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Von Neumann lattices of Wannier functions for Bloch electrons in a magnetic field

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The problem of Bloch electrons in a magnetic field in two dimensions can be reduced to a one-dimensional problem with a Hamiltonian $\hat{H}$ that is a periodic function of $\hat{x}$ and $\hat{p}$. Wannier functions can be defined for the sub-bands of the spectrum of this effective Hamiltonian. When the Chern class (quantized Hall conductance integer) of the sub-band is zero, the Weyl–Wigner formalism can be used to represent these Wannier functions by a von Neumann lattice. It is shown how this von Neumann lattice of Wannier functions can be defined for irrational as well as rational magnetic fields.

An important benefit from using the Weyl–Wigner formalism is that symmetries of the periodic potential are reflected by symmetries of the effective Hamiltonian in phase space. It is shown how the Wannier functions can be defined so that their Wigner functions have the point symmetries of the effective Hamiltonian.

An example of how these results can prove useful is given: if we take matrix elements of the Hamiltonian between the Wannier states of a sub-band, we derive a new effective Hamiltonian describing this sub-band, which is again a periodic function of coordinate and momentum operators. Since, by projecting onto a sub-band, we have also reduced the number of degrees of freedom, this operation is a renormalization group transformation. It is shown that the symmetry of the new effective Hamiltonian in phase space is the same as that of the original one. This preservation of symmetry helps to explain some unusual properties of the spectrum when the Hamiltonian has fourfold symmetry.

1. INTRODUCTION

This paper describes some results on Bloch electrons in a magnetic field in two dimensions, which are obtained by transforming the original two-dimensional problem on a lattice into a one-dimensional problem on a line. Since this transformation is not as well known as it might be, I will start by giving a brief description of how it works.

Peierls (1933) showed how to construct a single-band model for the problem of Bloch electrons in a magnetic field. If $\epsilon_n(\boldsymbol{k})$ is the Bloch dispersion relation for the nth band when the field $B = 0$, then the Peierls effective Hamiltonian describing the effect of a weak magnetic field is

$$\hat{H}_{\mathrm{eff}}^{(n)} = \epsilon_n\left(\frac{1}{\hbar}\hat{\boldsymbol{p}} - \frac{e}{\hbar}\boldsymbol{A}(\hat{\boldsymbol{r}})\right), \tag{1.1}$$

where $\boldsymbol{A}(\boldsymbol{r})$ is the vector potential. The basis set for this effective Hamiltonian is the set of lattice sites $\boldsymbol{R}$ corresponding to the lattice of Wannier functions for the crystal in the absence of a magnetic field. Although the Peierls Hamiltonian is only approximate, there is a function $\epsilon_n'(\boldsymbol{k})$ for which (1.1) is exact, and which tends toward $\epsilon_n(\boldsymbol{k})$ as $B \to 0$ (Blount 1962).

To reduce (1.1) to a one-dimensional effective Hamiltonian, we will choose $\boldsymbol{A}(\boldsymbol{r})$ to be the Landau gauge

$$\boldsymbol{A} = (0, Bx, 0), \tag{1.2}$$

and write

$$X = \left(\frac{1}{\hbar} p_y - \frac{eBx}{\hbar}\right) \mathscr{A}^{\frac{1}{2}}, \quad P = \frac{1}{\hbar} p_x \mathscr{A}^{\frac{1}{2}}, \tag{1.3}$$

where $\mathscr{A}$ is the area of unit cell. Since $\boldsymbol{A}(\boldsymbol{r})$ does not contain y, p_y is a good quantum number, and enters only as a parameter. The effective Hamiltonian (1.1) can now be written

$$\hat{H}_{\text{eff}}^{(n)} = \epsilon_n(\mathscr{A}^{-\frac{1}{2}}\hat{P}, \mathscr{A}^{-\frac{1}{2}}\hat{X}) = H(\hat{X}, \hat{P}), \tag{1.4}$$

where

$$[\hat{X}, \hat{P}] = \mathrm{i}\hbar^*, \quad \hbar^* = eB\mathscr{A}/\hbar. \tag{1.5}$$

We have expressed the original effective Hamiltonian in the form of a one-dimensional effective Hamiltonian $H(X, P)$ (equation (1.4)), which has been scaled so that the area of its unit cell in the (X, P) phase plane is $4\pi^2$. The 'Planck constant' in (1.5) is a dimensionless measure of the magnetic field: $\hbar^*/2\pi$ is the number of flux quanta per unit cell, and we will use the symbol β for this quantity. Because p_y enters as a parameter in X, the basis set for the new effective Hamiltonian (1.4) is the entire X axis. Thus the original two-dimensional problem on a lattice has been reduced to a one-dimensional problem on a line.

Apart from the simplification resulting from the reduction to a one-dimensional problem, there is another advantage in using the effective Hamiltonian (1.4). Symmetries of the Bloch dispersion relation $\epsilon_n(\boldsymbol{k})$ become symmetries of $H(X, P)$ in the phase plane; thus symmetries of the crystal lattice are represented in a transparent way. It is known that symmetries of the crystal lattice can have a dramatic effect on the nature of the spectrum and eigenstates when a magnetic field is applied (see Wilkinson 1984*a*, *b*).

We can also use a one-dimensional effective Hamiltonian, which is periodic in x and p, in the limit in which the lattice potential weakly perturbs a Landau level. In this case also, symmetries of the crystal lattice are represented by symmetries in the phase plane. Both types of one-dimensional effective Hamiltonian are discussed in more detail in Appendix A.

The Weyl–Wigner formalism for quantum mechanics provides a method for representing operators and density matrices as functions of phase-space coordinates. In §2 I introduce the Weyl association between operators and phase-space functions, and show that it is a natural tool to use in this problem, because the Weyl function of an operator transforms classically under translations, rotations and reflections in phase space (which correspond to equivalent operations in real space when $B = 0$). I will also introduce von Neumann lattices of states; these are sets of states with Wigner functions localized about the points of a lattice in

phase space. The main objective of this paper is to study the use of von Neumann lattices as a set of Wannier states for a sub-band of the spectrum of the effective Hamiltonian (1.4).

In §3, Wannier states for the effective Hamiltonian (1.4) will be introduced. These Wannier states can be defined whenever the dimensionless magnetic field β is rational, $\beta = p/q$. When $\beta = 1/q$ (i.e. $p = 1$), it is natural to try to represent these Wannier states as a von Neumann lattice in phase space. It is found that this is possible if and only if the Chern class (quantized Hall conductance integer) of the sub-band is zero. When this condition is satisfied, I will show how a von Neumann lattice of Wannier functions can be defined for irrational as well as rational fields. In §3 I also show how the states of the von Neumann lattice can be chosen so that the Wigner function of each state has the point symmetries of the effective Hamiltonian.

One motivation for studying Wannier functions stems from the fact that they are orthogonal to all states outside their own sub-band. Because of this, we can obtain an effective Hamiltonian describing a sub-band of the spectrum by taking matrix elements of the Hamiltonian between the Wannier states of that sub-band. This is essentially the same procedure as that used by Peierls to construct the original effective Hamiltonian (1.1) from Wannier states of the system when $B = 0$. The results of forming an effective Hamiltonian for a sub-band are, of course, entirely trivial when the magnetic field β is rational. When β is irrational, however, we find that the new effective Hamiltonian describing the sub-band is also a periodic function of position and momentum coordinates, like (1.4), but with a new value of $\hbar^*$. Since the number of degrees of freedom has also been reduced (by taking matrix elements between the states of one sub-band only), this operation is a renormalization group transformation. This renormalization group transformation will be described in §4, and it will be shown that if the von Neumann lattice of Wannier functions is prepared so that their Wigner functions have the point symmetry of the effective Hamiltonian, then the symmetry of the new effective Hamiltonian is the same as that of the original one. This preservation of symmetry has important implications for the structure of the spectrum and of the eigenstates. The renormalization group transformation that is described here is an exact version of an approximate method introduced previously by Suslov (1982) and Wilkinson (1984*a*).

2. The Weyl–Wigner formalism

In this section, I will introduce the Weyl–Wigner formalism and describe why it is useful for this problem. I introduce a set of operators that represent the rotation, translation and reflection symmetries of the effective Hamiltonian. I also describe the von Neumann lattice of states, which will be used in §3 to represent the Wannier functions of a sub-band.

2.1. *The Weyl correspondence and invariant quantization*

The Weyl correspondence (Weyl 1927) associates a function $A(x,p)$ to an operator $\hat{A}$; the operator is written

$$\hat{A} = \iint \mathrm{d}x\,\mathrm{d}p\, A(x,p)\,\hat{W}(x,p), \tag{2.1}$$

where the Weyl operator

$$\hat{W}(x,p) = \frac{\hbar}{2\pi}\iint \mathrm{d}X\,\mathrm{d}P \exp\left\{\frac{\mathrm{i}}{\hbar}\left[(p-\hat{p})\,P+(x-\hat{x})\,X\right]\right\}. \tag{2.2}$$

This operator basis is self inverse; if $W_{\mathrm{inv}}(x,p)$ is defined by

$$\mathrm{tr}\left[\hat{W}(x,p)\;\hat{W}_{\mathrm{inv}}(x',p')\right] = \delta(x-x')\,\delta(p-p') \tag{2.3}$$

then we find

$$\hat{W}_{\mathrm{inv}}(x,p) = \hat{W}(x,p). \tag{2.4}$$

Thus $A(x,p)$ is given by

$$A(x,p) = \mathrm{tr}\left[\hat{W}(x,p)\,\hat{A}\right]. \tag{2.5}$$

If the operator $\hat{A}$ is a density matrix, then $A(x,p)$ is called Wigner's function (Wigner 1932).

Basis operators other than (2.2) could be used (Mehta 1964), but the Weyl operator has some properties that make it especially suitable for analysing problems of Bloch electrons in a magnetic field. The Weyl correspondence has special properties with respect to linear canonical transformations. In one dimension these transformations take the form

$$\begin{bmatrix} x' \\ p' \end{bmatrix} = \tilde{M}\begin{bmatrix} x \\ p \end{bmatrix}, \quad \det \tilde{M} = 1, \tag{2.6}$$

and include rotations of the phase plane about the origin. The Weyl correspondence shows how to quantize the Hamiltonian in a way that is invariant under rotations of the phase plane, and also provides a classical representation of these rotations. This is very important in the present context since rotations in phase space correspond to rotations of the crystal lattice in real space.

There are two steps required to establish these results. First, note that linear transformations of phase space are generated by quadratic Hamiltonians $\mathscr{H}$. There is also a quantum evolution operator associated with $\mathscr{H}$, given by $\hat{U}(t) = \exp(\mathrm{i}\hat{\mathscr{H}}t/\hbar)$. Consider the time-dependent (Heisenberg) operator $\hat{A}(t) = \hat{U}(t)\,\hat{A}\,\hat{U}^{\dagger}(t)$. It can be shown that the Weyl function, $A_{\mathrm{W}}(x,p,t)$, of this operator evolves classically, i.e.

$$\frac{\partial A_{\mathrm{W}}}{\partial t} = \frac{\partial A_{\mathrm{W}}}{\partial x}\,\dot{x} + \frac{\partial A_{\mathrm{W}}}{\partial p}\,\dot{p} = \{A_{\mathrm{W}}, \mathscr{H}\}. \tag{2.7}$$

A proof of this result is given by Ozorio de Almeida & Hannay (1982) for the case in which A_{W} is a Wigner function; the general case is proved in just the same

way. The result only holds if $\mathscr{H}$ is quadratic, and if $A_{\mathrm{W}}(x,p,t)$ is obtained by using the Weyl operator (2.2).

The second point to note is that if the Hamiltonian of the system is expressed as a sum of functions h_i of linear combinations of x and p,

$$\hat{H} = H(\hat{x},\hat{p}) = \sum_i h_i(a_i\,\hat{x}+b_i\,\hat{p}), \tag{2.8}$$

then the Weyl function $H_{\mathrm{W}}(x,p)$ of the Hamiltonian is just the classical Hamiltonian

$$H_{\mathrm{W}}(x,p) = H(x,p) = \sum_i h_i(a_i\,x+b_i\,p). \tag{2.9}$$

Thus, since (by (2.7)) $H_{\mathrm{W}}(x,p)$ transforms classically under linear canonical transformations, and (by definition), so does the classical Hamiltonian $H(x,p)$, we see that if we express the Hamiltonian in the form (2.8), the results of quantizing this Hamiltonian are invariant under linear canonical transformations of phase space (2.6). Papers by Groenewold (1946), Baker (1958) and Balazs & Jennings (1983) contain many more useful results on the Weyl–Wigner formalism.

The effective Hamiltonian (1.4) can be expressed in the form (2.8) by writing it as a Fourier series. To avoid introducing too much notation, we will make a canonical transformation of the form (2.6), chosen so that the Hamiltonian is periodic on a square lattice in phase space of side 2π:

$$\hat{H} = H(\hat{x},\hat{p}) = \sum_{NM} h_{NM} \exp\{\mathrm{i}(N\hat{x}+M\hat{p})\}. \tag{2.10}$$

If the Hamiltonian originally had threefold rotational symmetry, shearing the phase space to make the lattice a square one disguises this symmetry. For this reason we will exclude these cases from consideration here; they do have some very interesting properties, however, which will be described in a later publication.

Now we evaluate the matrix elements of (2.10) in the x representation. The Schrödinger equation $\hat{H}\,|\psi\rangle = E\,|\psi\rangle$ becomes

$$\sum_M [\sum_N h_{NM} \exp\{\mathrm{i}(Nx+\tfrac{1}{2}M\hbar)\}]\,\psi(x+M\hbar) = E\psi(x), \tag{2.11}$$

i.e. the Schrödinger equation is a difference equation with periodic coefficients, with frequency $\beta = \hbar/2\pi$. Note that the Hamiltonian only couples a sequence of points x_n separated by a distance $\hbar$:

$$x_n = n\hbar+\delta. \tag{2.12}$$

The parameter δ is related to the quasi-momentum in the y-direction, p_y, in (1.3).

Finally, it may be helpful to give a specific example of an effective Hamiltonian. Suppose that the Bloch dispersion relation when $B = 0$ is

$$\epsilon(\boldsymbol{k}) = 2\alpha\cos k_x + \cos k_y. \tag{2.13}$$

The corresponding effective Hamiltonian is

$$\hat{H} = H(\hat{x},\hat{p}) = 2\cos\hat{p} + 2\alpha\cos\hat{x}, \tag{2.14}$$

and the Schrödinger equation (2.11) is

$$\psi(x+\hbar)+\psi(x-\hbar)+2\alpha\cos x\,\psi(x)=E\psi(x), \tag{2.15}$$

or

$$\psi_{n+1}+\psi_{n-1}+2\alpha\cos(2\pi\beta n+\delta)\,\psi_n=E\psi_n, \tag{2.16}$$

where $\psi_n=\psi(x_n)$. Equation (2.16) is known as Harper's equation (Harper 1955), and it may be useful to bear this simple model in mind in subsequent discussions.

2.2. *Symmetry operations in phase space*

Now we introduce operators that represent translations, rotations and reflections in phase space. The Weyl–Wigner functions of states and operators transform classically under the effect of these operators.

The operator

$$\hat{T}(X,P)=\exp\{\mathrm{i}(P\hat{x}-X\hat{p})/\hbar\} \tag{2.17}$$

shifts the Wigner function $W_\psi(x,p)$ of a state $|\psi\rangle$ through a vector (X,P) in the phase plane

$$W_{T\psi}(x,p)=W_\psi(x-X,p-P), \tag{2.18}$$

i.e. it plays the role of the translation operator in phase space. The composition

$$\hat{T}(X,P)\,\hat{T}(X',P')=\exp\{\mathrm{i}(X'P-XP')/2\hbar\}\,\hat{T}(X+X',P+P') \tag{2.19}$$

and the adjoint is

$$\hat{T}^\dagger(X,P)=\hat{T}(-X,-P). \tag{2.20}$$

The phase change on transporting a state anticlockwise about a circuit of area $\mathscr{A}$ is therefore $\mathscr{A}/\hbar$. The algebra of the phase-space translation operators is the same as that of the magnetic translation operators introduced by Peierls (1933).

The rotation operator has already been discussed; the operator

$$\hat{R}(\theta)=\exp\{\mathrm{i}(\hat{x}^2+\hat{p}^2+\hbar)\,\theta/2\hbar\} \tag{2.21}$$

rotates the Wigner function of a state clockwise through the angle θ. The factor of $\frac{1}{2}\hbar$ added to the harmonic oscillator Hamiltonian ensures that $\hat{R}(2\pi)=\hat{1}$ (instead of $-\hat{1}$ if this were omitted). If the Wigner function of a state $|\psi\rangle$ is localized in phase space near the origin, $\hat{R}(\theta)\,|\psi\rangle$ could be computed simply by expanding $|\psi\rangle$ in eigenstates of the harmonic oscillator Hamiltonian. If the Wigner function of $|\psi\rangle$ is not localized, however, this is impracticable, but $\hat{R}(\theta)\,|\psi\rangle$ can still be calculated quite easily by using the position-space representation of $\hat{R}(\theta)$ (Feynman & Hibbs 1965):

$$\left.\begin{aligned} |\psi'\rangle=\hat{R}(\theta)\,|\psi\rangle,\quad \psi'(x)=\int \mathrm{d}x'\,R(x,x',\theta)\,\psi(x),\\ R(x,x';\theta)=\left(\frac{1}{2\pi\mathrm{i}\hbar\sin\theta}\right)^{\frac{1}{2}}\exp\left\{\mathrm{i}\left[\frac{\theta}{2}+\frac{(x^2+x'^2)\cos\theta-2xx'}{2\hbar\sin\theta}\right]\right\}. \end{aligned}\right\} \tag{2.22}$$

Finally, a mirror symmetry about the line $p=0$ can be represented by the operation of taking the complex conjugate of the wavefunction. This symmetry will be denoted by the operator $\hat{M}$:

$$|\psi'\rangle=\hat{M}\,|\psi\rangle,\quad \psi'(x)=\psi^*(x). \tag{2.23}$$

2.3. *Two types of basis set*

The effective Hamiltonian (2.10) is invariant under a square lattice of translations in phase space, of side 2π. This suggests use of a basis set consisting of a set of functions $|n, m; \nu\rangle$, with the Wigner function of the state $|0, 0; \nu\rangle$ localized about a symmetry centre of this lattice, and the states $|n, m; \nu\rangle$ obtained by translating the state $|0, 0, \nu\rangle = |\nu\rangle$ by the vector $(2\pi n, 2\pi m)$:

$$|n, m, \nu\rangle = \hat{T}(2\pi n, 2\pi n)\,|\nu\rangle \tag{2.24}$$

(see figure 1). Such a set of states is a form of von Neumann lattice. Since the unit cell area is $4\pi^2$, we see that the number of states per unit Planck constant area is β, which is less than unity. The set of states (3.17) is therefore certainly incomplete. Our aim will, however, be to choose the generating state $|\nu\rangle$ in such a way that the von Neumann lattice (2.24) is a strictly complete basis for the νth sub-band of the spectrum of the effective Hamiltonian, and these states are therefore a form of Wannier function.

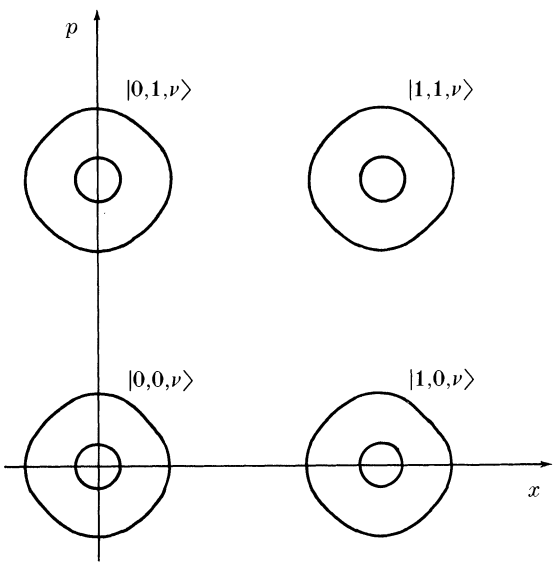

FIGURE 1. An illustration of the von Neumann lattice basis set, $|n, m; \nu\rangle$. The curves represent contours of the Wigner functions of the states.

The remainder of this section will describe how the von Neumann lattice states $|n, m; \nu\rangle$ can be transformed into another basis set, denoted by $|n; \delta; \nu\rangle$, which will be used in §3 to relate the von Neumann lattice to the conventional Wannier functions of the Schrödinger equation, (2.11) or (2.16).

To define the relation between the $|n, m; \nu\rangle$ and $|n; \delta; \nu\rangle$ basis sets we will consider a finite $(\mathcal{N} \times \mathcal{N})$ lattice of states in the phase plane

$$|n, m; \nu\rangle = \hat{T}(2\pi n, 2\pi m)\,|\nu\rangle, \quad \tfrac{1}{2}\mathcal{N} < n, m < \tfrac{1}{2}\mathcal{N}, \tag{2.25}$$

and later take the limit $\mathcal{N} \to \infty$. The $|n; \delta; \nu\rangle$ basis set is then given by

$$|n; \delta; \nu\rangle = \mathcal{N}^{-\frac{1}{2}} \sum_m \exp\{2\pi i(n\pi - \delta) m/\hbar\} |n, m; \nu\rangle, \tag{2.26}$$

where δ takes the values

$$\delta = l\hbar/\mathcal{N}, \quad l = 0, 1, \ldots, \mathcal{N}-1. \tag{2.27}$$

In the limit $\mathcal{N} \to \infty$, δ becomes a continuous variable, and it will become apparent that it is the same as the phase parameter δ introduced in (2.12).

The $|n; \delta; \nu\rangle$ states are, in effect, obtained by Fourier transforming the $|n, m; \nu\rangle$ states over m, and so are a unitary transformation of these states. To demonstrate the motivation for the definition (2.26), consider the position-space wavefunction of one of the $|n; \delta; \nu\rangle$ states:

$$\begin{aligned} \psi(x) &= \langle x | n; \delta; \nu\rangle \\ &= \mathcal{N}^{-\frac{1}{2}} \sum_m \exp\{2\pi i(n\pi - \delta) m/\hbar\} \langle x | n, m; \nu\rangle. \end{aligned} \tag{2.28}$$

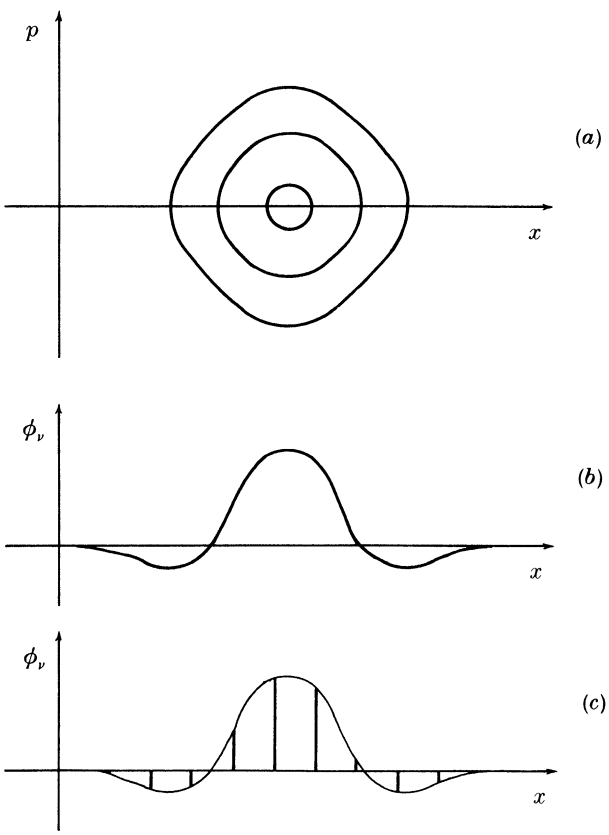

FIGURE 2. An illustration of the relation between the $|n, m; \nu\rangle$ basis and the $|n; \delta; \nu\rangle$ basis. (*a*) Contours of the Wigner function of the state $|n, 0; \nu\rangle$ in the phase plane. (*b*) Wavefunction of the state $|n, 0; \nu\rangle$. (*c*) Wavefunction of the state $|n; \delta; \nu\rangle$ is a Dirac δ-comb, sampling the wavefunction $\phi_\nu(x - 2\pi n)$ of the state $|n, 0; \nu\rangle$ with phase δ.

Now

$$\begin{aligned}\langle x\,|\,n,m;\,\nu\rangle &= \langle x\,|\,\hat{T}(2\pi n, 2\pi m)\,|\,\nu\rangle \\ &= \exp\left\{\frac{-2\pi^2 inm}{\hbar}\right\}\left\langle x\,\middle|\,\exp\left\{\frac{2\pi i m\hat{x}}{\hbar}\right\}\exp\left\{\frac{-2\pi i n\hat{p}}{\hbar}\right\}\middle|\,\nu\right\rangle \\ &= \exp\{-2\pi i(x+n\pi)\,m/\hbar\}\,\phi_\nu(x-2\pi n), \end{aligned} \tag{2.29}$$

where $\phi_\nu(x) = \langle x\,|\,\nu\rangle$, so that

$$\psi(x) = \mathscr{N}^{-\frac{1}{2}}\sum_m \exp\{2\pi i(x-\delta)\,m/\hbar\}\,\phi_\nu(x-2\pi n). \tag{2.30}$$

Thus, in the limit as $\mathscr{N}\to\infty$, $\psi(x)$ becomes the function $\phi_\nu(x)$ shifted through $2\pi n$ along the x-axis, and sampled on a comb of Dirac δ-functions at the points $x_k = k\hbar+\delta$ (see figure 2). Therefore the states $|\,n;\,\delta;\,\nu\rangle$, $|\,n';\,\delta';\,\nu\rangle$ are plainly orthogonal for $\delta\neq\delta'$. Also, since $\hat{H}$ contains only translation operators $\exp\{i\hat{Mp}\}$ shifting states by multiples M of $\hbar$, it is clear that $\hat{H}$ is diagonal with respect to δ. This fact makes the $|\,n;\,\delta;\,\nu\rangle$ basis important in intermediate stages of the calculations in §4.

3. Von Neumann lattices as Wannier functions

In this section the Wannier functions when β is a rational number of the form $\beta = 1/q$ are discussed, and it is shown how the generating state $|\,\nu\rangle$ of the von Neumann lattice can be chosen so that the $|\,n;\,\delta;\,\nu\rangle$ states are Wannier functions of a sub-band. The von Neumann lattice is only a useful basis set when the Chern class is zero; when M is non-zero the expansion of an arbitrary state in terms of the von Neumann lattice is not convergent. The von Neumann lattices of Wannier functions for irrational fields are also defined, and the method of constructing these states is shown. Finally, I show how the states $|\,\nu\rangle$ can be chosen so that their Wigner functions have the point symmetry of the effective Hamiltonian.

3.1. *Wannier functions when β is rational*

From the Schrödinger equation (2.11) or (2.16) we can see immediately that when β is rational, $\beta = p/q$, Bloch's theorem is applicable and the band is split into q sub-bands. Usually these sub-bands do not overlap and are separated from each other by finite gaps. (Harper's equation is special in this respect: since it is a second-order difference equation, the bands cannot overlap, but due to a physically non-generic symmetry the gaps can close; see Bellissard & Simon 1982.) When β is made irrational, the gaps in the spectrum persist for a sufficiently small change in β, but the structure of the spectrum and eigenstates changes dramatically. If we consider Harper's equation (2.16), and apply perturbation theory in α or $1/\alpha$, this suggests that the spectrum is a Cantor set (Avron & Simon 1981), although proving this is difficult (Simon 1982).

We will denote the Bloch states when β is rational by $|\,k,\,\delta;\,\nu\rangle$; k is the Bloch wavevector and ν is an index labelling the sub-band. The amplitudes ψ_n of these

wavefunctions are of the form

$$\psi_n = \exp\{ik\hbar n\}\, U_n(k, \delta, \nu), \tag{3.1}$$

where U_n is periodic with period q, $U_{n+q} = U_n$, and k has been normalized so that the wavefunction is periodic in k with period unity. We can form Wannier functions from these Bloch waves in the usual way by integrating over the wavevector. These Wannier functions are separated by a distance of q lattice sites along the x axis, i.e. their separation is $q\hbar$. If $\beta = 1/q$ (i.e. $p = 1$), then the separation of the Wannier functions in x is 2π, which suggests that they can be related to the von Neumann lattice introduced in §2.

To make the connection between the von Neumann lattice and the Wannier functions when $\beta = 1/q$, it is useful to consider the discrete amplitudes ψ_n to be obtained by sampling a continuous function $\psi_\nu(k, x)$ at regularly spaced intervals: let us write

$$\psi_n = \psi_\nu(k, x_n) \tag{3.2}$$

where

$$x_n = n\hbar + \delta, \quad \hbar = 2\pi\beta = 2\pi/q, \tag{3.3}$$

and the function $\psi_\nu(k, x)$ is of Bloch form

$$\psi_\nu(k, x+2\pi) = \mathrm{e}^{\mathrm{i}kx}\, \psi_\nu(k, x). \tag{3.4}$$

Apart from an overall phase, the Bloch states are periodic in δ with period $\hbar$, and in k with period unity. The analytic function $\psi_\nu(k, x)$ is not itself necessarily periodic in k however; in general it can be chosen to satisfy a periodicity condition of the form

$$\psi_\nu(k+1, x) = \mathrm{e}^{\mathrm{i}Mx/\hbar}\, \psi_\nu(k, x). \tag{3.5}$$

The integer M is a topological invariant, the Chern class, which characterizes the νth sub-band (Avron *et al.* 1983), and it is related to the quantized Hall conductance integer of the sub-band (Thouless *et al.* 1982); see Appendix B. Its interpretation is as follows: if the Bloch states have their overall phases fixed so that $|k, \delta; \nu\rangle$ is an analytic function of k and δ, then the phase change of the wavefunction on making a cycle around the edge of the 'Brillouin zone' in (k, δ) space is $2\pi M$. When M is non-zero, therefore, the Bloch states $|k, \delta; \nu\rangle$ cannot be expressed as an analytic and periodic function of k and δ: there must be some singularity in the phase of the Bloch states. When $\beta = 1/q$, it is usually the case that M is unity for one of the sub-bands and zero for the remainder (see Thouless *et al.* 1982; for Harper's equation with q even, the central pair of bands touch, and share the Hall current, but this degeneracy is destroyed by perturbations).

The value of the Chern class integer M has important implications for the Wannier functions. We will denote the Wannier states by the symbol $|n; \delta; \nu\rangle$, and the states introduced in §2 for which we used the same symbol can be identified with these Wannier states. The Bloch waves and Wannier functions are related by

$$\left.\begin{aligned} |k, \delta; \nu\rangle &= \mathscr{N}^{-\frac{1}{2}} \sum_n \mathrm{e}^{2\pi\mathrm{i}kn}\, |n; \delta; \nu\rangle, \\ |n; \delta; \nu\rangle &= \mathscr{N}^{-\frac{1}{2}} \sum_k \mathrm{e}^{-2\pi\mathrm{i}kn}\, |k, \delta; \nu\rangle. \end{aligned}\right\} \tag{3.6}$$

If $M = 0$, the wavefunction $|k, \delta; \nu\rangle$ can be obtained as an analtyic, periodic function of k and δ, and the Wannier states $|n; \delta; \nu\rangle$ are exponentially localized, and can be obtained by sampling an analytic, localized function $\phi_\nu(x)$ at a set of points x_k. If ψ_k are the amplitudes of the Wannier state $|n; \delta; \nu\rangle$, then

$$\psi_k = \phi_\nu(x_k - 2\pi n), \quad x_k = k\hbar + \delta. \tag{3.7}$$

Use of (3.2) in (3.6) gives $\phi_\nu(x)$ in terms of $\psi_\nu(k, x)$:

$$\phi_\nu(x) = \int \mathrm{d}k\, \psi_\nu(k, x). \tag{3.8}$$

If we identify the set of states $|n; \delta; \nu\rangle$ introduced in §2.3 with the Wannier functions, then by comparing (2.30) and (3.7), it is seen that $\phi_\nu(x)$ can be identified with the wavefunction of the state $|\nu\rangle$, which is used to generate the von Neumann lattice (2.24).

When M is non-zero, however, $\psi_\nu(k, x)$ cannot be an analytic, periodic function of k and an analytic function of x. The implications for the Wannier functions depend on how we choose the singularities of the phases of the Bloch waves. For instance, if we express $\psi_\nu(k, x)$ as an analytic function in x, it is not periodic in k (equation (3.5)), and so the Wannier states are a smooth function of δ, but are not well localized. Alternatively, we could make $\psi_\nu(k, x)$ analytic and periodic in k, but at the cost of introducing discontinuities along the x-axis at points separated by a distance $\hbar$. Then $\phi_\nu(x)$ would be well localized, but it would have discontinuities. Another possibility would be to introduce dislocations in the phase of the Bloch waves of total strength M. Then the function $\phi_\nu(x)$ would be neither well localized nor analytic (see figure 3).

3.2. *Von Neumann lattices and the Chern class*

Now we will consider in detail the question of whether a von Neumann lattice can be used as a Wannier function-like basis set for a sub-band when $\beta = 1/q$. In §3.1 we saw how to construct the wavefunction $\phi_\nu(x)$ of the state $|\nu\rangle$ so that the $|n; \delta; \nu\rangle$ states would be Wannier functions of the Schrödinger equation (2.11). We found that when the Chern class M is zero, we can choose $\phi_\nu(x)$ to be both well localized and an analytic function of x. The Wigner function of the state $|\nu\rangle$ will then be well localized in phase space.

If M is non-zero, however, the phase of the Bloch states $|k, \delta; \nu\rangle$ has singularities in the Brillouin zone, so that $\phi_\nu(x)$ is poorly localized or non-analytic, or both. This results in the Wigner function of the state $|\nu\rangle$ being poorly localized in x or p, or both. The Wigner function $W_\nu(x, p)$ will have power-law decay in at least one direction in phase space. The details of this depend on how we choose to arrange the singularities of the phase of the Bloch states. There must be either dislocation points, where the phase changes by $2\pi N$ on making a cycle about the point, with $\Sigma_i N_i = M$, or line discontinuities across which the phase of the Bloch waves changes abruptly. For the case in which the singularities are dislocation points, we can show that the Wigner function $W_\nu(x, p)$ of $|\nu\rangle$ has a r^{-4} decay law, where r measures distance in the phase plane. If there is a phase singularity along a line $\delta = \text{const.}$ or $k = \text{const.}$, the Wigner function decays as p^{-2} or x^{-2} respectively, and

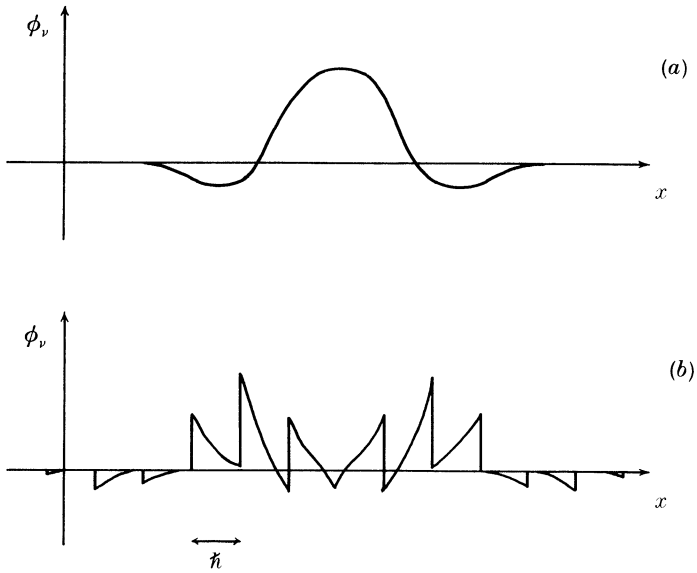

FIGURE 3. (*a*) When the Chern class is zero, the function $\phi_\nu(x)$ that defines the Wannier states is well localized and analytic. (*b*) When the Chern class is not equal to zero, $\phi_\nu(x)$ must be either not well localized, or non-analytic, or both. In this illustration, the Bloch states are an analytic, periodic function of k, but have discontinuities in δ. The function $\phi_\nu(x)$ is then well localized, but discontinuous.

is well localized in the other direction. These results are discussed in more detail in Appendix C.

If the von Neumann lattice is to be of any use as a basis set, the expansion of an arbitrary state $|\chi\rangle$ in the subspace spanned by the νth sub-band should be absolutely convergent. Thus, if we write

$$|\chi\rangle = \sum_{nm} a_{nm} |n, m; \nu\rangle, \tag{3.9}$$

the set of coefficients a_{nm} should satisfy

$$\sum_{nm} |a_{nm}| < \infty. \tag{3.10}$$

We will find that, because the Wigner functions of the states forming the von Neumann lattice are poorly localized when M is not zero, the condition (3.10) is not satisfied, and the von Neumann lattice is only a useful basis set when $M = 0$.

Since the states forming the von Neumann lattice are orthonormal (as they were derived from an orthogonal set of Wannier functions), we have $a_{nm} = \langle n, m; \nu | \chi \rangle$. We can find an expression for $|a_{nm}|$ in terms of the Wigner functions of the states $|\nu\rangle$ and $|\chi\rangle$: if $|a\rangle$ and $|b\rangle$ are two arbitrary states, then $|\langle a|b\rangle|^2 = \mathrm{tr}\,(\hat{\rho}_a \hat{\rho}_b)$, where $\hat{\rho}_a = |a\rangle\langle a|$, $\hat{\rho}_b = |b\rangle\langle b|$. Using (2.1), we have

$$\hat{\rho}_a = \iint \mathrm{d}x\,\mathrm{d}p\; W_a(x,p)\, \hat{W}(x,p), \tag{3.11}$$

where W_a is the Wigner function of $|a\rangle$ and $\hat{W}$ the Weyl operator. Then, using (2.3) and (2.4), we find

$$|\langle a|b\rangle|^2 = \iint \mathrm{d}x\,\mathrm{d}p\; W_a(x,p)\, W_b(x,p). \tag{3.12}$$

Hence we find

$$|a_{nm}|^2 = \iint \mathrm{d}x\,\mathrm{d}p\; W_\chi(x,p)\, W_\nu(x-2\pi n, p-2\pi m). \tag{3.13}$$

Knowing that the decay law of the Wigner function $W_\nu(x,p)$ is r^{-4} in two dimensions or x^{-2} in one dimension, we see that the coefficients a_{nm} decay as r^{-2} or x^{-1}, and the expansion (3.9) is therefore not convergent when M is not zero. These conclusions parallel those of Thouless (1984), who showed that the Wannier functions in two spatial dimensions are not well localized when the Hall conductance is not zero.

We could try to get over this problem by allowing non-orthogonal Wannier functions. Write

$$|n;\delta;\nu\rangle = \mathscr{N}^{-\frac{1}{2}} \sum_k \mathrm{e}^{2\pi \mathrm{i} nk} f(k,\delta)\,|k,\delta;\nu\rangle; \tag{3.14}$$

if $|f| = 1$ everywhere, then these states are the usual orthogonal Wannier functions, but if this constraint is dropped these states are no longer orthogonal. Suppose that the phases of the states $|k,\delta;\nu\rangle$ have been chosen so that there is a dislocation of strength M at the point (k^*, δ^*), where M is the Chern class. Let R be the distance from the point (k^*, δ^*) in the Brillouin zone. If we choose the function $f(k,\delta)$ so that near the dislocation point it vanishes as

$$f(k,\delta) \sim |R|^M, \tag{3.15}$$

then the state $f(k,\delta)\,|k,\delta;\nu\rangle$ is an analytic function of k and δ (but is not normalized). The Wannier functions (3.14) are then analytic functions of δ and are well localized, and the corresponding von Neumann lattice is made up of states with well localized Wigner functions. This set of states is still not of any use, however, since the expansion (3.9) still does not converge. Because the states forming the von Neumann lattice are no longer orthogonal, the coefficient a_{nm} is not given simply by $\langle n,m;\nu|\chi\rangle$; we find

$$a_{nm} = \mathscr{N}^{-\frac{1}{2}} \sum_k \sum_\delta (f(k,\delta))^{-1} \exp\{-2\pi\mathrm{i}[kn + (n\pi - \delta)\,m]\}\,\langle k,\delta;\nu|\chi\rangle \tag{3.16}$$

and hence

$$\sum_{nm} |a_{nm}|^2 = \frac{1}{N} \sum_k \sum_\delta \frac{|\langle k,\delta;\nu|\chi\rangle|^2}{|f(k,\delta)|^2}. \tag{3.17}$$

Because $f(k,\delta)$ has a zero at (k^*, δ^*) when $M \neq 0$, this quantity diverges for almost all states $|\chi\rangle$, and (3.10) will also diverge. Thus we conclude that von Neumann lattices can only be used as a basis set when the Chern class is zero, even if we are prepared to accept non-orthogonal basis states.

Finally, we comment that the non-orthogonal, localized states constructed using

(3.14) also have another disadvantage when $M \neq 0$, namely that they are not a complete set. Because $f(k, \delta)$ vanishes at (k^*, δ^*), the states (3.14) are all orthogonal to the Bloch state $|k^*, \delta^*; \nu\rangle$, so that this Bloch state cannot be reconstructed from these Wannier functions. There is an extensive mathematical literature of conventional von Neumann lattices of the type first described by von Neumann (1955) with one state per unit h area in phase space. This corresponds to the special case of $q = 1$ in our problem, so that there is only one sub-band, which has a Chern class $M = 1$. Several proofs have been published showing that these conventional von Neumann lattices are overcomplete by one state; see Bacry *et al.* (1976), Dana & Zak (1983), and references therein. There is no contradiction with the results of this paper, however, since these proofs only show that the conventional von Neumann lattice is an overcompleted basis for localized ($l^2(R)$) states, and the Bloch wave $|k^*, \delta^*; \nu\rangle$ is not in this space. Of course, the conventional von Neumann lattice is not of any use for numerical work since the expansion of typical states in terms of the von Neumann lattice does not converge.

3.3. *Wannier states and von Neumann lattices for irrational fields*

Up to this point, we have only considered von Neumann lattices of Wannier functions for rational magnetic fields, of the form $\beta = 1/q$. The discussion is now extended to irrational magnetic fields. When the magnetic field is changed from an initial rational value to some nearby irrational one, the gaps in the spectrum persist, but the eigenstates are no longer Bloch waves, so that the Wannier functions must be defined in a different way. We will require that our generalized von Neumann lattice of Wannier functions have the following properties.

(*a*) The states should tend toward those of the rational case as $\beta \to 1/q$.

(*b*) The states should be well localized in phase space (in the sense that their Wigner functions are localized).

(*c*) The states should form a strictly complete (i.e. complete but not overcomplete) basis for the νth sub-band.

(*d*) Every state should be orthogonal to every eigenstate not contained in the νth sub-band.

The motivation for (*c*) and (*d*) is that we want to decouple the νth sub-band from the rest of the spectrum, so that taking matrix elements of the Hamiltonian between these states provides a complete description of the sub-band. We will construct a set of states that satisfy these requirements by using a perturbative argument, in which the small parameter ϵ is the deviation of β from an initial rational value, $\epsilon = |\beta - 1/q|$, and we will only be able to show that these states are a complete set for sufficiently small ϵ. I will not give a fully detailed account of this work here, because a complete account of this and other work will be published elsewhere (Simon & Wilkinson 1985).

Our first step is to introduce a set of states satisfying all of the requirements except (*d*). We note that when the Chern class (quantized Hall conductance) is zero, the number of states per unit area in phase space remains constant as Planck's constant (the magnetic field) is altered; this result can be seen by using the Středa formula (Středa 1982). This suggests that we can still use a von Neumann lattice of states based on the same square lattice of spacing 2π. One way of justifying this

is to consider a finite but arbitrarily large system with periodic boundary conditions, with exactly the same number of von Neumann lattice states as are required to form a complete basis. These states are then a complete set provided they are linearly independent. Let $|\nu_0\rangle$ be the generating state of the von Neumann lattice when $\beta = \beta_0 = 1/q$, and $|\nu'\rangle = |\nu'(\beta)\rangle$ be any state which has a well localized Wigner function, and which tends toward the original generating state $|\nu_0\rangle$ as $\beta \to \beta_0 = 1/q$. The set of states

$$|n, m; \nu'\rangle = \hat{T}(2\pi n, 2\pi m)\,|\nu'\rangle \tag{3.18}$$

certainly satisfies conditions (*a*) and (*b*), and for sufficiently small $\epsilon = |\beta - 1/q|$ they are linearly independent, and therefore also satisfy (*c*). To see that this is the case, first note that in the rational case, $\beta_0 = 1/q$, the von Neumann lattice of Wannier functions is orthonormal. When we go to the irrational case, the normalization matrix is no longer exactly unity, and has additional terms of size $o(\epsilon)$. Since the states forming the lattice are well localized, the off-diagonal terms in the normalization matrix are short ranged, and the normalization matrix cannot suddenly become singular. For sufficiently small ϵ, therefore, the states (3.18) are linearly independent, and remain a complete set.

Now we will modify the states (3.18), so that they also satisfy condition (*d*). We will multiply the state $|\nu'\rangle$ by a projection operator $f_\nu(\hat{H})$ to obtain a new state $|\nu\rangle$, which will be used to generate our final basis set

$$|\nu\rangle = f_\nu(\hat{H})\,|\nu'\rangle, \tag{3.19}$$

$$|n, m; \nu\rangle = \hat{T}(2\pi n, 2\pi m)\, f_\nu(\hat{H})\,|\nu'\rangle. \tag{3.20}$$

In (3.19) $\hat{H}$ is the Hamiltonian (for the irrational field) and $f_\nu(E)$ is a function that is unity for values of E contained in the spectrum of the νth sub-band, and zero throughout the rest of the spectrum (again, we mean the spectrum at the irrational value of β). This ensures that condition (*d*) is satisfied.

We must check that in applying the projection operator we do not lose any of the properties (*a*), (*b*) and (*c*). It is easy to see that condition (*a*) is still satisfied. Condition (*b*) is rather more difficult, and causes us to be careful about how we choose the projection function $f_\nu(E)$. Because the νth sub-band is flanked by a pair of gaps, the function $f_\nu(E)$ can be chosen to be a smooth function of E (see figure 4). This implies that the projection operator $f_\nu(\hat{H})$ is localized, and the state $|\nu\rangle$ used to generate the lattice remains localized in phase space. A detailed discussion of this fact will be given in the forthcoming paper mentioned earlier. Lastly, consider condition *c*: we note that because $f_\nu(\hat{H})\,|\nu\rangle = |\nu\rangle$ exactly in the rational case, the state $|\nu\rangle$ differs from $|\nu'\rangle$ only by a small ($o(\epsilon)$) amount. Since the states of the von Neumann lattice also remain localized under a suitably chosen projection operator, they must still be linearly independent for sufficiently small ϵ, so that condition (*c*) is still satisfied.

Finally, we comment that a similar approach to forming generalized Wannier functions can be applied to many systems in which a part of the spectrum is isolated between a pair of gaps, and that translational invariance is not a

FIGURE 4. (*a*) The dark blocks represent the bands of the spectrum when $\beta = 1/q$. The νth sub-band is the central one of the three sub-bands shown. (*b*) When β is changed slightly, the spectrum is much more complicated, but the large gaps flanking the νth sub-band persist. (*c*) The projection function $f_\nu(E)$ can be chosen to be smooth, so that the projection operator is localized.

precondition for having well localized Wannier functions. This result was suggested in a paper by Kivelson (1982), but no general derivation was given.

3.4. *Symmetry of the von Neumann lattice*

It is desirable that the Wigner function of the state $|\nu\rangle$ used to generate the von Neumann lattice should have the point symmetries of the effective Hamiltonian. As well as being aesthetically satisfying, this will enable us to prove an important symmetry preservation principle for the renormalization group in §4. The Wigner function of $|\nu\rangle$ does not automatically have these symmetries, but because there is so much freedom in the way $|\nu\rangle$ is defined, it can be chosen in such a way as to satisfy these symmetry requirements. First I will show how, when β is rational, the phases of the Bloch waves can be chosen so that the Wigner function of $|\nu\rangle$ has all the required symmetries. Then I will show how these symmetries can be retained when we extend the definition of the von Neumann lattice to irrational values of β. Because we made a canonical transformation to make the lattice square, it is difficult to discuss cases in which the Hamiltonian originally had threefold or sixfold axes, so we will not consider these cases here. We will consider twofold and fourfold axes and mirror planes, as these are not affected by transforming to a square lattice.

When $\beta = 1/q$, The eigenstates are Bloch waves $|k, \delta; \nu\rangle$, and we find that the state $|\nu\rangle$ used to generate the von Neumann lattice is given by

$$|\nu\rangle = \mathcal{N}^{-1} \sum_k \sum_\delta |k, \delta; \nu\rangle. \tag{3.21}$$

In the limit $\mathcal{N} \to \infty$, therefore, the state $|\nu\rangle$ is obtained by integrating the Bloch waves over the 'Brillouin zone' in (k, δ) space. This equation (3.21) does not uniquely define $|\nu\rangle$ since the overall phases of the Bloch waves are arbitrary. I will show how to constrain these phases so that the Wigner function of $|\nu\rangle$ has the required symmetries; these constraints still do not uniquely determine $|\nu\rangle$.

We can simplify the notation slightly here by denoting the Bloch state $|k, \delta; \nu\rangle$ by $|\boldsymbol{K}\rangle$; we will suppose that the Chern class is zero, and that $|\boldsymbol{K}\rangle$ is analytic, periodic function of $\boldsymbol{K} = (k, \delta)$. The set of point symmetries is generated by a rotation R, and possibly also a reflection M, acting in the phase plane. In §2.2 the method of associating quantum mechanical operators $\hat{R}$ and $\hat{M}$ with these symmetry operations was shown. We find that when we apply a symmetry operator, for instance $\hat{R}$, to a Bloch state $|\boldsymbol{K}\rangle$, the result is (apart from an overall phase factor) a new Bloch state $|\boldsymbol{K}_{\mathrm{R}}\rangle$. We can see this by the following argument The Wigner function of the state $|k, \delta; \nu\rangle$ can be shown to consist of a square lattice of δ functions, located at the points $(x_{nm}, p_{nm}) = (\delta + n\hbar, k\hbar + m\hbar)$ in the phase plane, and the amplitudes of these δ functions are periodic in both n and m with a period of q lattice spacings. When we act on a state $|\boldsymbol{K}\rangle$ with an operator $\hat{R}$ or $\hat{M}$, the Wigner function of $|\boldsymbol{K}\rangle$ is transformed classically, so that this lattice of δ functions is rotated or reflected in the phase plane to give a new lattice, corresponding to another Bloch state $|\boldsymbol{K}_{\mathrm{R}}\rangle$ or $|\boldsymbol{K}_{\mathrm{M}}\rangle$. Thus we can write

$$\hat{R}|\boldsymbol{K}\rangle = \mathrm{e}^{\mathrm{i}\phi_{\mathrm{R}}(\boldsymbol{K})}|\boldsymbol{K}_{\mathrm{R}}\rangle, \quad \hat{M}|\boldsymbol{K}\rangle = \mathrm{e}^{\mathrm{i}\phi_{\mathrm{M}}(\boldsymbol{K})}|\boldsymbol{K}_{\mathrm{M}}\rangle, \tag{3.22}$$

where the phases $\phi_{\mathrm{R}}(\boldsymbol{K})$ and $\phi_{\mathrm{M}}(\boldsymbol{K})$ are analytic and periodic functions of $\boldsymbol{K}$.

Suppose we now make a phase transformation of the Bloch waves

$$|\boldsymbol{K}'\rangle = \mathrm{e}^{\mathrm{i}\theta(\boldsymbol{K})}|\boldsymbol{K}\rangle, \tag{3.23}$$

with $\theta(\boldsymbol{K})$ chosen so that $\phi_{\mathrm{K}}, \phi_{\mathrm{M}}$ vanish

$$\hat{R}|\boldsymbol{K}'\rangle = |\boldsymbol{K}'_{\mathrm{R}}\rangle, \quad \hat{M}|\boldsymbol{K}'\rangle = |\boldsymbol{K}'_{\mathrm{M}}\rangle. \tag{3.24}$$

The set of Bloch waves $|\boldsymbol{K}'\rangle$ is now completely invariant under all the point symmetry operations. The state $|\nu\rangle$ will then be invariant under $\hat{R}$, and if necessary also under $\hat{M}$,

$$\hat{R}|\nu\rangle = \hat{M}|\nu\rangle = |\nu\rangle, \tag{3.25}$$

and its Wigner function will therefore have all the required symmetries. The method for choosing the phase transformation $\theta(\boldsymbol{K})$ is discussed in Appendix D.

Now let us consider how the state $|\nu\rangle$ can be chosen to have the correct symmetries when β is made irrational. Recall from §3.3 that there are two steps involved; first we choose a state $|\nu'\rangle$ to act as the generating state of the von Neumann lattice. This state is arbitrary, apart from the property that it must tend toward a generating state $|\nu_0\rangle$ for the rational hold case as $\beta \to 1/q$. The second step is to act on the state $|\nu'\rangle$ with the projection operator $f_\nu(\hat{H})$ to ensure orthogonality between sub-bands.

First, let us consider the choice of the state $|\nu'\rangle$. Suppose that $|\nu_0\rangle$ is a generating state for the rational case $\beta = 1/q$, and has all the required symmetries in the phase

plane. We will define the state $|\nu'\rangle$ as follows: if $W_{\nu_0}(x,p)$ is the Wigner function of $|\nu_0\rangle$, we write

$$W_{\nu'}(x,p) = W_{\nu_0}(cx, cp), \tag{3.26}$$

where the scale factor c is chosen so that the Wigner function still represents the density matrix of a pure state after $\hbar = 2\pi\beta$ has been changed:

$$c = (\hbar_0/\hbar)^{\frac{1}{2}} = (\beta q)^{-\frac{1}{2}}. \tag{3.27}$$

The definition (3.26) of the state $|\nu'\rangle$ automatically ensures that it has the required symmetries. We must now show that the final generating state $|\nu\rangle = f_\nu(\hat{H})|\nu'\rangle$ also has these symmetries. Suppose that the projection operator is expanded as a power series in $\hat{H}$:

$$f_\nu(\hat{H}) = \sum_n A_n \hat{H}^n. \tag{3.28}$$

It can be shown that the product of two operators with a given set of point symmetries in phase space also has these symmetries. By using (3.28), therefore, the Wigner function of $|\nu\rangle$ can be written as a sum of terms, each having the point of symmetry of the Hamiltonian.

4. The renormalized effective Hamiltonian

In this section we take matrix elements of the Hamiltonian between the Wannier functions $|n;\delta;\nu\rangle$, and find that the resulting Schrödinger equation is a difference equation with periodic coefficients. We can interpret this Schrödinger equation as resulting from quantizing a new effective Hamiltonian, $\hat{H}^{(1)}$, which is also a periodic function of a phase-plane coordinates. If the Wigner function of the generating state $|\nu\rangle$ has the point symmetries of the original effective Hamiltonian, then the symmetry of $\hat{H}^{(1)}$ is the same as that of $\hat{H}$. This renormalization group can therefore preserve the symmetry of the Hamiltonian. The unusual spectrum associated with Hamiltonians with fourfold symmetry is explained by the attracting fixed points having twofold symmetry; because of the preservation of symmetry, fourfold symmetric Hamiltonians are stuck on a critical surface.

4.1. *Matrix elements in Wannier function basis*

Now we calculate matrix elements of the Hamiltonian $\hat{H}$ between the Wannier functions $|n;\delta;\nu\rangle$. When β is rational, of the form $\beta = 1/q$, these matrix elements are independent of n, as expected. When β is irrational, however, we will find that the Schrödinger equation in this reduced basis is again a difference equation with periodic coefficients (cf. Harper's equation (2.16)). Since, in the irrational case, the Wannier functions $|n;\delta;\nu\rangle$ are no longer exactly orthogonal within the band, we must also calculate the normalization matrix elements between these states.

We will express the matrix elements between the $|n;\delta;\nu\rangle$ states, i.e. the Wannier functions, in terms of states of the von Neumann lattice $|n,m;\nu\rangle$. This

allows the effects of symmetries to be investigated. Using the relation (2.26), we find

$$\langle n;\delta;\nu|\hat{H}|n';\delta';\nu\rangle$$

$$=\frac{1}{\mathcal{N}}\sum_{m}\sum_{m'}\exp\left\{\frac{-2\pi\mathrm{i}}{\hbar}(\delta' m'-\delta m)\right\}$$

$$\times\exp\left\{\frac{4\pi^2\mathrm{i}}{\hbar}\left(\frac{nm-n'm'}{2}\right)\right\}\langle n',m';\nu|\hat{H}|n,m;\nu\rangle$$

$$=\frac{1}{\mathcal{N}}\sum_{m}\sum_{m'}\exp\left\{\frac{-2\pi\mathrm{i}}{\hbar}(\delta' m'-\delta m)\right\}$$

$$\times\exp\left\{\frac{4\pi^2\mathrm{i}}{\hbar}\left(\frac{n+n'}{2}\right)(m'-m)\right\}\langle n'-n,m'-m;\nu|\hat{H}|0,0;\nu\rangle$$

$$=\frac{1}{\mathcal{N}}\sum_{\substack{j\\(j+J)\ \mathrm{mod}\ 2=0}}\sum_{J}\exp\left\{\frac{-2\pi\mathrm{i}}{\hbar}\left(\frac{\delta+\delta'}{2}\right)j\right\}\exp\left\{\frac{4\pi^2\mathrm{i}}{\hbar}\left(\frac{n+n'}{2}\right)j\right\}$$

$$\times\exp\left\{\frac{2\pi\mathrm{i}(\delta'-\delta)J}{\hbar}\right\}\langle n'-n,j;\nu|\hat{H}|\nu\rangle$$

$$=\frac{1}{\mathcal{N}}\sum_{J=-\infty}^{\infty}\exp\left\{\frac{2\pi\mathrm{i}(\delta'-\delta)J}{\hbar}\right\}\left[\sum_{j=0,\,\pm2,\,\pm4,\,\ldots}\exp\left\{\frac{2\pi\mathrm{i}}{\hbar}\left(\frac{\delta+\delta'}{2}\right)j\right\}\right.$$

$$\times\exp\left\{\frac{4\pi^2\mathrm{i}}{\hbar}\left(\frac{n+n'}{2}\right)j\right\}\langle n'-n,j,\nu|\hat{H}|\nu\rangle$$

$$+\sum_{j=1,\,1\pm2,\,1\pm4\ldots}\exp\left\{\frac{-2\pi\mathrm{i}}{\hbar}(\delta'-\delta)\right\}\exp\left\{\frac{-2\pi\mathrm{i}}{\hbar}\left(\frac{\delta+\delta'}{2}\right)j\right\}$$

$$\left.\times\exp\left\{\frac{4\pi^2\mathrm{i}}{\hbar}\left(\frac{n+n'}{2}\right)j\right\}\langle n'-n,j,\nu|\hat{H}|\nu\rangle\right]. \tag{4.1}$$

In the limit $\mathcal{N}\to\infty$, we can put

$$\frac{1}{\mathcal{N}}\sum_{J}\exp\left\{\frac{2\pi\mathrm{i}(\delta'-\delta)J}{\hbar}\right\}\xrightarrow[\mathcal{N}\to\infty]{}\Delta(\delta'-\delta)=\begin{cases}0 & \delta\neq\delta',\\ 1 & \delta=\delta',\end{cases} \tag{4.2}$$

so that in this limit

$$\langle n';\delta';\nu|\hat{H}|n;\delta;\nu\rangle$$

$$=\Delta(\delta'-\delta)\sum_{j}\exp\left\{\frac{-2\pi\mathrm{i}\delta j}{\hbar}\right\}\exp\left\{\frac{4\pi^2\mathrm{i}}{\hbar}\left(\frac{n+n'}{2}\right)j\right\}\langle n'-n,j;\nu|\hat{H}|\nu\rangle. \tag{4.3}$$

By setting $\hat{H}=\hat{1}$, we find a similar formula for the normalization operator.

$$\langle n';\delta';\nu|n;\delta;\nu\rangle=\Delta(\delta'-\delta)\sum_{j}\exp\left\{\frac{-2\pi\mathrm{i}\delta j}{\hbar}\right\}\exp\left\{\frac{4\pi^2\mathrm{i}}{\hbar}\left(\frac{n+n'}{2}\right)j\right\}\langle n'-n,j,\nu|\nu\rangle. \tag{4.4}$$

As expected, the Hamiltonian and normalization matrix are diagonal with respect to the label δ, and they are in the form of a Jacobi matrix with respect to n with

periodic coefficients. In the special case when $\hbar/2\pi = \beta = 1/q$, of course, we find that the matrix elements depend only on $n'-n$, so the Hamiltonian can be diagonalized by Bloch waves.

Now let us consider the constraints imposed by symmetry on the matrix elements appearing on the right side of (4.3) and (4.4). We can think of these matrix elements $H_{nm} = \langle n, m; \nu | \hat{H} | \nu \rangle$ and $N_{nm} = \langle n, m; \nu | \nu \rangle$ as points on a lattice (cf. figure 1). Because the Hamiltonian and normalization operators are Hermitian

$$H_{n,m} = H^*_{-n,-m}, \tag{4.5}$$

and similarly for N_{nm}. To use information about symmetries for the crystal lattice, we will assume that the state $|\nu\rangle$ has been defined so that its Wigner function has the point symmetries of the lattice. Fist, we consider rotational symmetries. If two lattice points, n, m and n', m' are related by a rotational symmetry of the effective Hamiltonian, we find that

$$H_{n'm'} = = H_{nm}. \tag{4.6}$$

It is obvious that the magnitudes of these quantities are the same, but it is less clear that they have the same phase. To prove (4.6), we need to show that

$$\hat{R}(\theta)\,\hat{T}(\boldsymbol{R}) = \hat{T}(\boldsymbol{R}')\,\hat{R}(\theta), \tag{4.7}$$

where $\boldsymbol{R}'$ is obtained from $\boldsymbol{R}$ by rotation through the angle θ. This relation is easily shown to be true for Gaussian coherent states, and since these operators act classically on the Wigner function of a state it is true for any state, apart from a complex phase factor. Because any state can be expanded in coherent states, (4.7) is therefore true in general. Since the Bloch dispersion relation, and therefore the effective Hamiltonian, have inversion symmetry we see from (4.5) and (4.6) that all of the coefficients H_{nm} and N_{nm} are real. Finally, if n, m and n', m' are points related by a reflection, we can show that

$$H_{n'm'} = H^*_{nm}. \tag{4.8}$$

Since all the coefficients are real, these coefficients are therefore equal. The final result is that all of the matrix elements H_{nm} and N_{nm} are real, and any pair related by any symmetry operation are equal.

It may be helpful to the reader to remark that, as β tends toward the original rational value $1/q$, the coefficients H_{nm} become the Fourier coefficients of the energy of the Bloch band as a function of k and δ:

$$\sum_{nm} H_{nm}\, \mathrm{e}^{2\pi \mathrm{i} k m}\, \mathrm{e}^{2\pi \mathrm{i}\delta n/\hbar} \xrightarrow[\beta \to 1/q]{} \epsilon_\nu(k, \delta). \tag{4.9}$$

Also, in the same limit,

$$N_{nm} \xrightarrow[\beta \to 1/q]{} \delta_{n0}\,\delta_{m0}. \tag{4.10}$$

4.2. *A new effective Hamiltonian*

Recall that we began with an effective Hamiltonian $H(\hat{x}, \hat{p})$, which was a periodic function of $\hat{x}$ and $\hat{p}$ (for example (2.14)), and expressed the Schrödinger equation as a difference equation with periodic coefficients (for example (2.16)). Later, when

we took matrix elements between the Wannier functions of a sub-band, we found that the Schrödinger equation remained in this form (see (4.3), (4.4)). Now we will invert our first operation and express the new Schrödinger equation in terms of an effective Hamiltonian and normalization operator that are periodic functions in phase space.

First it will be useful to introduce a new basis set $|n;\delta_1;\nu)$, which is in one to one correspondence with the $|n;\delta;\nu\rangle$ basis, but which is orthonormal,

$$(n';\delta_1';\nu|n;\delta_1;\nu) = \delta_{nn'}\Delta(\delta_1-\delta_1'). \tag{4.11}$$

This is just a formal device to enable us to represent the normalization matrix as an operator. We will find a new effective Hamiltonian operator $\hat{H}_\nu^{(1)}$ and normalization operator $\hat{N}_\nu^{(1)}$ whose matrix elements in the $|n;\delta_1;\nu)$ basis are the same as those of the original Hamiltonian $\hat{H}$ and the normalization matrix in the $|n;\delta;\nu\rangle$ basis.

The periodicity of the coefficients of the Jacobi matrices (4.3), (4.4) is different from the periodicity on the original Schrödinger equation (for example (2.16)). This suggests defining a new Planck constant $\hbar_1$, given by

$$\hbar_1 = 2\pi\beta_1, \quad \beta_1 = 1/\beta - [1/\beta], \quad \beta = \hbar/2\pi. \tag{4.12}$$

The square brackets in (4.12) denote the integer part of $1/\beta$. Also, by analogy with (3.7), we write

$$x_n^{(1)} = n\hbar_1 + \delta_1, \quad \delta_1 = \delta/\beta, \tag{4.13}$$

which defines the new coordinate $x^{(1)}$. Finally we define a new momentum $p^{(1)}$ by writing

$$[\hat{x}^{(1)}, \hat{p}^{(1)}] = \mathrm{i}\hbar_1. \tag{4.14}$$

Now let us introduce the operators $\hat{H}_\nu^{(1)}$ and $\hat{N}_\nu^{(1)}$, which we write in the form

$$\left.\begin{aligned}\hat{H}_\nu^{(1)} &= \sum_{NM} H_{NM\nu}^{(1)} \exp\{\mathrm{i}(N\hat{x}^{(1)} + M\hat{p}^{(1)})\},\\ \hat{N}_\nu^{(1)} &= \sum_{NM} N_{NM\nu}^{(1)} \exp\{\mathrm{i}(N\hat{x}^{(1)} + M\hat{p}^{(1)})\},\end{aligned}\right\} \tag{4.15}$$

which is analogous to the original effective Hamiltonian (1.4). Using (4.13), we have a correspondence between points along the $x^{(1)}$-axis and the states $|n;\delta_1;\nu)$. We define the matrix elements of $\hat{H}^{(1)}$ in the $|n;\delta;\nu)$ representation to be the matrix elements of this operator between corresponding states in the $x^{(1)}$ representation. Taking matrix elements of (4.15) in the $x^{(1)}$ representation, and using this definition, we find

$$\left.\begin{aligned}(n';\delta_1';\nu|\hat{H}_\nu^{(1)}|n;\delta_1;\nu) &= \Delta(\delta_1'-\delta_1)\\ &\quad\times\sum_j H_{j,n'-n,\nu}^{(1)} \exp\{\mathrm{i}j\delta_1\} \exp\{\tfrac{1}{2}\mathrm{i}(n+n')\hbar_1 j\}\\ (n';\delta_1';\nu|\hat{N}_\nu^{(1)}|n;d_1;n) &= \Delta(\delta_1'-\delta_1)\\ &\quad\times\sum_j N_{j,n'-n,\nu}^{(1)} \exp\{\mathrm{i}j\delta_1\} \exp\{\tfrac{1}{2}\mathrm{i}(n+n')\hbar_1 j\}\end{aligned}\right\} \tag{4.16}$$

Taking account of (4.12), (4.13), and comparing this result (4.16) with (4.3) and (4.4), we require that

$$\left.\begin{aligned}(n';\delta_1';\nu|\hat{H}_\nu^{(1)}|n;\delta_1;\nu) &= \langle n';\delta';\nu|\hat{H}|n;\delta;\nu\rangle,\\ (n';\delta_1';\nu|\hat{N}^{(1)}|n;\delta_1;\psi) &= \langle n';\delta';\nu|n;\delta;\psi\rangle.\end{aligned}\right\} \tag{4.17}$$

This gives us the Fourier coefficients of the effective Hamiltonian and normalization operators:

$$H^{(1)}_{NM\nu} = \langle N, M, \nu|\hat{H}|\nu\rangle, \quad N^{(1)}_{NM\nu} = \langle N, M, \nu|\nu\rangle. \tag{4.18}$$

This completes our renormalization group transformation; (4.15) and (4.18) define the new effective Hamiltonian, and (4.12) defines the new value of Planck's constant.

The renormalization group transformation preserves the symmetries of the Hamiltonian. In section 4.1, it was shown that the lattices of matrix elements $H_{nm} = \langle n, m, \nu|\hat{H}|\nu\rangle$ and $N_{nm} = \langle n, m, \nu|\nu\rangle$ have all the point symmetries of the effective Hamiltonian $\hat{H}$. Equation (4.18) shows that these matrix elements are just the Fourier coefficients of the new effective Hamiltonian, $\hat{H}^{(1)}$. Therefore $\hat{H}^{(1)}$ and $\hat{H}$ have the same symmetry in their respective phase spaces.

Finally, we note that it is possible to transform to an orthonormal basis, and so eliminate the normalization operator, $\hat{N}^{(1)}$. This can be done in the usual way, by multiplying both sides of the Schrödinger equation

$$(\hat{H}^{(1)} - E\hat{N}^{(1)})|\psi\rangle = 0 \tag{4.19}$$

by $(\hat{N}^{(1)})^{-\frac{1}{2}}$. Since $\hat{N}^{(1)}$ is assumed to be non-singular, $(\hat{N}^{(1)})^{-\frac{1}{2}}$ exists, and if we write $\hat{N}^{(1)} = \hat{1} + \hat{\epsilon}$, we can expand it in powers of $\hat{\epsilon}$. We recall that the product of two operators with a given phase-space symmetry (of their Weyl functions) also has this symmetry. Since the transformation to an orthonormal basis is expressed in terms of products of operators all having the same symmetry, the symmetry of the Hamiltonian $\hat{H}^{(1)}_\nu$is still preserved when we transform to an orthonormal basis.

4.3. *Implications of the renormalization group transformation*

The renormalization group transformation derived above describes each sub-band ν that has zero quantized Hall conductance in terms of a new effective Hamiltonian, $\hat{H}^{(1)}_\nu$, and a new dimensionless magnetic field β_1 (or a new 'Planck constant', $\hbar_1 = 2\pi\beta_1$). Every sub-band ν' of this new effective Hamiltonian that has zero Hall current can itself be described by a new effective Hamiltonian $\hat{H}^{(2)}_{\nu'}$, and dimensionless magnetic field β_2. The mapping of β is related to its continued fraction expansion

$$\beta = \cfrac{1}{n_1 + \cfrac{1}{n_2 + \cfrac{1}{n_3 + \ldots}}} = [n_1, n_2, n_3, \ldots]. \tag{4.20}$$

We find that $\beta_1 = [n_2, n_3, n_4, \ldots]$, $\beta_2 = [n_3, n_4, \ldots]$, etc. We stress that this transformation can only be iterated when the Chern class of every sub-band in the sequence is zero. Wannier functions can be defined for irrational fields when the

Chern class is non zero, but this has not been done in this paper because these Wannier functions cannot be represented as a von Neumann lattice. By using these Wannier functions, a renormalization group can be defined for these sub-bands also, but the renormalization of β is different from the scheme described above.

To understand the meaning of the new effective Hamiltonian, $\hat{H}_\nu^{(1)}$, it is useful to consider the limit in which β is very close to the original rational value, $1/q$. Noting (4.9) and (4.15), we see that

$$\hat{H}_\nu^{(1)}(\hat{x}^{(1)}, \hat{p}^{(1)}) \xrightarrow[\beta \to 1/q]{} \epsilon_\nu(\delta/2\pi\hbar_1, k/2\pi\hbar), \tag{4.21}$$

i.e. in this limit the renormalized Hamiltonian is derived from the dispersion relation $\epsilon_\nu(k, \delta)$ of the Bloch band when $\beta = 1/q$ by replacing δ and k with position and momentum operators $\hat{x}^{(1)}$ and $\hat{p}^{(1)}$. This is very similar to the Peierls substitution method for obtaining the original effective Hamiltonian (1.4) from the dispersion relation in zero field.

I have stressed that the renormalization group transformation preserves the symmetry of the effective Hamiltonian in phase space. The reason for emphasizing this point is that Hamiltonians with a fourfold symmetry in phase space have special properties, which the preservation of symmetry by the renormalization group transformation helps to explain. The most remarkable property of these Hamiltonians with fourfold symmetry is that the spectrum appears to be a *fractal* Cantor set of measure zero, with a remarkable hierarchical structure that is related to the continued fraction expansion of β (Wilkinson 1984*a*, *b*), whereas perturbation theory suggests that the spectrum should be a Cantor set of finite measure (Avron & Simon 1981). At first sight it appears that the renormalization group should always predict that the measure of the spectrum is zero: it derives a new Hamiltonian describing the structure of the spectrum between a pair of gaps (see figure 5), and there are gaps within the spectrum of this new Hamiltonian. The measure of the energies that are known not to lie on a gap might therefore be expected to decrease to zero. The mechanism of the renormalization group transformation can be reconciled with the expectation that the spectrum is normally a Cantor set of finite measure, however. If we assume that the Hamiltonian is mapped by the renormalization group transformation towards a fixed-point Hamiltonian with no gaps in the spectrum, then this apparent contradiction is resolved. Hamiltonians of the form $f(\alpha_1 x + \alpha_2 p)$, where f is a periodic function and α_1, α_2 constants, have no gaps in their spectrum and the fixed-point Hamiltonian would be of this type. Thus, under the action of the renormalization group transformation the periodic dependence of the Hamiltonian on one direction in phase space becomes weaker and weaker. Now recall that the renormalization group transformation preserves the symmetry of the Hamiltonian in phase space. If the initial Hamiltonian has fourfold symmetry, it cannot than be mapped towards a fixed-point Hamiltonian depending on only one phase-space coordinate, whereas a Hamiltonian without 'isotropic' symmetry can be mapped towards such a fixed point without a change of symmetry.

Thus the preservation of symmetry explains why the gaps in the spectrum do not become vanishingly small as we iterate the renormalization group

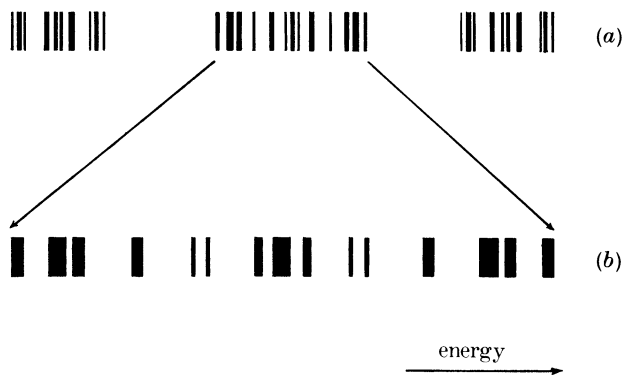

FIGURE 5. (*a*) The spectrum of the original Hamiltonian H. (*b*) The spectrum of the renormalized Hamiltonian $\hat{H}^1_\nu$ is the same as that part of the spectrum of $\hat{H}$ contained in the νth sub-band. By iterating the renormalization group transformation, the fine detail in the structure of the spectrum can be studied.

transformation for a Hamiltonian with fourfold symmetry. These results do not, unfortunately, provide a full explanation of why the measure of the spectrum is zero for these systems, since the von Neumann lattice, and therefore the renormalization group transformation, have only been defined for sub-bands for which the Chern class is zero. We can only use this renormalization group transformation to study those hierarchies of sub-bands for which the Chern class of every sub-band is zero.

The renormalization group scheme that has been described here is exact, in the sense that it could be implemented on a computer with the only approximations coming from numerical truncations. An approximate version of this method has previously been described by Suslov (1982) and independently by Wilkinson (1984*b*), who used W.K.B. methods to construct approximate Wannier functions and calculate approximate matrix elements in the semiclassical ($\hbar \to 0$) limit. In these papers the preservation of symmetry was only shown in an approximate way, in terms of W.K.B. theory, and it was not possible to give a precise criterion to determine for which sub-bands the von Neumann lattice of Wannier functions would exist. As well as providing an exact formalism for computation of this renormalization group, this paper has justified many of the results of the earlier work by proving that the preservation of symmetry is an exact result, and has provided a precise criterion for the existence of a suitable von Neumann lattice basis set in terms of the Chern class of the sub-band.

5. Conclusions and summary

Throughout this paper we have used a one-dimensional representation of the problem of Bloch electrons in two dimensions in a perpendicular magnetic field. The three-dimensional problem can be treated in a similar way, reducing it to a one-parameter family of one-dimensional Hamiltonians. We have discussed the two-dimensional problem primarily because it is more interesting; the Cantor set spectrum and the connections with the quantized Hall effect are special to the two-dimensional system.

It has been shown that the Weyl–Wigner formalism is a useful tool for the working on this problem, since it shows how to quantize the Hamiltonian correctly and how to represent symmetries of the effective Hamiltonian by classical symmetry transformations of the Wigner functions in phase space. This is possibly the only problem of physical interest for which the Weyl–Wigner formalism could be a useful computational tool, since it is very unusual for symplectic (linear canonical) transformations to have an important physical meaning.

We have considered the Wannier functions of the one-dimensional effective Hamiltonian, and it has been shown that they can be represented by a von Neumann lattice in phase space if an only if the Chern class (quantized Hall conductance integer) of the sub-band is zero.

Von Neumann lattices of Wannier functions can also be constructed even when the magnetic field is irrational, and the eigenstates of the Hamiltonian are not Bloch waves. In this case we take as our definition of Wannier functions that they should be a complete set for their own sub-band, and orthogonal to every state outside their own sub-band. Since a perturbative argument was used, this result has only been demonstrated for irrational fields β that are sufficiently close to a rational field of the form $\beta = 1/q$. At present there is no proof that a complete von Neumann lattice can be constructed for every value of β.

Dana & Zak (1985) have considered a problem related to the problem of defining Wannier functions for irrational fields. They have considered the problem of defining a set of N different lattices of localized basis states which should be capable of reproducing the Bloch waves of a set of N different bands. They conclude that this is possible if and only if the sum of the Chern classes of the N bands is zero.

It has also been shown that the states forming these von Neumann lattices can be chosen so that their Wigner functions have the point symmetries of the Hamiltonian. Threefold and sixfold symmetries have been excluded, partly because this would have required more complicated notation and partly because these cases have some special properties that will be discussed in a later publication.

Having succeeded in defining a set of Wannier functions for irrational fields, it is a natural step to calculate matrix elements of the Hamiltonian between these Wannier functions; this operation gives a new Schrödinger equation describing the νth sub-band only. We found that this new Schrödinger equation is a difference equation with periodic coefficients, and that it can be thought of as resulting from the quantization of a new effective Hamiltonian, which is also a periodic function of position and momentum. Thus each sub-band with zero quantized Hall conductance can be described by a renormalized effective Hamiltonian and Planck's constant. It is also possible to construct Wannier functions for irrational fields when the quantized Hall conductance of the sub-band is not zero, and this also leads to a renormalization group transformation, with a slightly different rule for the renormalization of the Planck constant. I did not describe this here, because the construction of the Wannier functions is quite complicated, and they cannot be represented as a von Neumann lattice. This work will be described in a joint paper with B. Simon.

The results of this paper are the first description of an exact renormalization group that can be used to analyse the fine structure of the Cantor set spectrum,

as well as providing information about the structure of the eigenstates. Previously Ostlund & Pandit (1984) have described an exact renormalization group applicable to Harper's equation, but since they used a transfer matrix approach in which the energy is a fixed parameter, their method cannot be used to analyse the scaling properties of the spectrum. Their method is also limited in that it does not allow for any natural representation of symmetries in phase space. It is also difficult to extend it beyond Harper's equation (2.16) to other difference equations of the form (2.11), which are not limited to having nearest-neighbour coupling.

An important formal property of the renormalization group transformation used has also been shown, that it preserves the point of symmetry of the effective Hamiltonian in the phase plane (again, the cases of threefold and sixfold symmetries have been excluded, which will be discussed elsewhere). It has been observed that when the effective Hamiltonian has an 'isotropic' symmetry in the phase plane (i.e. has 3, 4 or 6-fold point symmetry), then the spectrum has unusual fractal structure. The preservation of symmetry by the renormalization group suggests an explanation of this fact: normally the Hamiltonian is mapped towards a fixed point at which it depends on one phase–space coordinate, and the gaps in the spectrum become vanishingly small. When the Hamiltonian has an isotropic symmetry, however, this symmetry is preserved, and so that Hamiltonian cannot be mapped towards such a fixed point, which has only twofold rotational symmetry. The gaps then occupy a finite fraction of the range of the spectrum at every iteration, implying that the measure of the spectrum is zero.

I wish to thank Professor B. Simon, Professor D. J. Thouless and Professor M. V. Berry, F.R.S., for useful discussions. Some of the results of section 3.3 overlap with a joint paper to be written by B. Simon and myself.

A major part of this paper forms part of a Ph.D thesis of the University of Bristol, where I was supported by the S.E.R.C. I also wish to acknowledge the award of a Weingart Fellowship from the California Institute of Technology.

Appendix A

The results of this paper are based on two ideas. The first is that the true Hamiltonian

$$\hat{H} = [\hat{\boldsymbol{p}} - e\boldsymbol{A}(\hat{\boldsymbol{r}})]^2/2m + V(\boldsymbol{r}), \tag{A 1}$$

with $V(\hat{\boldsymbol{r}})$ a periodic function, can be replaced by an effective Hamiltonian $\hat{H}_{\text{eff}} = H(\hat{x}, \hat{p})$, with H a periodic function of x and p. The second is that symmetries of $V(x, y)$ in two-dimensional coordinate space are represented by symmetries of the one-dimensional Hamiltonian $H(x, p)$ in phase space. In the introduction I gave a simplified derivation of these two results, starting from the Peierls effective Hamiltonian. In this Appendix I list some further comments about the reduction to a one-dimensional representation. The author hopes to publish an expanded discussion of this representation in another paper.

(*a*) First we discuss the limits to the validity of the Peierls effective Hamiltonian (1.1).

As noted in the introduction, (1.1) is not an exact effective Hamiltonian. For sufficiently small magnetic fields, however, there exists a modified dispersion relation $\epsilon'_n(\boldsymbol{k})$, for which (1.1) gives an exact description of the effect of the magnetic field on the band. Blount (1962) has given the first few terms in the expansion of $\epsilon'_n(k)$ in terms of B

$$\epsilon'_n(\boldsymbol{k}) = \epsilon_n(\boldsymbol{k}) + B\epsilon^1_n(\boldsymbol{k}) + B^2\epsilon^2_n(\boldsymbol{k}) + \ldots . \tag{A 2}$$

Provided the potential $V(x, y)$ has centres on twofold symmetry, the first correction $\epsilon^1_n(\boldsymbol{k})$ is zero, so that the corrections to (1.1) are of order B^2.

The Peierls effective Hamiltonian should not be applied to degenerate or overlapping bands, since under these conditions it is not clear how an effective Hamiltonian can be defined to give an accurate description of the effect of the magnetic field on the bands. Also, for degenerate bands, the dispersion relation of each band need not itself have the full symmetry of the lattice, so that the assumed relation between symmetries of $\epsilon_n(\boldsymbol{k})$ and symmetries of $V(\boldsymbol{r})$ would not apply.

(*b*) It was also mentioned in the introduction that an effective Hamiltonian can also be derived when B is very large, and $V(x, y)$ is a weak perturbation, splitting the degeneracy of a Landau level.

In this case we use a basis of Landau states, labelled by a level number N and the x-coordinate of the centre of the state. If we take matrix elements of the Hamiltonian (A 1) between the states of a given Landau level (i.e. one fixed value of N), we find that the Schrödinger equation is a one-parameter family of difference equations with periodic coefficients. The Hamiltonian only couples Landau states with their x-label separated by a multiple of some quantity, which we will call $\hbar^*$, so that if we write $x_n = n\hbar^* + \delta$ the Schrödinger equation is a difference equation in n, parametrized by δ (Rauh 1974, 1975). We saw, in §2, that a Schrödinger equation of this type also arises when we quantize a one-dimensional Hamiltonian that is periodic in x and p. Thus we can derive an effective Hamiltonian $\hat{H}(\hat{x}, \hat{p})$ describing the effect of the potential $V(\boldsymbol{r})$ as a perturbation of the Nth Landau level. It can also be shown that the symmetry of this Hamiltonian in the phase plane is the same as the symmetry of the potential in real space (Wilkinson 1984*b*). Thus there is a relation between the symmetry of $V(x, y)$ in real space and that of $H(x, p)$ in phase space in both the high-magnetic field and the low-magnetic field.

(*c*) Finally we comment on the relation between the symmetry of the potential in real space and that of the effective Hamiltonian in phase space.

For the low field, the effective Hamiltonian (1.4) has the same symmetry in phase space as the Bloch dispersion relation $\epsilon_n(\boldsymbol{k})$ in $\boldsymbol{k}$ space. If we use the uncorrected form of $\epsilon_\nu(\boldsymbol{k})$, the symmetries of this function clearly reflect those of $V(\boldsymbol{r})$ (except that $\epsilon_n(\boldsymbol{k})$ always has inversion symmetry because of time-reversal invariance). If we incorporate the field-dependent corrections, (A 2), this is no longer obviously true. Similarly, for the high field, it is possible to derive a corrected effective Hamiltonian that gives an exact description of the splitting of the Landau level, including the effects of coupling to other Landau levels. In both cases, it should be verified that these corrections do not destroy the correspondence between the symmetry of the potential and that of the effective Hamiltonian. The author hopes to discuss this point in a later publication.

Appendix B

In the text the Chern class, defined by (3.5), is described as the Hall conductance integer of the sub-band. This remark needs some qualification. The Chern class of the true wavefunction in the magnetic Brillouin zone is always equal to the quantized Hall conductance integer (Thouless *et al.* 1982). This is not, however, always equal to the Chern class of the wavefunction of the effective Hamiltonian, as defined by (3.5). For the high field, the two definitions are the same, but for the low field, the Chern class of the true magnetic Bloch states differs from the Chern class defined by (3.5). The difference between these cases is due to differences in the relation between the solutions of the effective Schrödinger equation and the real one.

We will consider Harper's equation (2.16) as an example of an effective Schrödinger equation

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

and will compare the interpretation of the quantities involved for the high and low field.

First, let us consider the low field. Recall that the basis set used to derive the Peierls effective Hamiltonian is a lattice of Wannier functions for the crystal in zero magnetic field (modified by the appropriate phase factors because of the gauge $\boldsymbol{A}(\boldsymbol{r})$). Assume that the lattice is square, of unit spacing. The amplitude of the Wannier state at position (n, m) is $\psi_n \mathrm{e}^{\mathrm{i}m\delta}$. Thus δ ranges from 0 to 2π, and the amplitude ψ_n represents the amplitude of the solution on a row of fixed lattice sites. As mentioned earlier, β is the number of flux quanta per unit cell.

For the high field, the amplitudes ψ_n represent the amplitude of a particular Landau state, which moves along the x-axis as δ varies. In this case δ only ranges from 0 to $\hbar = 2\pi\beta$. The parameter β is now the inverse of the number of flux quanta per unit cell (Rauh 1974, 1975).

The amplitudes ψ_n therefore behave differently when we change the parameter δ. For the low field, they are fixed in space, whereas in the high field, they move through space as δ is varied. Thus, even though the same effective Hamiltonian can be used in each case, the periodicity of the wavefunctions in δ is different. For the high field the wavefunction is periodic in δ with period $\hbar = 2\pi\beta$, and when we increase δ by $\hbar$, we must associate ψ_{n+1} for the new value of δ with ψ_n for the old value. This is equivalent to using the representation introduced in §3, where amplitudes ψ_n are obtained by sampling a continuous function with phase δ. The definition of the Chern class introduced in §3 therefore corresponds to the Chern class of the true wavefunctions for the high field.

For the low field, the situation is different. The wavefunctions are now periodic in δ with period 2π, and when δ is increased by 2π, there is no need to re-assign the labels of the amplitudes ψ_n, because they have remained fixed in space. For this reason, the Chern class of the solutions is different even though the effective Hamiltonian (B 1) may be the same as for the high field.

Finally, I point out a couple of useful facts about the Chern class. First, Středa (1982) gives a very simple formula for the quantized Hall conductance:

$$\sigma_{xy} = e(\partial \mathcal{N}/\partial B). \tag{B 2}$$

In this expression $\mathcal{N}$ is the total number of states per unit area below a given gap in the spectrum, and σ_{xy} is the total Hall conductance of all the occupied bands. This formula usually provides the simplest way of calculating the Chern classes of the sub-bands. Secondly, we note that by using (B 2) we can make a connection between the Chern class and the gap-labelling theorem (Avron & Simon 1983). If μ is the fraction of the states of the band filled, then this theorem states that the filling fractions at the gaps in the spectrum are characterized by pairs of integers n, m:

$$\mu_{nm} = m + n\beta. \tag{B 3}$$

We can use (B 3) to calculate $\mathcal{N}$ in (B 2); note that the total number of states in the band changes with B for the high field, but is fixed for the low field. We find that for the low field the Hall conductance integer (the sum of the Chern classes of all the occupied bands) is n, whereas for the high field it is m. This clearly illustrates the difference between these two cases.

Appendix C

In this appendix, we examine the power-law decay of the Wigner function $W_\nu(x, p)$ and of the coefficients a_{nm} when the Chern class, M, is non-zero. Recall that the Wigner function of the state $|\nu\rangle$ cannot be made well localized because the Bloch states $|k, \delta; \nu\rangle$ cannot be obtained as an analytic and periodic function of k and δ. The singularities of the phase of the Bloch states can be either dislocation points or line discontinuities.

First we will consider the case in which the Bloch states have a line discontinuity. To see the relations between the tails of $W_\nu(x, p)$ and the wavefunction $\phi_\nu(x)$, we can use the formulae

$$|\phi_\nu(x)|^2 = \int \mathrm{d}p\, W_\nu(x, p), \tag{C 1}$$

$$|\tilde{\phi}_\nu(p)|^2 = \int \mathrm{d}x\, W_\nu(x, p). \tag{C 2}$$

In (C 2), $\tilde{\phi}_\nu(p)$ is the wavefunction of $|\nu\rangle$ in the p representation, and is the Fourier transform of $\phi_\nu(x)$. A discontinuity in the phase of the Bloch waves along a line $k = \text{const.}$ causes $\phi_\nu(x)$ to be poorly localized, with a $1/x$ decay. By (C 1), therefore, the Wigner function has a $1/x^2$ decay law. Similarly, a discontinuity along a line $\delta = \text{const.}$ causes $\phi_\nu(x)$ to be discontinuous, so that $\tilde{\phi}_\nu(p)$ has a $1/p$ decay law, and by (C 2) the Wigner function has a $1/p^2$ decay. Despite the Wigner function being well localized in the conjugate direction, these decays are so slow that the expansion (3.9) is not absolutely convergent. Any other type of line discontinuity leads to localization properties that are at least as bad as the two cases described.

Now let us consider the other type of phase singularity, the dislocation point. Consider a dislocation of strength N at the point (k^*, δ^*) in the Brillouin zone, and let (R, θ) be radial coordinates in the (k, δ)-plane measured from this point. Without loss of generality, we can assume that the phase of the Bloch wave is $N\theta$ in the neighbourhood of the dislocation:

$$|k, \delta; \nu\rangle = \mathrm{e}^{\mathrm{i}N\theta} |k^*, \delta^*; \nu\rangle + o(R). \tag{C 3}$$

Instead of calculating the power-law decay of the Wigner function, and deducing the decay law of the coefficients a_{nm}, in this case it is easier to calculate the amplitudes a_{nm} directly. Using (2.26), (3.6), and (3.9), we find

$$a_{nm} = \mathcal{N}^{-1} \sum_{\delta} \sum_{k} \exp\{-2\pi\mathrm{i}[k\hbar n + (n\pi - \delta)\, m]/\hbar\} \langle k, \delta; \nu | \chi\rangle. \tag{C 4}$$

In the limit $\mathcal{N} \to \infty$, the summations become integrals, and the amplitude a_{nm} is essentially just the Fourier coefficient of the periodic function $\langle k, \delta; \nu | \chi\rangle$. The decay of this Fourier transform at large n, m is determined by the singularity of this function at the point (k^*, δ^*). From (C 3), therefore, we see that the coefficient a_{nm} decays at the same rate at the Fourier transform of the function

$$f(R, \theta) = \mathrm{e}^{\mathrm{i}N\theta}. \tag{C 5}$$

The Fourier transform $\tilde{f}(k, \theta)$ of this function decays as $1/k^2$. The coefficients a_{nm} therefore have an inverse-square decay, so that once again the expansion (3.9) is not absolutely convergent. The Wigner function $W_\nu(x, p)$ has some complicated fine-grained structure, but this result, together with (3.13), shows that when $W_\nu(x, p)$ is smoothed out by convoluting it with $W_\chi(x, p)$, it has a $1/r^4$ decay law.

Appendix D

Recall that if the effective Hamiltonian has rotational or mirror symmetries, represented by operators $\hat{R}$ or $\hat{M}$, then the Bloch waves satisfy

$$\hat{R} |\boldsymbol{K}\rangle = \exp\{\mathrm{i}\phi_{\mathrm{R}}(\boldsymbol{K})\} |\boldsymbol{K}_{\mathrm{R}}\rangle, \tag{D 1}$$

$$\hat{M} |\boldsymbol{K}\rangle = \exp\{\mathrm{i}\phi_{\mathrm{M}}(\boldsymbol{K})\} |\boldsymbol{K}_{\mathrm{M}}\rangle. \tag{D 2}$$

The Bloch wave $|\boldsymbol{K}\rangle = |k, \delta; \nu\rangle$ is associated, via the operation of evaluating its Wigner function, with a lattice of points in phase space $(x_{nm}, p_{nm}) = (\delta + n\hbar, (k+m)\hbar)$. The 'rotated' Bloch state $|\boldsymbol{K}_{\mathrm{R}}\rangle$ resulting from the action of $\hat{R}$ on $|\boldsymbol{K}\rangle$ is identified by remembering that the rotation operator acts classically on this lattice of points.

Our aim is to find a phase transformation

$$|\boldsymbol{K}'\rangle = \mathrm{e}^{\mathrm{i}\theta(\boldsymbol{K})} |\boldsymbol{K}\rangle, \tag{D 3}$$

so that the phases $\phi_{\mathrm{R}}(\boldsymbol{K}), \phi_{\mathrm{M}}(\boldsymbol{K})$ vanish, i.e. $\hat{R} |\boldsymbol{K}'\rangle = |\boldsymbol{K}'_{\mathrm{R}}\rangle$, $\hat{M} |K'\rangle = |\boldsymbol{K}'_{\mathrm{M}}\rangle$. This requires that $\theta(\boldsymbol{K})$ satisfy the equations

$$\phi_{\mathrm{R}}(\boldsymbol{K}) = \theta(\boldsymbol{K}_{\mathrm{R}}) - \theta(\boldsymbol{K}), \tag{D 4}$$

$$\phi_{\mathrm{M}}(\boldsymbol{K}) = \theta(\boldsymbol{K}_{\mathrm{M}}) - \theta(\boldsymbol{K}). \tag{D 5}$$

I will not try to give a general prescription for solving these equations for $\theta(\boldsymbol{K})$, but, instead, will illustrate the method by finding $\theta(\boldsymbol{K})$ in two particular cases.

The first case we consider is when there is fourfold rotational symmetry, and no mirror symmetry, so that (D 2) and (D 5) do not apply. The angle $\theta(\boldsymbol{K})$ must be a linear combination of $\phi_{\mathrm{R}}(\boldsymbol{K})$, $\phi_{\mathrm{R}}(\boldsymbol{K}_{\mathrm{R}})$, $\phi_{\mathrm{R}}(\boldsymbol{K}_{\mathrm{R}^2})$, and $\phi_{\mathrm{R}}(\boldsymbol{K}_{\mathrm{R}^3})$. These four quantities are not linearly independent; because $\hat{R}^4 = \hat{1}$, we have

$$\phi_{\mathrm{R}}(\boldsymbol{K})+\phi_{\mathrm{R}}(\boldsymbol{K}_{\mathrm{R}})+\phi_{\mathrm{R}}(\boldsymbol{K}_{\mathrm{R}^2})+\phi_{\mathrm{R}}(\boldsymbol{K}_{\mathrm{R}^3}) = 0. \tag{D 6}$$

Let us choose to eliminate $\phi_{\mathrm{R}}(\boldsymbol{K}_{\mathrm{R}^3})$, and write $\theta(\boldsymbol{K})$ as a linear combination of the other three values. Substituting into (D 4), and solving for the coefficients, we find

$$\theta(\boldsymbol{K}) = -\tfrac{1}{4}[3\phi_{\mathrm{R}}(\boldsymbol{K})+2\phi_{\mathrm{R}}(\boldsymbol{K}_{\mathrm{R}})+\phi_{\mathrm{R}}(\boldsymbol{K}_{\mathrm{R}^2})]. \tag{D 7}$$

For our second example, we consider the case in which there is both twofold rotational symmetry and mirror symmetry. In this case, $\theta(\boldsymbol{K})$ must be a linear combination of the eight values of ϕ_{M} and ϕ_{R} at the four symmetry-related points, i.e. of $\phi_{\mathrm{R}}(\boldsymbol{K})$, $\phi_{\mathrm{R}}(\boldsymbol{K}_{\mathrm{R}})$, $\phi_{\mathrm{R}}(\boldsymbol{K}_{\mathrm{M}})$, $\phi_{\mathrm{R}}(\boldsymbol{K}_{\mathrm{RM}})$, and the corresponding values of ϕ_{M}. Using the results

$$\hat{R}^2 = 1, \quad \hat{M}^2 = \hat{1}, \quad \hat{R}\hat{M} = \hat{M}\hat{R}, \tag{D 8}$$

we can find linear relations between these eight phases, analogous to (D 6):

$$\phi_{\mathrm{R}}(\boldsymbol{K})+\phi_{\mathrm{R}}(\boldsymbol{K}_{\mathrm{R}}) = 0, \quad \phi_{\mathrm{R}}(\boldsymbol{K}_{\mathrm{M}})+\phi_{\mathrm{R}}(\boldsymbol{K}_{\mathrm{RM}}) = 0, \tag{D 9}$$

$$\phi_{\mathrm{M}}(\boldsymbol{K})+\phi_{\mathrm{M}}(\boldsymbol{K}_{\mathrm{M}}) = 0, \quad \phi_{\mathrm{M}}(\boldsymbol{K}_{\mathrm{R}})+\phi_{\mathrm{M}}(\boldsymbol{K}_{\mathrm{RM}}) = 0, \tag{D 10}$$

$$\phi_{\mathrm{R}}(\boldsymbol{K})+\phi_{\mathrm{M}}(\boldsymbol{K}_{\mathrm{R}}) = \phi_{\mathrm{M}}(\boldsymbol{K})-\phi_{\mathrm{R}}(\boldsymbol{K}_{\mathrm{M}}). \tag{D 11}$$

Let us take $\phi_{\mathrm{R}}(\boldsymbol{K})$, $\phi_{\mathrm{M}}(\boldsymbol{K})$, $\phi_{\mathrm{R}}(\boldsymbol{K}_{\mathrm{M}})$ as the three independent variables. We find that the following solution to (D 4) and (D 5)

$$\theta(\boldsymbol{K}) = \tfrac{1}{4}[\phi_{\mathrm{R}}(\boldsymbol{K})+\phi_{\mathrm{R}}(\boldsymbol{K}_{\mathrm{M}})-2\phi_{\mathrm{M}}(\boldsymbol{K})]. \tag{D 12}$$

The same methods can be used to find $\theta(\boldsymbol{K})$ in all the other cases. In the most complicated example, where there is fourfold symmetry and mirror symmetry, of the sixteen values of ϕ_{R} and ϕ_{M}, only six are linearly independent.

References

Avron, J. & Simon, B. 1981 *Phys. Rev. Lett.* **46**, 1166–1168.

Avron, J. & Simon, B. 1983 *Duke math. J.* **50**, 369–391.

Avron, J., Seiler, R. & Simon, B. 1983 *Phys. Rev. Lett.* **51**, 51–53.

Bacry, H., Grossman, A. & Zak, J. 1976 *Phys. Rev.* B **12**, 1118–1120.

Baker, G. A. Jr 1958 *Phys. rev.* **109**, 2198–2206.

Balazs, N. L. & Jennings, B. K. 1983 *Physica* **121**, 576–586.

Bellissard, J. & Simon, B. 1982 *J. funct. Anal.* **48**, 408–419.

Blount, E. I. 1962 *Phys. Rev.* **126**, 1636–1653.

Dana, I. & Zak, J. 1983 *Phys. Rev.* B **28**, 811–820.

Dana, I. & Zak, J. 1985 *Phys. Rev.* B **32**, 3612–3621.

Feynman, R. P. & Hibbs, A. R. 1965 *Quantum mechanics and path integrals.* New York: McGraw-Hill.

Groenewold, H. J. 1946 *Physica* **12**, 405–460.

Harper, P. G. 1955 *Proc. phys. Soc. Lond.* A **68**, 879–892.

Kivelson, S. 1982 *Phys. Rev.* B **26**, 4269–4277.
Mehta, C. L. 1964 *J. Math. Phys.* **5**, 677–686.
Ostlund, S. & Pandit, R. 1984 *Phys. Rev.* B **29**, 1394–1414.
Ozorio de Almeida, A. M. & Hannay, J. H. 1982 *Ann. Phys.* **138**, 115–154.
Peierls, R. 1933 *Z. Phys.* **80**, 763–791.
Rauh, A. 1974 *Physics Status Solidi* B **65**, K 131–135.
Rauh, A. 1975 *Physics Status Solidi* B **69**, K 9–13.
Simon, B. 1982 *Adv. appl. Math.* **3**, 463–490.
Simon, B. & Wilkinson, M. 1985 (In preparation.)
Středa, P. 1982 *J. Phys.* C **15**, L 717–721.
Suslov, I. M. 1982 *Zh. éksp. teor. Fiz.* **83**, 1079–1088 (transl. as *Soviet Phys. JETP* **56**, 612–617).
Thouless, D. J., Kohmoto, M., Nightingale, M. P. & den Nijs, M. 1982 *Phys. Rev. Lett.* **49**, 405–408.
Thouless, D. J. 1984 *J. Phys.* C **17**, 325–328.
von Neumann, J. 1955 *Mathematical foundations of quantum mechanics.* Princeton University Press.
Weyl, H. 1927 *Z. Phys.* **46**, 1–46.
Wigner, E. P. 1932 *Phys. Rev.* **40**, 749–759.
Wilkinson, M. 1984*a* *Proc. R. Soc. Lond.* A **391**, 305–350.
Wilkinson, M. 1984*b* Ph.D. thesis, University of Bristol.