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Conserved and broken symmetries in the renormalization of the phase space lattice Hamiltonian

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Abstract. The phase space lattice Hamiltonian is a realistic model for Bloch electrons in a magnetic field. It has a fractal spectrum when the lattice has centres of threefold or fourfold rotational symmetry. This fact has been explained using a renormalization group (RG) method, assuming that the RG transformation preserves the symmetry of the Hamiltonian. The symmetry preservation property has previously been demonstrated for fourfold rotation; the threefold case is considerably more difficult to analyse. In this paper we present a simplified form of the RG equations which clearly exhibits the threefold symmetry preservation. We also discuss the case of sixfold rotational symmetry, for which the symmetry of the Hamiltonian may be reduced to threefold under the action of the RG.

1. Introduction

The phase space lattice Hamiltonian takes the form

$$\hat{H} = \sum_n \sum_m H_{nm} \hat{T}(n\overline{h}, m\overline{h}) \qquad H_{nm} = H^*_{-n-m} \tag{1.1}$$

where the operators $\hat{T}(X, P)$ are Weyl operators, which we formally write as

$$\hat{T}(X, P) = \exp[\mathrm{i}(P\hat{x} - X\hat{p})/\overline{h}] \tag{1.2}$$

and which are defined by the relation $\hat{T}(X, P)\psi(x) = \exp[\mathrm{i}P(x - \frac{1}{2}X)/\overline{h}]\psi(x - X)$. The coefficients H_{nm} are assumed to be short ranged, in that they decrease rapidly as $|n|, |m| \to \infty$. The Hamiltonian is represented by a periodic function $H(x, p)$ with Fourier coefficients H_{nm}, which is obtained by replacing $\hat{x}$ and $\hat{p}$ by numbers x and p: equations (1.1) and (1.2) then correspond to the Weyl quantization of $H(x, p)$. The phase space lattice Hamiltonian is of physical importance because it is an effective Hamiltonian describing the effect of a magnetic field on an electron in a periodic potential [1–3].

Rotational symmetries of the periodic potential in coordinate space correspond to rotational symmetries of the Hamiltonian function $H(x, p)$ in the phase plane [4], and in this paper we will be largely concerned with the implications of these symmetries for the spectrum of the phase space lattice Hamiltonian. The spectrum obtained by quantization using the Weyl scheme is invariant under linear canonical transformations of the phase space. We can therefore map a triangular lattice to a square lattice by an area-preserving shear. After making such a transformation, the operator $\hat{R}_6$ representing a sixfold rotation has the property

$$\hat{R}_6 \hat{T}(X, P) = \hat{T}(P, P - X)\hat{R}_6 \tag{1.3}$$

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and the condition for (1.1) to be invariant under a sixfold rotation of the phase plane is

$$H_{m,m-n} = H_{n,m}. \tag{1.4}$$

The operator $\hat{R}_6$ can be expressed as the exponential of a quadratic form in the operators $\hat{x}$ and $\hat{p}$, but for the purposes of this paper (1.3) is sufficient to define $\hat{R}_6$. The corresponding fourfold symmetry relations are

$$\hat{R}_4\hat{T}(X, P) = \hat{T}(P, -X)\hat{R}_4 \tag{1.5}$$

$$H_{m,-n} = H_{n,m}. \tag{1.6}$$

The spectrum of (1.1) depends upon the number theoretical properties of β, the ratio of $2\pi\hbar$ to the area of a primitive unit cell in the (x, p) plane. When β is the ratio of two integers p/q, the spectrum is a set of q bands (some of which may touch or overlap), whereas when β is irrational, the spectrum is a Cantor set [5–7]. For most choices of the Fourier coefficients H_{nm}, and for most irrational β, the Cantor set spectrum appears to have a non-zero measure. A very surprising result is that the Cantor set spectrum is a fractal set of zero measure when the Hamiltonian $H(x, p)$ has centres of threefold or fourfold symmetry in the (x, p) plane. This observation has proved very difficult to explain in general, although much progress has been made with Harper's model, where the only non-zero coefficients are $H_{10} = H_{01} = H_{-1,0} = H_{0,-1} = 1$, and in some closely related models [8–10].

Renormalization group (RG) methods have proved useful for understanding the nature of the spectrum and eigenstates. The RG transformation has been implemented in an approximate form, using WKB methods to estimate matrix elements, in [11–15]. Our discussion will be based upon an exact implementation, described in detail in [16, 17], using a formulation developed in [18, 19]. When β is close to the rational value p/q, the spectrum can be divided into q subsets, which cluster around the bands of the rational spectrum. The RG transformation constructs an effective Hamiltonian, also in the form of a phase space lattice Hamiltonian, whose spectrum corresponds to one of these subsets.

The formulae for the RG transformation will be cast in a form which is very similar to those for a tight-binding effective Hamiltonian, representing a single band of a system without a magnetic field. The tight-binding effective Hamiltonian can be constructed from the Wannier functions: the fundamental Wannier function is obtained by integrating the Bloch states $|B(\boldsymbol{k})\rangle$over the Brillouin zone

$$|\phi\rangle = \int_{\mathrm{BZ}} \mathrm{d}\boldsymbol{k}\, |B(\boldsymbol{k})\rangle \tag{1.7}$$

and a lattice of Wannier functions spanning the band can be constructed by applying translation operators:

$$|\phi(\boldsymbol{R})\rangle = \hat{T}(\boldsymbol{R})|\phi\rangle \tag{1.8}$$

where $\boldsymbol{R}$ is a lattice vector, and $\hat{T}(\boldsymbol{r}) = \exp[\mathrm{i}\hat{\boldsymbol{p}} \cdot \boldsymbol{r}/\hbar]$ is the translation operator for a displacement $\boldsymbol{r}$. The Wannier states $|\phi(\boldsymbol{R})\rangle$ form an orthonormal set which spans the states of the band. The tight-binding effective Hamiltonian is

$$\hat{H}_{\mathrm{eff}} = \sum_{\boldsymbol{R}} H(\boldsymbol{R})\hat{T}(\boldsymbol{R}) \tag{1.9}$$

where the hopping coefficients are

$$H(\boldsymbol{R}) = \langle\phi|\hat{T}(\boldsymbol{R})\hat{H}|\phi\rangle \tag{1.10}$$

(these are also the Fourier coefficients of the dispersion relation $E(\boldsymbol{k})$ of the band).

The renormalised effective Hamiltonian is similar to (1.9), with the translation operators replaced by Weyl operators. The analogy is strengthened if it can be shown that the coefficients $H(\boldsymbol{R})$ are given by a formula analogous to (1.10). The coefficients were obtained in this form in [18], in the special case where the Chern integer M (a topological invariant describing the quantized Hall conductance [20] of the band) is zero, but extension to non-zero Chern integers was not possible, because of difficulties in defining the Wannier functions when $M \neq 0$ [21]. In [16], it was shown how satisfactory Wannier functions can be defined when $M \neq 0$, and in section 2 we show how the equation for the amplitudes defining the renormalised Hamiltonian can be cast in the form of (1.10).

The fact that a threefold or fourfold rotational symmetry implies a zero measure Cantor set spectrum has been explained using the RG transformation, using the following argument [18]. The spectrum of the Hamiltonian (1.1) is a subset of the range of the periodic function $H(x, p)$. A finite fraction f of this range can usually be shown to lie in gaps of the spectrum. If this fraction does not approach zero as the RG transformation is iterated, the spectrum is a set of zero measure. The spectrum of $\hat{H}$ is equal to the full range of the function $H(x, p)$ if this function depends only upon one linear combination of x and p, i.e. if $H(x, p) = h(\alpha x - \alpha' p)$; for example if $H(x, p) = h(x)$, then the eigenstates of the Hamiltonian have wavefunctions $\psi(x) = \delta(x - X)$ with eigenvalues $h(X)$. If the Hamiltonian is mapped into this form by the RG transformation, the spectrum will be a Cantor set of non-zero measure. A Hamiltonian of this form has twofold symmetry in the (x, p) plane. The existence of a Cantor set spectrum of zero measure is established by showing that the RG transformation preserves threefold or fourfold rotational symmetries of $H(x, p)$, making any hypothesized attractor with only twofold symmetry inaccessible.

In the case where the Hamiltonian has fourfold symmetry, it has been shown explicitly that the renormalised Hamiltonian can be constructed so that it has the same symmetry [16]. In sections 3 and 4 of this paper we consider the more difficult case where the Hamiltonian has threefold or sixfold rotation centres; this has already been analysed using the semiclassical version of the RG transformation [13, 15], but the proof that the RG transformation can be constructed to show preservation of threefold symmetry exactly has only recently become possible. Our calculation combines the simplified RG equations obtained in section 2 with results obtained recently by one of us [22] on the form of the sixfold rotation operator for Wannier states of the Hamiltonian (1.1). In the case where the Hamiltonian has sixfold symmetry there are usually nearly degenerate bands, which require a separate analysis, given in sections 5 and 6: in these cases the sixfold symmetry is broken, and the renormalized Hamiltonian has only threefold centres.

2. A simplified formulation of the RG equations

2.1. A review of the RG equations

We start by reviewing the exact RG procedure, described in [19, 16]. When $\beta = p/q$ the spectrum consists of a set of q bands, which we assume are non-overlapping. If β is close to p/q, then for sufficiently small $\Delta\beta = \beta - p/q$ it is possible to identify a subset of the spectrum which is associated with the ν^{th} band of the rational spectrum. The RG method constructs an effective Hamiltonian $\hat{H}^{(\nu)}$ for which the spectrum corresponds to that subset of the spectrum of $\hat{H}$ which is associated with the νth band. The effective Hamiltonian is similar in form to $\hat{H}$, except the Fourier coefficients are replaced by their renormalized values $H^{(\nu)}_{nm}$, and the operators $\hat{x}$, $\hat{p}$ are replaced by operators with a commutator defined

by a renormalized Planck constant $\overline{h}_\nu$:

$$\hat{H}^{(\nu)} = \sum_n \sum_m H^{(\nu)}_{nm} \hat{T}'(n\overline{h}'_\nu, m\overline{h}'_\nu) \tag{2.1}$$

$$\hat{T}'_\nu(X, P) = \exp[\mathrm{i}(P\hat{x}' - X\hat{p}')/\overline{h}'_\nu] \qquad [\hat{x}', \hat{p}'] = \mathrm{i}\overline{h}'_\nu. \tag{2.2}$$

This renormalization is implemented by the following procedure. A set of generalized Wannier states is constructed out of the Bloch states $|B_\nu(k, \delta)\rangle$ of the νth band of the spectrum when β takes the rational value p/q. These Bloch states can be written in the form

$$\langle x|B_\nu(k, \delta)\rangle = \sum_n \exp[\mathrm{i}kx/\overline{h}]U_\nu(x; k)\delta(x - n\overline{h} - \delta) \tag{2.3}$$

where $U_\nu(x; k) = U_\nu(x + 2\pi; k)$. In general, the Bloch states $|B_\nu(k, \delta)\rangle$ are not available as analytic and periodic functions of k and δ, but the phases of the Bloch states can be chosen so that

$$\begin{aligned} &|B_\nu(k, \delta + \overline{h})\rangle = |B_\nu(k, \delta)\rangle \\ &|B_\nu(k + \kappa_\nu, \delta)\rangle = \exp[2\pi\,\mathrm{i}M_\nu\delta/\overline{h}]|B_\nu(k, \delta)\rangle. \end{aligned} \tag{2.4}$$

Here M_ν is the Chern number, which corresponds to the quantized Hall effect integer of the band [20], and κ_ν is the size of the Brillouin zone for the νth band, which will be specified later. Although the Bloch states are not a periodic function of (k, δ) unless $M_\nu = 0$, the states $\hat{T}(0, -qM_\nu k)|B_\nu(k, \delta)\rangle$ are periodic. The generalized Wannier states are a set of localized states $|\phi_\mu\rangle$, with $\mu = 1, \ldots, |N_\nu|$, where N_ν satisfies

$$pN_\nu + qM_\nu = 1. \tag{2.5}$$

The M_ν are always such that N_ν is an integer, and the integer N_ν determines $\kappa_\nu = 2\pi M_\nu + \overline{h}N_\nu$: we have $\kappa_\nu \to 2\pi/q$ in the rational limit $\beta \to p/q$. The generalized Wannier states are constructed, for rational values of $\beta = p/q$, as follows

$$\begin{aligned} |\phi_\mu\rangle = \frac{q^2}{4\pi^2 pN_\nu} \sum_{\mu'=1}^{|N_\nu|} &\exp[2\pi\,\mathrm{i}\mu\mu'/N_\nu]\hat{T}(2\pi\mu'/N_\nu, 0) \\ &\times \int_0^{2\pi/q} \mathrm{d}k \int_0^{2\pi p/q} \mathrm{d}\delta \exp[\mathrm{i}qk\mu']\hat{T}(0, -qM_\nu k)|B_\nu(k, \delta)\rangle. \end{aligned} \tag{2.6}$$

Having constructed the generalized Wannier states using (2.6), a set of generalized Bloch functions are obtained, which are defined even for irrational values of β:

$$\begin{aligned} |B_\nu(k, \delta)\rangle = \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} \sum_{\mu=1}^{|N_\nu|} &\exp\left[-\frac{2\pi\,\mathrm{i}}{\overline{h}}\left(m\delta + \frac{n(k + \mu\overline{h})}{N_\nu}\right)\right] \\ &\times \hat{T}(0, 2\pi m)\hat{T}(2\pi n/N_\nu, 0)\hat{T}(0, 2\pi M_\nu k/\kappa_\nu)\hat{P}_\nu|\phi_\mu\rangle \end{aligned} \tag{2.7}$$

where $\hat{P}_\nu$ is a projection operator, which projects into the subspace spanned by the νth band of the spectrum of $\hat{H}$ at the irrational value of β (the definition and role of this projection operator are discussed in detail in [19]).

The crucial observation in the construction of the RG transformation is that the matrix elements of $\hat{H}$ in the basis formed by the generalized Bloch states turn out to be exactly the same as the matrix elements of an operator $\hat{H}'$, similar to (2.1)

$$\hat{H}' = \sum_n \sum_m H'_{nm} \hat{T}'(n\overline{h}'_\nu, m\overline{h}'_\nu) \tag{2.8}$$

in the basis formed by the eigenstates of the position operator $\hat{x}'$. The renormalized Planck constant $\overline{h}'_\nu$ is given by

$$\overline{h}'_\nu = 2\pi\beta'_\nu \qquad \beta'_\nu = \frac{q\beta - p}{N_\nu\beta + M_\nu} \tag{2.9}$$

and the Fourier coefficients H'_{nm} are given by a linear transformation of those of $\hat{H}$

$$H'_{nm} = \sum_{N=-\infty}^{\infty}\sum_{M=-\infty}^{\infty} H_{NM}\tau_{nm}^{NM}. \tag{2.10}$$

The coefficients τ_{nm}^{NM} defining the renormalization of operators are expressed in terms of the generalized Wannier states as follows

$$\begin{aligned}\tau_{nm}^{NM} &= (-1)^{p(mN+nM-qnm)}\sum_{\mu=1}^{|N_\nu|}\langle\phi_\mu|\hat{\tau}_{nm}^{NM}|\phi_\mu\rangle \\ \hat{\tau}_{nm}^{NM} &= \hat{t}(M-mq, N-nq)\hat{T}((-2\pi n + N\kappa_\nu)/N_\nu, (-2\pi m + M\kappa_\nu)\overline{h}/\kappa_\nu)\end{aligned} \tag{2.11}$$

where $\hat{t}(n_x, n_p)$ is an operator acting on the labels of the Wannier states:

$$\hat{t}(n_x, n_p)|\phi_\mu\rangle = \exp\left[\frac{2\pi\,\mathrm{i}M_\nu}{N_\nu}\left(\mu - \frac{1}{2}n_x\right)n_y\right]|\phi_{\mu-n_x}\rangle. \tag{2.12}$$

Note that the $\hat{t}(n_x, n_p)$ operators have a similar non-commuting algebra to the Weyl operators (1.2):

$$\hat{t}(n_x, n_p)\hat{t}(n'_x, n'_p) = \exp\left[\frac{2\pi\,\mathrm{i}M_\nu}{N_\nu}\frac{(n'_x n_p - n'_p n_x)}{2}\right]\hat{t}(n_x + n'_x, n_p + n'_p). \tag{2.13}$$

As well as constructing a renormalized representation $\hat{H}'$ of the Hamiltonian using (2.8) and the subsequent equations, we also construct a renormalized representation $\hat{N}'$of the normalization operator by taking matrix elements of the identity operator. The subset of the spectrum spanned by the νth band is then that of the effective Hamiltonian

$$\hat{H}^{(\nu)} = \hat{N}'^{-1/2}\hat{H}'\hat{N}'^{-1/2} \tag{2.14}$$

which is obtained in the form of the Fourier expansion (2.1).

2.2. A simplified formulation of the RG equations

In this paper we will find it convenient to express the above results in a considerably simplified form. First, we shall redefine the renormalized Planck constant by adding pq, so that (2.9) is replaced by a new definition

$$\overline{h}'_\nu = 2\pi\beta'_\nu \qquad \beta'_\nu = \frac{q\beta - p}{N_\nu\beta + M_\nu} + pq. \tag{2.15}$$

The effect of this change is equivalent to multiplying all of the Fourier coefficients H'_{nm} of the renormalized Hamiltonian by the factor $(-1)^{pqnm}$.

A more fundamental change is that we will introduce a Hilbert space which is a Cartesian sum of $|N_\nu|$ copies of the Hilbert space for the real line. We use parentheses to denote state vectors in this space: the symbol $|\Phi)$ represents a vector in the extended Hilbert space which corresponds to the set of $|N_\nu|$ vectors $|\phi_\mu\rangle$, $\mu = 1, \ldots, |N_\nu|$ in the space of functions on the real line. The Dirac bracket for states $|\Phi)$ and $|\Psi)$ is defined to be

$$(\Phi|\Psi) = \sum_{\mu=1}^{|N_\nu|}\langle\phi_\mu|\psi_\mu\rangle. \tag{2.16}$$

We define a set of translation operators $\hat{\mathcal{T}}_{nm}$ in the extended Hilbert space as follows

$$\hat{\mathcal{T}}_{nm} = \hat{t}(-mq, -nq)\hat{T}(-2\pi n/N_\nu, -2\pi m\bar{h}/\kappa_\nu). \tag{2.17}$$

This expression defines the generalized translation operators $\hat{\mathcal{T}}(\boldsymbol{R})$ for sites on a lattice (the non-lattice translations will not be required in this paper). These operators have the same non-commutative algebra as the Weyl operators

$$\hat{\mathcal{T}}_{nm}\hat{\mathcal{T}}_{n'm'} = \exp\left[2\pi \mathrm{i}\gamma\left(\frac{nm' - mn'}{2}\right)\right]\hat{\mathcal{T}}_{n+n',m+m'} \tag{2.18}$$

where (recalling (2.15))

$$\gamma = \frac{2\pi p - q\bar{h}}{\kappa_\nu} + pq = \beta'_\nu. \tag{2.19}$$

The geometry of the lattice labelled by the integers (n, m) (i.e. whether it is square, triangular, or lower symmetry) need not be specified at this stage.

We also define an operator which represents the Hamiltonian in the extended Hilbert space:

$$\hat{\mathcal{H}} = \sum_N \sum_M H_{NM}\hat{t}(M, N)\hat{T}(N\kappa_\nu/N_\nu, M\bar{h}). \tag{2.20}$$

This operator commutes with the translation operators:

$$\hat{\mathcal{H}} = \hat{\mathcal{T}}_{nm}\hat{\mathcal{H}}\hat{\mathcal{T}}^{+}_{nm}. \tag{2.21}$$

With these definitions, the formula for the Fourier coefficients of the renormalized Hamiltonian is remarkably simple

$$H'_{nm} = (\Phi|\hat{\mathcal{T}}_{nm}\hat{\mathcal{H}}|\Phi) \tag{2.22}$$

where $|\Phi)$ is the state vector in the extended Hilbert space formed from the generalized Wannier functions.

Formula (2.22) can be simplified further by associating the pair of integers (n, m) with a lattice vector $\boldsymbol{R} = n\boldsymbol{a}_1 + m\boldsymbol{a}_2$, where the $\boldsymbol{a}_i$ are basis vectors for the lattice. A straightforward calculation shows that the effect of operator $\hat{T}(2\pi pn, 2\pi pm)$ on a set of Bloch states is equivalent to that of applying the operator $\hat{\mathcal{T}}_{nm}$ to the corresponding Wannier states, i.e. $\hat{\mathcal{T}}_{nm}$ is the image of the operator $\hat{T}(2\pi pn, 2\pi pm)$ under the mapping defined by (2.6). It is therefore natural to choose the lattice formed by the vectors $\boldsymbol{R}$ to have a unit cell of area $(2\pi p)^2$, and to write the RG equations in the form

$$\begin{aligned} &\hat{H}' = \sum_{\boldsymbol{R}} H'(\boldsymbol{R})\hat{T}'(\tilde{\boldsymbol{R}}) \qquad \tilde{\boldsymbol{R}} = \frac{\bar{h}'_\nu}{2\pi p}\boldsymbol{R} \\ &H'(\boldsymbol{R}) = (\Phi|\hat{\mathcal{T}}(\boldsymbol{R})\hat{\mathcal{H}}|\Phi). \end{aligned} \tag{2.23}$$

This equation is closely analogous to equation (1.10) for the hopping coefficients defining the Hamiltonian for a periodic potential without a magnetic field, in the tight-binding representation.

3. Symmetric Wannier functions

3.1. Wannier functions without a magnetic field

In this section we show how to construct Wannier functions which are symmetric under rotational symmetry operations. There are several complications in the case of the phase

space lattice Hamiltonian. We will therefore consider first a two-dimensional system with periodic potential without a magnetic field. The eigenstates of the Hamiltonian $\hat{H}$ are Bloch states, with wavevector $\boldsymbol{k} = (k_1, k_2)$. We assume that the energy bands $\mathcal{E}(\boldsymbol{k})$ are non-overlapping, non-degenerate, and that the eigenstates are a periodic function of $\boldsymbol{k}$. A Wannier state $|\phi\rangle$ can be generated by integrating the Bloch states $|B(\boldsymbol{k})\rangle$ over the Brillouin zone: see equation (1.7). The Bloch states can be recovered from the set of Wannier states translated through lattice vectors $\boldsymbol{R}$ as follows

$$|B(\boldsymbol{k})\rangle = \sum_{\boldsymbol{R}} \exp[\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}]\hat{T}(\boldsymbol{R})|\phi\rangle \tag{3.1}$$

where the translation operator $\hat{T}(\boldsymbol{R}) = \exp[\mathrm{i}\hat{\boldsymbol{p}}\cdot\boldsymbol{R}]$ commutes with the Hamiltonian.

The Wannier states are not invariant under gauge transformations of the Bloch waves, of the form

$$|B(\boldsymbol{k})\rangle \to |B'(\boldsymbol{k})\rangle = \exp[\mathrm{i}\theta(\boldsymbol{k})]|B(\boldsymbol{k})\rangle. \tag{3.2}$$

The gauge function $\theta(\boldsymbol{k})$ must be such that the gauge-transformed Bloch states remain periodic: it can be written

$$\begin{aligned} &\theta(\boldsymbol{k}) = \boldsymbol{k}\cdot\boldsymbol{R} + \tilde{\theta}(\boldsymbol{k}) \\ &\tilde{\theta}(\boldsymbol{k}+\boldsymbol{K}) = \tilde{\theta}(\boldsymbol{k}) \end{aligned} \tag{3.3}$$

where $\boldsymbol{R}$ is any lattice vector, and $\boldsymbol{K}$ any reciprocal lattice vector (satisfying $\boldsymbol{K}\cdot\boldsymbol{R} = 2\pi n$, for some integer n).

We will also assume that the Hamiltonian $\hat{H}$ has an N-fold rotational symmetry:

$$\hat{H} = \hat{R}\hat{H}\hat{R}^{+} \qquad \hat{R}^N = \hat{I} \tag{3.4}$$

where $\hat{I}$ is the identity operator. Our objective will be to establish the existence of Wannier states which are rotationally symmetric. It is easily verified that

$$\hat{R}|B(\boldsymbol{k})\rangle = \exp[\mathrm{i}\theta(\boldsymbol{k})]|B(\boldsymbol{k}_R)\rangle \tag{3.5}$$

where $\theta(\boldsymbol{k})$ satisfies (3.3), and $\boldsymbol{k}_R$ is the rotated Bloch wavevector. We will seek to construct a gauge transformation such that

$$\hat{R}|B'(\boldsymbol{k})\rangle = \exp[2\pi\mathrm{i}L/N]|B'(\boldsymbol{k}_R)\rangle \tag{3.6}$$

where the gauge transformation is of the form (3.2) with $\theta(\boldsymbol{k})$ replaced by $\chi(\boldsymbol{k})$ and $\boldsymbol{R}$ by another vector $\boldsymbol{r}$:

$$\begin{aligned} &|B'(\boldsymbol{k})\rangle = \exp[\mathrm{i}\chi(\boldsymbol{k})]|B(\boldsymbol{k})\rangle \\ &\chi(\boldsymbol{k}) = \tilde{\chi}(\boldsymbol{k}) + \boldsymbol{k}\cdot\boldsymbol{r} \end{aligned} \tag{3.7}$$

and $\tilde{\chi}(\boldsymbol{k})$ is periodic on the Brillouin zone. Substituting (3.8) into (3.6), and comparing it with (3.6), we find

$$\frac{2\pi L}{N} = \chi(\boldsymbol{k}) - \chi(\boldsymbol{k}_R) + \theta(\boldsymbol{k}) = \tilde{\chi}(\boldsymbol{k}) - \tilde{\chi}(\boldsymbol{k}_R) + \tilde{\theta}(\boldsymbol{k}) + \boldsymbol{k}\cdot(\boldsymbol{r} - \boldsymbol{r}_{R^{-1}} + \boldsymbol{R}) \tag{3.8}$$

where we have used the relation $\boldsymbol{k}_R\cdot\boldsymbol{r} = \boldsymbol{k}\cdot\boldsymbol{r}_{R^{-1}}$. In order to solve this equation we must have

$$\boldsymbol{r} - \boldsymbol{r}_{R^{-1}} + \boldsymbol{R} = \boldsymbol{0} \tag{3.9}$$

where $\boldsymbol{R}$ is a lattice vector, and $\boldsymbol{r}$ should also be a lattice vector if the gauge-transformed Bloch states are to remain periodic on the Brillouin zone. For an arbitrary lattice vector $\boldsymbol{R}$, the vector $\boldsymbol{r}$ which solves (3.9) will not always be a lattice vector. Inspection of figure 1(*a*) shows that in the case of fourfold rotations on a unit square lattice, $\boldsymbol{r}$ may be the vector

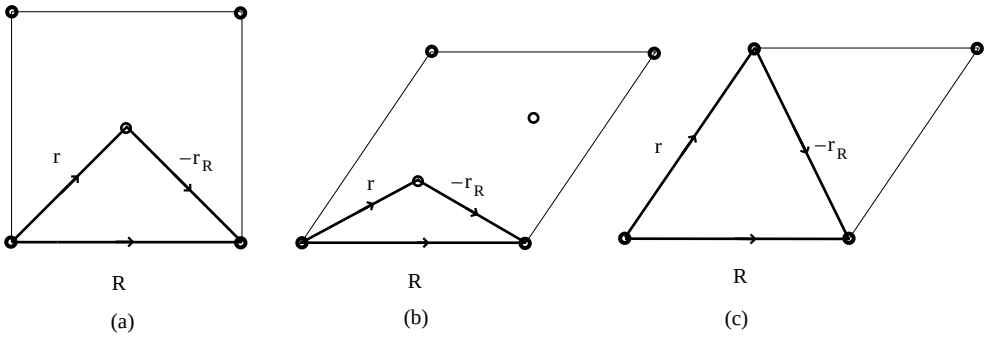

Figure 1. The vector $\boldsymbol{r}$ which solves (3.9) can represent a displacement from one symmetry centre to another inequivalent centre in the case of (*a*) fourfold or (*b*) threefold rotations. In the case of sixfold rotation, the translation is always to an equivalent centre (*c*).

$(\frac{1}{2}, \frac{1}{2})$: note that although the vector $\boldsymbol{r}$ is not a lattice vector, it does represent a translation from the origin to another centre of fourfold symmetry. Similarly, in the case of threefold rotations on a triangular lattice (figure 1(*b*)), the vector $\boldsymbol{r}$ may not be a lattice vector, but it always represents a translation to another centre of threefold rotational symmetry. In the case of sixfold rotational symmetry on a triangular lattice, there is only one centre of symmetry in each unit cell, but in this case the vector $\boldsymbol{r}$ solving (3.10) is always a lattice vector (figure 1(*c*)).

If (3.9) is not satisfied by a lattice vector, it is impossible to construct a gauge transformation which enables the Wannier functions to be made N-fold symmetric about the origin. Instead, consider a rotation operator $\hat{R}'$ with the centre of rotation shifted by a vector $\boldsymbol{r}$:

$$\begin{aligned}\hat{R}' &= \hat{T}(-\boldsymbol{r})\hat{R}\hat{T}(\boldsymbol{r}) \\ &= \hat{T}(-\boldsymbol{r}+\boldsymbol{r}_R)\hat{R}.\end{aligned} \tag{3.10}$$

This satisfies

$$\hat{R}'|B(\boldsymbol{k})\rangle = \exp[\mathrm{i}(\theta(\boldsymbol{k}) + (\boldsymbol{k}-\boldsymbol{k}_R)\cdot\boldsymbol{r})]|B(\boldsymbol{k}_R)\rangle \tag{3.11}$$

so that $\theta(\boldsymbol{k})$ in (3.5) is replaced by

$$\theta'(\boldsymbol{k}) = \theta(\boldsymbol{k}) - \boldsymbol{k}\cdot\boldsymbol{R} = \tilde{\theta}(\boldsymbol{k}). \tag{3.12}$$

By choosing $\boldsymbol{r}$ so that (3.9) is satisfied, the term linear in $\boldsymbol{k}$ is removed from (3.3). We noted above that the vector $\boldsymbol{r}$ which solves (3.9) is always a lattice vector, or a translation to another centre with at least as high a degree of rotational symmetry.

As well as considering the linear part of the gauge transformation, we must also consider the periodic part, $\tilde{\chi}(\boldsymbol{k})$. It will be useful to consider the Fourier expansion of the $\tilde{\chi}(\boldsymbol{k})$, which we write in the form

$$\tilde{\chi}(\boldsymbol{k}) = \sum_{\boldsymbol{R}} \tilde{\chi}(\boldsymbol{R})\exp[\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}] \tag{3.13}$$

and a similar expansion for $\tilde{\theta}(\boldsymbol{k})$ with coefficients $\tilde{\theta}(\boldsymbol{R})$. We find that the Fourier coefficients satisfy the recurrence relation (for $\boldsymbol{R} \neq \boldsymbol{0}$)

$$\tilde{\chi}(\boldsymbol{R}_R) = \tilde{\theta}(\boldsymbol{R}) + \tilde{\chi}(\boldsymbol{R}). \tag{3.14}$$

Iteration of (3.14) determines $N-1$ coefficients from an arbitrarily chosen $\tilde{\chi}(\boldsymbol{R})$. We remark that the solution is not unique, because many of the Fourier coefficients are arbitrary, and that consistency of this solution requires

$$\sum_{n=0}^{N-1} \tilde{\theta}(\boldsymbol{k}_{R^n}) = 2\pi L \tag{3.15}$$

for some integer L: this follows from (3.5) if $\hat{R}^N = \hat{I}$.

We have now shown how to construct Bloch states satisfying (3.6) for rotation about one N-fold symmetry centre, in the case of a two-dimensional periodic potential without magnetic field: the Wannier function (1.7) is then automatically an eigenfunction of the rotation operator about the same symmetry centre, with the same eigenvalue.

3.2. Symmetric Bloch states for the phase space lattice

We now consider how to extend this calculation to the case of the phase space lattice Hamiltonian. We will show how an equation analogous to (3.6) can be satisfied by choosing a suitable gauge for the Bloch states. In the argument presented above, we assumed that:

(a) the Bloch states lie on a Brillouin zone which is a unit cell of the reciprocal lattice;

(b) the rotation operator $\hat{R}$ maps one Bloch state into another Bloch state;

(c) the Bloch states are periodic and analytic on the Brillouin zone.

The only point at which we used (c) was when (1.7) was used to construct the Wannier function. If we confine ourselves to ensuring that (3.6) is satisfied, we do not require this assumption.

The Brillouin zone for the phase space lattice Hamitonian is (in the rational case) a rectangle in (k, δ) space with sides $2\pi/q$ along the k-axis and $2\pi p/q$ along the δ-axis: unless $p = 1$, it is not therefore a reciprocal of the square phase space lattice of side $2\pi p$ describing the translational symmetry of the Bloch states. Also, the rotation operator $\hat{R}$ maps a single Bloch state $|B(k, \delta)\rangle$ into a superposition of p different Bloch states $|B(k', \delta' + j\bar{h}/p)\rangle$, $j = 0, \ldots, p-1$. We will now consider how to redefine the Brillouin zone and rotation operator so that assumptions (a) and (b) hold for $p \neq 1$.

We can define Bloch states on a Brillouin zone of dimension $2\pi/q$ in both the k and δ directions by considering a vector $|B(k, \delta)\}$ of p Bloch states:

$$|B(k, \delta)\} = (|B(k, \delta)\rangle, |B(k, \delta + 2\pi/q)\rangle, \ldots, |B(k, \delta + 2\pi(p-1)/q)\rangle) \tag{3.16}$$

with $0 \leqslant k, \delta < 2\pi/q$: we will use the notation $|\ldots\}$ for vectors in a Hilbert space of functions defined on a space consisting of the Cartesian sum of p copies of the real line.

It is now necessary to construct rotation operators $\hat{\mathcal{R}}^{(B)}$ which map Bloch states $|B(k, \delta)\}$ into other Bloch states, with the same periodicity properties:

$$\hat{\mathcal{R}}^{(B)}|B(k, \delta)\} = \exp[\mathrm{i}\theta(k, \delta)]|B(k', \delta')\} \tag{3.17}$$

where $\theta(k, \delta)$ consists of a part which is periodic on the Brillouin zone, and possibly a linear part, analogous to (3.3). The case of a fourfold rotation was discussed in [16]: the first element of the rotated Bloch state $|B(k, \delta)\}$ is given by

$$|B(k', \delta')\rangle = \frac{1}{\sqrt{p}} \exp\left[\frac{\mathrm{i}q^2 M_v k\delta}{2\pi p}\right] \sum_{j=1}^{p} \hat{R}|B(k, \delta)\rangle \tag{3.18}$$

where $(k', \delta') = (\delta, -k)$: this defines the operator $\hat{\mathcal{R}}_4^{(B)}$. The analogous formula for the case of sixfold rotation is given in [22].

Having defined rotation operators $\hat{\mathcal{R}}_4^{(B)}$ and $\hat{\mathcal{R}}_6^{(B)}$ for the Bloch states, the arguments above can be applied directly. If the linear term in $\theta(k,\delta)$ is present, it represents a translation of the Bloch states through a lattice vector $\boldsymbol{R}$. (The lattice reciprocal to the square Brillouin zone of side $2\pi/q$ is a square lattice of side $2\pi p$: cf the comments preceding (2.23).) The linear term can be eliminated by considering a rotation about a point $\boldsymbol{r}$, where $\boldsymbol{r}$ is related to $\boldsymbol{R}$ by (3.9). The Bloch states can, therefore, be given N-fold rotational symmetry about a point translated by $\boldsymbol{r}$ from the origin in phase space. It is therefore possible to calculate a gauge in which

$$\hat{\mathcal{R}}_N'^{(B)}|B(k,\delta)\} = \exp[\mathrm{i}\theta(k,\delta)]|B(k',\delta')\} \tag{3.19}$$

where $\hat{\mathcal{R}}_N'^{(B)}$ is the rotation operator about the shifted symmetry centre.

The form of the translation operator $\hat{\mathcal{T}}(\boldsymbol{R})$ of the Wannier states $|\Phi)$ has only been determined for lattice translations in this paper. The symmetry of the Wannier states can, however, still be characterized in the following way, using (3.10):

$$|\Phi) = \exp[2\pi\mathrm{i}L/N]\hat{\mathcal{T}}(\boldsymbol{R})\hat{\mathcal{R}}_N|\Phi) \tag{3.20}$$

where L is an integer and $\hat{\mathcal{R}}_N$ is a rotation operator for the Wannier functions, conjugate to that of the Bloch states: its specific form will be discussed in the next section.

4. Symmetry preservation for simple bands

4.1. Fourfold rotations

In this section we show how the symmetry preservation property of the renormalized Hamiltonian is obtained, using rotation operators representing the symmetry of the Wannier functions. We first review the case of fourfold symmetry, using the new notations defined in section 2: this leads to a considerable simplification of the proof of fourfold symmetry preservation given in [16].

In the case of fourfold symmetry, the integers (n,m) labelling the translation operators (2.17) must be mapped onto a square lattice: we write

$$\boldsymbol{R} \to 2\pi p(n\boldsymbol{e}_1 + m\boldsymbol{e}_2) \tag{4.1}$$

where the $\boldsymbol{e}_i$ are orthonormal basis vectors, and the RG equations may be represented in the form (2.23). A $\pi/2$ rotation in the lattice of points $\boldsymbol{R}$ is represented by the following transformation of the integer labels:

$$(n,m) \underset{R_4}{\longrightarrow} (m,-n). \tag{4.2}$$

The generalized rotation operator, which realizes this transformation, was obtained in [16]: for rational β it takes the form

$$\hat{\mathcal{R}}_4 = \hat{S}(pN_\nu)\hat{R}_4\hat{r}_4. \tag{4.3}$$

Here (4.4) $\hat{S}(\eta)$ is a squeezing operator, defined by its effect upon a coordinate space wavefunction,

$$\langle x|\hat{S}(\eta)|\psi\rangle = \eta^{1/2}\langle \eta x|\psi\rangle \tag{4.4}$$

and $\hat{r}_4$ is a discrete Fourier transform acting over the labels μ:

$$\hat{r}_4|\Phi) = \left\{ \frac{1}{\sqrt{|N_\nu|}} \sum_{\mu'=1}^{|N_\nu|} \exp[2\pi\mathrm{i}M_\nu\mu\mu'/N_\nu]|\phi'_{\mu'}\rangle \,\middle|\, \mu = 1,\ldots,|N_\nu| \right\}. \tag{4.5}$$

The rotation operator $\hat{\mathcal{R}}_4$ is the image of the rotation operator $\hat{\mathcal{R}}_4^{(B)}$ of the Bloch states, defined by (3.17), under transformation (2.6) which converts from Bloch to Wannier states, i.e. if the Bloch states are rotated using the operator $\hat{\mathcal{R}}_4^{(B)}$, then the Wannier functions generated using (2.6) are rotated by rotation opertors $\hat{\mathcal{R}}_4$ defined in (4.3) [16].

If the Hamiltonian has fourfold symmetry, i.e. if $\hat{H} = \hat{R}_4 \hat{H} \hat{R}_4^{-1}$, we find that its representation in the extended Hilbert space is also symmetric under the operator $\hat{\mathcal{R}}_4$, in the rational limit:

$$\hat{\mathcal{H}} = \hat{\mathcal{R}}_4 \hat{\mathcal{H}} \hat{\mathcal{R}}_4^{-1}. \tag{4.6}$$

If the Hamiltonian has fourfold symmetry, the arguments leading to equation (3.20) show that the Bloch states can be gauged so that the Wannier functions satisfy

$$\hat{\mathcal{T}}(\boldsymbol{R}) \hat{\mathcal{R}}_4 |\Phi) = \exp[2\pi \mathrm{i} L/4] |\Phi) \tag{4.7}$$

for some lattice vector $\boldsymbol{R}$, and by shifting the origin of the phase space lattice we can ensure that $\boldsymbol{R} = \boldsymbol{0}$. Substituting (4.7) into formula (2.22) for the Fourier coefficient of the renormalized Hamiltonian, and using (4.6), we then find that the Fourier coefficients of the renormalized Hamiltonian satisfy $H'_{-m,n} = H'_{nm}$: in view of the correspondence defined in (4.2), this implies that

$$H'(\boldsymbol{R}_{R_4}) = H'(\boldsymbol{R}) \tag{4.8}$$

where $\boldsymbol{R}$ represents a vector in the (x, p) phase plane. The renormalized Hamiltonian is therefore also fourfold symmteric in the rational case:

$$\hat{H}' = \hat{R}'_4 \hat{H}' \hat{R}'^{-1}_4 \tag{4.9}$$

where $\hat{R}'_4$ is the operator $\hat{R}_4$, with $\overline{h}$ replaced by $\overline{h}'_\nu$. For irrational β, the representation of the Hamiltonian in the extended Hilbert space, $\hat{\mathcal{H}}$, is invariant under the fourfold rotation operator

$$\hat{\mathcal{R}}'_4 = \hat{S}(\overline{h} N_\nu / \kappa_\nu) \hat{R}_4 \hat{r}_4 \tag{4.10}$$

(which reduces to (4.3) in the rational limit, $\overline{h}/2\pi \to p/q$). It was shown in [16] that, if relation (4.7) is satisfied in the rational case, then in the irrational case a similar relation applies for the operator $\hat{\mathcal{R}}'_4$, and a Wannier state $|\Phi')$, which is obtained by a scaling of the original Wannier state

$$|\Phi') = \hat{S}(\eta) |\Phi) \qquad \eta = \sqrt{\frac{2\pi}{q\kappa_\nu}}. \tag{4.11}$$

If these Wannier functions are used in the RG equation (2.23), it follows that fourfold rotational symmetry is also preserved in the irrational case.

4.2. Threefold and sixfold rotations

We can now extend this approach to the case of sixfold rotations (and results for threefold rotations are obtained immediately by applying $\hat{\mathcal{R}}_6$ twice).

In the case of sixfold rotations, we choose to assign the following correspondence between lattice points and pairs of integers

$$\boldsymbol{R} \to 2\pi p \left(\frac{\sqrt{3}}{2} n a \boldsymbol{e}_1 + \left(m - \frac{1}{2} n \right) a \boldsymbol{e}_2 \right) \tag{4.12}$$

where $a = (2/\sqrt{3})^{1/2}$ is chosen to normalize the area of the unit cell to $(2\pi p)^2$. A $\pi/3$ rotation is therefore represented by the following transformation on the integer pairs

$$(n, m) \underset{R_6}{\longrightarrow} (m - n, n). \tag{4.13}$$

The rotation operator for sixfold rotations defined in this way was given in [20]: in the rational case

$$\hat{\mathcal{R}}_6 = \hat{T}(0, \alpha\pi p N_\nu)\hat{Q}(pqN_\nu M_\nu)\hat{S}(pN_\nu)\hat{R}_6\hat{r}_6\hat{t}(0, \alpha N_\nu/2) \tag{4.14}$$

where α takes the values 0, 1 if $N_\nu \times M_\nu$ is even or odd respectively, and the operators $\hat{Q}(s)$, $\hat{R}_6$ and $\hat{r}_6$ are defined by the relations

$$\hat{Q}(s) = \exp[-\mathrm{i}s\hat{x}^2/2\overline{h}] \tag{4.15}$$

$$\hat{R}_6 = \hat{R}_4\hat{Q}(1) \tag{4.16}$$

$$\hat{r}_6|\Phi) = \left\{ \frac{1}{\sqrt{N_\nu}} \sum_{\mu'=1}^{|N_\nu|} \exp[2\pi\mathrm{i}M_\nu(\mu\mu' - \mu'^2/2)/N_\nu]|\phi_\mu\rangle \middle| \mu = 1, \ldots, |N_\nu| \right\}. \tag{4.17}$$

These operators satisfy the relations

$$\hat{Q}(s)\hat{T}(X, P) = \hat{T}(X, P + sX)\hat{Q}(s) \tag{4.18}$$

$$\hat{R}_6\hat{T}(X, P) = \hat{T}(P, P - X)\hat{R}_6 \tag{4.19}$$

$$\hat{r}_6\hat{t}(n, m) = \hat{t}(m, n - m)\hat{r}_6 \tag{4.20}$$

implying that $\hat{Q}(s)$ represents a shear of the phase space, and $\hat{R}_6$, $\hat{r}_6$ are sixfold rotations.

If the Hamiltonian $\hat{H}$ is symmetric under a sixfold rotation, $\hat{H} = \hat{R}_6\hat{H}\hat{R}_6^{-1}$, then it is found that its representation in the extended Hilbert space is also symmetric, under the operator $\hat{\mathcal{R}}_6$, in the rational limit, i.e. $\hat{\mathcal{H}} = \hat{\mathcal{R}}_6\hat{\mathcal{H}}\hat{\mathcal{R}}_6^{-1}$. In the irrational case the operator $\hat{\mathcal{H}}$ is invariant under the rotation operator

$$\hat{\mathcal{R}}_6' = \hat{T}(0, \alpha\pi\overline{h}N_\nu/\kappa_\nu)\hat{Q}(\overline{h}qN_\nu M_\nu/\kappa_\nu)\hat{S}(\overline{h}N_\nu/\kappa_\nu)\hat{R}_6\hat{r}_6\hat{t}(0, \alpha N_\nu/2). \tag{4.21}$$

As argued earlier, the Bloch states can always be gauged such that (3.6) is satisfied, which implies that the Wannier functions $|\Phi)$ satisfy $\hat{\mathcal{R}}_6|\Phi) = \exp[2\pi\mathrm{i}L/6]|\Phi)$. A set of Wannier functions $|\Phi')$, which satisfy a similar relation with the operator $\hat{\mathcal{R}}_6'$, can be obtained by the following transformation:

$$|\Phi') = \hat{S}(\eta)\hat{T}(\alpha\pi(\eta - 1), \alpha\pi pN_\nu(\eta - 1))|\Phi) \tag{4.22}$$

where η takes the same value as in (4.11).

The sixfold rotation operator does not, in general, commute with the translations $\hat{\mathcal{T}}(\boldsymbol{R})$: we find

$$\hat{\mathcal{R}}_6\hat{\mathcal{T}}(\boldsymbol{R})\hat{\mathcal{R}}_6^{-1} = \exp[\mathrm{i}\boldsymbol{k} \wedge \tilde{\boldsymbol{R}}/\overline{h}_\nu']\hat{\mathcal{T}}(\boldsymbol{R}_{R_6}) \tag{4.23}$$

where

$$\exp[\mathrm{i}\boldsymbol{k} \wedge \tilde{\boldsymbol{R}}/\overline{h}_\nu'] = \exp[-\mathrm{i}m\alpha\pi N_\nu\beta_\nu'] \tag{4.24}$$

(note that this factor equals unity in the rational limit $\overline{h} \to 2\pi p/q$). The Fourier coefficients of the renormalized Hamiltonian therefore satisfy

$$H(\boldsymbol{R}) = (\Phi'|\hat{\mathcal{T}}(\boldsymbol{R})\hat{\mathcal{H}}|\Phi') = H(\boldsymbol{R}_{R_6})\exp[\mathrm{i}\boldsymbol{k} \wedge \tilde{\boldsymbol{R}}/\overline{h}_\nu']. \tag{4.25}$$

It follows that the renormalized Hamiltonian satisfies

$$\hat{R}_6\hat{H}\hat{R}_6^{-1} = \hat{T}(\boldsymbol{k})\hat{H}\hat{T}^{-1}(\boldsymbol{k}) \tag{4.26}$$

i.e. the effect of rotating the renormalized Hamiltonian is equivalent to applying a translation in the phase plane through a distance $\boldsymbol{k}$. This implies that the effective Hamiltonian has a sixfold centre which is translated away from the origin, if $\alpha = 1$, in the irrational case.

5. The honeycomb lattice: degenerate bands

Here we consider the case where $H(x, p)$ has sixfold symmetry. The discussion in section 3 indicated that the Bloch states of a simple band can always be gauged so that the corresponding Wannier functions have sixfold rotational symmetry. The following argument makes this result appear paradoxical. In the semiclassical limit, $\overline{h} \to 0$, the Wannier states correspond to localized states with their Wigner functions concentrated on contours of the Hamiltonian function $H(x, p)$. For lattices with sixfold symmetry, the contours of $H(x, p)$ are of two types: they may enclose centres of either sixfold symmetry or threefold symmetry. We might therefore expect that for some bands there is no gauge for which the Wannier functions have higher than threefold rotational symmetry.

The resolution of this paradox at first appears to be simple. There are two contours with threefold symmetry per unit cell, related by an inversion about the centre of sixfold symmetry. The threefold contours form a honeycomb lattice, containing two types of site, labelled A and B, which are not equivalent under a translation, but which are equivalent under inversion about a sixfold centre. It might therefore be expected that the bands associated with these contours would be degenerate, so that well defined Wannier functions could not be constructed from the Bloch states of a single band. In fact, numerical experiments show that for a Hamiltonian with sixfold symmetry there are typically no degenerate bands. The paradox remains: semiclassical arguments suggest that Wannier functions should have no higher than threefold symmetry, whereas section 3 gave a proof that sixfold symmetry is attainable.

In order to explain the resolution of this paradox, we consider the case of a Hamiltonian containing a symmetry breaking parameter θ: the symmetry is sixfold at $\theta = 0$, and threefold for other values of θ. An example is the model

$$H(x, p; \theta) = \cos(x - \theta) + \cos\left(\frac{1}{2}x + \frac{\sqrt{3}}{2}p\right) + \cos\left(\frac{1}{2}x - \frac{\sqrt{3}}{2}p\right) \qquad (5.1)$$

(which was previously considered in [13], using a semiclassical analysis). For non-zero values of θ, there are three non-equivalent centres of threefold symmetry per unit cell, any one of which could be the centre of threefold symmetry for a Wannier function associated with a simple band. When $\theta = 0$, there is only one possible symmetry centre for a simple band, namely the one centre of sixfold symmetry. The centre of symmetry for the Wannier functions of bands associated with the other two symmetry centres must therefore jump discontinuously as $\theta \to 0$. The only mechanism for such a jump is if bands become degenerate. It follows that if there are not degenerate bands at $\theta = 0$, there must be degeneracies between bands for values of θ close to 0. We verified this argument by searching for a degeneracy between the lowest two bands of the Hamiltonian corresponding to (5.1), with $p/q = \frac{1}{20}$: a degeneracy was located at $\theta^* \approx 9.6 \times 10^{-6}$.

The construction of the RG transformation assumes the existence of bands which are well separated from their neighbours. The arguments above show that when $H(x, p)$ has sixfold symmetry, there can exist pairs of bands which are either degenerate or nearly degenerate. In order to deal with this situation, we describe how to construct sets of Wannier functions which span the two nearly degenerate bands, and show how the renormalization procedure must be modified to deal with this case.

First, consider how to generate a set of well localized Wannier functions which span two degenerate or nearly degenerate bands. We assume that we have available a symmetry breaking parameter θ as considered above, and that the bands become degenerate at $\pm\theta^*$. We choose a value of θ which satisfies $|\theta| > \theta^*$ so that the Wannier functions of the two

bands can be symmetrized about the threefold centres. We term the Wannier functions $|\Phi_1)$, $|\Phi_2)$ for the two symmetry centres respectively, and assume that the Bloch states have been gauged so that

$$\hat{T}(\boldsymbol{R})\hat{\mathcal{R}}_3|\Phi_L) = \exp[2\pi \mathrm{i}J/3]|\Phi_L) \tag{5.2}$$

where J is an integer, $\boldsymbol{R}$ is a lattice vector, $\hat{\mathcal{R}}_3 = \hat{\mathcal{R}}_6^2$ describes $2\pi/3$ rotations, and L takes the values 1 or 2. The next step is to project these Wannier states into the subspace of $\hat{H}(\theta)$ spanned by both bands of the Hamiltonian for $\theta = 0$

$$|\Phi_1') = f(\hat{H}(0))|\Phi_1') \tag{5.3}$$

and similarly for $|\Phi_2')$, where $f(E)$ is a function with arbitrarily many continuous derivatives, which is unity for all values of E which contain spectrum from the two bands of $\hat{H}(0)$ which are of interest, and zero for the rest of the spectrum. Because of the hypothesis that θ^* is small, the primed Wannier functions are close to the unprimed ones. Note that after applying the projection operator, the Wannier functions are still symmetric with respect to the operators $\hat{\mathcal{R}}_3$, because this operator is also a symmetry of the Hamiltonian $\hat{H}$. It is desireable that the Wannier functions $|\Phi_2')$ should be related to $|\Phi_1')$ by an inversion (twofold rotation) $\hat{\mathcal{R}}_2$ about the sixfold symmetry centre, which we also take to be the origin: we therefore write

$$|\Phi_{\bar{L}}') = \hat{\mathcal{R}}_2|\Phi_L') \tag{5.4}$$

where $\bar{1} = 2$, $\bar{2} = 1$, and the inversion $\hat{\mathcal{R}}_2 = \hat{\mathcal{R}}_4^2$. We can take the state $|\Phi_1')$, calculated as described above, and use this equation to define $|\Phi_2')$.

We now use the set of states $\hat{\mathcal{T}}_{nm}|\Phi_L')$ as a basis for expansion of the set of eigenstates spanned by the two bands. The results summarized in section 2 can be applied directly: the matrix elements of the Hamiltonian in the basis formed by translations of the Wannier functions $|\Phi_1')$, $|\Phi_2')$ are the same as those of an effective Hamiltonian $\hat{H}'_{AB}$, which is in the form of (2.1). The renormalized Hamitonian describing the two bands can therefore be written in the form of a 2×2 matrix, each element of which is an operator of the form (2.1):

$$\begin{aligned} \hat{H}' &= \sum_{\boldsymbol{R}} \tilde{H}'(\boldsymbol{R})\hat{T}(\tilde{\boldsymbol{R}}) \\ \tilde{H}'(\boldsymbol{R}) &= \begin{pmatrix} H'_{11}(\boldsymbol{R}) & H'_{12}(\boldsymbol{R}) \\ H'_{21}(\boldsymbol{R}) & H'_{22}(\boldsymbol{R}) \end{pmatrix} \end{aligned} \tag{5.5}$$

where

$$H'_{LL'}(\boldsymbol{R}) = (\Phi'_L|\hat{\mathcal{T}}(\boldsymbol{R})\hat{\mathcal{H}}|\Phi'_{L'}). \tag{5.6}$$

This can also be written in the form

$$\begin{aligned} \hat{H}' &= \sum_{L=1,2}\sum_{L'=1,2}\sum_{\boldsymbol{R}} H'_{LL'}(\boldsymbol{R})\hat{P}_{LL'}\hat{T}'(\tilde{\boldsymbol{R}}) \\ \hat{P}_{LL'} &= |L\rangle\langle L'| \end{aligned} \tag{5.7}$$

where this Hamiltonian acts on the Hilbert space of vectors $|L, x\rangle$, where x is the coordinate and L takes the values $1, 2$.

The Hamiltonian $\hat{H}'$ is defined in (5.5) so that it acts on a double triangular lattice. It is more desirable to define it on a single honeycomb lattice, as this reflects the distribution of the Wannier states of the two bands. We therefore apply a unitary transformation

$$\hat{H}' \to \hat{H}'' = \hat{U}\hat{H}'\hat{U}^{-1}$$
$$\hat{U} = \sum_{L=1,2} |L\rangle\hat{T}'(\tilde{\boldsymbol{r}}_L)\langle L| \tag{5.8}$$

where $\tilde{\boldsymbol{r}}_L = (-1)^L\tilde{\boldsymbol{r}}$ is a vector representing the displacement of the Lth triangular sublattice, relative to the centre of sixfold symmetry centre of the honeycomb lattice. The transformed Hamiltonian is

$$\hat{H}'' = \sum_{\boldsymbol{R}}\sum_{L=1,2}\sum_{L'=1,2}\hat{H}'_{LL'}(\boldsymbol{R})\exp[\mathrm{i}(\boldsymbol{R}\wedge(\boldsymbol{r}_L+\boldsymbol{r}_{L'}))/2\overline{h}']|L\rangle\hat{T}'(\tilde{\boldsymbol{R}}+\tilde{\boldsymbol{r}}_L-\tilde{\boldsymbol{r}}_{L'})\langle L'|. \tag{5.9}$$

Note that the vectors $\tilde{\boldsymbol{R}}+\tilde{\boldsymbol{r}}_L-\tilde{\boldsymbol{r}}_{L'}$ are displacements between points in the two triangular sublattices of a honeycomb lattice. We can therefore write

$$\hat{H}'' = \sum_{\boldsymbol{R}_{LL'}} H''(\boldsymbol{R}_{LL'})|L\rangle\hat{T}'(\tilde{\boldsymbol{R}}_{LL'})\langle L'| \tag{5.10}$$

where the sum runs over all vectors $\boldsymbol{R}_{LL'}$ connecting the two sublattices ($L, L' = 1, 2$) of a honeycomb lattice. The coefficients $H''(\boldsymbol{R}_{LL'})$ are matrices determined by the comparison of (5.9) and (5.10); their symmetry will be considered in the next section.

6. Symmetry breaking

The effective Hamiltonian (5.11) is defined upon a honeycomb lattice. In this section we characterize its rotational symmetries, and discuss methods by which this Hamiltonian can be further reduced to an effective Hamiltonian on a simple lattice, of the form of (2.1).

The effect of a sixfold rotation of the honeycomb lattice about the centre of sixfold symmetry is to rotate the vectors $\boldsymbol{R}_{LL'}$ by $\pi/3$, and to exchange the labels of the sublattices, L, L'. We therefore represent the sixfold rotations of the renormalized Hamiltonian on the honeycomb lattice by the operator

$$\hat{R}''_6 = \begin{pmatrix} 0 & \hat{R}_6 \\ \hat{R}_6 & 0 \end{pmatrix} \tag{6.1}$$

and, using (5.8), the corresponding rotation operator for the Hamiltonian in the representation (5.5) is

$$\hat{R}'_6 = \begin{pmatrix} 0 & \hat{T}(\tilde{\boldsymbol{r}})\hat{R}_6\hat{T}(\tilde{\boldsymbol{r}}) \\ \hat{T}(-\tilde{\boldsymbol{r}})\hat{R}_6\hat{T}(-\tilde{\boldsymbol{r}}) & 0 \end{pmatrix}. \tag{6.2}$$

In the appendix we show that, provided the Wannier states $|\Phi_L)$ satisfy (5.2) and the Hamiltonian $\hat{H}$ has sixfold symmetry, then

$$H'(\boldsymbol{R}_{LL'}) = H'(\boldsymbol{R}^{(R_6)}_{LL'}) \tag{6.3}$$

where $\boldsymbol{R}^{(R_6)}_{LL'}$ is the vector obtained by a $\pi/3$ rotation of $\boldsymbol{R}_{LL'}$. This implies that $\hat{H}''$ is invariant under the sixfold rotation operator $\hat{R}''_6$. In this sense, the honeycomb lattice Hamiltonian does preserve the symmetry of the original Hamiltonian; a similar discussion of this point has been given by Kerdelhue [15].

The calculation of the effective Hamiltonian (5.10) does not, however, represent a complete renormalization of the problem: this requires a reduction of (5.10) or (5.5) to a block diagonal form, in which each of the diagonal elements is a Hamiltonian similar to

(2.1). To effect this reduction, we start with representation (5.5) rather than (5.10), because the translation operators contributing to the elements of (5.5) span a simple lattice (of the form which occurs in the single band-effective Hamiltonian (2.1)), whereas those of (5.10) span the honeycomb lattice. We can effect this reduction to block diagonal form by applying a unitary transformation generated by a Hamiltonian $\hat{G}$ which is of the same form as (5.5) (i.e. a 2×2 matrix of linear combinations of lattice translation operators), and which is also invariant under the symmetry operation $\hat{R}'_6$:

$$\hat{H}'_d = \begin{pmatrix} \hat{H}_1 & 0 \\ 0 & \hat{H}_2 \end{pmatrix} = \exp[\mathrm{i}\hat{G}]\hat{H}' \exp[-\mathrm{i}\hat{G}]. \tag{6.4}$$

Each of the diagonal elements of the operator $\hat{H}'_d$ is a renormalized operator describing one of the two subbands used to construct the Wannier states $|\Phi_1)$, $|\Phi_2)$.

The Hamiltonian $\hat{H}'_d$ is invariant under the symmetry operator $\hat{R}'_6$, but this does not imply that each renormalized Hamiltonian $\hat{H}_1$ or $\hat{H}_2$ has sixfold symmetry, because each of these operators is mapped into the other by the action of the sixfold rotational symmetry operator (6.2). The symmetry of $\hat{H}_1$ and $\hat{H}_2$ becomes apparent when we consider the operator describing threefold rotational symmetry

$$\hat{R}'_3 = \hat{R}'^2_6 = \begin{pmatrix} \hat{T}(\tilde{\boldsymbol{r}})\hat{R}_3\hat{T}^+(\tilde{\boldsymbol{r}}) & 0 \\ 0 & \hat{T}^+(\tilde{\boldsymbol{r}})\hat{R}_3\hat{T}(\tilde{\boldsymbol{r}}) \end{pmatrix}. \tag{6.5}$$

Because this matrix is in diagonal form, it describes a symmetry of the operators $\hat{H}_1$ and $\hat{H}_2$: they are invariant under threefold rotations about centres shifted from the origin by $\tilde{\boldsymbol{r}}$ and $-\tilde{\boldsymbol{r}}$ respectively. The renormalization procedure therefore exhibits a surprising symmetry breaking: the symmetry of the sixfold invariant Hamiltonian is reduced to threefold when there are degenerate or nearly degenerate bands.

We remark that this symmetry breaking was previously observed [13] in a semiclassical analysis of (5.1) with $\theta = 0$: the semiclassical limit corresponds to the case $p = 1$ and $q \gg 1$. In this limit, only the nearest-neighbour interactions between sites on the honeycomb lattice are significant, and $\hat{H}''^2$ is well approximated by a Hamiltonian on a simple triangular lattice. This was found to be also of the form of (5.1), but with $\theta \neq 0$, implying that the original sixfold symmetry had been broken to threefold.

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Appendix

Consider the effect of the sixfold rotation operator (6.1) on the Hamiltonain (5.10). Applying the sixfold rotation maps the operator $|L\rangle\hat{T}(\tilde{\boldsymbol{R}}_{LL'})\langle L'|$ into $|\bar{L}\rangle\hat{T}(\tilde{\boldsymbol{R}}^{R_6}_{LL'})\langle\bar{L}|$. It follows that the Hamiltonian (5.1) is invariant under the sixfold rotation (6.1) if

$$H''(\boldsymbol{R}_{LL'}) = H''(\boldsymbol{R}^{(R_6)}_{LL'}) \tag{A.1}$$

where the superscript (R_6) denotes rotation of a vector by $\pi/3$. We will prove that this result holds if the original Hamiltonian $\hat{H}$ has sixfold symmetry about the origin, and if the Wannier functions $|\Phi_L)$ have threefold symmetry in the form of (5.2).

We start with some preliminary remarks and definitions concerning vectors. The vector $\boldsymbol{R}_{LL'}$ can be written as

$$\boldsymbol{R}_{LL'} = \boldsymbol{R} + \boldsymbol{r}_{L'} - \boldsymbol{r}_L \tag{A.2}$$

where $\boldsymbol{r}_L = -(-1)^L \boldsymbol{r}$. Also, we write

$$\boldsymbol{r}_L^{(R_6)} = \boldsymbol{r}_{\bar{L}} + (-1)^L \boldsymbol{F} \tag{A.3}$$

where $\boldsymbol{F}$ is a lattice vector. We then find that

$$\begin{aligned} \boldsymbol{R}_{LL'}^{(R_6)} &= \boldsymbol{R}^{(R_6)} + \boldsymbol{F}_{\bar{L}\bar{L}'} + \boldsymbol{r}_{\bar{L}'} - \boldsymbol{r}_{\bar{L}} \\ \boldsymbol{F}_{\bar{L}\bar{L}'} &= \boldsymbol{F}[(-1)^{\bar{L}} - (-1)^{\bar{L}'}] \end{aligned} . \tag{A.4}$$

These relations will be used in (A.7) below.

We now turn to the proof of (A.1). The Wannier states satisfy

$$|\Phi_L) = \exp[2\pi \mathrm{i} J/3] \hat{\mathcal{R}}_3 \hat{\mathcal{T}}((-1)^{L+1}\boldsymbol{F})|\Phi_L) \tag{A.5}$$

implying that

$$|\Phi_L) = \hat{\mathcal{R}}_6^{-1} \hat{\mathcal{T}}((-1)^L \boldsymbol{F})|\Phi_{\bar{L}}) \tag{A.6}$$

since $\hat{\mathcal{R}}_2^{-1}\hat{\mathcal{T}}(\boldsymbol{R})\hat{\mathcal{R}}_2 = \hat{\mathcal{T}}(-\boldsymbol{R})$ and $\hat{\mathcal{R}}_3\hat{\mathcal{R}}_2 = \hat{\mathcal{R}}_6^{-1}$. The proof of (A.1) is now straightforward:

$$\begin{aligned} H''(\boldsymbol{R}_{LL'}) &= (\Phi_L|\hat{\mathcal{T}}(\boldsymbol{R})\hat{\mathcal{H}}|\Phi_{L'}) \exp[\mathrm{i}(\boldsymbol{R} \wedge (\boldsymbol{r}_L + \boldsymbol{r}_{L'})/2\overline{h}'_\nu] \\ &= (\Phi_{\bar{L}}|\hat{\mathcal{T}}((-1)^{L+1}\boldsymbol{F})\hat{\mathcal{R}}_6\hat{\mathcal{T}}(\boldsymbol{R})\hat{\mathcal{R}}_6^{-1}\hat{\mathcal{T}}((-1)^{L'}\boldsymbol{F})\hat{\mathcal{H}}|\Phi_{\bar{L}'}) \\ &\quad \times \exp[\mathrm{i}\boldsymbol{R}^{(R_6)} \wedge ((\boldsymbol{r}_{\bar{L}} + \boldsymbol{r}_{\bar{L}'}) + \boldsymbol{F}((-1)^{\bar{L}} + (-1)^{\bar{L}'}))/2\overline{h}'_\nu] \\ &= (\Phi_{\bar{L}}|\hat{\mathcal{T}}(\boldsymbol{R}^{(R_6)} + \boldsymbol{F}_{\bar{L}\bar{L}'})\hat{\mathcal{H}}|\Phi_L) \exp[\mathrm{i}\boldsymbol{R}^{(R_6)} \wedge (\boldsymbol{r}_{\bar{L}} + \boldsymbol{r}_{\bar{L}'})/2\overline{h}'_\nu] \\ &= H''((\boldsymbol{R}^{(R_6)} + \boldsymbol{F}_{\bar{L}\bar{L}'})_{\bar{L}\bar{L}'}) = H''((\boldsymbol{R}_{LL'})^{(R_6)}). \end{aligned} \tag{A.7}$$

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