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Generalized Wannier function and renormalization of Harper's equation

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Abstract. Harper's equation, a model for Bloch electrons in a magnetic field, has a band spectrum when the dimensionless magnetic field β is a rational number p/q. This paper considers the definition of generalized Wannier functions, which can be used to represent the Bloch bands of the spectrum of the rational Harper equation by means of a von Neumann lattice. One representation of these Bloch bands can be extended to the irrational case, and taking matrix elements in this basis leads to a renormalization-group transformation acting on the Hamiltonian. The results in the present paper considerably extend a previous analysis of this renormalization-group transformation, in that the formalism is suitable for systematic calculations of the renormalized Hamiltonian, and that the transformation preserves the rotational symmetry of the Harper Hamiltonian in phase space.

1. Introduction

1.1. Physical background

Harper's equation

$$\psi_{n+1} + \psi_{n-1} + 2\cos(2\pi\beta n + \delta)\psi_n = E\psi_n \tag{1.1}$$

is a Schrödinger equation in the form of a difference equation with periodic coefficients. It is a realistic single-band model for an electron moving in a plane, with a spatially periodic potential, and a uniform magnetic field perpendicular to the plane. It was originally derived [1] using the Peierls substitution [2], and it can also be obtained by taking matrix elements of the Hamiltonian in a Landau level basis [3, 4]. In the Landau level picture, the parameter β is given by $\beta = h/eBA$, where B is the magnetic field, A is the area of the unit cell, h is the Planck constant and e is the electron charge. In the Peierls substitution picture, β is given by the reciprocal of this quantity. Throughout this paper it will be assumed that (1.1) represents a perturbed Landau level.

Harper's equation is of considerable mathematical interest because of the structure of its spectrum. When β is the ratio of two integers, there is a band spectrum with q non-overlapping bands, with dispersion relations $\mathcal{E}_\nu(k, \delta)$ (where k is the Bloch wavevector and ν an index labelling the band). When β is irrational, the spectrum is a Cantor set of zero measure, with an intricate non-self-similar hierarchical structure, which was predicted by Azbel [5] and observed in numerical experiments by Hofstadter [6]. Various techniques

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have been used to analyse the structure of the spectrum: methods which are applicable to a general class of models representing Bloch electrons in a magnetic field include semiclassical approaches [5, 7–11] and renormalization-group methods [12–18]. There are also a variety of bounds and exact equalities which are specific to Harper's equation and a small class of related models described by three-term recursion relations [19–22]. This paper is a synthesis of two different renormalization-group approaches described in earlier papers [14, 15] by the same author. The primary motivation for the work reported here was to deal with some technical difficulties with the method described in [15], which have been a barrier to further applications of this approach.

The ideas developed in this paper will refer more naturally to another representation of the Hamiltonian corresponding to the Schrödinger equation (1.1) as a function of operators $\hat{x}$ and $\hat{p}$ satisfying the canonical commutation relation. The Hamiltonian

$$\hat{H} = H(\hat{x}, \hat{p}) = 2(\cos\hat{p} + \cos\hat{x}) \tag{1.2}$$

is equivalent to (1.1) if it is quantized using the Weyl rule and if

$$[\hat{x}, \hat{p}] = \mathrm{i}\hbar \qquad \hbar = 2\pi\beta. \tag{1.3}$$

The rôle of the Weyl quantization rule in representing Bloch electrons in a magnetic field by Hamiltonians such as (1.3) is discussed in [23], where it is shown that rotational symmetries of the crystal lattice are represented by rotational symmetries of the Hamiltonian in phase space. In this paper, the symbol h will be used for the physical Planck constant, and $\hbar$ for the dimensionless quantity $2\pi\beta$.

This paper will make extensive use of phase-space representations such as (1.2), and the following operators, which will be termed phase-space translation operators, will play an important rôle:

$$\hat{T}(X, P) = \exp[\mathrm{i}(P\hat{x} - X\hat{p})/\hbar]. \tag{1.4}$$

These operators have a non-commutative algebra

$$\begin{aligned}\hat{T}(X_1, P_1)\hat{T}(X_2, P_2) &= \exp[\mathrm{i}(X_2P_1 - X_1P_2)/2\hbar]\hat{T}(X_1 + X_2, P_1 + P_2)\\ &= \exp[\mathrm{i}(X_2P_1 - X_1P_2)/\hbar]\hat{T}(X_2, P_2)\hat{T}(X_1, P_1)\end{aligned} \tag{1.5}$$

and they are relevant to this problem because their algebra is of the same form as that of the magnetic translation operators introduced by Zak [24].

As well as applying to Harper's equation, the results will be applicable to a class of Hamiltonians which can be represented as a Fourier series, with coefficients H_{nm}:

$$\hat{H} = \sum_{n=-\infty}^{\infty}\sum_{m=-\infty}^{\infty} H_{nm}\exp[\mathrm{i}(m\hat{x} - n\hat{p})] = \sum_{n=-\infty}^{\infty}\sum_{m=-\infty}^{\infty} H_{nm}\hat{T}(n\hbar, m\hbar). \tag{1.6}$$

The Fourier coefficients are assumed to decay rapidly as $n, m \to \infty$.

1.2. Discussion of earlier work

This paper is primarily a development of a renormalization-group method discussed in [15]. In this earlier paper it is shown that the spectrum of Harper's equation in the neighbourhood of a rational value (p/q, say) of β can be approximated by quantizing the dispersion relations $\mathcal{E}_\nu(k,\delta)$ of the q bands of the rational spectrum, by means of the Peierls substitutions $qk \to \hat{x}'$, $q\delta \to \hat{p}'$. The canonical operators $\hat{x}'$ and $\hat{p}'$ have a renormalized Planck constant $\hbar' = 2\pi\beta'$, which depends on the quantized Hall conductance integer M_ν of the band (the quantized Hall effect for this problem is analysed in [25]). The dependence of β' on M_ν explains the 'clustering rules' discovered empirically by Hofstadter [6].

These results were derived by introducing a set of generalized Bloch states $|B_\nu(k,\delta)\rangle$, which are defined for irrational β, and which are obtained from the rational Bloch states by varying the phase parameter δ as a function of position. In the limit $\beta \to p/q$, the matrix elements of the Hamiltonian in the basis of generalized Bloch states are the same as those of a renormalized Hamiltonian which is obtained by a Peierls substitution of the dispersion relation.

There are a variety of difficulties with the method described in the earlier paper, which the calculations presented here overcome.

(i) The method presented in [15] cannot readily be adapted to calculate corrections to the lowest-order approximation, $\hat{H}_{\rm eff} \sim \mathcal{E}_\nu(\hat{x}'/q, \hat{p}'/q)$.

(ii) The phases of the Bloch states are arbitrary, and the results of the renormalization-group transformation depend upon the choice of these phases: it is necessary to quantify the effect of gauge transformations which change the relative phases of the Bloch waves.

(iii) It is desirable to find a form of the renormalization-group transformation which preserves the four-fold rotational symmetry of the Harper Hamiltonian.

This latter point is particularly important, because if the rotational symmetry is preserved, the spectrum is expected to be a Cantor set of measure zero, whereas if this symmetry is not preserved by the renormalization-group transformation, the spectrum could be a Cantor set of finite measure [14, 15].

Another earlier paper [14] showed how the renormalization-group transformation can be set up in a way which naturally preserves the rotational symmetry of the Hamiltonian, using a generalized Bloch-state basis constructed out of Wannier functions translated throughout phase space to form a generalized von Neumann lattice. This calculation was restricted to the case where the quantized Hall conductance integer M_ν of the band is zero; this restriction arises because it is not possible to construct conventional Wannier functions when $M_\nu \neq 0$ [26]. The calculations presented here involve the construction of a von Neumann lattice of generalized Wannier functions, which can be defined for arbitrary values of M_ν. There are considerable technical complications because the construction of the von Neumann lattice is necessarily anisotropic, and the symmetry of the Hamiltonian is obscured at intermediate points of the calculation.

1.3. Plan of paper and summary of new results

This paper describes a refinement of the earlier calculations which is much more suitable for explicit calculation of the corrections to the renormalized effective Hamiltonian as a series in $\Delta\beta = \beta - p/q$, and which shows how the rotational symmetry of the Hamiltonian can be explicitly preserved by the renormalization-group transformation. The plan of the paper is as follows.

In section 2, it is shown how the Bloch bands of the rational case can be characterized in a way which makes it possible to extend the definition of the Bloch states to irrational values of β. It is shown that the Bloch bands of the rational dispersion relations can be derived from a set of N_ν normalizable functions, where N_ν is related to the quantized Hall conduction integer M_ν by the formula $1 = pN_\nu + qM_\nu$. Section 3 shows how these normalizable functions can be used to form a set of generalized Wannier states $|\phi_\mu^{(\nu)}\rangle$: the Bloch waves are generated from these Wannier functions by using translation operators of the form (1.4) to generate von Neumann lattices, and combining the states of the von Neumann lattices with the appropriate phases.

Section 4 considers the calculation of matrix elements of the Hamiltonian and similar operators in the basis formed by the generalized Bloch states. These matrix elements are those of a difference operator in the Bloch wavevector k, with periodic coefficients. Explicit formulae for the Fourier coefficients are obtained in terms of the matrix elements $\langle\phi_{\mu'}^{(\nu)}|\hat{T}(X,P)|\phi_\mu^{(\nu)}\rangle$. Section 5 shows that the matrix elements of the Hamiltonian are the same as those of a renormalized operator, periodic in canonical variables $\hat{x}'$, $\hat{p}'$, with a renormalized commutator $[\hat{x}', \hat{p}'] = i\hbar'$. The renormalized operator is related to the original by a linear transformation of the Fourier coefficients defined in (1.6).

Section 6 studies the effect of a $\pi/2$ rotation of the Hamiltonian in phase space. For a particular choice of gauge (defining the relationship between the phase of rotated and unrotated Bloch states), the Wannier functions $|\phi_\mu^{(R\nu)}\rangle$ of the rotated Hamiltonian are obtained in terms of those of the original Hamiltonian $|\phi_\mu^{(\nu)}\rangle$. If the Hamiltonian is invariant under rotation, these relations are shown to imply a rotational invariance of the renormalized Hamiltonian. The rotational invariance depends on a surprising operator identity discussed in appendix B.

Finally, section 7 summarizes the important results, and points to future work on this problem.

2. Generalized Bloch states

In this section the Bloch states of the rational case are characterized, and their extension to irrational β is described. For clarity of presentation, and because of necessary changes in notation, there is some overlap between this section and [15]; the approach adopted here is, however, more transparent and the result in section 2.3 is entirely new.

2.1. Bloch states obtained by sampling an analytic function

When β is the ratio of two integers, $\beta = p/q$, Harper's equation has a translational invariance corresponding to increasing n by q. In this 'rational' case, Bloch's theorem is applicable and the eigenstates are Bloch waves, with a Bloch wavevector k:

$$\psi_n = \exp(ikn)U_n(k,\delta) \qquad U_{n+q} = U_n. \tag{2.1}$$

The eigenvalues form q non-overlapping bands, with dispersion relation $\epsilon_\nu(k,\delta)$, where the index $\nu = 1,\ldots,q$ labels the bands. The eigenstates are periodic, up to a complex phase, in both k and δ, with periods $2\pi/q$ and $2\pi p/q$, respectively. It will be useful to represent the Bloch states by means of Dirac bra and ket vectors; the ket vector $|B_\nu(k,\delta)\rangle$ will be used to represent the Bloch state in the νth band with wavevector k and phase parameter δ. The Bloch states are only defined up to a multiplicative complex phase factor $e^{i\theta(k,\delta)}$. It is possible to choose the phases of the Bloch states such that they are an analytic function of the parameters k and δ. It may not, however, be possible to choose the phases so that the Bloch waves are periodic on the Brillouin zone. The states can always be made precisely periodic in δ, but states separated by the period of the Brillouin zone in the k direction may differ by a phase factor:

$$|B_\nu(k+2\pi/q,\delta)\rangle = \exp[\mathrm{i}\chi(\delta)]|B_\nu(k,\delta)\rangle$$
$$|B_\nu(k,\delta+2\pi p/q)\rangle = |B_\nu(k,\delta)\rangle. \tag{2.2}$$

Because of the periodicity in δ, $\chi(\delta+2\pi p/q)-\chi(\delta)=2\pi M_\nu$ for some integer M_ν. The integer M_ν is termed the Chern character of the fibre-bundle formed by the Bloch states, and the quantized Hall conductance carried by the νth band is $\sigma_{xy}^{(\nu)}=M_\nu e^2/h$ [25]. It will be convenient to choose the phase $\chi(\delta)$ as follows

$$\chi(\delta)=M_\nu q\delta/p. \tag{2.3}$$

If the Bloch states are an analytic function of δ, the amplitudes ψ_n defining the Bloch states can be obtained by sampling an analytic function $\psi_\nu(x;k)$:

$$\psi_n=\psi_\nu(x_n;k) \qquad x_n=2\pi\beta n+\delta. \tag{2.4}$$

The Bloch states produced by this construction are clearly periodic in δ. For consistency with (2.1), the function $\psi_\nu(x;k)$ is a Bloch function:

$$\psi_\nu(x;k)=\mathrm{e}^{\mathrm{i}kx/2\pi\beta}U_\nu(x;k) \qquad U_\nu(x+2\pi p;k)=U_\nu(x;k). \tag{2.5}$$

Harper's equation is unchanged under the transformations $\delta\to\delta+2\pi/q$, $n\to n-\Delta n$, where Δn satisfies $p\Delta n+q\Delta m=1$ for some integer Δm. This implies that, with an appropriate choice of phase of the Bloch waves, $U_\nu(x+2\pi\Delta m;k)=U_\nu(x;k)$. Comparing this with (2.5), it is clear that, with a suitable choice of phases,

$$U_\nu(x+2\pi;k)=U_\nu(x;k). \tag{2.6}$$

When (2.6) is satisfied, the following representation for the function $\psi_\nu(x;k)$ can be used:

$$\psi_\nu(x;k)=\sum_{n=-\infty}^{\infty}a_n(k)\mathrm{e}^{\mathrm{i}(k+n\hbar)x/\hbar} \tag{2.7}$$

where $\hbar\equiv 2\pi\beta$. Equation (2.7) can also be written in the form

$$\psi_\nu(x;k)=\langle x|\psi_\nu(k)\rangle \qquad |\psi_\nu(k)\rangle=\sum_{n=-\infty}^{\infty}a_n(k)|k+n\hbar\rangle \tag{2.8}$$

where $|k\rangle$ denotes an eigenstate of the momentum operator: $\hat{p}=-\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}x}$, $\hat{p}|k\rangle=k|k\rangle$.

We now consider how to make (2.8) consistent with (2.2) and (2.3). Because x and δ are related by (2.4), the phase in (2.2) depending on δ becomes a phase depending on x:

$$\psi_\nu(x;k+2\pi/q)=\exp[\mathrm{i}qM_\nu x/p]\psi_\nu(x;k). \tag{2.9}$$

From (2.9), shifting k by $2\pi/q$ increases the momentum k of the state by $M_\nu q\hbar/p=2\pi M_\nu$: therefore

$$|\psi_\nu(k+2\pi/q)\rangle=\sum_{n=-\infty}^{\infty}a_n(k)|k+n\hbar+2\pi M_\nu\rangle. \tag{2.10}$$

To summarize: equation (2.4) relates the amplitudes ψ_n to an analytic function $\psi_\nu(x;k)$. The Bloch wave property of $\psi_\nu(x;k)=\langle x|\psi_\nu(k)\rangle$ and the periodicity in k are described by (2.8) and (2.10), respectively.

2.2. Generalized Bloch states

It will be useful to define generalized Bloch states for which β need not be a rational number. Generalized Bloch states can be defined which are periodic (up to a phase) in a Brillouin zone of size $\Delta\delta = \hbar$ in the δ parameter, and $\Delta k = \kappa_\nu$ in the k parameter (where κ_ν will be determined shortly). The generalized Bloch states are defined by a set of amplitudes ψ_n which are obtained by sampling the continuous function $\psi_\nu(x;k)$ as prescribed by (2.4). When β is irrational, the $|\psi_n|$ form a quasiperiodic rather than a periodic sequence. Equations (2.5)–(2.8) continue to be valid for the generalized Bloch states. Equations (2.9) and (2.10) must be replaced by

$$\psi_\nu(x;k+\kappa_\nu) = \mathrm{e}^{2\pi\mathrm{i}M_\nu x/\hbar}\psi_\nu(x;k) \tag{2.11}$$

and

$$|\psi_\nu(k+\kappa_\nu)\rangle = \sum_{n=-\infty}^{\infty} a_n(k)|k+n\hbar+2\pi M_\nu\rangle \tag{2.12}$$

indicating that the periodicity of the Brillouin zone in k is now κ_ν.

The value of κ_ν can be determined as follows. From (2.8),

$$|\psi_\nu(k+\kappa_\nu)\rangle = \sum_{n=-\infty}^{\infty} a_n(k+\kappa_\nu)|k+\kappa_\nu+n\hbar\rangle \tag{2.13}$$

and consistency between (2.12) and (2.13) therefore requires

$$\kappa_\nu = 2\pi M_\nu + N_\nu\hbar \tag{2.14}$$

for some integer N_ν.

It is desirable to define generalized Bloch states which approach the Bloch eigenstates in the limit $\beta \to p/q$: this requires that $\kappa_\nu \to 2\pi/q$ in this limit, and (2.14) therefore implies that N_ν satisfies

$$1 = qM_\nu + pN_\nu. \tag{2.15}$$

The gap labelling theorem [27] and the Středa formula [28] imply that a solution of (2.15) exists for which N_ν is an integer.

In the limit $\beta \to p/q$, the generalized Bloch states resemble the usual Bloch states, but with a slowly varying value of the phase parameter δ. These states may be useful as a basis set for expansion of an eigenstate of the Hamiltonian. Born–von Karman boundary conditions are applied to a finite number $\mathcal{N}_x$ of n values, the values of k are restricted to be multiples of

$$\Delta k = 2\pi/\mathcal{N}_x. \tag{2.16}$$

The values of the phase parameter δ will also be assumed to be quantized, so that it takes $\mathcal{N}_y$ discrete values

$$\delta = l\hbar/\mathcal{N}_y \qquad l = 1,\ldots,\mathcal{N}_y. \tag{2.17}$$

This corresponds to considering the problem of Bloch electrons in a magnetic field on a finite-sized rectangular lattice, with a total of $\mathcal{N}_x\mathcal{N}_y$ states in the Landau level [23]. In [15] it was shown that the generalized Bloch states have the correct density of states to form a complete set for a band of the spectrum when β is irrational.

2.3. *Representation of Bloch waves using normalizable functions*

It will be useful to represent the generalized Bloch states in terms of a set of normalizable functions instead of the Bloch functions $\psi_\nu(x;k)$. It will now be shown that the function $\psi_\nu(x;k)$ can be generated from a set of exactly N_ν normalizable functions. In section 3, these functions will be associated with a set of Wannier states $|\phi_\mu^{(\nu)}\rangle$, $\mu = 1, \ldots, N_\nu$.

Comparison of (2.12) and (2.13) gives a recurrence relation connecting the functions $a_n(k)$:

$$a_n(k) = a_{n-N_\nu}(k + \kappa_\nu). \tag{2.18}$$

A solution of (2.18) can be obtained in the form $a_n(k) = F(k + \alpha n)$: it is found that $\alpha = \kappa_\nu / N_\nu$, i.e. $a_n(k) = F(k + \kappa_\nu n / N_\nu)$. Only coefficients a_n with values of n separated by N_ν are related by (2.18). A set of N_ν different functions are therefore required

$$a_{nN_\nu+\mu}(k) = F_\mu^{(\nu)}(k + n\kappa_\nu) \qquad \mu = 1, \ldots, N_\nu. \tag{2.19}$$

This shows that the set of functions $a_n(k)$ can be generated from N_ν normalizable functions $F_\mu^{(\nu)}(k)$.

3. Generalized von Neumann lattices

In this section, it will be shown that the generalized Bloch states can be obtained from a set of N_ν overlapping generalized von Neumann lattices. This will be derived from an alternative representation of the Bloch states.

3.1. *A new representation of the Bloch states*

In section 2, the generalized Bloch states were regarded as being defined by a discrete set of coefficients ψ_n. In this section, another viewpoint will be adopted: the generalized Bloch states will be regarded as a set of functions on the real line, of the form

$$\langle x | B_\nu(k,\delta)\rangle = \sum_{n=-\infty}^{\infty} \psi_n \tilde{\delta}(x - x_n) \qquad x_n = n\hbar + \delta \tag{3.1}$$

where $\tilde{\delta}(x)$ is a suitably defined delta function, and $\psi_n = \psi_\nu(x_n;k)$. Note that this representation is very closely related to the k–q representation [29]; the difference is that a plane wave e^{ikx} in the k–q representation is replaced by a Bloch wave $\psi_\nu(x;k)$.

To simplify the discussion of the definition and normalization of $\tilde{\delta}(x)$, it will be assumed that δ takes $\mathcal{N}_y$ discrete values given by (2.17), and the relationship between the states $|B_\nu(k,\delta)\rangle$ and $|\psi_\nu(k)\rangle$ will be defined as follows

$$\begin{aligned} |B_\nu(k,\delta)\rangle &= \frac{1}{\mathcal{N}_y^{1/2}} \sum_{m=1}^{\mathcal{N}_y} e^{-2\pi i m\delta/\hbar} e^{2\pi i m\hat{x}/\hbar} |\psi_\nu(k)\rangle \\ &= \frac{1}{\mathcal{N}_y^{1/2}} \sum_{m=1}^{\mathcal{N}_y} e^{-2\pi i m\delta/\hbar} \hat{T}(0, 2\pi m) |\psi_\nu(k)\rangle \end{aligned} \tag{3.2}$$

where $\hat{T}(X, P)$ is the phase-space translation operator (1.4). Note that, according to (3.2), δ behaves as a Bloch wavevector for translations along the momentum axis in phase space.

According to (3.1), the overlap between two of the generalized Bloch states, $|B_\nu(k,\delta)\rangle$ and $|B_{\nu'}(k',\delta')\rangle$, should vanish if $\delta \neq \delta' \bmod \hbar$. It will be instructive to verify this explicitly:

$$\begin{aligned}\langle B_{\nu'}(k',\delta')|B_\nu(k,\delta)\rangle &= \frac{1}{\mathcal{N}_y}\sum_{m=1}^{\mathcal{N}_y}\sum_{m'=1}^{\mathcal{N}_y}\exp[2\pi\mathrm{i}(m'\delta'-m\delta)/\hbar]\langle\psi_{\nu'}(k')|\hat{T}^+(0,2\pi m')\hat{T}(0,2\pi m)|\psi_\nu(k)\rangle \\ &= \frac{1}{\mathcal{N}_y}\sum_{m=1}^{\mathcal{N}_y}\sum_{m'=1}^{\mathcal{N}_y}\exp\left[-\frac{2\pi\mathrm{i}}{\hbar}\left(\frac{m+m'}{2}\right)(\delta-\delta')\right] \\ &\quad\times\exp\left[-\frac{2\pi\mathrm{i}}{\hbar}\left(\frac{\delta+\delta'}{2}\right)(m'-m)\right]\langle\psi_{\nu'}(k')|\hat{T}(0,2\pi(m-m'))|\psi_\nu(k)\rangle. \end{aligned} \tag{3.3}$$

The summation variables m and m' in (3.3) can be replaced by

$$j = m - m' \qquad J = \left(\frac{m+m'}{2}\right). \tag{3.4}$$

It will be assumed that the matrix element in the right-hand side of (3.3) decays very rapidly as $|j| = |m-m'| \to \infty$. The summations in (3.4) will be replaced by a sum over j from $-\infty$ to ∞, and a sum over $\mathcal{N}_y$ values of J, taking integer values if j is even, and half-integer values if j is odd. For a sufficiently rapid decay of the matrix elements, the error incurred by altering the summations is $\mathrm{O}(1/\mathcal{N}_y)$

$$\begin{aligned}\langle B_{\nu'}(k',\delta')|B_\nu(k,\delta)\rangle &= \frac{1}{\mathcal{N}_y}\sum_{j=-\infty}^{\infty}\exp\left[-\frac{2\pi\mathrm{i}}{\hbar}\left(\frac{\delta+\delta'}{2}\right)j\right]\langle\psi_{\nu'}(k')|\hat{T}(0,2\pi j)|\psi_\nu(k)\rangle \\ &\quad\times\sum_J\exp[-2\pi\mathrm{i}J(\delta'-\delta)/\hbar] + \mathrm{O}(1/\mathcal{N}_y). \end{aligned} \tag{3.5}$$

It is useful to define the symbol $\Delta(\delta-\delta')$ as follows

$$\Delta(\delta-\delta') \equiv \frac{1}{\mathcal{N}_y}\sum_{J=1}^{\mathcal{N}_y}\mathrm{e}^{2\pi\mathrm{i}(\delta-\delta')J/\hbar} = \begin{cases}1 & \delta = \delta' \bmod \hbar \\ 0 & \delta \neq \delta' \bmod \hbar\end{cases} \tag{3.6}$$

where the second equality holds if the values of δ and δ' have the discrete values given by (2.17). Note that the symbol $\Delta(\delta-\delta')$ is really a version of the Kronecker delta symbol, with the arguments represented as real variables, discretized by (2.17), rather than as integers. With this definition, the final expression is

$$\begin{aligned}\langle B_{\nu'}(k',\delta')|B_\nu(k,\delta)\rangle &= \Delta(\delta-\delta')\sum_{j=-\infty}^{\infty}(-1)^{Nj}\exp\left[-\frac{2\pi\mathrm{i}}{\hbar}\left(\frac{\delta+\delta'}{2}\right)j\right] \\ &\quad\times\langle\psi_{\nu'}(k')|\hat{T}(0,2\pi j)|\psi_\nu(k)\rangle \end{aligned} \tag{3.7}$$

where $\delta-\delta' = N\hbar$, and, in this and subsequent expressions, the $\mathrm{O}(1/\mathcal{N}_y)$ error term is dropped, because only the limit $\mathcal{N}_y \to \infty$ is required. The term $(-1)^{Nj}$ arises because, when j is odd, the summation in (3.5) is over half-integer values of J. This result confirms the orthogonality of states with different values of δ.

3.2. Generalized von Neumann lattice basis

Using (3.2), (2.8) and (2.19), the generalized Bloch state $|B_\nu(k,\delta)\rangle$ can be written in the form

$$|B_\nu(k,\delta)\rangle = \frac{1}{\mathcal{N}_y{}^{1/2}} \sum_{m=1}^{\mathcal{N}_y} \mathrm{e}^{-2\pi i m\delta/\hbar} \hat{T}(0, 2\pi m) \sum_{\mu=1}^{N_\nu} |\psi_\mu^{(\nu)}(k)\rangle$$

$$|\psi_\mu^{(\nu)}(k)\rangle = \sum_{n=-\infty}^{\infty} F_\mu^{(\nu)}(k + n\kappa_\nu)|k + (nN_\nu + \mu)\hbar\rangle. \tag{3.8}$$

The states $|\psi_\mu^{(\nu)}(k)\rangle$ are Bloch states, with periodicity $2\pi/N_\nu$, and are periodic (up to a phase factor) in k with period κ_ν; shifting k by κ_ν corresponds to a boost of their momentum by $2\pi M_\nu$ (cf (2.12)). A set of Wannier functions will now be identified for the Bloch states $|\psi_\mu^{(\nu)}(k)\rangle$. The Bloch states can be expressed in the form of an integral

$$|\psi_\mu^{(\nu)}(k)\rangle = \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} \mathrm{d}k'\, \delta(k' - k - (nN_\nu + \mu)\hbar) F_\mu^{(\nu)}(\alpha k' + \gamma)|k'\rangle. \tag{3.9}$$

Comparing with (3.8), α and γ must be chosen so that $\alpha k' + \gamma = k + n\kappa_\nu$ when $k' = k + (nN_\nu + \mu)\hbar$: this gives $\alpha = \kappa_\nu/N_\nu\hbar$, $\gamma = -(\kappa_\nu\mu\hbar + 2\pi M_\nu k)/N_\nu\hbar$. Now the Poisson summation formula will be used to re-write the sum of delta functions in (3.9):

$$\sum_{n=-\infty}^{\infty} \delta(k' - k - (nN_\nu + \mu)\hbar) = \frac{-1}{N_\nu\hbar} \sum_{m=-\infty}^{\infty} \exp[2\pi i m(k' - k - \mu\hbar)/N_\nu\hbar]. \tag{3.10}$$

Using this result, (3.9) can be re-written in the form

$$|\psi_\mu^{(\nu)}(k)\rangle = \frac{-1}{N_\nu\hbar} \sum_{m=-\infty}^{\infty} \mathrm{e}^{-2\pi i m(k+\mu\hbar)/N_\nu\hbar} \int_{-\infty}^{\infty} \mathrm{d}k'\, F_\mu^{(\nu)}(\alpha k' + \gamma)\mathrm{e}^{2\pi i m k'/N_\nu\hbar}|k'\rangle. \tag{3.11}$$

Noting that the momentum eigenstates $|k\rangle$ satisfy $\hat{T}(X,0)|k\rangle = \mathrm{e}^{-iXk/\hbar}|k\rangle$, equation (3.11) can be written in the form

$$|\psi_\mu^{(\nu)}(k)\rangle = \frac{-1}{N_\nu\hbar} \sum_{m=-\infty}^{\infty} \exp[-2\pi i m(k + \mu\hbar)/N_\nu\hbar]\hat{T}(-2\pi m/N_\nu, 0)|\phi_\mu^{(\nu)}(k)\rangle \tag{3.12}$$

where

$$|\phi_\mu^{(\nu)}(k)\rangle = \int_{-\infty}^{\infty} \mathrm{d}k'\, F_\mu^{(\nu)}\left(\frac{\kappa_\nu(k' - \mu\hbar) - 2\pi M_\nu}{N_\nu\hbar}\right)|k'\rangle. \tag{3.13}$$

The states $|\phi_\mu^{(\nu)}(k)\rangle$ clearly have a localized wavefunction if the $F_\mu^{(\nu)}(k)$ are analytic functions. Equation (3.13) implies that the state $|\phi_\mu^{(\nu)}(k)\rangle$ is a type of Wannier function, from which the Bloch wave $|\psi_\mu^{(\nu)}(k)\rangle$ can be generated. It is desirable to remove the k-dependence of the Wannier functions. This can be achieved by writing

$$|\phi_\mu^{(\nu)}(k)\rangle = \hat{T}(0, 2\pi M_\nu k/\kappa_\nu)|\phi_\mu^{(\nu)}\rangle$$

$$|\phi_\mu^{(\nu)}\rangle = \int_{-\infty}^{\infty} \mathrm{d}k'\, F_\mu^{(\nu)}\left(\frac{\kappa_\nu k' - \mu\hbar}{N_\nu\hbar}\right)|k'\rangle. \tag{3.14}$$

Combining (3.14), (3.12) and (3.8) gives the following representation of the $|B_\nu(k,\delta)\rangle$ states:

$$|B_\nu(k,\delta)\rangle = C\sum_{\mu=1}^{N_\nu}\sum_{n=-\infty}^{\infty}\sum_{m=-\infty}^{\infty}\exp\left[-\frac{2\pi\mathrm{i}}{\hbar}\left(m\delta+\frac{n(k+\mu\hbar)}{N_\nu}\right)\right]$$
$$\times\hat{T}(0,2\pi m)\hat{T}(-2\pi n/N_\nu,0)\hat{T}(0,2\pi M_\nu k/\kappa_\nu)|\phi_\mu^{(\nu)}\rangle \quad (3.15)$$

where C is a normalization constant. The generalized Bloch states can therefore be formed from a set of N_ν overlapping generalized von Neumann lattices, generated by applying phase-space translation operators to a set of N_ν generalized Wannier functions $|\phi_\mu^{(\nu)}\rangle$. If the Wannier states $|\phi_\mu^{(\nu)}\rangle$ are suitably normalized, the normalization multiplier in (3.15) can be written

$$C = (\mathcal{N}_x\mathcal{N}_y)^{-1/2}. \quad (3.16)$$

Note that, except when $N_\nu = 1$, the von Neumann lattices of states in (3.15) are denser in the X direction than the P direction and, when M_ν is non-zero, the states move in the P direction as the wavevector k in the X direction increases. Physically, this movement can be interpreted as a Hall current flowing in response to a weak electric field, represented by an adiabatic variation of the wavevector [25, 30]. The symmetry of the original phase-space Hamiltonian (1.2) is therefore completely lost at this point in the analysis, except for the special case when $N_\nu = 1$ and $M_\nu = 0$ (which only occurs if $p = 1$).

4. Matrix elements of translation operators

4.1. Evaluation of matrix elements

The Hamiltonian $\hat{H}$, and other operators of interest such as projections of the Hamiltonian of the form $\hat{P} = f(\hat{H})$ (where $f(x)$ is a suitable smooth function [15]), can all be expressed as a superposition of phase-space translation operators $\hat{T}(N\hbar, M\hbar)$, such as (1.6). In this section, matrix elements of these translation operators will be evaluated in the basis of generalized Bloch states $|B_\nu(k,\delta)\rangle$.

Using representation (3.15):

$$\langle B_\nu(k',\delta')|\hat{T}(X,P)|B_\nu(k,\delta)\rangle = |C|^2\sum_{\mu'=1}^{N_\nu}\sum_{\mu=1}^{N_\nu}\sum_{m'}\sum_{m}\sum_{n'}\sum_{n}$$
$$\times\exp\left[\frac{2\pi\mathrm{i}}{\hbar}(m'\delta'-m\delta)\right]\exp\left[\frac{2\pi\mathrm{i}}{N_\nu\hbar}(k'n'-kn)\right]$$
$$\times\exp\left[\frac{2\pi\mathrm{i}}{N_\nu}(\mu'n'-\mu n)\right]\langle\phi_{\mu'}^{(\nu)}|\hat{\tau}|\phi_\mu^{(\nu)}\rangle \quad (4.1)$$

where $\hat{\tau}$ is a product of translation operators

$$\hat{\tau} = \hat{T}(0,-2\pi M_\nu k'/\kappa_\nu)\hat{T}(2\pi n'/N_\nu,0)\hat{T}(0,-2\pi m')\hat{T}(X,P)\hat{T}(0,2\pi m)$$
$$\times\hat{T}(-2\pi n/N_\nu,0)\hat{T}(0,2\pi M_\nu k/\kappa_\nu) \quad (4.2)$$

which can be evaluated using (1.5) as follows

$$\hat{\tau} = e^{i\Theta}\hat{T}(-2\pi(n-n')/N_\nu + X, 2\pi(m-m') + 2\pi M_\nu(k-k')/\kappa_\nu + P) \tag{4.3}$$

with

$$\Theta = \frac{2\pi M_\nu}{\hbar}\left(\frac{k+k'}{2\kappa_\nu}\right)\left[\frac{2\pi}{N_\nu}(n-n') - X\right] - \frac{2\pi}{N_\nu\hbar}\left(\frac{n+n'}{2}\right)[2\pi(m-m') + P] - \frac{2\pi}{\hbar}\left(\frac{m+m'}{2}\right)X. \tag{4.4}$$

In (4.1), it is convenient to sum over the variables

$$l = n - n' \qquad L = \frac{n+n'}{2} \qquad j = m - m' \qquad J = \frac{m+m'}{2}. \tag{4.5}$$

Transforming the sums in the same manner as the transformations leading from (3.3) to (3.5), specializing to $X = N\hbar$, $P = M\hbar$, and using (4.4) and (4.5) gives

$$\begin{aligned}\langle B_\nu(k',\delta')|\hat{T}(N\hbar, M\hbar)|B_\nu(k,\delta)\rangle &= |C|^2 \sum_J \exp[-2\pi i(\delta - \delta' + N\hbar)J/\hbar] \\ &\times \sum_j \exp\left[-\frac{2\pi i}{\hbar}\left(\frac{\delta+\delta'}{2}\right)j\right] \\ &\times \sum_{\mu'=1}^{N_\nu}\sum_{\mu=1}^{N_\nu}\sum_L \exp\left[-\frac{2\pi i}{N_\nu\hbar}(k - k' + 2\pi j + (\mu - \mu' + M)\hbar)L\right] \\ &\times \sum_l \exp\left[-2\pi i\left(\frac{k+k'}{2\kappa_\nu}\right)\{((\kappa_\nu - 2\pi M_\nu)/N_\nu\hbar)l + M_\nu N\}\right] \\ &\times \exp\left[-\frac{2\pi i}{N_\nu}\left(\frac{\mu+\mu'}{2}\right)l\right] \\ &\times \langle\phi_{\mu'}^{(\nu)}|\hat{T}(-2\pi l/N_\nu + N\hbar, 2\pi j + M\hbar + 2\pi M_\nu(k-k')/\kappa_\nu)|\phi_\mu^{(\nu)}\rangle. \end{aligned} \tag{4.6}$$

The sums over the dummy indices J and L are only non-zero if, respectively, the following two conditions are met:

$$\begin{aligned} &\delta - \delta' + N\hbar = 0 \bmod \hbar \\ &k - k' + 2\pi j + (\mu - \mu' + M)\hbar = 0 \bmod N_\nu\hbar = N'N_\nu\hbar \end{aligned} \tag{4.7}$$

for some integer N'. Provided both δ and δ' are in the range 0 to $\hbar$, as implied by (2.17), the matrix elements can therefore be written in the form

$$\begin{aligned}&\langle B_\nu(k',\delta')|\hat{T}(N\hbar, M\hbar)|B_\nu(k,\delta)\rangle \\ &\quad = \Delta(\delta - \delta')\sum_{j=-\infty}^{\infty}\sum_{l=-\infty}^{\infty}\sum_{N'=-\infty}^{\infty}\sum_{\mu=1}^{N_\nu}\sum_{\mu'=1}^{N_\nu}(-1)^{Nj+N'l} \\ &\quad\times \Delta(k - k' + 2\pi j + (\mu - \mu' + M - N'N_\nu)\hbar)\exp[-2\pi i\delta j/\hbar] \\ &\quad\times \exp\left[-2\pi i\left(\frac{k+k'}{2\kappa_\nu}\right)(l + NM_\nu)\right]\exp\left[-\frac{2\pi i}{N_\nu}\left(\frac{\mu+\mu'}{2}\right)l\right] \\ &\quad\times \langle\phi_{\mu'}^{(\nu)}|\hat{T}(-2\pi m/N_\nu + N\hbar, -2\pi(np + M_\nu l) + M\hbar + 2\pi M_\nu(k-k')/\kappa_\nu)|\phi_\mu^{(\nu)}\rangle \end{aligned} \tag{4.8}$$

where $\Delta(x)$ is defined by (3.6), and the factor $(-1)^{Nj+N'l}$ takes account of the fact that the sums are over half-integer values of J and L when, respectively, j and l are odd. Also, (2.15) has been used to simplify the argument of one of the complex exponentials.

Condition (4.7) can also be written

$$k - k' = l\kappa_\nu + n\Delta k$$
$$\Delta k = 2\pi p - q\hbar \tag{4.9}$$

where l and n are integers (distinct from the dummy integers used in summations in some earlier expressions). Comparing (4.7) and (4.9),

$$-j = M_\nu l + np \qquad N'N_\nu = \mu - \mu' + M - nq + lN_\nu \tag{4.10}$$

and using (2.15),

$$\frac{\partial(j, N')}{\partial(n, l)} = \det\begin{pmatrix} -p & -M_\nu \\ -q/N_\nu & 1 \end{pmatrix} = -\frac{1}{N_\nu}. \tag{4.11}$$

This shows that, provided 2π and $\hbar$ are not rationally related, the summations over n and l cover N_ν times as many values of $k - k'$ as the summations over j, N'. Varying μ' in (4.7) between 1 and N_ν multiplies the number of distinct values of $k - k'$ by N_ν. The summations over j, N' and μ' in (4.8) can therefore be replaced by summations over n and l. Making this replacement, changing the summation variable m to $m - M_\nu N$, and renaming a dummy index gives

$$\langle B_\nu(k', \delta')|\hat{T}(N\hbar, M\hbar)|B_\nu(k, \delta)\rangle = \Delta(\delta - \delta') \sum_{n=-\infty}^{\infty} \sum_{l=-\infty}^{\infty} \Delta(k - k' - l\kappa_\nu - n\Delta k)$$
$$\times \exp[2\pi \mathrm{i}\delta(M_\nu l + pn)/\hbar] \sum_{m=-\infty}^{\infty} \exp\left[-2\pi \mathrm{i}\left(\frac{k + k'}{2\kappa_\nu}\right) m\right] (-1)^{lm} \tau_{nm}^{NM} \tag{4.12}$$

where

$$\tau_{nm}^{NM} = (-1)^{pnN} \sum_{\mu=1}^{N_\nu} (-1)^{(m-NM_\nu)(\mu-\mu'+M-nq)/N_\nu} \exp\left[-\frac{2\pi \mathrm{i}}{N_\nu}\left(\frac{\mu + \mu'}{2}\right)(m - M_\nu N)\right]$$
$$\times \langle \phi_{\mu'}^{(\nu)}|\hat{T}(-2\pi(m - NM_\nu)/N_\nu + N\hbar, -2\pi(np + M_\nu l)$$
$$+ M\hbar + 2\pi M_\nu(k - k')/\kappa_\nu)|\phi_\mu^{(\nu)}\rangle \tag{4.13}$$

and

$$\mu' = (\mu + M - nq) \bmod N_\nu. \tag{4.14}$$

Equation (4.12) shows that the matrix elements are in the form of a difference operator in the k variables, with coefficients which are periodic with period κ_ν. Equation (4.13) gives the mth Fourier coefficient of the term-coupling wavevector k to $k' = k + n\Delta k$, in terms of the matrix elements of the localized states $|\phi_\mu^{(\nu)}\rangle$.

4.2. A more symmetric expression for the Fourier coefficients

The formula for the Fourier coefficients (4.13) which defines the matrix elements will now be written in a more compact and symmetric form. Using (2.14), (2.15) and (4.9) to simplify the arguments of the translation operator in (4.13), and using (2.15) to simplify the phase factors gives:

$$\tau_{nm}^{NM} = \sum_{\mu=1}^{N_\nu}(-1)^{p(nN+mM-qnm)} \exp\left[-\frac{2\pi \mathrm{i} M_\nu}{N_\nu}(\mu - \tfrac{1}{2}(nq-M))(mq-N)\right]$$
$$\times \langle\phi_{\mu'}^{(\nu)}|\hat{T}((-2\pi m + N\kappa_\nu)/N_\nu, (-2\pi n + M\kappa_\nu)\hbar/\kappa_\nu)|\phi_\mu^{(\nu)}\rangle. \tag{4.15}$$

This result can be further simplified by introducing operators $\hat{t}(\lambda_1, \lambda_2)$ which are defined, for integer values of λ_1 and λ_2, by the relation

$$\hat{t}(\lambda_1, \lambda_2)|\phi_\mu^{(\nu)}\rangle = \exp\left[\frac{2\pi \mathrm{i} M_\nu}{N_\nu}(\mu - \tfrac{1}{2}\lambda_1)\lambda_2\right]|\phi_{\mu-\lambda_1}^{(\nu)}\rangle. \tag{4.16}$$

The operators $\hat{t}(\lambda_1, \lambda_2)$ are clearly analogous to the phase-space translation operators $\hat{T}(X, P)$ in that they have the same type of non-commutative algebra:

$$\hat{t}(\lambda_1, \lambda_2)\hat{t}(\lambda_1', \lambda_2') = \exp\left[\frac{2\pi \mathrm{i} M_\nu}{N_\nu}\left(\frac{\lambda_2\lambda_1' - \lambda_1\lambda_2'}{2}\right)\right]\hat{t}(\lambda_1 + \lambda_1', \lambda_2 + \lambda_2'). \tag{4.17}$$

Also, note that the $\hat{t}(\lambda_1, \lambda_2)$ operators commute with the phase-space translations $\hat{T}(X, P)$. Making use of definition (4.21), the coefficient τ_{nm}^{NM} can be written in the form

$$\tau_{nm}^{NM} = (-1)^{p(nN+mM-qnm)}\sum_{\mu=1}^{N_\nu}\langle\phi_\mu^{(\nu)}|\hat{\mathcal{T}}_{nm}^{NM}|\phi_\mu^{(\nu)}\rangle$$

$$\hat{\mathcal{T}}_{nm}^{NM} = \hat{t}(M - nq, N - mq)\hat{T}((-2\pi m + N\kappa_\nu)/N_\nu, (-2\pi n + M\kappa_\nu)\hbar/\kappa_\nu). \tag{4.18}$$

Note that the coefficients τ_{nm}^{NM} can all be obtained from a set of N_ν^2 functions $W_{nn'}^{(\nu)}(\mathcal{X}, \mathcal{P})$, defined by

$$W_{nn'}^{(\nu)}(\mathcal{X}, \mathcal{P}) = \sum_{\mu=1}^{N_\nu}\langle\phi_\mu^{(\nu)}|\hat{t}(n, n')\hat{T}(\mathcal{X}/N_\nu, \mathcal{P}\hbar/\kappa_\nu)|\phi_\mu^{(\nu)}\rangle. \tag{4.19}$$

In terms of the functions $W_{nn'}^{(\nu)}(\mathcal{X}, \mathcal{P})$, the coefficients τ_{nm}^{NM} can be written in a form in which the pairs of integer labels N, M and n, m appear in a symmetric pattern:

$$\tau_{nm}^{NM} = (-1)^{p(nN+mM-qnm)}W_{n_x n_p}^{(\nu)}(\mathcal{X}, \mathcal{P}) \tag{4.20}$$

with

$$n_x = M - nq \qquad n_p = N - mq$$
$$\mathcal{X} = -2\pi m + N\kappa_\nu \qquad \mathcal{P} = -2\pi n + M\kappa_\nu. \tag{4.21}$$

It is surprising that the arguments of the $\hat{T}(X, P)$ operator in (4.19) should have to be multiplied by different factors in order to obtain (4.20) in this symmetric form. This asymmetry in the definition of $W_{nn'}^{(\nu)}(\mathcal{X}, \mathcal{P})$ suggests that it may be difficult to make it reflect a four-fold symmetry of the crystal lattice. This apparent difficulty is resolved in section 6.

5. Renormalization-group transformation

5.1. A renormalization-group mapping of operators

In section 4, it was shown that the matrix elements of the Hamiltonian (1.6), when expressed in terms of the generalized Bloch states, are in the form of a difference operator in the k variable, with step length Δk and with periodic coefficients with period κ_ν. This new representation of the Hamiltonian is therefore very similar to the original Harper's equation. In this section, it will be shown that the matrix elements are equivalent to those of a 'renormalized' Hamiltonian of the form

$$\hat{H}'^{(\nu)} = \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} H'^{(\nu)}_{nm} \exp[\mathrm{i}(n\hat{p}' - m\hat{x}')] = \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} H'^{(\nu)}_{nm} \hat{T}'_{nm} \tag{5.1}$$

where

$$[\hat{x}', \hat{p}'] = \mathrm{i}\hbar' \qquad \hbar' = 2\pi\beta' = 2\pi\Delta k/\kappa_\nu. \tag{5.2}$$

Because the allowed values of δ (specified by (2.17)) satisfy $0 < \delta \leqslant \hbar$, the matrix elements (4.12) are only non-zero when $\delta = \delta'$. The k values will be considered to form a continuum from $-\infty$ to ∞, but only values $0 < k \leqslant \kappa_\nu$ are physically distinct. When expanding a state in terms of the $|B_\nu(k, \delta)\rangle$ basis, only values which are related by (4.9) are required, since only these values are coupled by the Hamiltonian. Moreover, only states with differing values of n are required, because states with k differing by multiples of κ_ν are physically equivalent: for this reason only the case where $l = 0$ in (4.12) is required.

Accordingly, attention will be restricted to a subset of the generalized Bloch states where $k = k_0 + n\Delta k$ (and n is an integer). If 2π is not rationally related to $\hbar$, it is useful to make a phase transformation of these states:

$$|\chi_n\rangle = \exp[2\pi\mathrm{i}\delta pn/\hbar]|B_\nu(k_0 + n\Delta k, \delta)\rangle. \tag{5.3}$$

When $\hbar$ is rationally related to 2π, this set of states is closed, and (5.3) would be inconsistent in that it would equate a state to a multiple of itself which would typically be different from unity; for this reason the subsequent discussion of this section is specific to irrational values of β. Using (4.12), the matrix elements of the translation operator $\hat{T}_{NM} = \hat{T}(N\hbar, M\hbar)$ are then

$$\langle\chi_{n+\Delta n}|\hat{T}_{NM}|\chi_n\rangle = \sum_{m=-\infty}^{\infty} \exp\left[\frac{2\pi\mathrm{i}}{\kappa_\nu}((n + \tfrac{1}{2}\Delta n)\Delta k + k_0)m\right] \tau^{NM}_{\Delta nm}. \tag{5.4}$$

Note that the choice of the phase transformation in (5.3) makes (5.4) independent of δ.

The matrix elements (5.4) will now be compared with those of the operator

$$\hat{\tau}'_{NM} = \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} \tau^{NM}_{nm} \exp[\mathrm{i}(n\hat{p}' - m\hat{x}')] = \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} \tau^{NM}_{nm} \hat{T}'_{nm} \tag{5.5}$$

in the basis of eigenstates of x'. These matrix elements are

$$\langle x'_1|\hat{\tau}'_{NM}|x'_2\rangle = \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} \tau^{NM}_{nm} \exp\left[\mathrm{i}\left(\frac{x'_1 + x'_2}{2}\right)m\right] \langle x'_1|x'_2 + n\hbar'\rangle. \tag{5.6}$$

Now restricting attention to the subset of $|x'\rangle$ states $|\chi'_n\rangle = |x'_0 + n\hbar'\rangle$, the non-zero matrix elements in (5.6) are

$$\langle \chi'_{n+\Delta n}|\hat{\tau}'_{NM}|\chi'_n\rangle = \sum_{n=-\infty}^{\infty}\sum_{m=-\infty}^{\infty} \exp\left[\mathrm{i}(x'_0 + (n+\tfrac{1}{2}\Delta n)\hbar')m\right]\tau^{NM}_{\Delta nm}. \qquad (5.7)$$

If $\hbar'$ is identified with $2\pi\Delta k/\kappa_\nu$, and x'_0 with k_0/κ_ν, these matrix elements are exactly the same as those in (5.4). The original translation operator $\hat{T}_{NM}$ is therefore renormalized into a sum $\hat{\tau}'_{NM}$ of translation operators $\hat{T}'_{nm}$, with a renormalized Planck constant $\hbar'$. The same reasoning holds for any operator such as Hamiltonian (1.6) which is a sum of the translation operators $\hat{T}_{NM}$. The renormalized Hamiltonian (5.1) is therefore specified by the Fourier coefficients

$$H'^{(\nu)}_{nm} = \sum_{N=-\infty}^{\infty}\sum_{M=-\infty}^{\infty} H_{NM}\tau^{NM}_{nm}. \qquad (5.8)$$

5.2. Simple results for the renormalization-group coefficients in the rational limit

It is difficult to write down general results for the coefficients τ^{NM}_{nm} in (5.8) which define the renormalization-group transformation. In the rational limit $\hbar \to 2\pi p/q$ however, these coefficients satisfy some simple relationships.

In the rational case $\beta = p/q$, the generalized Bloch states reduce to exact eigenstates, and the matrix elements of $\hat{H}$ are, using (4.12) and setting $l = 0$, $\Delta k = 0$:

$$\begin{aligned}\langle B_\nu(k',\delta')|\hat{H}|B_\nu(k,\delta)\rangle &= \Delta(\delta-\delta')\Delta(k-k') \sum_{N=-\infty}^{\infty}\sum_{M=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}\sum_{m=-\infty}^{\infty} \\ &\quad\times \exp[-2\pi\mathrm{i}\delta np/\hbar]\exp[-2\pi\mathrm{i}km/\kappa_\nu]H_{NM}\tau^{NM}_{nm} \\ &= \Delta(\delta-\delta')\Delta(k-k')\delta_{\nu\nu'}\mathcal{E}_\nu(k,\delta) \end{aligned} \qquad (5.9)$$

where $\mathcal{E}_\nu(k,\delta)$ is the dispersion relation for the νth band, which has Fourier coefficients $\mathcal{E}^{(\nu)}_{nm}$. Comparing (5.8) and (5.9), it is clear that the set of coefficients $\hat{H}^{(\nu)}_{nm}$ defining the renormalized Hamiltonian therefore approach the Fourier coefficients $\mathcal{E}^{(\nu)}_{nm}$ of the dispersion relation in the rational limit, and that this gives a sum rule for the coefficients τ^{NM}_{nm}:

$$H'^{(\nu)}_{nm} = \sum_{N=-\infty}^{\infty}\sum_{M=-\infty}^{\infty} H_{NM}\tau^{NM}_{nm} \to \mathcal{E}^{(\nu)}_{nm} \qquad (5.10)$$

in the limit $\hbar \to 2\pi p/q$. Similarly, in the rational limit, the Bloch states are orthogonal

$$\langle B_{\nu'}(k',\delta')|B_\nu(k,\delta)\rangle = \Delta(k-k')\Delta(\delta-\delta')\delta_{\nu\nu'} \qquad (5.11)$$

implying that

$$\tau^{00}_{nm} \to \delta_{n0}\delta_{m0} \qquad (5.12)$$

as $\hbar \to 2\pi p/q$. By considering matrix elements of integer powers of $\hat{H}$, it is also possible to derive further sum rules analogous to (5.10) relating the coefficients τ^{NM}_{nm} to Fourier coefficients of the dispersion relation.

The two results (5.10) and (5.12) were obtained less formally in [15]. It follows directly from these results that the renormalized Hamiltonian is obtained from the dispersion relation $\mathcal{E}_\nu(k,\delta)$ by a Peierls substitution.

6. Rotational symmetry

The symmetry between $\hat{x}$ and $\hat{p}$ of the Harper Hamiltonian is obscured in the Wannier function representation of the Bloch states (3.15). This is a necessary feature of the construction of these states, because it is desirable to keep the Bloch states strictly periodic in at least one of the Bloch wavevectors (k, δ), and if the Chern number M_ν is non-zero the periodicity must be lost in the other variable. The aim of this section is to consider the effect of a $\pi/2$ rotation in the phase plane on the $|B_\nu(k,\delta)\rangle$ states, and to calculate the transformation of the Wannier functions $|\phi_\mu^{(\nu)}\rangle$ generated by this rotation. It will be shown that, provided the phases of the Bloch states are chosen to satisfy a particular condition, the function $W_{nn'}^{(\nu)}(\mathcal{X}, \mathcal{P})$ defined by (4.19) is symmetric under rotations if the Hamiltonian also has this symmetry.

6.1. Rotation of Bloch states

The operator describing a $\pi/2$ rotation in the phase plane is the Fourier transform operator (with an additional scaling by a factor of $\hbar$). This operator will be denoted by $\hat{R}$:

$$\langle x|\hat{R}|\psi\rangle = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \mathrm{d}x'\, \mathrm{e}^{\mathrm{i}xx'/\hbar} \langle x'|\psi\rangle. \tag{6.1}$$

This operator rotates phase-space translation operators by $\pi/2$:

$$\hat{R}\hat{T}(X, P) = \hat{T}(-P, X)\hat{R}. \tag{6.2}$$

Now consider the effect of applying the rotation operator to a Bloch eigenstate $|B_\nu(k,\delta)\rangle$ in the rational case. Clearly

$$\hat{H}_\mathrm{R}\hat{R}|B_\nu(k,\delta)\rangle = \mathcal{E}_\nu(k,\delta)\hat{R}|B_\nu(k,\delta)\rangle \tag{6.3}$$

where $\hat{H}_\mathrm{R} = \hat{R}\hat{H}\hat{R}^{-1}$ is an operator which can be obtained from $\hat{H}$ by rotating the arguments of all of the component translation operators by $\pi/2$. The state $\hat{R}|B_\nu(k,\delta)\rangle$ must, therefore, be a linear combination of Bloch eigenstates of the rotated Hamiltonian $\hat{H}_\mathrm{R}$ with the same energy $\mathcal{E}_\nu(k,\delta)$. The case where $\hat{H}_\mathrm{R} = \hat{H}$ will be of particular interest.

Instead of considering the effect of a rotation on a single Bloch eigenstate, the effect of the rotation operator on a particular linear combination of Bloch eigenstates will be analysed: this linear combination is of the form

$$|S_\nu(k,\delta)\rangle = \frac{1}{\sqrt{p}} \sum_{j=1}^{p} |B_\nu(k, \delta + 2\pi j/q)\rangle. \tag{6.4}$$

It will be shown that

$$\hat{R}|S_\nu(k,\delta)\rangle = |B_\nu'^{(\mathrm{R})}(k',\delta')\rangle \tag{6.5}$$

where $|B_\nu'^{(\mathrm{R})}(k,\delta)\rangle$ is obtained by a gauge transformation from the Bloch state $|B_\nu^{(\mathrm{R})}(k,\delta)\rangle$ of the rotated Hamiltonian $\hat{H}_\mathrm{R}$

$$|B_\nu'^{(\mathrm{R})}(k,\delta)\rangle = \mathrm{e}^{\mathrm{i}\theta(k,\delta)}|B_\nu^{(\mathrm{R})}(k,\delta)\rangle \tag{6.6}$$

and the transformation of the Bloch wavevectors k and δ, induced by the rotation operator, is

$$k' = \delta \qquad \delta' = -k. \tag{6.7}$$

The effect of the rotation operator on the sum of Bloch states $|S_\nu(k,\delta)\rangle$ defined by (6.4) is therefore to produce a single Bloch eigenstate $|B_\nu'^{(\mathrm{R})}(k',\delta')\rangle$ of the rotated Hamiltonian $\hat{H}_{\mathrm{R}}$. The transformed Bloch wavevectors are related by a $\pi/2$ rotation in the Brillouin zone (6.7), and the phase of the rotated Bloch states differs by a gauge transformation (6.6) from Bloch states of the standard form (3.15).

It will now be verified that $\hat{R}|S_\nu(k,\delta)\rangle$ is a single Bloch state. Specializing (3.15) to the rational case ($\hbar = 2\pi p/q$, $\kappa_\nu = 2\pi/q$), and splitting the sum over n into a double sum over n' and μ', with $n = N_\nu n' + \mu'$:

$$\begin{aligned}|S_\nu(k,\delta)\rangle = \frac{C}{\sqrt{p}} \sum_{j=1}^{p} \sum_{m} \exp[-\mathrm{i}qm\delta/p] \exp[-2\pi \mathrm{i}mj/p] \hat{T}(0, 2\pi m) \\ \times \sum_{n'} \sum_{\mu=1}^{N_\nu} \sum_{\mu'=1}^{N_\nu} \exp[-\mathrm{i}qk(n'N_\nu + \mu')/pN_\nu] \exp[-2\pi \mathrm{i}\mu(n'N_\nu + \mu')/N_\nu] \\ \times \hat{T}(-2\pi n, 0) \hat{T}(-2\pi\mu'/N_\nu, 0) \hat{T}(0, qM_\nu k) |\phi_\mu^{(\nu)}\rangle\end{aligned} \tag{6.8}$$

where C is the normalization factor (3.16). This state vanishes except when m is a multiple of p. Using (1.5) and (2.15) to commute translation operators and simplify phase factors, and renaming the dummy indices, this reduces to

$$\begin{aligned}|S_\nu(k,\delta)\rangle = C \sum_m \mathrm{e}^{\mathrm{i}qkm/p} \hat{T}(2\pi m, 0) \sum_n \mathrm{e}^{-\mathrm{i}q\delta n} \hat{T}(0, 2\pi np) \hat{T}(0, qM_\nu k) \\ \times \sum_{\mu=1}^{N_\nu} \exp[-\mathrm{i}qk\mu] |\chi_\mu^{(\nu)}\rangle\end{aligned} \tag{6.9}$$

where

$$|\chi_\mu^{(\nu)}\rangle = \sqrt{p}\hat{T}(-2\pi\mu/N_\nu, 0) \sum_{\mu'=1}^{N_\nu} \exp[-2\pi \mathrm{i}\mu\mu'/N_\nu] |\phi_{\mu'}^{(\nu)}\rangle. \tag{6.10}$$

Applying the rotation operator to this state gives (using (6.2))

$$\begin{aligned}\hat{R}|S_\nu(k,\delta)\rangle = C \sum_m \exp[-\mathrm{i}q\delta' m/p] \hat{T}(0, 2\pi m) \sum_n \exp[-\mathrm{i}qk'n] \hat{T}(-2\pi pn, 0) \hat{T}(qM_\nu\delta', 0) \\ \times \sum_{\mu=1}^{N_\nu} \exp[\mathrm{i}q\delta'\mu] |\Phi_\mu^{(\mathrm{R}\nu)}\rangle\end{aligned} \tag{6.11}$$

where

$$|\Phi_\mu^{(\mathrm{R}\nu)}\rangle = \sqrt{p}\hat{T}(0, -2\pi\mu/N_\nu) \sum_{\mu'=1}^{N_\nu} \exp[-2\pi \mathrm{i}\mu\mu'/N_\nu] \hat{R}|\phi_{\mu'}^{(\nu)}\rangle \tag{6.12}$$

and k' and δ' are given by (6.7). The summation over m plays the same rôle as that in (3.2), indicating that the wavefunction of this state is zero except at positions $x_n = n\hbar + \delta'$; also, k' is clearly a Bloch wavevector. This state is therefore a Bloch state of the rotated Hamiltonian, similar to the standard form (3.15), and differing from it by at most a gauge transformation.

6.2. *An alternative Wannier function representation*

In the previous subsection, it was shown that a Bloch wave can also be represented in the form (6.11). This is an alternative representation to (3.15) in terms of a different set of Wannier functions $|\Phi_\mu^{(\nu)}\rangle$:

$$|B'_\nu(k,\delta)\rangle = C\sum_m \exp[-\mathrm{i}q\delta m/p]\hat{T}(0,2\pi m)\sum_n \exp[-\mathrm{i}qkn]\hat{T}(-2\pi pn,0)\hat{T}(qM_\nu\delta,0) \times \sum_{\mu=1}^{N_\nu}\exp[\mathrm{i}q\mu\delta]|\Phi_\mu^{(\nu)}\rangle. \tag{6.13}$$

The periodicity of this new representation of the Bloch states is described by the relations

$$|B'_\nu(k+2\pi/q,\delta)\rangle = |B'_\nu(k,\delta)\rangle$$
$$|B'_\nu(k,\delta+2\pi p/q)\rangle = \exp[-\mathrm{i}qM_\nu k]|B'_\nu(k,\delta)\rangle \tag{6.14}$$

which is different from the periodicity properties of the previous Wannier function representation (3.15) (cf (2.2) and (2.3)):

$$|B_\nu(k+2\pi/q,\delta)\rangle = \exp[\mathrm{i}qM_\nu\delta/p]|B_\nu(k,\delta)\rangle$$
$$|B_\nu(k,\delta+2\pi p/q)\rangle = |B_\nu(k,\delta)\rangle. \tag{6.15}$$

The phase $\theta(k,\delta)$ appearing in gauge transformation (6.6) therefore satisfies the equations

$$\theta(k+2\pi/q,\delta)-\theta(k,\delta) = -qM_\nu k$$
$$\theta(k,\delta+2\pi p/q)-\theta(k,\delta) = -qM_\nu\delta/p. \tag{6.16}$$

The solution of these equations is of the form $\theta(k,\delta) = \alpha k\delta + \chi(k,\delta)$, where $\chi(k,\delta)$ is periodic with periods $\Delta k = \Delta\delta = 2\pi/q$ and, by inspection, the coefficient of $k\delta$ is $\alpha = -q^2M_\nu/2\pi p$. The phases of the Bloch waves will be chosen so that the following condition is satisfied:

$$|B'^{(\mathrm{R})}_\nu(k,\delta)\rangle = \exp[-\mathrm{i}q^2M_\nu k\delta/2\pi p]|B_\nu^{(\mathrm{R})}(k,\delta)\rangle. \tag{6.17}$$

Note that, given a choice of gauge for the $|B_\nu(k,\delta)\rangle$ states, this relationship defines, via (6.4) and (6.5), the phase of the $|B_\nu^{(\mathrm{R})}(k,\delta)\rangle$ states.

6.3. *Rotations of Wannier functions*

Two expansions for Bloch states in terms of Wannier functions have been given, which will be termed type I (defined by (3.15)), and type II (defined by (6.13)). Equation (6.12) gives the type II Wannier functions of the rotated Hamiltonian $\hat{H}_\mathrm{R}$ in terms of the type I Wannier functions of $\hat{H}$. Now the type I Wannier functions of the rotated Hamiltonian $|\phi_\mu^{(\mathrm{R}\nu)}\rangle$ will be determined in terms of the unrotated set $|\phi_\mu^{(\nu)}\rangle$. The result will be expressed as a rotation operator for the set of Wannier functions.

Appendix A gives a formula for the type I Wannier functions $|\phi_\mu^{(\nu)}\rangle$ in terms of the Bloch states $|B_\nu(k,\delta)\rangle$. The approach will be to use this formula with the Bloch waves $|B_\nu^{(\mathrm{R})}(k,\delta)\rangle$ obtained from gauge transformation (6.17) of the $|B_\nu'^{(\mathrm{R})}(k,\delta)\rangle$ states: the latter will be expanded in terms of the type II Wannier functions, which are given by (6.12). Combining (A.4) and (6.17) gives

$$|\phi_\mu^{(\mathrm{R}\nu)}\rangle = \frac{q^2}{4\pi^2 p N_\nu C}\sum_{\mu'=1}^{N_\nu}\exp[2\pi i\mu\mu'/N_\nu]\hat{T}(2\pi\mu'/N_\nu,0)$$
$$\times\int_0^{2\pi/q}\mathrm{d}k\int_0^{2\pi p/q}\mathrm{d}\delta\,\exp[iqk\mu']\exp[iq^2M_\nu k\delta/2\pi p]$$
$$\times\,\hat{T}(0,-qM_\nu k)|B_\nu'^{(\mathrm{R})}(k,\delta)\rangle \tag{6.18}$$

and the Bloch states of the rotated Hamiltonian are obtained by substituting (6.12) and (6.13) into (6.18). Using a result (B.3) proved in appendix B, this can be written

$$|\phi_\mu^{(\mathrm{R}\nu)}\rangle = -\frac{1}{\sqrt{N_\nu}}\sum_{\mu'=1}^{N_\nu}\exp[2\pi \mathrm{i}\mu\mu'/N_\nu]\hat{T}(2\pi\mu'/N_\nu,0)\hat{T}(0,2\pi p\lambda)\hat{T}(2\pi\mu'/N_\nu,0)$$
$$\times\,\hat{S}(pN_\nu)\hat{R}\hat{T}(-2\pi\lambda/N_\nu,0)\sum_{\lambda'=1}^{N_\nu}\exp[2\pi\mathrm{i}\lambda\lambda'/N_\nu]|\phi_{\lambda'}^{(\nu)}\rangle \tag{6.19}$$

where $\hat{S}(\eta)$ is a unitary operator which stretches the x axis by a factor of η

$$\langle x|\hat{S}(\eta)|\psi\rangle = \sqrt{\eta}\langle\eta x|\psi\rangle. \tag{6.20}$$

Commuting a pair of $\hat{T}$ operators, and using (6.2) and (B.9) to commute all of the $\hat{T}$ operators to the left of the $\hat{S}$ and the $\hat{R}$, this reduces to

$$|\phi_\mu^{(\mathrm{R}\nu)}\rangle = -\frac{1}{\sqrt{N_\nu}}\sum_{\mu'=1}^{N_\nu}\sum_{\lambda=1}^{N_\nu}\exp[2\pi\mathrm{i}(\mu+q\lambda)\mu'/N_\nu]\sum_{\lambda'=1}^{N_\nu}\exp[-2\pi\mathrm{i}\lambda\lambda'/N_\nu]\hat{S}(pN_\nu)\hat{R}|\phi_{\lambda'}^{(\nu)}\rangle. \tag{6.21}$$

The sum over μ' vanishes unless $q\lambda+\mu = 0 \bmod N_\nu$; using (2.15) this condition can also be expressed as $\lambda = -M_\nu\mu \bmod N_\nu$, so that

$$|\phi_\mu^{(\mathrm{R}\nu)}\rangle = -\frac{1}{\sqrt{N_\nu}}\sum_{\mu'=1}^{N_\nu}\exp[2\pi\mathrm{i}M_\nu\mu\mu'/N_\nu]\hat{S}(pN_\nu)\hat{R}|\phi_{\mu'}^{(\nu)}\rangle. \tag{6.22}$$

The rotation operator for the type I Wannier functions is therefore a composition of a phase-space rotation, a stretching and a discrete Fourier transform acting on the μ labels. It will be convenient to introduce an operator $\hat{r}$ for this discrete Fourier transform:

$$\hat{r}|\phi_\mu\rangle = -\frac{1}{N_\nu^{1/2}}\sum_{\mu'=1}^{N_\nu}\exp[2\pi\mathrm{i}M_\nu\mu\mu'/N_\nu]|\phi_{\mu'}\rangle. \tag{6.23}$$

Note that the operator $\hat{r}$ acts on a set of states $\{|\phi_\mu\rangle,\ \mu=1,\ldots,N_\nu\}$ rather than upon a single state. With this notation, (6.23) can be written

$$|\phi_\mu^{(\mathrm{R}\nu)}\rangle = \hat{S}(pN_\nu)\hat{R}\hat{r}|\phi_\mu^{(\nu)}\rangle. \tag{6.24}$$

The composition of three operators in (6.24) is a rotation operator for the set of Wannier functions. Note that this form for the rotation operator depends on the phases of the Wannier functions being chosen so that (6.17) is satisfied.

6.4. Implications of rotational symmetry: the rational case

If the Hamiltonian has rotational symmetry such that $\hat{H} = \hat{H}_{\rm R}$, then the rotated Bloch states must be equal to the unrotated states, up to a phase. In appendix C, it is shown that there exist gauges for which the rotated and unrotated states differ by a fixed phase $\theta(k, \delta) = \pi L/2$, where L is an integer. In the following considerations, it will be assumed that such a choice of gauge has been made. This implies that the rotated Wannier functions $|\phi_\mu^{({\rm R}\nu)}\rangle$ must be identical to the $|\phi_\mu^{(\nu)}\rangle$ set, apart from a phase factor:

$$|\phi_\mu^{(\nu)}\rangle = {\rm i}^L \hat{S}(pN_\nu)\hat{R}(\hbar_0)\hat{r}|\phi_\mu^{(\nu)}\rangle. \tag{6.25}$$

In this equation the fact that the rotation operator $\hat{R}$ depends on $\hbar$ has been shown explicitly, and for the rational case we set $\hbar = \hbar_0 = 2\pi p/q$. It will now be shown that this implies that the function $W_{nn'}^{(\nu)}(\mathcal{X}, \mathcal{P})$ defined by (4.19) has rotational symmetry in the rational case.

As a preliminary, consider the commutation of operator $\hat{r}$ defined in (6.23) with the translation operator $\hat{t}(n, n')$ defined by (4.16):

$$\hat{r}\hat{t}(n, n') = \hat{t}(-n', n)\hat{r}. \tag{6.26}$$

Note that this is analogous to commutation rule (6.2) for the $\hat{R}$ and $\hat{T}(X, P)$ operators. In the rational case, the function $W_{nn'}^{(\nu)}(X, P)$ is given by setting $\hbar/\kappa_\nu = p$ in (4.19), substituting (6.25) into (4.19), and using (6.2), (6.26) and (B.9) to commute operators:

$$\begin{aligned} W_{nn'}^{(\nu)}(\mathcal{X}, \mathcal{P}) &= \sum_{\mu=1}^{N_\nu} \langle\phi_\mu^{(\nu)}|\hat{r}^+\hat{R}^+\hat{S}^+(pN_\nu)\hat{t}(n, n')\hat{T}(\mathcal{X}/N_\nu, p\mathcal{P})\hat{S}(pN_\nu)\hat{R}\hat{r}|\phi_\mu^{(\nu)}\rangle \\ &= \sum_{\mu=1}^{N_\nu} \langle\phi_\mu^{(\nu)}|\hat{t}(-n', n)\hat{T}(-\mathcal{P}/N_\nu, \mathcal{X}p)|\phi_\mu^{(\nu)}\rangle = W_{-n'n}^{(\nu)}(-\mathcal{P}, \mathcal{X}). \end{aligned} \tag{6.27}$$

This result implies that, provided the phases of the Bloch states are suitably chosen, the function $W_{nn'}^{(\nu)}(\mathcal{X}, \mathcal{P})$ has exact rotational symmetry in the rational case, under a combined rotation of the n, n' and $\mathcal{X}, \mathcal{P}$ variables. Comparing with (4.20) and (4.21), this implies that the renormalization coefficients τ_{nm}^{NM} satisfy the symmetry relation $\tau_{m,-n}^{-M,N} = \tau_{nm}^{NM}$. From (5.8), it is clear that this symmetry ensures that the symmetry of the Fourier coefficients of the Hamiltonian $H_{-M,N} = H_{NM}$, is also found in the Fourier coefficients of the renormalized Hamiltonian: $H'^{(\nu)}_{-m,n} = H'^{(\nu)}_{nm}$. A four-fold rotational symmetry of the classical Hamiltonian (or other operator) is therefore preserved by the renormalization-group transformation in the rational limit $\hbar \to 2\pi p/q$.

6.5. Preservation of rotational symmetry in the irrational case

The four-fold symmetry of $W_{nn'}^{(\nu)}(\mathcal{X}, \mathcal{P})$ can also be preserved in the irrational case by a suitable modification of the Wannier functions.

If β is irrational, the translation operator in (6.27) is replaced by $\hat{T}(\mathcal{X}/N_\nu, \mathcal{P}\hbar/\kappa_\nu)$. It is easy to verify that this symmetry relation would continue to hold if the Wannier functions satisfied the transformation law

$$|\phi_\mu^{(\nu)}\rangle = {\rm i}^L \hat{S}(\hbar N_\nu/\kappa_\nu)\hat{R}\hat{r}|\phi_\mu^{(\nu)}\rangle. \tag{6.28}$$

Given a set of Wannier functions for the rational case satisfying (6.25), a set of states $|\phi_\mu'^{(\nu)}\rangle$ satisfying (6.28) can easily be generated by scaling them by a factor η:

$$|\phi_\mu'^{(\nu)}\rangle = \hat{S}(\eta)|\phi_\mu^{(\nu)}\rangle. \tag{6.29}$$

Note that the rotation operator satisfies

$$\hat{R}(\hbar) = \hat{S}(\hbar_0/\hbar)\hat{R}(\hbar_0) \tag{6.30}$$

which follows from the definitions (6.1) and (6.20). Requiring that $|\phi_\mu^{(\nu)}\rangle = \hat{S}^+(\eta)|\phi_\mu'^{(\nu)}\rangle$ satisfies (6.25), and using (6.30) and (B.10), the required scaling factor is found:

$$\eta = \sqrt{2\pi/q\kappa_\nu}. \tag{6.31}$$

Note that this approaches unity when $\beta \to p/q$. If the Wannier functions are re-scaled according to (6.29) and (6.31), the functions $W_{nn'}^{(\nu)}(\mathcal{X}, \mathcal{P})$ are transformed as follows

$$\begin{aligned} W_{nn'}^{(\nu)}(\mathcal{X}, \mathcal{P}) \to W_{nn'}'^{(\nu)}(\mathcal{X}, \mathcal{P}) &= \sum_{\mu=1}^{N_\nu} \langle\phi_\mu'^{(\nu)}|\hat{t}(n, n')\hat{T}(\mathcal{X}/N_\nu, \mathcal{P}\hbar/\kappa_\nu)|\phi_\mu'^{(\nu)}\rangle \\ &= \sum_{\mu=1}^{N_\nu} \langle\phi_\mu^{(\nu)}|\hat{S}^+(\eta)\hat{t}(n, n')\hat{T}(\mathcal{X}/N_\nu, \mathcal{P}\hbar/\kappa_\nu)\hat{S}(\eta)|\phi_\mu^{(\nu)}\rangle = W_{nn'}^{(\nu)}(\eta\mathcal{X}, \eta\mathcal{P}). \end{aligned} \tag{6.32}$$

In order to preserve a four-fold symmetry of the Hamiltonian in the renormalization-group transformation, the phases of the Bloch waves should be chosen according to the prescription in appendix C. The function $W_{nn'}^{(\nu)}(\mathcal{X}, \mathcal{P})$ then has the correct symmetry in the rational case. In the irrational case, the arguments of this function should be scaled with the factor η, as prescribed by (6.31) and (6.32).

7. Summary and discussion

This paper has been concerned with the definition of a generalized Bloch basis for Harper's equation, and with the evaluation of matrix elements of the Hamiltonian in this basis, showing that they are the same as the matrix elements of a renormalized operator. It is a more refined and formal version of arguments presented in [15]. The new results contained in this paper are summarized below, and the important formulae are enumerated.

A significant new result, introduced in section 2, is that the generalized Bloch states can be generated from a set of N_ν normalizable functions $F_\mu^{(\nu)}(k)$, where N_ν, defined by (2.15), is the gap labelling integer conjugate to the Hall conductance integer M_ν. In section 3, it was shown that these normalizable functions can be used as a set of Wannier functions $|\phi_\mu^{(\nu)}\rangle$ for a von Neumann lattice representation of the Bloch states. This von Neumann lattice representation is inherently anisotropic (except for the special case where $N_\nu = 1$ and $M_\nu = 0$, which was treated in [14]). This anisotropy is a source of severe difficulty in setting up a version of the renormalization-group transformation which preserves the four-fold symmetry of the Hamiltonian.

An explicit formula for the matrix elements of translation operators in the basis of generalized Bloch states (4.12) is derived in section 4 and, in section 5, this is used to obtain the Fourier coefficients which characterize renormalized operators. After a long calculation, these Fourier coefficients are expressed in terms of matrix elements of the form $\langle\phi_\mu^{(\nu)}|\hat{t}(n,n')\hat{T}(\mathcal{X}/N_\nu,\mathcal{P}\hbar/\kappa_\nu)|\phi_\mu^{(\nu)}\rangle$, where $\hat{t}(n,n')$ is a translation operator acting on the μ labels. The final formulae for the Fourier coefficients, (4.18) or (4.20) and (4.21), are quite simple and symmetric in form, but they do not respect the isotropy of the lattice because the arguments of the operator $\hat{T}(X,P)$ are scaled by different amounts.

Section 6 considered the effect of $\pi/2$ rotations of the Hamiltonian in phase space. The relationship of the Wannier states $|\phi_\mu^{(\mathrm{R}\nu)}\rangle$ of the rotated Hamiltonian to the unrotated set $|\phi_\mu^{(\nu)}\rangle$ is given by (6.24), under the assumption that the Bloch states are chosen to satisfy a particular gauge relationship (6.17). The rotation operator for the Wannier functions contains a Fourier-transform operator $\hat{R}$, and a discrete Fourier transform $\hat{r}$ over the μ labels, both of which might be expected. The surprising feature of this result is that it also contains a 'stretching' operator $\hat{S}(pN_\nu)$. In sections 6.4 and 6.5 it is shown that this stretching operator cancels out the apparent anisotropy in the formulae for the matrix elements, and that the function $W_{nn'}^{(\nu)}(\mathcal{X},\mathcal{P})$ defining the renormalization coefficients τ_{nm}^{NM} can be made rotationally invariant. A four-fold symmetry of the Hamiltonian is therefore preserved by the renormalization-group transformation.

The constraints on the choice of gauge imposed in section 2 and appendix C still do not give a unique choice. An exact formulation of the renormalization-group transformation requires evaluation of matrix elements of the projection operator $\hat{P}$ for a band, and of the projected Hamiltonian $\hat{H}_P = \hat{P}\hat{H}\hat{P}$ [15]. The calculation of the expansion of the effective Hamiltonian in powers of $\beta - p/q$ is complicated by the fact that the result is not unique; gauge transformations of the Bloch states determine canonical transformations of the renormalized effective Hamiltonian. This question will be treated in detail in a subsequent paper.

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Appendix A. Wannier states from Bloch functions

This appendix describes how to invert (3.15) to express the Wannier functions in terms of the Bloch functions. The calculation is specific to the rational case.

First consider the state

$$\hat{T}(0,-qM_\nu k)|B_\nu(k,\delta)\rangle = C\sum_{m=-\infty}^{\infty}\exp[-\mathrm{i}qm\delta/p]\hat{T}(0,2\pi m) \times\sum_{n=-\infty}^{\infty}\exp[-\mathrm{i}qkn]\hat{T}(-2\pi n/N_\nu,0)\sum_{\mu=1}^{N_\nu}\exp[-2\pi\mathrm{i}\mu n/N_\nu]|\phi_\mu^{(\nu)}\rangle. \qquad (\mathrm{A}.1)$$

This state is clearly periodic in both k and δ. It is useful to consider the following integral

$$|I_\mu\rangle = \frac{1}{C}\int_0^{2\pi/q}\mathrm{d}k\int_0^{2\pi p/q}\mathrm{d}\delta\,\exp[\mathrm{i}qk\mu]\hat{T}(0,-qM_\nu k)|B_\nu(k,\delta)\rangle = \frac{4\pi^2 p}{q^2}\sum_{\mu'=1}^{N_\nu}\exp[-2\pi\mathrm{i}\mu\mu'/N_\nu]\hat{T}(-2\pi\mu/N_\nu,0)|\phi_{\mu'}^{(\nu)}\rangle. \qquad (\mathrm{A}.2)$$

This result relates a sum of Wannier functions to an integral over the Brillouin zone. A single Wannier function can be obtained from the $|I_\mu\rangle$ states by performing a further summation:

$$\frac{1}{N_\nu}\sum_{\lambda=1}^{N_\nu}\exp[2\pi\mathrm{i}\lambda\mu/N_\nu]\hat{T}(2\pi\lambda/N_\nu,0)|I_\lambda\rangle = \frac{4\pi^2 p}{q^2}|\phi_\mu^{(\nu)}\rangle. \tag{A.3}$$

Combining the above results gives an expression for the Wannier functions in terms of the Bloch states

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

This expression is analogous to the standard method for constructing conventional Wannier functions by means of an integration over the Brillouin zone, and it reduces to the standard result when $M_\nu = 0$ and $N_\nu = 1$.

Appendix B. An operator identity

The operator

$$\hat{O}(k,\delta) = \exp[\mathrm{i}q^2M_\nu k\delta/2\pi p]\sum_{n=-\infty}^{\infty}\sum_{m=-\infty}^{\infty}\exp[-\mathrm{i}q(kpn+\delta m)/p]$$
$$\times\hat{T}(0,2\pi m - qM_\nu k)\hat{T}(-2\pi pn + qM_\nu\delta,0) \tag{B.1}$$

is easily shown to be periodic in k and δ: $\hat{O}(k+2\pi/q,\delta) = \hat{O}(k,\delta) = \hat{O}(k,\delta+2\pi p/q)$. The aim of this appendix is to evaluate the Fourier coefficients of this operator:

$$\hat{O}_{NM} = \int_0^{2\pi/q}\mathrm{d}k\int_0^{2\pi p/q}\mathrm{d}\delta\ \exp[\mathrm{i}q(kpN+\delta M)/p]\hat{O}(k,\delta) \tag{B.2}$$

and to relate them to a unitary operator $\hat{S}(\eta)$ which describes a dilation of the x coordinate axis by a factor of η: $\langle x|\hat{S}(\eta)|\psi\rangle = \sqrt{\eta}\langle\eta x|\psi\rangle$. It will be shown that, when $\hbar = 2\pi p/q$,

$$\hat{O}_{NM} = -\frac{4\pi^2 p}{q^2}\frac{1}{\sqrt{pN_\nu}}\hat{T}(0,2\pi M)\hat{T}(2\pi N/N_\nu,0)\hat{S}(pN_\nu). \tag{B.3}$$

To derive this result, consider the coordinate representation of $\hat{O}_{NM}|\psi\rangle$ for an arbitrary state $|\psi\rangle$:

$$\langle x|\hat{O}(k,\delta)|\psi\rangle = \exp[\mathrm{i}q^2M_\nu k(\delta - x)/2\pi p]\sum_{m=-\infty}^{\infty}\exp[\mathrm{i}qm(x-\delta)/p]$$
$$\times\sum_{n=-\infty}^{\infty}\exp[-\mathrm{i}qkn]\langle x+2\pi pn - qM_\nu\delta|\psi\rangle. \tag{B.4}$$

Using the Poisson summation formula, the sum over m can be expressed as a sum over delta functions:

$$\langle x|\hat{O}(k,\delta)|\psi\rangle = -\frac{2\pi p}{q}\exp[\mathrm{i}q^2 M_\nu k(\delta - x)/2\pi p]\sum_{m=-\infty}^{\infty}\delta(x - 2\pi pm/q - \delta)$$

$$\times\sum_{n=-\infty}^{\infty}\exp[-\mathrm{i}qkn]\langle x + 2\pi pn - qM_\nu\delta|\psi\rangle. \tag{B.5}$$

Now note that, for any function $f(\delta)$:

$$\sum_{m=-\infty}^{\infty}\int_0^{2\pi p/q}\mathrm{d}\delta\, f(\delta)\delta(x - 2\pi pm/q - \delta) = \int_{-\infty}^{\infty}\mathrm{d}\delta\, f(\delta)\delta(x-\delta) = f(x). \tag{B.6}$$

It follows that

$$\int_0^{2\pi p/q}\mathrm{d}\delta\exp[\mathrm{i}qM\delta/p]\langle x|\hat{O}(k,\delta)|\psi\rangle$$

$$= -\frac{2\pi p}{q}\exp[\mathrm{i}qMx/p]\sum_{n=-\infty}^{\infty}\exp[-\mathrm{i}qkn]\langle x + 2\pi pn - qM_\nu x|\psi\rangle. \tag{B.7}$$

Finally, integrating over k gives

$$\hat{O}_{NM} = -\frac{2\pi p}{q}\exp[\mathrm{i}qMx/p]\int_0^{2\pi/q}\mathrm{d}k\exp[\mathrm{i}qkN]\sum_{n=-\infty}^{\infty}\exp[-\mathrm{i}kn]\langle x - 2\pi pn + qM_\nu x|\psi\rangle$$

$$= -\frac{4\pi^2 p}{q}\exp[\mathrm{i}qMx/p]\langle x - 2\pi pN - qM_\nu x|\psi\rangle$$

$$= -\frac{4\pi^2 p}{q}\frac{1}{\sqrt{pN_\nu}}\exp[\mathrm{i}qMx/p]\langle x - 2\pi N/N_\nu|\hat{S}(pN_\nu)|\psi\rangle$$

$$= -\frac{4\pi^2 p}{q}\frac{1}{\sqrt{pN_\nu}}\langle x|\hat{T}(0,2\pi M)\hat{T}(2\pi N/N_\nu,0)S(pN_\nu)|\psi\rangle \tag{B.8}$$

from which (B.3) follows immediately.

It is useful to note the rule for commuting the $\hat{S}$ and $\hat{T}$ operators:

$$\hat{S}(\eta)\hat{T}(X,P) = \hat{T}(X/\eta, P\eta)\hat{S}(\eta). \tag{B.9}$$

This result is easily obtained from definitions (1.6) and (6.20), by calculating the matrix element $\langle x|\hat{T}(X,P)\hat{S}(\eta)|\psi\rangle$. Similarly,

$$\hat{R}\hat{S}(\eta) = \hat{S}(1/\eta)\hat{R}. \tag{B.10}$$

Appendix C. Construction of a rotationally invariant gauge

In section 6.2, it was shown that the Bloch states of the rotated Hamiltonian can be obtained from those of the unrotated Hamiltonian as follows

$$|B_\nu^{(R)}(k',\delta')\rangle = \frac{1}{\sqrt{p}}\exp[iq^2 M_\nu k\delta/2\pi p]\hat{R}\sum_{j=1}^{p}|B_\nu(k,\delta+2\pi j/q)\rangle = \hat{\mathcal{R}}_B|B_\nu(k,\delta)\rangle \qquad (C.1)$$

where k' and δ' are given by (6.7), and the second equality defines the rotation operator for the Bloch states $\mathcal{R}_B$. If $\hat{H}_R = \hat{H}$, the rotated Bloch states must be equal to the unrotated states, apart from a phase factor:

$$|B_\nu^{(R)}(k,\delta)\rangle = \exp[i\theta(k,\delta)]|B_\nu(k,\delta)\rangle \qquad (C.2)$$

where $\theta(k+2\pi/q,\delta) = \theta(k,\delta) = \theta(k,\delta+2\pi/q)$. A gauge transformation of the Bloch states will now be constructed for which the function $\theta(k,\delta)$ is a constant, i.e. a function $\chi(k,\delta)$ will be determined such that the gauge-transformed states

$$|B'_\nu(k,\delta)\rangle = \exp[i\chi(k,\delta)]|B_\nu(k,\delta)\rangle \qquad (C.3)$$

satisfy

$$|B'^{(R)}_\nu(k,\delta)\rangle = \hat{\mathcal{R}}_B|B'_\nu(-\delta,k)\rangle = \exp(i\theta_0)|B'_\nu(k,\delta)\rangle. \qquad (C.4)$$

where θ_0 is a constant. Combining (C.2), (C.3) and (C.4) gives a relationship between the functions $\chi(k,\delta)$ and $\theta(k,\delta)$:

$$\chi(k,\delta) = \chi(-\delta,k) + \theta(-\delta,k) - \theta_0. \qquad (C.5)$$

To construct the solution of this equation, the function $\chi(k,\delta)$ is Fourier expanded

$$\chi(k,\delta) = \sum_{n=-\infty}^{\infty}\sum_{m=-\infty}^{\infty}\chi_{nm}\exp[iq(nk+m\delta)] \qquad (C.6)$$

and $\theta(k,\delta)$ is expanded in the same manner with coefficients θ_{nm}. In terms of the Fourier coefficients, (C.5) reads

$$\chi_{nm} = \chi_{m,-n} + \theta_{m,-n} - \delta_{n0}\delta_{m0}\theta_0. \qquad (C.7)$$

Except for the special case of χ_{00}, the coefficient χ_{nm} is related to three other coefficients, $\chi_{m,-n}$, $\chi_{-n,-m}$ and $\chi_{-m,n}$ by (C.7). The choice of one of the coefficients (χ_{nm}, say) is arbitrary, but once this has been chosen the other three coefficients are determined by three iterations of (C.7). Coefficient χ_{00} is arbitrary.

For this to be a consistent solution, a fourth iteration of (C.7) should give the original coefficient χ_{nm}. Clearly, this requires that the four Fourier coefficients θ_{nm}, $\theta_{m,-n}$, $\theta_{-n,-m}$ and $\theta_{-m,n}$ should sum to zero for all (n,m) except $(0,0)$: equivalently

$$\theta(k,\delta) + \theta(\delta,-k) + \theta(-k,-\delta) + \theta(-\delta,k) = \text{constant}. \qquad (C.8)$$

This condition is satisfied if $\hat{\mathcal{R}}_B^4|B_\nu(k,\delta)\rangle = |B_\nu(k,\delta)\rangle$ *in which case the constant in* (C.8) is $2\pi L$, where L is an integer. Equation (C.8) can be verified as follows. In section 6.3, the Wannier functions of the rotated Hamiltonian were shown to be related to those of the unrotated Hamiltonian by application of an operator

$$\hat{\mathcal{R}}_\phi = \hat{r}\hat{S}(pN_\nu)\hat{R}. \qquad (C.9)$$

It is clear that $\hat{\mathcal{R}}_\phi^4 = \hat{I}$, where $\hat{I}$ is the identity operator. The Wannier functions of the four-times rotated Hamiltonian are therefore identical to those of the unrotated Bloch states, and the four-times rotated Bloch states must therefore be identical to the original states: this verifies (C.8). A solution for the gauge transformation $\chi(k,\delta)$ can therefore be found such that the phase change under rotation of Bloch states, defined by (C.2), is $\theta = \pi L/2$.

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