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A six-fold rotation operator for the Wannier functions of the phase-space lattice Hamiltonian

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Abstract. We consider a set of localized Wannier functions which can be used to describe the Bloch bands of one-dimensional Hamiltonians whose associated Weyl function is periodic under a hexagonal lattice of translations in phase space. These Hamiltonians can be used to describe electrons on two-dimensional hexagonal lattices penetrated by a magnetic field. The effect on the Wannier functions of a $\pi/3$ rotation of the phase plane is considered. The resulting transformation is found to be surprisingly complicated when the quantized Hall conductance integer for the Bloch band is non-zero.

1. Introduction

This paper considers a calculation of the properties of a set of Wannier functions for the phase-space lattice Hamiltonian (defined by Wilkinson in an earlier paper [1]) under a $\pi/3$ rotation of the phase plane. The details of the construction of these Wannier functions are complicated and readers are referred to [1] for a discussion of their evaluation.

These Wannier functions are relevant for describing Bloch solutions of Hamiltonians which are periodic functions of the operators $\hat{x}$ and $\hat{p}$. Hamiltonians of this form [2] (or their related Schrödinger equations [3–5]) occur in the problem of two-dimensional Bloch electrons in a magnetic field where the commutator $[\hat{x}, \hat{p}] = \mathrm{i}\hbar$ and $\hbar$ is related to the dimensionless parameter β which measures the ratio of the flux quantum (h/e) to the flux through a unit cell of the potential (BA). [2–4] concern perturbations of electrons in Landau levels due to a periodic potential, in this case $\beta = h/eBA$. [5] concerns electrons perturbed by a weak magnetic field, in which case $\beta = eBA/h$. In the case where the unit cell has area $4\pi^2$ then $\hbar = 2\pi\beta$. Bloch solutions exist if the parameter β is a rational number.

The Hamiltonian may have rotational symmetries in its phase plane. These symmetries are important in determining the structure of the spectrum of the Hamiltonian; for irrational β the spectrum is believed to be a Cantor set of zero measure if the Hamiltonian has centres of three-, four- or six-fold symmetry in the phase plane [6–10]. This result can be demonstrated if the rotational properties of the Wannier functions are known [1, 17]. The symmetries of the phase plane arise naturally when the two-dimensional periodic potential possesses such symmetries [11]. In order to study the effects of these symmetries it will be useful to understand the effect of such a rotation on a set of basis states for the eigenfunctions of the Hamiltonian. For rational β Bloch's theorem is applicable and the eigenstates of $\hat{H}$ are Bloch states $|B_\nu(k, \delta)\rangle$, where k and δ are Bloch wavevectors. It is not, in general, possible to construct a complete basis of well localized Wannier functions for Bloch bands

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in the presence of magnetic fields [12] by simply integrating over the Bloch wavevectors. However, Wilkinson [1] has shown how a set of generalized Wannier functions may be defined that do form a complete basis for the Bloch band (the details of which are given in the following section). If we apply $\hat{R}_i$, an ith-(three, four or six)fold rotation operator, to the Bloch states $|B_\nu(k,\delta)\rangle$ of the Hamiltonian, the resulting states will be eigenfunctions of the rotated Hamiltonian $\hat{H}^{(R_i)} = \hat{R}_i \hat{H} \hat{R}_i^{-1}$. The natural expectation is that the Wannier functions constructed from these new Bloch states will be related to the initial Wannier function by the relation

$$|\tilde{\phi}\rangle = \hat{R}_i|\phi\rangle. \tag{1.1}$$

Surprisingly it turns out that this is only valid when the quantized Hall conductance integer for the νth Bloch band, M_ν, is zero. (Thouless *et al* [13] discuss the role of the integer M_ν in the Hall effect of periodic systems and show that M_ν is the Chern integer of the Bloch band.)

When M_ν is non-zero we have a set of $|N_\nu|$ Wannier functions, $|\phi_\mu^{(\nu)}\rangle, \mu = 1, \ldots, |N_\nu|$ [1], where N_ν is an integer related to M_ν by $1 = qM_\nu + pN_\nu$. In the four-fold case it is found [1] that

$$|\tilde{\phi}_\mu^{(\nu)}\rangle = \hat{S}(pN_\nu)\hat{R}_4\hat{r}_4|\phi_\mu^{(\nu)}\rangle \tag{1.2}$$

where $\hat{S}(\eta)$ is a unitary operator which stretches the x-axis by a factor η and $\hat{r}_4$ is a rotation operator acting on the labels of the Wannier functions. The full definitions of these operators will be given later. In this work we compute the transformation of the Wannier functions under a six-fold rotation of the Bloch states. We find that the rotation operator has still more complicated features

$$|\tilde{\phi}_\mu^{(\nu)}\rangle = \hat{T}(0, \alpha\pi pN_\nu a)\hat{Q}(-q^2M_\nu^2/\sqrt{3})\hat{S}(pN_\nu)\hat{R}_6\hat{r}_6\hat{t}(0, \alpha N_\nu/2)|\phi_\mu^{(\nu)}\rangle. \tag{1.3}$$

Here $a = (2/\sqrt{3})^{1/2}$, $\hat{Q}$ is an operator which shears the phase space, $\hat{T}$ is a phase-space translation operator, $\hat{t}$ is a translation operator acting on the labels of the Wannier functions and α takes the value 0 or 1 if $N_\nu \times M_\nu$ is an even or odd number, respectively.

Section 2 describes the set of Wannier functions introduced by Wilkinson [1]. These Wannier functions are constructed for Hamiltonians defined on a square lattice in phase space. In section 3 a Hamiltonian defined on a hexagonal lattice in phase space is introduced and the properties are characterized under six-fold rotations. It is shown how this Hamiltonian can be unitarily transformed to a Hamiltonian defined on a square lattice and how the Wannier functions are related to those on the square lattice. It is also shown how a six-fold rotation operator on the hexagonal lattice is represented on the square lattice. Section 4 considers the effect on the square lattice Wannier functions of such a rotation of the Bloch states and constructs a rotation operator for the Wannier functions, from this a rotation operator for the hexagonal lattice Wannier functions can be obtained.

2. Phase-space Wannier functions

We summarize here the relevant results from [1]. Hamiltonians defined on a square lattice in phase space are considered. The area of the unit cell in the phase plane of the classical Hamiltonian is taken as $4\pi^2$. The Hamiltonian takes the form

$$H(\hat{x}, \hat{p}) = \sum_{nm} H_{nm}\hat{T}(n\overline{h}, m\overline{h})$$

where

$$\hat{T}(X,P) = \exp[\mathrm{i}(P\hat{x} - X\hat{p})/\hbar]. \tag{2.1}$$

$\hat{T}(X,P)$ is a phase-space translation operator and will be widely used in the following work. These operators have a non-commutative algebra of the same form as the magnetic translation operators introduced by Zak [14].

$$\hat{T}(X_1,P_1)\hat{T}(X_2,P_2) = \exp[\mathrm{i}(X_2P_1 - X_1P_2)/2\hbar]\hat{T}(X_1+X_2,P_1+P_2). \tag{2.2}$$

When $\beta = p/q$, the Bloch states $|D_\nu(k,\delta)\rangle$ of the Hamiltonian (2.1) can be obtained from a set of $|N_\nu|$ Wannier functions $|\Phi_\mu^{(\nu)}\rangle$. (We will reserve the notation $|B_\nu(k,\delta)\rangle$ and $|\phi_\mu^{(\nu)}\rangle$ for the Bloch and Wannier states of Hamiltonians defined on hexagonal lattices.)

$$|D_\nu(k,\delta)\rangle = C\sum_{\mu=1}^{|N_\nu|}\sum_{n=-\infty}^{\infty}\sum_{m=-\infty}^{\infty}\exp\left[-\frac{2\pi\mathrm{i}}{\hbar}\left(m\delta + \frac{n(k+\mu\hbar)}{N_\nu}\right)\right] \times\hat{T}(0,2\pi m)\hat{T}(-2\pi n/N_\nu,0)\hat{T}(0,qM_\nu k)|\Phi_\mu^{(\nu)}\rangle \tag{2.3}$$

C is a normalization constant. If the Wigner function of the Wannier states $|\Phi_\mu^{(\nu)}\rangle$ is smooth and localized in phase space then these Bloch states have the following periodicity properties

$$|D_\nu(k+2\pi/q,\delta)\rangle = \exp[\mathrm{i}qM_\nu\delta/p]|D_\nu(k,\delta)\rangle$$
$$|D_\nu(k,\delta+2\pi p/q)\rangle = |D_\nu(k,\delta)\rangle. \tag{2.4}$$

The Wannier states can be obtained from the Bloch states $|D_\nu(k,\delta)\rangle$ by inverting the relation (2.3)

$$|\Phi_\mu^{(\nu)}\rangle = \frac{q^2}{4\pi^2\sqrt{p}N_\nu C}\sum_{\mu'=1}^{|N_\nu|}\exp[2\pi\mathrm{i}\mu\mu'/N_\nu]\,\hat{T}(2\pi\mu'/N_\nu,0) \times\int_0^{2\pi/q}\mathrm{d}k\int_0^{2\pi/q}\mathrm{d}\delta\;\exp[\mathrm{i}qk\mu']\,\hat{T}(0,-qM_\nu k)|S_\nu(k,\delta)\rangle \tag{2.5}$$

where

$$|S_\nu(k,\delta)\rangle = \frac{1}{\sqrt{p}}\sum_{j=1}^{p}|D_\nu(k,\delta+2\pi j/q)\rangle. \tag{2.6}$$

$|S_\nu(k,\delta)\rangle$ is also a valid Bloch state of the Hamiltonian (2.1). It should be noted that the Wannier function depends on the choice of gauge for the Bloch states. A gauge transformation may be applied to the Bloch states $|B_\nu(k,\delta)\rangle \to \exp[\mathrm{i}\theta(k,\delta)]|B_\nu(k,\delta)\rangle$ and the Wannier functions constructed from these states will still be smooth and well localized provided (2.4) still holds. We shall also introduce here a translation operator analagous to the phase-space translation operator (2.1) which acts on the labels of the Wannier functions

$$\hat{t}(n_1,n_2)|\Phi_\mu^{(\nu)}\rangle = \exp\left[\frac{2\pi\mathrm{i}M_\nu}{N_\nu}\left(\mu - \tfrac{1}{2}n_1\right)n_2\right]|\Phi_{\mu-n_1}^{(\nu)}\rangle. \tag{2.7}$$

These operators have a similar algebra to the translation operators $\hat{T}(X,P)$ introduced in (2.1)

$$\hat{t}(n_1,n_2)\hat{t}(n_1',n_2') = \exp\left[\frac{2\pi\mathrm{i}M_\nu}{N_\nu}\left(\frac{n_2n_1' - n_1n_2'}{2}\right)\right]\hat{t}(n_1+n_1',n_2+n_2') \tag{2.8}$$

n_1 is clearly restricted to integer values. We will place no such restriction on n_2 in this paper.

3. Mapping of hexagonal-lattice Hamiltonian to square lattice

In this section we describe how to relate the eigenstates of Hamiltonians defined on a hexagonal lattice to those of a Hamiltonian of the form (2.1). A general quantum Hamiltonian defined on a hexagonal lattice can be obtained by quantizing the following classical Hamiltonian, expressed as a Fourier sum, under the Weyl quantization

$$H^{(H)}(x, p) = \sum_{nm} H_{nm} \exp[\mathrm{i}a((m - \tfrac{1}{2}n)x - \tfrac{\sqrt{3}}{2}np)] \tag{3.1}$$

which can be expressed, in terms of the phase-space translation operators, as

$$H^{(H)}(\hat{x}, \hat{p}) = \sum_{nm} H_{nm} \hat{T}(\tfrac{\sqrt{3}}{2}n\hbar a, (m - \tfrac{1}{2}n)\hbar a). \tag{3.2}$$

In these expressions $a = (2/\sqrt{3})^{1/2}$ and is chosen to ensure that the unit cell of the Hamiltonian in the classical phase space has area $4\pi^2$. If $\hbar = 2\pi\beta = 2\pi p/q$ then the eigenfunctions of (3.2) are Bloch states.

The Weyl quantization [15] allows one to quantize the Hamiltonian in such a way that it is invariant under linear transformations of the phase plane. Among such transformations (which are generated by the action of quadratic Hamiltonians) are rotations and shearings of the phase plane. This property of the Weyl quantization is important in this context because rotations and shearings of the classical phase space correspond to analogous transformations of the crystal lattice in real space [11], [16] and [17] contain discussions of these points and other results on the Weyl quantization.

A $\pi/3$ rotation is generated by the operator $\hat{R}_6$ whose effect on the translation operators is defined by

$$\hat{R}_6\hat{T}(X, P) = \hat{T}(\tfrac{1}{2}X + \tfrac{\sqrt{3}}{2}P, \tfrac{1}{2}P - \tfrac{\sqrt{3}}{2}X)\hat{R}_6. \tag{3.3}$$

The operator $\hat{R}_6$ can be represented as

$$\hat{R}_6 = \exp[-\mathrm{i}(\hat{x}^2 + \hat{p}^2 + \hbar)\pi/6\hbar] \tag{3.4}$$

which is an operator that rotates the Wigner function [18] of a state clockwise through $\pi/3$ rad. Applying this operator to the Hamiltonian defined in (3.2) we see that the Hamiltonian is symmetric under this rotation if $H_{nm} = H_{m-n,n}$.

Now we consider a sequence of unitary transformations that map the Hamiltonian (3.2), defined on a hexagonal lattice, onto one of the form (2.1). First we will shear the lattice, this has the effect on the classical phase space of transforming the phase-space coordinates to

$$x \rightarrow x' = x \qquad p \rightarrow p' = p - \tfrac{1}{\sqrt{3}}x. \tag{3.5}$$

The operator which generates this shearing of the quantum Hamiltonian is

$$\hat{Q}(s) = \exp[-\mathrm{i}s\hat{x}^2/2\hbar] \qquad s = \tfrac{1}{\sqrt{3}} \tag{3.6}$$

and

$$\hat{Q}(s)\hat{T}(X, P) = \hat{T}(X, P + sX)\hat{Q}(s). \tag{3.7}$$

Under this transformation the Hamiltonian is now defined on a rectangular lattice

$$H^{(R)}(\hat{x}, \hat{p}) = \sum_{nm} H_{nm} \hat{T}(\tfrac{\sqrt{3}}{2}n\hbar a, m\hbar a). \tag{3.8}$$

We will now complete the transformation to a square lattice by the action of an operator $\hat{S}(1/a)$. $\hat{S}(\eta)$ is a unitary operator which stretches the x-axis by a factor η, and is defined by the relation

$$\langle x|\hat{S}(\eta)|\psi\rangle = \sqrt{|\eta|}\langle \eta x|\psi\rangle. \tag{3.9}$$

The operators $\hat{S}(\eta)$ and $\hat{T}(X,P)$ have the following commutation rule

$$\hat{S}(\eta)\hat{T}(X,P) = \hat{T}\left(\frac{X}{\eta}, P\eta\right)\hat{S}(\eta). \tag{3.10}$$

After this operation the Hamiltonian is in the form (2.1) which we will call $\hat{H}^{(S)}$ and, for rational β, $\hat{H}^{(S)}$ has Bloch eigenstates $|D_\nu(k,\delta)\rangle$.

The states $\hat{Q}(-s)\hat{S}(a)|D_\nu(k,\delta)\rangle$ are, therefore, eigenstates of the Hamiltonian $\hat{H}^{(H)}$. The Wannier functions for Bloch states on the hexagonal lattice $|\phi_\mu^{(\nu)}\rangle$ can, similarly, be obtained from the Wannier functions for the square-lattice Hamiltonian $|\Phi_\mu^{(\nu)}\rangle$. In terms of these Wannier states the eigenstates of (3.2) can be found:

$$|B_\nu(k,\delta)\rangle = \hat{Q}(-s)\hat{S}(a)|D_\nu(k,\delta)\rangle = C\sum_{\mu=1}^{|N_\nu|}\sum_{n=-\infty}^{\infty}\sum_{m=-\infty}^{\infty}\exp\left[-\frac{2\pi\mathrm{i}}{\hbar}\left(m\delta + \frac{n(k+\mu\hbar)}{N_\nu}\right)\right]$$
$$\times\hat{T}(0,2\pi ma)\hat{T}(-2\pi n/aN_\nu, \pi na/N_\nu)\hat{T}(0,qM_\nu ka)|\phi_\mu^{(\nu)}\rangle. \tag{3.11}$$

It can easily be shown that the rotation operator in the new phase space which represents a six-fold rotation in the old space is defined by the relation

$$\hat{R}\hat{T}(X,P) = \hat{T}(P, P-X)\hat{R}. \tag{3.12}$$

In other words $\hat{R}$ can be thought of as a 90° rotation followed by a shearing $\hat{Q}(1)$. This operator can be represented on the x-axis as

$$\langle x|\hat{R}|\psi\rangle = \frac{1}{\sqrt{2\pi\hbar}}\exp[-\mathrm{i}x^2/2\hbar]\int_{-\infty}^{\infty}\mathrm{d}x'\,\exp[\mathrm{i}xx'/\hbar]\langle x'|\psi\rangle. \tag{3.13}$$

4. Calculation of rotation operator for Wannier functions

In this section we consider the effect of the rotation operator of (3.12) on the states $|S_\nu(k,\delta)\rangle$ of a Hamiltonian of the form (2.1). Readers are reminded that everything in this section up until the last two equations is concerned with the square-lattice Hamiltonian. We will notate the Bloch states of Hamiltonians of the form (2.1) by $|D_\nu(k,\delta)\rangle$ and the Wannier states constructed from them by $|\Phi_\mu^{(\nu)}\rangle$. We will keep the notation of $|B_\nu(k,\delta)\rangle$ and $|\phi_\mu^{(\nu)}\rangle$ to results pertaining to the Hamiltonian (3.2).

We shall see that the states obtained by rotating the Bloch states $|S_\nu(k,\delta)\rangle$ are in the form of Bloch states with different Bloch wavevectors. We will regauge the new Bloch states such that they obey the gauge condition (2.4). These Bloch states will then be used as a basis from which to construct the Wannier functions according to the prescription (2.5). We are then able to calculate the transformation of the Wannier functions $|\Phi_\mu^{(\nu)}\rangle$ generated by the rotation.

We will consider applying the rotation operator to a particular linear combination of degenerate Bloch states $|S_\nu(k,\delta)\rangle$ defined in (2.6). From [1] this vector can be written

$$|S_\nu(k,\delta)\rangle = C\sum_m \mathrm{e}^{\mathrm{i}qkm/p}\hat{T}(2\pi m,0)\sum_n \mathrm{e}^{-\mathrm{i}q\delta n}\hat{T}(0,2\pi np)\hat{T}(0,qM_\nu k)$$
$$\times\sum_{\mu=1}^{|N_\nu|}\exp[-\mathrm{i}qk\mu]|\chi_\mu\rangle \tag{4.1}$$

where

$$|\chi_\mu^{(\nu)}\rangle = \sqrt{p}\hat{T}(-2\pi\mu/N_\nu, 0)\sum_{\mu'=1}^{|N_\nu|}\exp[-2\pi\mathrm{i}\mu\mu'/N_\nu]|\Phi_{\mu'}^{(\nu)}\rangle. \tag{4.2}$$

If we now apply the rotation operator to this vector then after some manipulation we find using (3.12), that

$$\hat{R}|S_\nu(k,\delta)\rangle = C\sum_m \mathrm{e}^{-\mathrm{i}qkm/p}\hat{T}(0, 2\pi m)\sum_n \mathrm{e}^{\mathrm{i}qn(k-\delta+\pi p)}\hat{T}(2\pi np, 0)$$
$$\times\hat{T}(qM_\nu k, qM_\nu k)\sum_{\mu=1}^{|N_\nu|}\mathrm{e}^{-\mathrm{i}qk\mu}\hat{R}|\chi_\mu\rangle = |\tilde{D}_\nu(k', \delta')\rangle. \tag{4.3}$$

Now the sum over m indicates that the wavefunction is only non-zero at positions $x_n = n\overline{h}+k$ and $k' = k - \delta + \pi p$ is a Bloch wavevector for translations in the x direction. This state is, then, of the form of a Bloch state.

Now if we consider the periodicity properties of this Bloch state $|\tilde{D}_\nu(k', \delta')\rangle$ then we find that

$$|\tilde{D}_\nu(k + 2\pi/q, \delta)\rangle = |\tilde{D}_\nu(k, \delta)\rangle$$
$$|\tilde{D}_\nu(k, \delta + 2\pi p/q)\rangle = \exp[\mathrm{i}qM_\nu(\delta - k - p\pi)]|\tilde{D}_\nu(k, \delta)\rangle. \tag{4.4}$$

In order to construct smooth well localized Wannier functions (2.5) we require that the Bloch states $\{|\tilde{D}_\nu(k, \delta)\rangle\}$ have the periodicity properties described in (2.4). To achieve this we apply a gauge transformation

$$|\tilde{D}'_\nu(k, \delta)\rangle = \exp[\mathrm{i}\theta(k, \delta)]|\tilde{D}_\nu(k, \delta)\rangle. \tag{4.5}$$

The function $\theta(k, \delta)$ satisfies the relationships

$$\begin{aligned}\theta(k + 2\pi/q, \delta) - \theta(k, \delta) &= -qM_\nu\delta/p \\ \theta(k, \delta + 2\pi p/q) - \theta(k, \delta) &= qM_\nu(\delta - k - \pi p).\end{aligned} \tag{4.6}$$

We consider a gauge function $\theta(k, \delta) = \epsilon_1 k\delta + \epsilon_2\delta^2 + \epsilon_3\delta$ and choosing the variables ϵ_1, ϵ_2 to satisfy (4.6) we find that

$$\epsilon_1 = -q^2M_\nu/2\pi p \qquad \epsilon_2 = q^2M_\nu/4\pi p. \tag{4.7}$$

This leaves us with a relation for ϵ_3

$$\pi pM_\nu + 2\pi p\epsilon_3/q = -\pi pqM_\nu. \tag{4.8}$$

Now we must choose ϵ_3 to satisfy (4.8). However, since phase changes of 2π are unimportant, it is only necessary for the two sides of (4.8) to agree up to some arbitrary multiple of 2π. For convenience later on we will choose values of ϵ_3 depending on whether the product $N_\nu \times M_\nu$ is an odd or an even number

$$\epsilon_3 = qN_\nu/2 \qquad N_\nu \times M_\nu = \text{odd}$$
$$\epsilon_3 = 0 \qquad N_\nu \times M_\nu = \text{even}.$$

If we use the states $|\tilde{D}'_\nu(k, \delta)\rangle$ as a base to build the Wannier functions according to (2.5), and using (4.1), (4.2), (4.3), (4.7) and (4.8) we have

$$|\tilde{\Phi}_\mu^{(\nu)}\rangle = \frac{q^2}{4\pi^2\sqrt{p}N_\nu C}\sum_{\mu'=1}^{|N_\nu|}\mathrm{e}^{2\pi\mathrm{i}\mu\mu'/N_\nu}\hat{T}(2\pi\mu'/N_\nu, 0)$$

$$\times\int_0^{2\pi/q}\mathrm{d}k\int_0^{2\pi p/q}\mathrm{d}\delta\,\mathrm{e}^{\mathrm{i}qk\mu'}\mathrm{e}^{\mathrm{i}q^2M_\nu k\delta/2\pi p}\mathrm{e}^{\mathrm{i}q^2M_\nu\delta^2/4\pi p}\mathrm{e}^{\mathrm{i}\epsilon_3\delta}\hat{T}(0,-qM_\nu k)$$
$$\times C\sum_m \mathrm{e}^{-\mathrm{i}q\delta m/p}\sum_n \mathrm{e}^{\mathrm{i}qnk}\hat{T}(0,2\pi m)\hat{T}(2\pi np,0)\hat{T}(qM_\nu\delta,qM_\nu\delta)$$
$$\times\sum_{\lambda=1}^{|N_\nu|}\mathrm{e}^{-\mathrm{i}q\delta\lambda}\hat{T}(0,2\pi\lambda/N_\nu)\sum_{\lambda'=1}^{|N_\nu|}\mathrm{e}^{-2\pi\mathrm{i}\lambda\lambda'/N_\nu}\hat{R}|\Phi_{\lambda'}^{(\nu)}\rangle. \tag{4.10}$$

Using a result that we prove in the appendix this can be rewritten

$$|\tilde{\Phi}_\mu^{(\nu)}\rangle = \frac{q^2}{4\pi^2\sqrt{p}N_\nu}\sum_{\mu'=1}^{|N_\nu|}\sum_{\lambda=1}^{|N_\nu|}\mathrm{e}^{2\pi\mathrm{i}\mu\mu'/N_\nu}\hat{T}(2\pi\mu'/N_\nu,0)\hat{O}_{\mu',-\lambda p}\hat{T}(0,2\pi\lambda/N_\nu)$$
$$\times\sum_{\lambda'=1}^{|N_\nu|}\mathrm{e}^{-2\pi\mathrm{i}\lambda\lambda'/N_\nu}\hat{R}|\Phi_{\lambda'}^{(\nu)}\rangle \tag{4.11}$$

where

$$\hat{O}_{NM} = \frac{4\pi^2 p}{q}\frac{1}{\sqrt{p}N_\nu}\hat{Q}(pqN_\nu M_\nu)\hat{T}(0,2\pi m)\hat{T}(0,\epsilon_3\overline{h})$$
$$\times\hat{T}(0,2\pi pqM_\nu N)\hat{T}(-2\pi N/N_\nu,0)\hat{S}(pN_\nu). \tag{4.12}$$

Now substituting for $\hat{O}_{NM}$ and commuting operators this expression simplifies, provided that ϵ_3 takes the values indicated earlier, to give

$$|\tilde{\Phi}_\mu^{(\nu)}\rangle = \frac{1}{N_\nu\sqrt{N_\nu}}\sum_{\mu'=1}^{|N_\nu|}\sum_{\lambda=1}^{|N_\nu|}\sum_{\lambda'=1}^{|N_\nu|}\mathrm{e}^{2\pi\mathrm{i}\mu\mu'qM_\nu/N_\nu}\mathrm{e}^{-2\pi\mathrm{i}\lambda\lambda'/N_\nu}\mathrm{e}^{2\pi\mathrm{i}\mu'q\lambda/N_\nu}$$
$$\times\mathrm{e}^{-\mathrm{i}\pi q^2\mu'^2M_\nu/N_\nu}\mathrm{e}^{-\mathrm{i}\mu'q\alpha\pi}\hat{T}(0,\alpha\pi pN_\nu)\hat{Q}(pqN_\nu M_\nu)\hat{S}(pN_\nu)\hat{R}|\Phi_{\lambda'}^{(\nu)}\rangle \tag{4.13}$$

where $\alpha = 1$ if $N_\nu \times M_\nu$ is odd and zero otherwise. Performing the summation over λ we can further simplify this expression to leave us with

$$|\tilde{\Phi}_\mu^{(\nu)}\rangle = \hat{R}_\Phi|\Phi_\mu^{(\nu)}\rangle \tag{4.14}$$

where

$$\hat{R}_\Phi = \hat{T}(0,\alpha\pi pN_\nu)\hat{Q}(pqN_\nu M_\nu)\hat{S}(pN_\nu)\hat{R}\hat{u}. \tag{4.15}$$

The operator $\hat{u}$ acts on the labels of the Wannier functions as follows

$$\hat{u}|\Phi_\mu^{(\nu)}\rangle = \frac{1}{\sqrt{N_\nu}}\sum_{\mu'=1}^{|N_\nu|}\mathrm{e}^{2\pi\mathrm{i}M_\nu[\mu\mu'-\frac{1}{2}\mu'^2]/N_\nu}\mathrm{e}^{\mathrm{i}\pi M_\nu\alpha\mu'}|\Phi_{\mu'}^{(\nu)}\rangle. \tag{4.16}$$

The definition of $\hat{u}$ in (4.16) contains three terms in the exponent. The first two resemble a Fourier transform and a shearing (which constitutes a six-fold rotation on the square lattice). The third can be considered as a translation operator (2.7) acting on the Wannier function. We therefore define $\hat{u} = \hat{r}\hat{t}(0,\alpha N_\nu/2)$ where

$$\hat{r}|\Phi_\mu^{(\nu)}\rangle = \frac{1}{\sqrt{N_\nu}}\sum_{\mu'=1}^{|N_\nu|}\mathrm{e}^{2\pi\mathrm{i}M_\nu(\mu\mu'-\mu'^2/2)/N_\nu}|\Phi_\mu^{(\nu)}\rangle. \tag{4.17}$$

If we consider the commutation of this operator $\hat{r}$ with the translation operator $\hat{t}(n_1,n_2)$ we find that

$$\hat{t}(n_1,n_2)\hat{r} = \hat{r}\hat{t}(n_2,n_2-n_1) \tag{4.18}$$

which is reminiscent of the commutation of $\hat{R}$ and $\hat{T}(X, P)$ defined in (3.12). So $\hat{r}$ is a rotation operator acting on the labels of the Wannier functions, and in terms of this we can write the total rotation operator for the Wannier functions as

$$\hat{R}_\Phi = \hat{T}(0, \alpha\pi p N_\nu)\hat{Q}(pqN_\nu M_\nu)\hat{S}(pN_\nu)\hat{R}\hat{r}\hat{t}(0, \alpha N_\nu/2). \tag{4.19}$$

The rotation operator for the Wannier functions of the hexagonal lattice $|\phi_\mu^{(\nu)}\rangle$ can be obtained by performing the operation

$$\hat{R}_\phi = \hat{Q}(-s)\hat{S}(a)\hat{R}_\Phi\hat{S}(1/a)\hat{Q}(s). \tag{4.20}$$

s and a take the values $1/\sqrt{3}$ and $(2/\sqrt{3})^{1/2}$, respectively. Applying these operations we find

$$\hat{R}_\phi = \hat{T}(0, \alpha\pi p N_\nu a)\hat{Q}(-q^2 M_\nu^2/\sqrt{3})\hat{S}(pN_\nu)\hat{R}_6\hat{r}_6\hat{t}(0, \alpha N_\nu/2). \tag{4.21}$$

This, then, is the form of the six-fold rotation operator for the set of Wannier states $|\phi_\mu^{(\nu)}\rangle$ defined in section 3.

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Appendix

In order to proceed from (4.10) we will derive an expression relating the Fourier coefficients $\hat{O}_{NM}$ of the operator

$$\begin{aligned}\hat{O}(k, \delta) = {}& e^{iq^2 M_\nu k\delta/2\pi p} e^{-iq^2 M_\nu \delta^2/4\pi p} e^{i\epsilon_3\delta}\hat{T}(0, -qM_\nu k)\\ &\times \sum_{n'}\sum_{m'} e^{-iq\delta m'/p} e^{iqn'k}\hat{T}(0, 2\pi m')\hat{T}(2\pi n' p, 0)\hat{T}(qM_\nu\delta, qM_\nu\delta)\end{aligned} \tag{A.1}$$

to a stretching and shearing of the phase plane.

Taking $m' = m + JM_\nu p$ and $n' = n + JM_\nu$ where J is an arbitrary integer and considering $\langle x|\hat{O}(k, \delta)|\psi\rangle$ when $x = J\hbar + \delta$ we have

$$\begin{aligned}\langle x|\hat{O}(k, \delta)|\psi\rangle = {}& \frac{-2\pi p}{q}\delta(x - J\hbar - \delta) e^{-iq^2 M_\nu x^2/4\pi p} e^{i\epsilon_3 x}\\ &\times \sum_n e^{iqnk}\langle x|\hat{T}(qM_\nu x, qM_\nu x)\hat{T}(2\pi np, 0)|\psi\rangle\\ = {}& \frac{-2\pi p}{q}\delta(x - J\hbar - \delta) e^{iq^2 M_\nu x^2/4\pi p} e^{i\epsilon_3 x} e^{iq^2 M_\nu^2 x^2 q/4\pi p} e^{inq^2 M_\nu x}\\ &\times\langle pN_\nu x|\hat{T}(2\pi np, 0)|\psi\rangle\\ = {}& \frac{-2\pi p}{q}\frac{1}{\sqrt{p}N_\nu}\delta(x - J\hbar - \delta) e^{-iq^2 M_\nu N_\nu x^2/4\pi} e^{-iq^2 M_\nu nx} e^{i\epsilon_3 x}\\ &\times\langle x|\hat{T}(2\pi n/N_\nu, 0)\hat{S}(pN_\nu)|\psi\rangle.\end{aligned} \tag{A.2}$$

Now we will compute the Fourier coefficients of $\hat{O}(k, \delta)$

$$\hat{O}_{NM} = \int_0^{2\pi p/q} d\delta\, e^{iqM\delta/p}\int_0^{2\pi/q} dk\, e^{ikN}\,\hat{O}(k, \delta) \tag{A.3}$$

we find

$$\langle x|\hat{O}_{NM}|\psi\rangle = \frac{4\pi^2 p}{q}\frac{1}{\sqrt{p}N_\nu}\mathrm{e}^{\mathrm{i}qM_\nu x/p}\mathrm{e}^{-\mathrm{i}q^2M_\nu nx}\mathrm{e}^{-\mathrm{i}q^2M_\nu x^2/4\pi p}\mathrm{e}^{\mathrm{i}\epsilon_3 x} \times\langle x|\hat{T}(-2\pi N/N_\nu, 0)\hat{S}(pN_\nu)|\psi\rangle \tag{A.4}$$

which is identical to (4.12).

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