed in section 3. If the Bloch states satisfy (6.1), the state $|C(\boldsymbol{k})\rangle = \hat{T}(-pM\boldsymbol{k} \cdot \boldsymbol{A}_2/2\pi)|B(\boldsymbol{k})\rangle$ is periodic on the Brillouin zone of the superlattice spanned by $p\boldsymbol{A}_1$, $\boldsymbol{A}_2$, and the Wannier functions $|\chi(\boldsymbol{R})\rangle$ are obtained by integrating the state $|C(\boldsymbol{k})\rangle$ with weight $\exp[\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{R}]$. In the case of standard Wannier functions, all of the Wannier states are obtained be applying translation operators to a single fundamental Wannier state. In the magnetic case, the full set of Wannier states is obtained by applying lattice translations to $|N|$ fundamental type I Wannier states, $|\chi_\mu\rangle = |\chi(\mu\boldsymbol{A}_1)\rangle$, $\mu = 0, \ldots, |N| - 1$, where N satisfies $pN + qM = 1$. The Bloch states are obtained from the type I fundamental Wannier functions using (3.10):

$$\begin{aligned}|B(\boldsymbol{k})\rangle = \sum_{\boldsymbol{R}=n_1\boldsymbol{A}_1+n_2\boldsymbol{A}_2} &\exp[-\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{R}]\hat{T}(n_2\boldsymbol{A}_2)\hat{T}(n_1\boldsymbol{A}_1)\hat{T}\left(\frac{pM}{2\pi}(\boldsymbol{k} \cdot \boldsymbol{A}_1)\boldsymbol{A}_2\right) \\ &\times \sum_{\mu} \exp[-\mathrm{i}p\mu(\boldsymbol{k} \cdot \boldsymbol{A}_1)]|\chi_\mu\rangle.\end{aligned} \tag{6.2}$$

A somewhat more natural representation of the Bloch states uses an alternative set of fundamental Wannier states: the type II Wannier states are defined by

$$|\phi_\mu\rangle = \frac{1}{N} \sum_{\mu'=0}^{|N|-1} \exp[-2\pi \mathrm{i}\mu\mu'/N]\hat{T}(-\mu'\boldsymbol{A}_1/N)|\chi_{\mu'}\rangle. \tag{6.3}$$

One advantage of using the type II Wannier states is that the summation over μ no longer depends upon $\boldsymbol{k}$; the Bloch states are given in terms of the type II states by the relation

$$|B(\boldsymbol{k})\rangle = \sum_{\boldsymbol{R}=n_1\boldsymbol{A}_1/N+n_2\boldsymbol{A}_2} \sum_{\mu=0}^{|N|-1} \exp[-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}] \exp[2\pi\mathrm{i}n_1\mu/N] \times \hat{T}(n_2\boldsymbol{A}_2)\hat{T}(n_1\boldsymbol{A}_1/N)\hat{T}\left(\frac{pM}{2\pi}(\boldsymbol{k}\cdot\boldsymbol{A}_1)\boldsymbol{A}_2\right)|\phi_\mu\rangle. \tag{6.4}$$

The other advantage of the type II Wannier states is that their transformations under a change of lattice basis vectors are simpler.

Sections 4 and 5 discussed the effects of making a transformation of the set of basis vectors for the lattice. The transformation of the basis vectors is characterized by an integer-valued unimodular matrix $\tilde{N}$, which can be constructed from a combination of rotations $\tilde{R}$ and shears $\tilde{S}(n)$:

$$\tilde{N} = \tilde{S}(n_1)\tilde{R}\tilde{S}(n_2)\tilde{R}\tilde{S}(n_3) \qquad \tilde{S}(n) = \begin{pmatrix} 1 & n \\ 0 & 1 \end{pmatrix} = [\tilde{S}(1)]^n \qquad \tilde{R} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{6.5}$$

The action of the rotation and shear transforms on the Wannier functions is characterized by operators $\hat{S}(\tilde{\alpha})$ and $\hat{s}(\alpha)$, discussed in appendix B, which are characterized by a symplectic transformation $\tilde{M}$ in the space of magnetic translations. The transformation of type I Wannier functions corresponding to an elementary rotation of the lattice basis, and the associated symplectic transformation are

$$\begin{aligned} |\chi'_\mu\rangle &= \frac{1}{\sqrt{p}} \sum_{\mu'=0}^{|N|-1} \exp\left[-\frac{2\pi\mathrm{i}q\mu\mu'}{N}\right] \hat{T}(\mu\boldsymbol{A}_2/N)\hat{S}(\tilde{\alpha})\hat{T}(-\mu'\boldsymbol{A}_1/N)|\chi_{\mu'}\rangle \\ \tilde{M} &= \begin{pmatrix} (pN)^{-1} & 0 \\ 0 & pN \end{pmatrix}. \end{aligned} \tag{6.6}$$

The transformation for the shearing transformation, and associated symplectic transformation are

$$|\chi'_\mu\rangle = \hat{s}(\alpha)\hat{T}(pn\mu\boldsymbol{A}_2)\hat{T}\big(Mn(\mathcal{N} - \tfrac{1}{2}p)\boldsymbol{A}_2\big)|\chi_\mu\rangle \qquad \tilde{M} = \begin{pmatrix} 1 & 0 \\ qMn & 1 \end{pmatrix}. \tag{6.7}$$

(The constant $\mathcal{N}$ is defined by equation (4.20).)

The corresponding transformations for the type II Wannier functions have the satisfying feature that the translation operators dependent upon the indices μ, μ' are eliminated. The transformation of type II Wannier functions corresponding to elementary rotation of the lattice basis is

$$|\phi'_\mu\rangle = \frac{1}{\sqrt{p}} \sum_{\mu'=0}^{|N|-1} \exp[-2\pi\mathrm{i}M\mu\mu'/N]\hat{S}(\tilde{\alpha})|\phi_{\mu'}\rangle \tag{6.8}$$

and that corresponding to a shear $\tilde{S}(n)$ is

$$\begin{aligned} |\phi'_\mu\rangle &= \sum_{\mu'=0}^{|N|-1} K(\mu-\mu')\hat{s}(\alpha)\hat{T}\big(Mn(\mathcal{N} - \tfrac{1}{2}p\boldsymbol{A}_2)\big)|\phi_{\mu'}\rangle \\ K(\nu) &= \frac{1}{N} \sum_{\lambda=0}^{|N|-1} \exp\left[-\frac{2\pi\mathrm{i}}{N}\big(\tfrac{1}{2}qn\lambda^2 + \nu\lambda - \tfrac{1}{2}qnN\lambda\big)\right]. \end{aligned} \tag{6.9}$$

It is a surprising feature that the symplectic transformation $\tilde{M}$ associated with the transformation of the Wannier states is different from the symplectic transformation $\tilde{N}$ which describes the change of lattice basis vectors.

If the Hamiltonian has rotational symmetry, there exist operators acting on the Wannier functions which represent this symmetry; Wannier functions may be chosen which are invariant under the action of these operators. The definition of these symmetry operations involves a reassignment of the lattice basis vectors, and they are therefore related to the results in section 5 of this paper. These symmetry operators have been constructed for fourfold and sixfold rotations of the phase-space lattice Hamiltonian model in references [2] and [14] respectively. These papers contain results related to a special case of equations (6.8) and (6.9) respectively.

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Appendix A

The system under consideration is a single particle of charge $-e$ moving in a periodic potential $V(\boldsymbol{r})$ with a uniform magnetic field $\boldsymbol{B}$ applied along the z-axis. Spin, relativistic and many-body effects are not considered. The Schrödinger equation for this system is

$$\begin{aligned} &\hat{H}|\psi\rangle = \left[\frac{1}{2m}\big(\hat{\boldsymbol{p}} - e\boldsymbol{A}(\boldsymbol{r})\big)^2 + V(\boldsymbol{r})\right]|\psi\rangle = E|\psi\rangle \\ &\boldsymbol{\nabla}\times\boldsymbol{A} = \boldsymbol{B} = B\boldsymbol{e}_3 \\ &V(\boldsymbol{r}+\boldsymbol{R}) = V(\boldsymbol{r}) \qquad \boldsymbol{R} = n_1\boldsymbol{A}_1 + n_2\boldsymbol{A}_2 \end{aligned} \tag{A.1}$$

where the basis vectors of the periodic potential are $\boldsymbol{A}_i$, $i = 1, 2$. The vector potential $\boldsymbol{A}(\boldsymbol{r}) = (A_1(\boldsymbol{r}), A_2(\boldsymbol{r}))$ will always be chosen to be linear in $\boldsymbol{r}$, specified by a matrix $\tilde{\mathcal{B}}$ with elements $\mathcal{B}_{ij}$:

$$A_i(\boldsymbol{r}) = \sum_{j=1,2}\mathcal{B}_{ij}r_j \qquad \boldsymbol{A}(\boldsymbol{r}) = \tilde{\mathcal{B}}\boldsymbol{r}. \tag{A.2}$$

One reason for this restriction being useful is that when $\boldsymbol{A}(\boldsymbol{r})$ is linear, the Hamiltonian can be subjected to linear canonical transformations without any ambiguity arising in its quantization. The two most common choices of $\tilde{\mathcal{B}}$ are given by

$$\begin{aligned} &\text{Landau gauge: } \boldsymbol{A} = (0, Bx, 0) \\ &\text{symmetric gauge: } \boldsymbol{A} = (-\tfrac{1}{2}By, \tfrac{1}{2}Bx, 0). \end{aligned} \tag{A.3}$$

The Schrödinger equation (A.1) is much harder to solve than the corresponding problem with no magnetic field applied, since the Hamiltonian is no longer trivially invariant under a translation through a lattice vector $\boldsymbol{R}$. In order to see how the symmetry of the lattice is contained in (A.1), it is necessary to understand the effects of translation in the presence of a magnetic field. Consider a change of variable $\boldsymbol{r} \to \boldsymbol{r}' = \boldsymbol{r} - \boldsymbol{R}$ in the Hamiltonian:

because $V(\boldsymbol{r}) = V(\boldsymbol{r}')$, this is equivalent to making a change in the vector potential to

$$\begin{aligned} &\boldsymbol{A}(\boldsymbol{r}) = \boldsymbol{A}(\boldsymbol{r}' + \boldsymbol{R}) = \boldsymbol{A}(\boldsymbol{r}') + \tilde{\mathcal{B}}\boldsymbol{R} = \boldsymbol{A}(\boldsymbol{r}') + \boldsymbol{\nabla}_{\boldsymbol{r}'}\Phi \\ &\Phi(\boldsymbol{r}') = (\tilde{\mathcal{B}}\boldsymbol{R}) \cdot \boldsymbol{r}'. \end{aligned} \tag{A.4}$$

The corresponding gauge transformation of a wavefunction $\psi(\boldsymbol{r})$ which solves the time-independent Schrödinger equation at energy E is

$$\psi(\boldsymbol{r}') \to \psi'(\boldsymbol{r}') = \exp[\mathrm{i}e\Phi(\boldsymbol{r}')/\hbar]\psi(\boldsymbol{r}'). \tag{A.5}$$

Expressing this in terms $\boldsymbol{r}$, and ignoring an irrelevant multiplicative factor, a translated solution of the Schrödinger equation is

$$\psi'(\boldsymbol{r}) = \exp[\mathrm{i}e(\tilde{\mathcal{B}}^{\mathrm{T}}\boldsymbol{r}) \cdot \boldsymbol{R}/\hbar]\psi(\boldsymbol{r} - \boldsymbol{R}) \tag{A.6}$$

which is also a solution with energy E.

Now a set of operators, $\hat{T}(\boldsymbol{R})$, will be introduced, which generate translations of the form (A.6); these operators are called the magnetic translation operators. A convenient choice of these operators is given by

$$\hat{T}(\boldsymbol{R}) = \exp\left[-\frac{\mathrm{i}}{\hbar}\left(\hat{\boldsymbol{p}} - e\tilde{\mathcal{B}}^{\mathrm{T}}\boldsymbol{r}\right) \cdot \boldsymbol{R}\right]. \tag{A.7}$$

The effect of this operator on $\psi(\boldsymbol{r})$ is to transform it into the state $\psi'(\boldsymbol{r})$ given by (A.6), multiplied by an unimportant overall phase. This operator is analogous to the ordinary translation operator, with the generator $-\boldsymbol{\nabla}$ replaced by $-\boldsymbol{\nabla} + (\mathrm{i}e/\hbar)\tilde{\mathcal{B}}^{\mathrm{T}}\boldsymbol{r}$. Note that it is only for linear gauges that a generator for infinitesimal translations can be explicitly identified.

Since $\hat{\boldsymbol{r}}$ and $\hat{\boldsymbol{p}}$ do not commute, pairs of magnetic translation operators do not in general commute; using the Baker–Cambell–Hausdorff formula, their composition law is found to be

$$\hat{T}(\boldsymbol{R})\hat{T}(\boldsymbol{R}') = \exp\left[\frac{\mathrm{i}e}{2\hbar}\boldsymbol{B} \cdot (\boldsymbol{R} \times \boldsymbol{R}')\right]\hat{T}(\boldsymbol{R} + \boldsymbol{R}'). \tag{A.8}$$

Note that the phase change θ on translating the solution in a clockwise sense about a circuit of area $\mathcal{A}$ is

$$\theta = \frac{2\pi e\mathcal{A}B}{h} \tag{A.9}$$

which is 2π times the number of flux quanta within the circuit.

Although the magnetic translation operators do not commute with each other, it is clear from their construction that they commute with the Hamiltonian for vectors $\boldsymbol{R}$ that are lattice translations, and therefore provide a mathematical description of the symmetry of the system.

Appendix B

In this appendix the composition relation for the operators $\hat{T}(\boldsymbol{R})$ will be written as

$$\begin{aligned} \hat{T}(\boldsymbol{R})T(\boldsymbol{R}') &= \exp\left[\frac{\mathrm{i}}{2\hbar}(R_1R_2' - R_2R_1')\right]\hat{T}(\boldsymbol{R} + \boldsymbol{R}') \\ &= \exp\left[\frac{\mathrm{i}}{2\hbar}(\boldsymbol{R} \times \boldsymbol{R}')\right]\hat{T}(\boldsymbol{R} + \boldsymbol{R}') = \exp\left[\frac{\mathrm{i}}{2\hbar}(\boldsymbol{R}'^{\,\mathrm{T}}\tilde{J}\boldsymbol{R})\right]\hat{T}(\boldsymbol{R} + \boldsymbol{R}') \end{aligned} \tag{B.1}$$

where the second equality defines the cross product, and where

$$\tilde{J} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}. \tag{B.2}$$

It will be shown that the operator

$$\begin{aligned}\hat{S}(\tilde{\alpha}) &= \int \mathrm{d}\boldsymbol{x}\, \exp\left[\frac{\mathrm{i}}{2\hbar}\left(\boldsymbol{x}^{\mathrm{T}}\tilde{\alpha}\boldsymbol{x}\right)\right]\hat{T}(\boldsymbol{x}) \\ &= \int_{-\infty}^{\infty}\mathrm{d}x_1 \int_{-\infty}^{\infty}\mathrm{d}x_2\, \exp\left[\frac{\mathrm{i}}{2\hbar}\left(\alpha_{11}x_1^2 + \alpha_{22}x_2^2 + 2\alpha_{12}x_1x_2\right)\right]\hat{T}(x_1, x_2)\end{aligned} \tag{B.3}$$

satisfies

$$\hat{T}(\boldsymbol{R}') = \exp[\mathrm{i}\Phi(\tilde{\alpha}, \boldsymbol{R})]\hat{S}^{-1}(\tilde{\alpha})\hat{T}(\boldsymbol{R})\hat{S}(\tilde{\alpha}) \tag{B.4}$$

where $\boldsymbol{R}'$ is related to $\boldsymbol{R}$ by a symplectic transformation:

$$\boldsymbol{R}' = \tilde{M}(\tilde{\alpha})\boldsymbol{R} \qquad \det(\tilde{M}) = 1 \tag{B.5}$$

and $\Phi(\tilde{\alpha}, \boldsymbol{R})$ is a phase which will be specified later. The symplectic matrix is given by

$$\begin{aligned}\tilde{M} &= (2\tilde{\alpha} + \tilde{J})^{-1}(2\tilde{\alpha} - \tilde{J}) \\ &= \frac{1}{\alpha_{11}\alpha_{22} - \alpha_{12}^2 + \frac{1}{4}}\begin{pmatrix} \alpha_{11}\alpha_{22} - (\alpha_{12} - \frac{1}{2})^2 & \alpha_{22} \\ -\alpha_{11} & \alpha_{11}\alpha_{22} - (\alpha_{12} + \frac{1}{2})^2 \end{pmatrix}.\end{aligned} \tag{B.6}$$

To demonstrate this result, consider the following operator:

$$\hat{S}' = \hat{T}(\boldsymbol{R})\hat{S}(\tilde{\alpha})\hat{T}(-\boldsymbol{R}') \tag{B.7}$$

where no relation between $\boldsymbol{R}$ and $\boldsymbol{R}'$ is assumed at this stage. Inserting the definition (B.3), and using (B.1) to write the result as an integral over a single translation operator, then changing variables, gives

$$\begin{aligned}\hat{S}' = \exp&\left[\frac{\mathrm{i}}{2\hbar}\left((\boldsymbol{R}' - \boldsymbol{R})^{\mathrm{T}}\tilde{\alpha}(\boldsymbol{R}' - \boldsymbol{R}) - \boldsymbol{R}^{\mathrm{T}}\tilde{J}\boldsymbol{R}'\right)\right]\int \mathrm{d}\boldsymbol{x}\, \exp\left[\frac{\mathrm{i}}{2\hbar}(\boldsymbol{x}^{\mathrm{T}}\tilde{\alpha}\boldsymbol{x})\right] \\ &\times\ \exp\left[\frac{\mathrm{i}}{2\hbar}\left(2(\boldsymbol{R}' - \boldsymbol{R})^{\mathrm{T}}\tilde{\alpha}\boldsymbol{x} + (\boldsymbol{R} + \boldsymbol{R}') \times \boldsymbol{x}\right)\right]\hat{T}(\boldsymbol{x}).\end{aligned} \tag{B.8}$$

The operator $\hat{S}'$ is proportional to $\hat{S}(\tilde{\alpha})$ if the phases which are linear in $\boldsymbol{x}$ vanish; in this case, equation (B.8) can be rearranged to give (B.4). This leads to the following relation:

$$2\tilde{\alpha}(\boldsymbol{R}' - \boldsymbol{R}) = \tilde{J}(\boldsymbol{R}' + \boldsymbol{R}) \tag{B.9}$$

which can be solved to give $\boldsymbol{R}' = (R_1', R_2')$ in terms of $\boldsymbol{R}$; this gives (B.5), (B.6). The phase appearing in (B.4) is given by

$$\Phi(\tilde{\alpha}, \boldsymbol{R}) = \frac{\boldsymbol{R}^{\mathrm{T}}\tilde{K}\boldsymbol{R}}{2\hbar} \qquad \tilde{K} = -(\tilde{M} - \tilde{I})^{\mathrm{T}}\tilde{\alpha}(\tilde{M} - \tilde{I}) + \tilde{J}\tilde{M}. \tag{B.10}$$

It is convenient to give a formula for the case where the phase factor in (B.2) contains terms which are linear in $\boldsymbol{x}$; define

$$\hat{S}(\tilde{\alpha}, \boldsymbol{b}) = \int \mathrm{d}\boldsymbol{x}\, \exp\left[\frac{\mathrm{i}}{2\hbar}\boldsymbol{x}^{\mathrm{T}}\tilde{\alpha}\boldsymbol{x}\right]\exp\left[\frac{\mathrm{i}}{\hbar}\boldsymbol{b}\cdot\boldsymbol{x}\right]\hat{T}(\boldsymbol{x}). \tag{B.11}$$

Making a change of variable $\boldsymbol{x}' = \boldsymbol{x} - \boldsymbol{a}$, then applying (B.1) gives, for an arbitrary choice of $\boldsymbol{a}$,

$$\hat{S}(\tilde{\alpha}, \boldsymbol{b}) = \exp\left[\frac{\mathrm{i}}{2\hbar}\left(\boldsymbol{a}^{\mathrm{T}}\tilde{\alpha}\boldsymbol{a} + 2\boldsymbol{a}\cdot\boldsymbol{b}\right)\right] \times \int \mathrm{d}\boldsymbol{x}' \exp\left[\frac{\mathrm{i}}{2\hbar}\boldsymbol{x}'^{\,\mathrm{T}}\left(2\tilde{\alpha}\boldsymbol{a} + 2\boldsymbol{b} + \tilde{J}\boldsymbol{a}\right)\right] \exp\left[\frac{\mathrm{i}}{2\hbar}(\boldsymbol{x}'^{\,\mathrm{T}}\tilde{\alpha}\boldsymbol{x}')\right]\hat{T}(\boldsymbol{x}')\hat{T}(\boldsymbol{a}). \tag{B.12}$$

If $\boldsymbol{a}$ is chosen such that the term for which the component of the phase linear in $\boldsymbol{x}$ vanishes, equation (B.12) gives

$$\hat{S}(\tilde{\alpha}, \boldsymbol{b}) = \exp[\mathrm{i}\Theta(\tilde{\alpha}, \boldsymbol{b})]\hat{S}(\tilde{\alpha})\hat{T}(\tilde{\beta}\boldsymbol{b}) \qquad \tilde{\beta} = -(\tilde{\alpha} + \tfrac{1}{2}\tilde{J})^{-1} \tag{B.13}$$

and the phase factor is

$$\Theta(\tilde{\alpha}, \boldsymbol{b}) = \frac{\boldsymbol{b}^{\mathrm{T}}\tilde{K}'\boldsymbol{b}}{2\hbar} \qquad \tilde{K}' = \tilde{\beta}^{\mathrm{T}}\tilde{\alpha}\tilde{\beta} + 2\tilde{\beta}. \tag{B.14}$$

Another operator closely related to $\hat{S}(\tilde{\alpha})$ will be required; this is defined by

$$\hat{s}(\alpha) = \int_{-\infty}^{\infty} \mathrm{d}x \, \exp\left[\frac{\mathrm{i}\alpha x^2}{2\hbar}\right]\hat{T}(x\boldsymbol{A}_2). \tag{B.15}$$

Following the same approach as was used for the operator $\hat{S}(\tilde{\alpha})$, it is easily shown that $\hat{s}(\alpha)$ satisfies

$$\hat{T}(\boldsymbol{R}') = \hat{s}^{-1}(\alpha)\hat{T}(\boldsymbol{R})\hat{s}(\alpha) \tag{B.16}$$

where $\boldsymbol{R}$ is an arbitrary vector, and $\boldsymbol{R}'$ is given by

$$\boldsymbol{R}' = \tilde{M}(\alpha)\boldsymbol{R} \qquad \tilde{M}(\alpha) = \begin{pmatrix} 1 & 0 \\ -\alpha^{-1} & 0 \end{pmatrix}. \tag{B.17}$$

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