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First order correction to the renormalization of the phase space lattice Hamiltonian

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Abstract. We develop a renormalization group analysis for a Hamiltonian which is a periodic function of $\hat{x}$ and $\hat{p}$; this is a model for Bloch electrons in a magnetic field, and includes Harper's model as a special case. The eigenfunctions are Bloch waves when β, the ratio of $\overline{h}/2\pi$ to the area of the unit cell, is a rational number p/q. The renormalization procedure produces an effective Hamiltonian $\hat{H}_{\rm eff}$ for a subset of the spectrum, which can be expanded in $\Delta\beta = \beta - p/q$. The zeroth-order term has been obtained in earlier papers; here we obtain the first-order term of this expansion in terms of the q-dimensional vectors $|u(k, \delta))$ which define the rational Bloch states (k and δ are Bloch wavevectors).

The effective Hamiltonian is not invariant under gauge transformations $\exp[i\theta(k, \delta)d\tau]$ multiplying the vector $|u(k, \delta))$. We show that the infinitesimal gauge transformation is equivalent to evolving $\hat{H}_{\rm eff}$ under a gauge Hamiltonian obtained (to lowest order in $\Delta\beta$) by quantizing $\theta(k, \delta)$.

1. Introduction

In this paper we develop a renormalization group (RG) analysis introduced in a sequence of earlier papers [1–3], which provides a powerful method for investigating the properties of Harper's model [4] for Bloch electrons in a magnetic field. The renormalized Hamiltonian can be expressed as a power series expansion about any rational value p/q of the commensurability parameter β. The earlier papers only give explicit formulae for the zeroth-order term; this is not sufficient to determine the spectrum in the limit $\beta \to p/q$, because the first-order correction modifies the Bohr–Sommerfeld quantization condition. In this paper we give an explicit formula for the first-order contribution: the RG procedure then provides a very complete description of the spectrum.

Our results are applicable to the Hamiltonian

$$\hat{H} = \sum_n \sum_m H_{nm}\ \hat{T}(n\overline{h}, m\overline{h}) = \sum_n \sum_m H_{nm}\ \exp[i(m\hat{x} - n\hat{p})] \qquad (1.1a)$$

$$H_{-n,-m} = H^*_{nm} \qquad (1.1b)$$

where the coefficients H_{nm} decay rapidly as $|n|, |m| \to \infty$, and where the operator $\hat{T}(X, P)$ is a phase-space translation operator, defined by

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

The Hamiltonian (1.1) can be viewed as either a periodic function of x and p with Fourier coefficients H_{nm}, or alternatively as a sum of terms describing hopping between sites on

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a lattice, with amplitude H_{nm} to hop by (n, m). The translation operators $\hat{T}(X, P)$ have a non-commutative algebra

$$\hat{T}(X_1, P_1)\hat{T}(X_2, P_2) = \exp[\mathrm{i}(X_2 P_1 - X_1 P_2)/2\bar{h}]\hat{T}(X_1 + X_2, P_1 + P_2) \tag{1.3}$$

which is isomorphic to that of the 'magnetic translation group' describing an electron moving in a plane with a perpendicular magnetic field [5, 6]. The Hamiltonian (1.1) is therefore a reasonable model for an electron moving in a plane with a perpendicular magnetic field and a periodic potential energy $V(x, y)$, and it provides a realistic effective Hamiltonian for this problem in the limit of weak potential V [7–9], and also in the limit where the magnetic field is a weak perturbation [10, 4, 11, 12]. An important parameter is the ratio β of $2\pi\bar{h}$ to the area $(4\pi^2)$ of the unit cell; in the small V limit this parameter equals the ratio of the area of a flux quantum to that of the unit cell of the potential $V(x, y)$. The extensively studied Harper model [4] corresponds to a special case of our Hamiltonian, in which the only non-zero coefficients are $H_{10} = H_{01} = 1$ (and their symmetry related images implied by (1.1*b*)); some of the remarkable properties of this model are discussed in review papers by Simon [13] and Sokoloff [14], and references to some more recent papers are given in [3].

Several authors have described RG methods applicable to (1.1) based upon semi-classical approximations [15–18]. By contrast, the results presented in this paper are based upon an exact procedure for writing down an effective Hamiltonian for a subset of the spectrum, which collapses onto a Bloch band when β is rational. This method was introduced in [1] for the special case in which the Hall conductance integer M_ν of the νth band is zero, and it was later reformulated [2] to allow general values of M_ν (the quantized Hall effect for this system was discussed by Thouless *et al* [19], who show that M_ν is the Chern integer of the Bloch band). The development used in [2] is not convenient for systematic calculations of corrections to the effective Hamiltonian, and the calculations presented here are based upon a more refined approach, which is described in [3].

The Schrödinger equation corresponding to (1.1) can be written

$$\sum_N \sum_M H_{NM} \exp[-\mathrm{i}NM\bar{h}/2] \exp[\mathrm{i}Mx_n]\psi_{n-N} = E\psi_n \tag{1.4}$$

where $\psi_n = \psi(x_n)$ and $x_n = n\bar{h} + \delta$. If β is a rational number p/q then the coefficients of the difference equation (1.4) are periodic in n with period q, and the solutions of this equation can be written as Bloch waves $\psi_n(k, \delta) = \exp[\mathrm{i}kn]\ u_n(k, \delta)$ where k is a Bloch wavevector and $u_{n+q} = u_n$. Equation (1.4) is easily transformed into an eigenvalue equation for the vector $\{u_n\}$ and the dispersion relation $\mathcal{E}(k, \delta)$: because both the coefficients of the matrix and the eigenvector are periodic in n, the q distinct elements of the periodic vector $\{u_n\}$ can be obtained as an eigenvector of a $q \times q$ matrix, $\tilde{H}(k, \delta)$. We will use the notation $|u_\nu(k, \delta)\rangle$ for the q-dimensional eigenvectors of this matrix; the q eigenvalues are the dispersion relations $\mathcal{E}_\nu(k, \delta)$ ($\nu = 1, \ldots, q$ is the band index). In [1, 3] it was shown that δ is a Bloch wavevector for translations in the $\hat{p}$ direction in the phase plane.

The RG transformation produces a new effective Hamiltonian $\hat{H}_{\mathrm{eff}}^{(\nu)}$, similar to (1.1), which describes a subset of the spectrum which collapses onto the νth Bloch band in the rational limit $\beta \to p/q$. The renormalized effective Hamiltonian can be expanded as a power series:

$$\hat{H}_{\mathrm{eff}}^{(\nu)} = \hat{H}_0^{(\nu)} + \Delta\bar{h}\hat{H}_1^{(\nu)} + \mathrm{O}(\Delta\bar{h}^2) \qquad \Delta\bar{h} = 2\pi(\beta - p/q)\,. \tag{1.5}$$

The contributions $\hat{H}_i^{(\nu)}$ are periodic functions of operators $\hat{x}'$ and $\hat{p}'$ which have a renormalized commutator; $[\hat{x}', \hat{p}'] = \mathrm{i}\bar{h}'_\nu$. In the earlier papers, it was shown that the zeroth-order term is obtained by quantizing the dispersion relation $\mathcal{E}_\nu(k, \delta)$:

$$\hat{H}_0^{(\nu)} = \mathcal{E}_\nu(\hat{x}'/q, \hat{p}'/q) \tag{1.6}$$

(periodic functions are understood to be quantized by evaluating their Fourier coefficients and associating them with an operator using an expansion of the form (1.1*a*); this is the Weyl quantization [20]). The formula for the renormalization of $\bar{h}$ depends on the Chern integer M_ν of the band

$$\bar{h}'_\nu = 2\pi\beta'_\nu, \quad \beta'_\nu = \frac{q\beta - p}{\beta N_\nu + M_\nu} \tag{1.7}$$

where N_ν is conjugate to the Chern integer M_ν under the relation

$$pN_\nu + qM_\nu = 1\,. \tag{1.8}$$

In this paper we obtain for the first time the first-order correction $\hat{H}_1^{(\nu)}$, which is expressed conveniently in terms of the eigenvector $|u_\nu(k, \delta))$ of the $q \times q$ matrix representing the Hamiltonian in the rational case. We find that $\hat{H}_1^{(\nu)}$ is obtained by quantizing the following function of (k, δ) by the substitutions $k \to \hat{x}'/q$, $\delta \to \hat{p}'/q$:

$$\begin{aligned}
H_1^{(\nu)}(k, \delta) &= H_{1a}^{(\nu)}(k, \delta) + H_{1b}^{(\nu)}(k, \delta) + H_{1c}^{(\nu)}(k, \delta) \\
H_{1a}^{(\nu)}(k, \delta) &= \frac{\mathrm{i}}{2}\left[\left(\frac{\partial u_\nu}{\partial \delta}\middle|\mathcal{E}_\nu(k, \delta) - \tilde{H}(k, \delta)\middle|\frac{\partial u_\nu}{\partial k}\right) - \left(\frac{\partial u_\nu}{\partial k}\middle|\mathcal{E}_\nu(k, \delta) - \tilde{H}(k, \delta)\middle|\frac{\partial u_\nu}{\partial \delta}\right)\right] \\
H_{1b}^{(\nu)}(k, \delta) &= \mathrm{i}\left(u_\nu\middle|\frac{\partial u_\nu}{\partial k}\right)\frac{\partial \mathcal{E}_\nu}{\partial \delta} - \mathrm{i}\left(u_\nu\middle|\frac{\partial u_\nu}{\partial \delta}\right)\frac{\partial \mathcal{E}_\nu}{\partial k} \\
H_{1c}^{(\nu)}(k, \delta) &= \frac{kqN_\nu}{2\pi}\frac{\partial \mathcal{E}_\nu}{\partial k}\,.
\end{aligned} \tag{1.9}$$

The vector $|u_\nu(k, \delta))$ is assumed to be given as an analytic function of k and δ, and it is periodic in k and δ apart from a phase factor $\exp[\mathrm{i}\chi]$, which will be specified later. The expression $H_{1a}^{(\nu)}$ in (1.9) was previously discovered by Bellissard and Rammal [21], who wrote down an expansion of the effective Hamiltonian about the extrema of the dispersion relation; in their theory the meaning of this term is only defined at the extrema of the band. Later, Helffer and Sjöstrand [18] identified the term $H_{1b}^{(\nu)}$ in a semi-classical calculation: their effective Hamiltonian differs from ours in that it does not contain the term $H_{1c}^{(\nu)}$, and it is quantized using a different value of $\bar{h}'$. Remarkably, Helffer and Sjöstrand's formulae give the same Bohr–Sommerfeld quantization condition as our effective Hamiltonian, but their semi-classical approximations are not valid in a small range of energy centred on the separatrix of the Hamiltonian. Our expression is valid throughout the band, including the separatrix.

The vector $|u_\nu(k, \delta))$ can be subjected to a 'gauge transformation'

$$|u_\nu(k, \delta)) \to |u'_\nu(k, \delta)) = \exp[\mathrm{i}\theta(k, \delta)]\,|u_\nu(k, \delta))\,. \tag{1.10}$$

The expressions $H_{1a}^{(\nu)}$ and $H_{1c}^{(\nu)}$ are gauge invariant, but $H_{1b}^{(\nu)}$ is not. We will consider the effect of an infinitesimal gauge transformation with phase $\theta(k, \delta)\mathrm{d}\tau$ periodic on the

Brillouin zone ($0 \leqslant k \leqslant 2\pi/q$, $0 \leqslant \delta \leqslant 2\pi/q$). We show that this is equivalent (to lowest order in $\Delta\hbar$) to evolving the effective Hamiltonian for time $\mathrm{d}\tau$ under the dynamics of a 'gauge Hamiltonian', obtained by quantizing $q^2\Delta\hbar\,\theta(k,\delta)$. Because evolution of an operator leaves its eigenvalues unchanged, the gauge transformation does not alter the spectrum of the effective Hamiltonian.

The form of $H_1^{(\nu)}$ given in (1.9) is not symmetric between k and δ. We note that, allowing for a more general gauge transformation of the vectors $|u_\nu(k,\delta)\rangle$, we can write this term in a symmetric form

$$H_1^{(\nu)}(k,\delta) = H_{1a}^{(\nu)} + \mathbf{A}\wedge\nabla\mathcal{E}_\nu(k,\delta) \qquad \mathbf{A} = \mathrm{i}(u|\nabla u) + \mathbf{A}' \tag{1.11}$$

where ∇ represents a vector operator $(\frac{\partial}{\partial k}, \frac{\partial}{\partial \delta})$, and where $\mathbf{A}'$ is chosen such that $\mathbf{A}$ is periodic and

$$\int_0^{2\pi/q}\mathrm{d}k\int_0^{2\pi/q}\mathrm{d}\delta\ \nabla\wedge\mathbf{A} = 0\,. \tag{1.12}$$

The formulation of the renormalization group transformation is considerably simpler in the case where the Hall conductance integer is $M_\nu = 0$. For this reason we confine our detailed discussion of the lengthy calculations leading to (1.9) to this special case: we will summarize the formulae describing the RG procedure for $M_\nu = 0$ in section 2, before presenting the analysis leading to (1.9) in sections 3 to 5. In section 6 we indicate how the calculation proceeds in the general case. Section 7 discusses the effects of gauge transformations, and section 8 describes some numerical tests of our results.

2. The renormalization-group method

Here we will summarize the equations which define the renormalization-group transformation. The general form of these equations, which are given in [3], are quite complicated; in this section we will quote the simplified form of these equations which are obtained in the special case where $p = 1$ and $M_\nu = 0$, before discussing the general case in section 6. This case was originally discussed in [1], but we will follow the slightly different notation of [3] for consistency with the results of section 6. We will use the notation (3.N.M) to refer to equation (N.M) of [3].

When β is the ratio of two integers p/q, the eigenvectors of the Hamiltonian (1.1) are Bloch waves, for which the wavefunction can be obtained by sampling an analytic, periodic function $U_\nu(x;k)$ as follows:

$$\langle x|B_\nu(k,\delta)\rangle = \sum_{n=-\infty}^{\infty}\exp[\mathrm{i}kx/\hbar]\ u_n(k,\delta)\ \delta(x-n\hbar-\delta)$$
$$u_n(k,\delta) = U_\nu(x_n;k) \qquad x_n = n\hbar+\delta \qquad U_\nu(x+2\pi;k) = U_\nu(x;k) \tag{2.1}$$

(this is discussed in subsection 2.1 of [3]). Note that writing the Bloch waves in this form has implications for the gauge of the vectors $|u_\nu(k,\delta)$. The rational Bloch states are eigenstates both of the Hamiltonian, and of operators which translate by multiples of the lattice periodicity:

$$\hat{H}_0\,|B_\nu(k,\delta)\rangle = \mathcal{E}_\nu(k,\delta)\,|B_\nu(k,\delta)\rangle \tag{2.2a}$$

$$\hat{T}_0(-2\pi m,-2\pi n)\,|B_\nu(k,\delta)\rangle = (-1)^{nmq}\exp[-\mathrm{i}q(n\delta-mk)]\,|B_\nu(k,\delta)\rangle\,. \tag{2.2b}$$

The subscript zeros indicate that the translation operator and the Hamiltonian are evaluated in the rational case, $\overline{h} = \overline{h}_0 \equiv 2\pi p/q$; (2.2*b*) follows from (1.3) and (3.3.15). If $M_\nu = 0$, the Bloch waves can be gauged such that they are periodic in k and δ over the Brillouin zone. We can form a basis Wannier function which will then be both analytic and spatially localized by integrating over k and δ:

$$|\phi^{(\nu)}\rangle = \int_0^{2\pi/q} \mathrm{d}k \int_0^{2\pi/q} \mathrm{d}\delta \; |B_\nu(k,\delta)\rangle \tag{2.3}$$

(this result is a special case of (3.A.4), which applies when $p = 1$ and $M_\nu = 0$).

The renormalization procedure uses the Wannier functions as a basis for representing the effective Hamiltonian of a sub-band where β is close to p/q. The Wannier states are projected into the band by applying a projection operator $\hat{P}$

$$\hat{P}_\nu = f_\nu(\hat{H}) = \sum_n |\psi_n\rangle \; f_\nu(E_n) \; \langle\psi_n| \tag{2.4}$$

where $|\psi_n\rangle$ and E_n are the eigenstates and eigenvalues of the Hamiltonian $\hat{H}$, and $f_\nu(E)$ is a function that is unity if E lies within the ν^{th} band of the spectrum, and zero if E lies within other parts of the spectrum [2]. Note that we are projecting the Wannier functions at $\overline{h}_0$ onto the exact eigenstates at $\overline{h}$.

The matrix elements of the Hamiltonian and the identity operators in a basis formed by the projected Wannier states $\hat{T}(2\pi n, 2\pi m)\hat{P}|\phi\rangle$ are the same as matrix elements of the following operators:

$$\begin{aligned}\hat{H}'_\nu &= \sum_N \sum_M H^{(\nu)}_{NM} \; \exp[\mathrm{i}(M\hat{x}' - N\hat{p}'] = \sum_N \sum_M H^{(\nu)}_{NM} \; \hat{T}(N\overline{h}'_\nu, M\overline{h}'_\nu) \\ \hat{N}'_\nu &= \sum_N \sum_M N^{(\nu)}_{NM} \; \exp[\mathrm{i}(M\hat{x}' - N\hat{p}'] = \sum_N \sum_M N^{(\nu)}_{NM} \; \hat{T}(N\overline{h}'_\nu, M\overline{h}'_\nu)\end{aligned} \tag{2.5}$$

with $[\hat{x}', \hat{p}'] = \mathrm{i}\overline{h}'_\nu$. These relations are equivalent to (3.5.1), but we have corrected a sign ambiguity. Using (1.7), we find that when $p = 1$ and $M_\nu = 0$, the renormalized Planck constant is given by

$$\overline{h}'_\nu = 2\pi\beta' \qquad \beta' = 1/\beta - [1/\beta] \tag{2.6}$$

($[X]$ means integer part of X). The Fourier coefficients defining the renormalized Hamiltonian and normalization operators in (2.6) are given by

$$\begin{aligned}H^{(\nu)}_{nm} &= (-1)^{mnq} \langle\phi^{(\nu)}|\hat{P}\,\hat{T}(-2\pi m, -2\pi n)\,\hat{H}\;\hat{P}|\phi^{(\nu)}\rangle \\ N^{(\nu)}_{nm} &= (-1)^{mnq} \langle\phi^{(\nu)}|\hat{P}\,\hat{T}(-2\pi m, -2\pi n)\,\hat{P}|\phi^{(\nu)}\rangle\end{aligned} \tag{2.7}$$

which are obtained by specializing (3.4.15) and (3.5.8).

The eigenenergies of this renormalized Hamiltonian operator can be obtained from the relation $(\hat{H}'_\nu - E\hat{N}'_\nu)|\psi\rangle = 0$. It is possible to transform $\hat{H}'_\nu$ to an orthonormal basis by multiplying the above equation from the left by $(\hat{N}'_\nu)^{-1}$:

$$\hat{H}^{(\nu)}_{\mathrm{eff}} = (\hat{N}'_\nu)^{-1}\hat{H}'_\nu\,. \tag{2.8}$$

Equation (2.8) gives an effective Hamiltonian which provides an exact representation of the subset of the spectrum which collapses onto the νth band in the rational limit. We will expand the Fourier coefficients (2.7) to first order in $\Delta\bar{h} = 2\pi\Delta\beta$ around $\bar{h}_0 = 2\pi p/q$, and then use (2.8) to determine the expansion of $\hat{H}^{(\nu)}_{\rm eff}$. Because $\hat{P}$, $\hat{H}$ and $\hat{T}(-2\pi m, -2\pi n)$ are all functions of $\bar{h}$, to first order we have for the Fourier coefficients of the Hamiltonian

$$\begin{aligned} H^{(\nu)}_{nm} = (-1)^{mnq}\langle\phi^{(\nu)}|\hat{P}_0\hat{H}_0\hat{T}_0(-2\pi m, -2\pi n)\hat{P}_0|\phi^{(\nu)}\rangle \\ + (-1)^{mnq}\Delta\bar{h}\bigg[\langle\phi^{(\nu)}|\bigg(\frac{\partial\hat{P}}{\partial\bar{h}}\bigg|_0 \hat{H}_0\hat{T}_0(-2\pi m, -2\pi n)\hat{P}_0 \\ + \hat{P}_0\hat{H}_0\hat{T}_0(-2\pi m, -2\pi n)\frac{\partial\hat{P}}{\partial\bar{h}}\bigg|_0\bigg)|\phi^{(\nu)}\rangle \\ + \langle\phi^{(\nu)}|\bigg(\hat{P}_0\frac{\partial\hat{H}}{\partial\bar{h}}\bigg|_0\hat{T}_0(-2\pi m, -2\pi n)\hat{P}_0 \\ + \hat{P}_0\hat{H}_0\frac{\partial\hat{T}}{\partial\bar{h}}\bigg|_0(-2\pi m, -2\pi n)\hat{P}_0\bigg)|\phi^{(\nu)}\rangle\bigg] + {\rm O}(\Delta\bar{h}^2)\,. \end{aligned} \tag{2.9}$$

In (2.9) the subscript zeros indicates that all these quantities are to be evaluated at $\bar{h}_0 = 2\pi p/q$. There exists an analogous expression for the Fourier coefficients of the normalization operator. From (2.2) and (2.3), and recognizing that $\hat{P}_0|B_\nu(k,\delta)\rangle = |B_\nu(k,\delta)\rangle$, we see that the zeroth-order term is simply the (nm)th Fourier coefficient of the dispersion relation $\mathcal{E}_\nu(k,\delta)$ [1,3]. In section 3 we show that the first-order term involving the derivative of the projection operator vanishes. The other terms can be expressed in terms of the q-dimensional vectors $|u_\nu(k,\delta))$ defining the rational Bloch states; some results required to relate these vectors to the Wannier states are established in section 4. In section 5 we evaluate the first-order correction in (2.9), and obtain the effective Hamiltonian using (2.7) and (2.8).

3. First-order effect of the projection operator

Our aim in this section is to show the term in (2.9) involving the derivative $\partial\hat{P}/\partial\bar{h}$ vanishes. We can write the projection operator as a Fourier transform

$$\hat{P} = f(\hat{H}) = \int_{-\infty}^{\infty}{\rm d}t\ \tilde{f}(t)\exp[-{\rm i}\hat{H}t/\bar{h}] = \int_{-\infty}^{\infty}{\rm d}t\ \tilde{f}(t)\ \hat{U}(t) \tag{3.1}$$

where $\hat{U}(t) = \exp[-{\rm i}\hat{H}t/\bar{h}]$ is the propagator. We will write the Hamiltonian in the form $\hat{H} = \hat{H}_0 + \Delta\hat{H} + {\rm O}(\Delta\bar{h}^2)$, where $\hat{H}$ is the Hamiltonian with commensurability β and $\hat{H}_0$ is the Hamiltonian at rational commensurability $\beta_0 = p/q$. In the limit $\beta \to \beta_0$, the difference between these two operators is small for x close to the origin, but grows to be O(1) at large values of x. Because we are interested in the effect of the projection operator upon a Wannier function which is localized around $x = 0$, we are justified in applying perturbation theory in $\Delta\hat{H}$. To develop this perturbation theory, we note that $\hat{U}$ satisfies a 'Dyson equation'

$$\hat{U}(t) = \hat{U}_0(t) - \frac{\rm i}{\bar{h}}\int_0^t{\rm d}t'\ \hat{U}_0(t-t')\,\Delta\hat{H}\ \hat{U}(t') \tag{3.2}$$

where $\hat{U}_0(t) = \exp[-\mathrm{i}\hat{H}_0 t/\overline{h}]$ and $\Delta\hat{H} = \frac{\partial\hat{H}}{\partial\overline{h}}\Delta\overline{h}$. We can obtain the first-order term in the perturbation expansion in $\Delta\overline{h}$ by replacing the $\hat{U}$ in the RHS of (3.2) by $\hat{U}_0$. From this we can calculate the expansion of the projection operator, which we will write as $\hat{P} = \hat{P}_0 + \Delta\hat{P} + \mathrm{O}(\Delta\overline{h}^2)$. In order to calculate the first-order corrections to the Fourier coefficients $H^{(\nu)}_{nm}$ and $N^{(\nu)}_{nm}$ due to the expansion of the projection operator, (2.9) shows that we must evaluate

$$\begin{aligned}\langle\phi^{(\nu)}|\frac{\partial\hat{P}}{\partial\overline{h}}\bigg|_0 &\hat{H}_0\hat{T}_0(-2\pi m, -2\pi n)|\phi^{(\nu)}\rangle \\ &= -\frac{\mathrm{i}}{\overline{h}}(-1)^{mnq}\int_{-\infty}^{\infty}\mathrm{d}t\ \tilde{f}(t)\int_0^t \mathrm{d}t'\ \langle\phi^{(\nu)}|\hat{U}_0(t-t')\frac{\partial\hat{H}}{\partial\overline{h}}\bigg|_0 \\ &\quad\times\hat{U}_0(t')\hat{H}_0\hat{T}_0(-2\pi m, -2\pi n)|\phi^{(\nu)}\rangle \end{aligned} \tag{3.3}$$

and its complex conjugate. Expressing the Wannier functions as integrals over Bloch waves using (2.3), and using (2.2), we have

$$\begin{aligned}\langle\phi^{(\nu)}|\frac{\partial\hat{P}}{\partial\overline{h}}\bigg|_0 &\hat{H}_0\hat{T}_0(-2\pi m, -2\pi n)|\phi^{(\nu)}\rangle \\ &= -\frac{\mathrm{i}}{\overline{h}}(-1)^{mnq}\int_0^{2\pi/q}\mathrm{d}k\int_0^{2\pi/q}\mathrm{d}k'\int_0^{2\pi/q}\mathrm{d}\delta\int_0^{2\pi/q}\mathrm{d}\delta'\ \exp[-\mathrm{i}q(n\delta - mk)] \\ &\quad\times\mathcal{E}_\nu(k,\delta)\langle B_\nu(k',\delta')|\frac{\partial\hat{H}}{\partial\overline{h}}\bigg|_0|B_\nu(k,\delta)\rangle \\ &\quad\times\int_{-\infty}^{\infty}\mathrm{d}t\ \tilde{f}(t)\int_0^t\mathrm{d}t'\ \exp[-\mathrm{i}\mathcal{E}_\nu(k',\delta')(t-t')/\overline{h}]\ \exp[-\mathrm{i}\mathcal{E}_\nu(k,\delta)t'/\overline{h}]\,. \end{aligned} \tag{3.4}$$

We will write the first set of t-independent terms as $C(k,k',\delta,\delta')$. If $\mathcal{E}_\nu(k,\delta)\neq\mathcal{E}_\nu(k',\delta')$ then performing the integrations over t' and then t gives

$$\begin{aligned}\langle\phi^{(\nu)}|\frac{\partial\hat{P}}{\partial\overline{h}}\bigg|_0 &\hat{H}_0\hat{T}_0(-2\pi m, -2\pi n)|\phi^{(\nu)}\rangle \\ &= \mathrm{i}\overline{h}\int_0^{2\pi/q}\mathrm{d}k\int_0^{2\pi/q}\mathrm{d}k'\int_0^{2\pi/q}\mathrm{d}\delta \\ &\quad\times\int_0^{2\pi/q}\mathrm{d}\delta'\ C(k,k'\delta,\delta')\ \frac{f(\mathcal{E}_\nu(k,\delta)) - f(\mathcal{E}_\nu(k',\delta'))}{\mathcal{E}_\nu(k,\delta)-\mathcal{E}_\nu(k',\delta')}\,. \end{aligned} \tag{3.5}$$

Now since both $\mathcal{E}_\nu(k,\delta)$ and $\mathcal{E}_\nu(k',\delta')$ are within the ν^{th} sub-band of the original spectrum then $f(\mathcal{E}_\nu(k,\delta)) - f(\mathcal{E}_\nu(k',\delta')) = 1 - 1 = 0$, so both this term and its conjugate vanish, provided the denominator in (3.5) does not vanish. If $\mathcal{E}_\nu(k,\delta) = \mathcal{E}_\nu(k',\delta')$, we have

$$\begin{aligned}\langle\phi^{(\nu)}|\frac{\partial\hat{P}}{\partial\overline{h}}\bigg|_0 &\hat{H}_0\hat{T}_0(-2\pi m, -2\pi n)|\phi^{(\nu)}\rangle \\ &= \int_0^{2\pi/q}\mathrm{d}k\int_0^{2\pi/q}\mathrm{d}k'\int_0^{2\pi/q}\mathrm{d}\delta\int_0^{2\pi/q}\mathrm{d}\delta'\ C(k,k',\delta,\delta') \\ &\quad\times\int_{-\infty}^{\infty}\mathrm{d}t\ \tilde{f}(t)\,t\ \exp[-\mathrm{i}t\mathcal{E}_\nu(k,\delta)/\overline{h}] \end{aligned} \tag{3.6}$$

and we can write the time integral as

$$\mathrm{i}\overline{h}\frac{\partial}{\partial E}\int_{-\infty}^{\infty}dt\ \exp[-\mathrm{i}\mathcal{E}_\nu(k,\delta)t/\overline{h}]\,\tilde{f}(t)=\mathrm{i}\overline{h}\frac{\partial}{\partial E}f(\mathcal{E}_\nu(k,\delta)) \tag{3.7}$$

which vanishes because $f(E)$ is a constant if E is within the νth band. We have demonstrated that there is no first-order correction to the Fourier coefficients of the Hamiltonian due to the perturbation of the projection operator. An analogous argument produces the same result for the Fourier coefficients of the normalization operator; we can therefore ignore the term containing $\partial\hat{P}/\partial\overline{h}$ in (2.9). Also, note that because $\hat{P}_0|\phi^{(\nu)}\rangle=|\phi^{(\nu)}\rangle$, the projection operator can be dropped from the other first-order terms of (2.9).

4. Representation by finite matrices

In this section we shall introduce a number of relations between matrix elements in a basis of Bloch states defined on the real line by (2.1), and matrix elements in a basis of q-dimensional vectors. We notate vectors in the Hilbert space of states defined on the real line by the Dirac bracket $|\cdots\rangle$, and those in the Hilbert space of q-dimensional vectors by a rounded bracket $|\cdots)$.

In (2.1) we introduced a representation of the Bloch state $|B(k,\delta)\rangle$ on the real x-axis (in this section we will drop the band label ν). We will introduce another Bloch-like state vector

$$\langle x|C(k,\delta)\rangle=\sum_{n=-\infty}^{\infty}\exp(\mathrm{i}kx/\overline{h})\ v_n(k,\delta)\ \delta(x-n\overline{h}-\delta) \tag{4.1}$$

where the set $\{v_n\}$ is formed by periodic repetition of the elements of another q-dimensional vector $|v(k,\delta))$; we will assume that, by analogy with (2.1), the $\{v_n\}$ are obtained by sampling a periodic, analytic function $V(x;k)$. We will require matrix elements of $\hat{x}$ and $\hat{p}$ between the states $|B(k,\delta)\rangle$ and $|C(k,\delta)\rangle$. We will also consider the case in which $|C(k,\delta)\rangle=\hat{A}|B(k,\delta)\rangle$ where $\hat{A}$ can be represented by a Fourier expansion

$$\hat{A}=\sum_N\sum_M A_{NM}\ \hat{T}(N\overline{h},M\overline{h}) \tag{4.2}$$

and show how $\hat{A}$ can be represented by a $q\times q$ matrix. We shall simply quote the results here, the proofs of the results in subsections 4.1 and 4.2 are dealt with in appendices A and B.

4.1. Matrix elements of canonical operators

The overlap of two vectors is given by

$$\langle C(k',\delta')|B(k,\delta)\rangle=\delta(\delta-\delta')\,\delta(k-k')\ (v(k,\delta)|u(k,\delta)) \tag{4.3}$$

where

$$(v(k',\delta')|u(k,\delta))=\sum_{i=1}^{q}v_n^*(k',\delta')u_n(k,\delta)\,. \tag{4.4}$$

The matrix elements of $\hat{p}$ are

$$\langle C(k',\delta')|\hat{p}|B(k,\delta)\rangle = \mathrm{i}\hbar\frac{\partial}{\partial\delta}\bigg[\delta(\delta-\delta')\delta(k-k')\exp[\mathrm{i}(k\delta-k'\delta')/\hbar]\ (v(k',\delta')|u(k,\delta))\bigg]$$
$$+\,k\delta(\delta-\delta')\delta(k-k')(v(k,\delta)|u(k,\delta))$$
$$-\,\mathrm{i}\hbar\delta(\delta-\delta')\delta(k-k')\left(v(k,\delta)\middle|\frac{\partial u}{\partial\delta}(k,\delta)\right) \tag{4.5}$$

and the matrix elements of $\hat{x}$ are

$$\langle C(k',\delta')|\hat{x}|B(k,\delta)\rangle = -\mathrm{i}\hbar\frac{\partial}{\partial k}\bigg[\delta(\delta-\delta')\delta(k-k')\exp[\mathrm{i}(k\delta-k'\delta')/\hbar]\ (v(k',\delta')|u(k,\delta))\bigg]$$
$$+\,\mathrm{i}\hbar\delta(\delta-\delta')\delta(k-k')\left(v(k,\delta)\middle|\frac{\partial u}{\partial k}(k,\delta)\right). \tag{4.6}$$

It should be noted that although these results are similar in structure, there is a term in (4.5) which has no parallel in (4.6). This asymmetry is a consequence of the constraints on the gauge of the $|u(k,\delta))$ which are implied by writing (2.1).

We remark that (4.5) and (4.6) are similar in structure to the matrix elements of the position operator in a basis of conventional Bloch states, as discussed in [11].

4.2. Matrix elements of periodic operators

Here we relate an operator $\hat{A}$ which is periodic in $\hat{x}$ and $\hat{p}$, to a $q\times q$ matrix $\tilde{A}(k,\delta) = \{A_{nm}(k,\delta)\}$; we require that if $|C(k,\delta)\rangle = \hat{A}|B(k,\delta)\rangle$, then $v_n = \sum_{m=1}^{q} A_{nm}u_m$. The details of the derivations are contained in appendix B. In terms of the Fourier coefficients of $\hat{A}$ defined by (4.2), we find

$$A_{nm}(k,\delta) = \sum_{j=-\infty}^{\infty} A'_{n,m+jq}(k,\delta)$$
$$A'_{nm}(k,\delta) = \sum_{M} A_{n-m,M}\exp[-\mathrm{i}k(n-m)]\exp[\mathrm{i}M\delta]\exp[\mathrm{i}M(n+m)\hbar/2]\,. \tag{4.7}$$

We also define three new operators $\hat{A}_\delta$, $\hat{A}_k$ and $\hat{A}_{k,\delta}$ acting on the Hilbert space of operators on the real line, which can be thought of as derivatives of $\hat{A}$ with respect to δ, k and k,δ. They are defined by the relations

$$\left(u(k',\delta')\ \middle|\ \frac{\partial\tilde{A}}{\partial\delta}\ \middle|\ v(k,\delta)\right) = \langle B(k',\delta')|\hat{A}_\delta|C(k,\delta)\rangle$$
$$\left(u(k',\delta')\ \middle|\ \frac{\partial\tilde{A}}{\partial k}\ \middle|\ v(k,\delta)\right) = \langle B(k',\delta')|\hat{A}_k|C(k,\delta)\rangle \tag{4.8}$$
$$\left(u(k',\delta')\ \middle|\ \frac{\partial^2\tilde{A}}{\partial\delta\partial k}\ \middle|\ v(k,\delta)\right) = \langle B(k',\delta')|\hat{A}_{\delta,k}|C(k,\delta)\rangle\,.$$

It follows from (4.7) that the operators are related to the Fourier coefficients of $\hat{A}$ by

$$\hat{A}_k = -\mathrm{i}\sum_{NM} NA_{NM}\ \hat{T}(N\hbar, M\hbar)$$
$$\hat{A}_\delta = \mathrm{i}\sum_{NM} MA_{NM}\ \hat{T}(N\hbar, M\hbar) \tag{4.9}$$
$$\hat{A}_{\delta,k} = \sum_{NM} NMA_{NM}\ \hat{T}(N\hbar, M\hbar)\,.$$

5. First-order correction to the effective Hamiltonian

We shall now use the results in section 4 to calculate the first-order corrections to the Fourier coefficients $H_{nm}^{(\nu)}$, $N_{nm}^{(\nu)}$ of the renormalized Hamiltonian and normalization operators. The results will be written in terms of the eigenvector $|u_\nu(k,\delta)\rangle$ of the $q\times q$ matrix $\tilde{H}(k,\delta)$ representing the Hamiltonian, constructed using (4.7). We shall write these first-order correction terms as $\Delta H_{nm}^{(\nu)}$ and $\Delta N_{nm}^{(\nu)}$. Considering (2.9), and remembering that for the first-order corrections we can ignore the projection operators, we have

$$\begin{aligned}\Delta H_{nm}^{(\nu)} &= (-1)^{mnq}\Delta\overline{h}\langle\phi^{(\nu)}|\frac{\partial\hat{H}}{\partial\overline{h}}\bigg|_0 \hat{T}_0(-2\pi m,-2\pi n)|\phi^{(\nu)}\rangle \\ &\quad + (-1)^{mnq}\Delta\overline{h}\langle\phi^{(\nu)}|\hat{H}_0\frac{\partial}{\partial\overline{h}}\hat{T}(-2\pi m,-2\pi n)\bigg|_0|\phi^{(\nu)}\rangle \\ &= (I_1+I_2)\Delta\overline{h} \qquad (5.1a)\end{aligned}$$

$$\Delta N_{nm}^{(\nu)} = (-1)^{mnq}\Delta\overline{h}\langle\phi^{(\nu)}|\frac{\partial}{\partial\overline{h}}\hat{T}(-2\pi m,-2\pi n)\bigg|_0|\phi^{(\nu)}\rangle \qquad (5.1b)$$

(the terms I_1, I_2 correspond to the two Dirac brackets in (5.1*a*)). To proceed we need to consider derivatives of the Hamiltonian and translation operators with respect to $\overline{h}$. We will consider the operators $\hat{x}$ and $\hat{p}$ in the coordinate representation so $\hat{x}=x$, $\hat{p}=-\mathrm{i}\overline{h}\frac{\partial}{\partial x}$; differentiating $\hat{T}(-2\pi m,-2\pi n)$ gives

$$\frac{\partial\hat{T}}{\partial\overline{h}}(-2\pi m,-2\pi n) = \frac{2\pi}{\overline{h}^2}ni(\pi m+\hat{x})\hat{T}(-2\pi m,-2\pi n)\,. \qquad (5.2)$$

Also, for the Hamiltonian (1.1) we have (using equation (4.9))

$$\begin{aligned}\frac{\partial\hat{H}}{\partial\overline{h}} &= -\frac{\mathrm{i}}{\overline{h}}\sum_N\sum_M N\,H_{NM}\exp[\mathrm{i}(M\hat{x}-N\hat{p})]\hat{p} - \frac{\mathrm{i}}{2}\sum_N\sum_M H_{NM}NM\exp[\mathrm{i}(M\hat{x}-N\hat{p})] \\ &= \frac{1}{\overline{h}}\hat{H}_k\,\hat{p} - \frac{\mathrm{i}}{2}\hat{H}_{\delta,k} \qquad (5.3)\end{aligned}$$

We are now in a position to evaluate the terms in (5.1); using equations (4.3)–(4.5), the integral I_1 is

$$\begin{aligned}I_1 &= \int_0^{2\pi/q}\mathrm{d}k'\int_0^{2\pi/q}\mathrm{d}k\int_0^{2\pi/q}\mathrm{d}\delta\int_0^{2\pi/q}\mathrm{d}\delta'\;\exp[-\mathrm{i}q(n\delta-mk)] \\ &\quad\times\langle B_\nu(k',\delta')|\left(\frac{1}{\overline{h}}\hat{H}_k\hat{p}+\frac{\mathrm{i}}{2}\hat{H}_{k,\delta}\right)|B_\nu(k,\delta)\rangle \\ &= \int_0^{2\pi/q}\mathrm{d}k\int_0^{2\pi/q}\mathrm{d}\delta\left[\frac{k}{\overline{h}}\left(u_\nu(k,\delta)\left|\frac{\partial\tilde{H}}{\partial k}\right|u_\nu(k,\delta)\right)\right. \\ &\quad - \mathrm{i}\left(u_\nu(k,\delta)\left|\frac{\partial\tilde{H}}{\partial k}\right|\frac{\partial u_\nu}{\partial\delta}(k,\delta)\right) \\ &\quad \left.-\frac{\mathrm{i}}{2}\left(u_\nu(k,\delta)\left|\frac{\partial^2\tilde{H}}{\partial k\partial\delta}\right|u_\nu(k,\delta)\right)\right]\exp[-\mathrm{i}q(n\delta-mk)]\,. \qquad (5.4)\end{aligned}$$

Similarly, using equation (4.6) we have

$$
\begin{aligned}
I_2 = \frac{2\pi \mathrm{i} n}{\hbar^2} \int_0^{2\pi/q} \mathrm{d}k' \int_0^{2\pi/q} \mathrm{d}\delta' \int_0^{2\pi/q} \mathrm{d}k \int_0^{2\pi/q} \mathrm{d}\delta\, \mathcal{E}_\nu(k',\delta') \\
\times \langle B_\nu(k',\delta')|\hat{x}|B_\nu(k,\delta)\rangle\ \exp[-\mathrm{i}q(n\delta - mk)] \\
+ \frac{2\pi^2 \mathrm{i} nm}{\hbar^2} \int_0^{2\pi/q} \mathrm{d}k \int_0^{2\pi/q} \mathrm{d}\delta\, \mathcal{E}_\nu(k,\delta) \exp[-\mathrm{i}q(n\delta - mk)] \\
= \int_0^{2\pi/q} \mathrm{d}k \int_0^{2\pi/q} \mathrm{d}\delta \left[\frac{2\pi^2}{\hbar^2} \mathrm{i} nm - \frac{2\pi}{\hbar} n \left(u_\nu(k,\delta) \middle| \frac{\partial u_\nu}{\partial k}(k,\delta) \right)\right] \\
\times \mathcal{E}_\nu(k,\delta) \exp[-\mathrm{i}q(n\delta - mk)]\,.
\end{aligned}
\tag{5.5}
$$

We can simplify this expression by writing the multipliers in (5.5) as derivatives of the exponential factor with respect to k and δ. Noting that $\mathcal{E}_\nu(k,\delta)$ is periodic across the Brillouin zone in both directions, as is the overlap $(u_\nu|\partial u_\nu/\partial k)$ in the gauge we have defined for the $|u_\nu(k,\delta))$ in (2.1); we can therefore integrate by parts and write (5.5) as

$$
\begin{aligned}
I_2 = \int_0^{2\pi/q} \mathrm{d}k \int_0^{2\pi/q} \mathrm{d}\delta \left[\frac{\mathrm{i}}{2} \frac{\partial^2 \mathcal{E}_\nu}{\partial k \partial \delta}(k,\delta) + \mathrm{i} \frac{\partial}{\partial \delta} \left(u_\nu(k,\delta) \middle| \frac{\partial u_\nu}{\partial k}(k,\delta) \right) \mathcal{E}_\nu(k,\delta)\right] \\
\times \exp[-\mathrm{i}q(n\delta - mk)]\,.
\end{aligned}
\tag{5.6}
$$

Before combining I_1 and I_2 we will re-write (5.4). By starting with the eigenvalue equation $\tilde{H}(k,\delta)|u(k,\delta)) = \mathcal{E}_\nu(k,\delta)|u(k,\delta))$ and differentiating with respect to k and then δ, the following two identities can be derived:

$$
\left(u_\nu(k,\delta) \middle| \frac{\partial \tilde{H}}{\partial k}(k,\delta) \middle| u_\nu(k,\delta) \right) = \frac{\partial \mathcal{E}_\nu}{\partial k}(k,\delta)
\tag{5.7a}
$$

$$
\begin{aligned}
\mathrm{i} \left(u_\nu(k,\delta) \middle| \frac{\partial \tilde{H}}{\partial k} \middle| \frac{\partial u_\nu}{\partial \delta}(k,\delta) \right) \\
= \frac{\mathrm{i}}{2} \left[\left(\frac{\partial u_\nu}{\partial k} \middle| \mathcal{E}_\nu - \tilde{H} \middle| \frac{\partial u_\nu}{\partial \delta} \right) - \left(\frac{\partial u_\nu}{\partial \delta} \middle| \mathcal{E}_\nu - \tilde{H} \middle| \frac{\partial u_\nu}{\partial k} \right) \right] \\
- \frac{\mathrm{i}}{2} \left(u_\nu \middle| \frac{\partial^2 \tilde{H}}{\partial k \partial \delta} \middle| u_\nu \right) + \frac{\mathrm{i}}{2} \frac{\partial^2 \mathcal{E}_\nu}{\partial k \partial \delta} + \mathrm{i} \frac{\partial \mathcal{E}_\nu}{\partial k} \left(u_\nu \middle| \frac{\partial u_\nu}{\partial \delta} \right).
\end{aligned}
\tag{5.7b}
$$

Note that the first term in the RHS of (5.7b) is the expression $H_{1a}^{(\nu)}$ appearing in (1.9). We now combine the two terms which make up $\Delta H_{nm}^{(\nu)}$: the terms involving double derivatives of the dispersion relation $\mathcal{E}_\nu(k,\delta)$ and the Hamiltonian $\tilde{H}(k,\delta)$ cancel, leaving

$$
\begin{aligned}
\Delta H_{nm}^{(\nu)} = \Delta\hbar \int_0^{2\pi/q} \mathrm{d}k \int_0^{2\pi/q} \mathrm{d}\delta \left[\mathrm{i} \left(u_\nu \middle| \frac{\partial u_\nu}{\partial k} \right) \frac{\partial \mathcal{E}_\nu}{\partial \delta} - \mathrm{i} \left(u_\nu \middle| \frac{\partial u_\nu}{\partial \delta} \right) \frac{\partial \mathcal{E}_\nu}{\partial k} \right. \\
\left. + H_{1a}^{(\nu)} + \mathrm{i}\mathcal{E}_\nu \frac{\partial}{\partial \delta} \left(u_\nu \middle| \frac{\partial u_\nu}{\partial k} \right) + \frac{k}{\hbar} \frac{\partial \mathcal{E}_\nu}{\partial k} \right] \exp[-\mathrm{i}q(n\delta - mk)]\,.
\end{aligned}
\tag{5.8}
$$

A similar calculation leads to

$$
\Delta N_{nm}^{(\nu)} = \Delta\hbar \int_0^{2\pi/q} \mathrm{d}k \int_0^{2\pi/q} \mathrm{d}\delta \left[\mathrm{i} \frac{\partial}{\partial \delta} \left(u_\nu \middle| \frac{\partial u_\nu}{\partial k} \right) \right] \exp[-\mathrm{i}q(n\delta - mk)]
\tag{5.9}
$$

for the correction to the Fourier coefficients of the normalization operator.

We now use (2.8) to calculate the effective Hamiltonian $\hat{H}^{(\nu)}_{\rm eff} = (\hat{N}'_\nu)^{-1}\hat{H}'_\nu$; writing $\hat{H}'_\nu = \mathcal{E}_\nu + \partial\hat{H}'_\nu\Delta\hbar + {\rm O}(\Delta\hbar^2)$ and $\hat{N}'_\nu = \hat{I} + \partial\hat{N}'_\nu\Delta\hbar + {\rm O}(\Delta\hbar^2)$, where $\hat{\mathcal{E}}_\nu$ is the operator obtained by quantizing $\mathcal{E}_\nu(k,\delta)$, we have

$$\hat{H}^{(\nu)}_{\rm eff} = \hat{\mathcal{E}}_\nu + (\partial\hat{H}'_\nu - \partial\hat{N}'_\nu\hat{\mathcal{E}}_\nu)\Delta\hbar + {\rm O}(\Delta\hbar^2)\,. \tag{5.10}$$

In appendix C we prove that, to zeroth order in $\Delta\hbar$, the product of operators $\hat{A}\,\hat{B}$ is given by quantizing the product $A(k,\delta)\,B(k,\delta)$. This means that the first-order correction to the Fourier coefficients of the effective Hamiltonian is given by subtracting

$$(\partial N'_\nu\mathcal{E})_{nm} = \int_0^{2\pi/q}{\rm d}k\int_0^{2\pi/q}{\rm d}\delta\left[{\rm i}\frac{\partial}{\partial\delta}(u|\frac{\partial u}{\partial k})\right]\mathcal{E}_\nu(k,\delta)\exp[-{\rm i}q(n\delta-mk)] \tag{5.11}$$

from $\Delta H^{(\nu)}_{nm}$. The final expression for the Fourier coefficients of the first-order contribution to the effective Hamiltonian is therefore

$$(H_1^{(\nu)})_{nm} = \int_0^{2\pi/q}{\rm d}k\int_0^{2\pi/q}{\rm d}\delta\ \exp[-{\rm i}q(n\delta-mk)]\ H_1^{(\nu)}\,. \tag{5.12}$$

where

$$H_1^{(\nu)} = H_{1a}^{(\nu)} + {\rm i}\left(u_\nu\left|\frac{\partial u_\nu}{\partial k}\right.\right)\frac{\partial\mathcal{E}_\nu}{\partial\delta} - {\rm i}\left(u_\nu\left|\frac{\partial u_\nu}{\partial\delta}\right.\right)\frac{\partial\mathcal{E}_\nu}{\partial k} + \frac{kq}{2\pi}\frac{\partial\mathcal{E}_\nu}{\partial k}\,. \tag{5.13}$$

This establishes (1.9) in the special case where $M_\nu = 0$ and $p = 1$.

6. Extension to non-zero Chern integer

6.1. General form of the renormalization-group equations

In this section we discuss how to generalize the derivation of (1.9) to the case where the Chern integer M_ν is non-zero. We will first summarize some of the important results from [3], again using the notation (3.N.M) to denote equation (N.M) of that paper.

Although $|B_\nu(k,\delta)\rangle$ can not be made periodic in k and δ unless $M_\nu = 0$, a gauge can be chosen such that the state vector $|C_\nu(k,\delta)\rangle = \hat{T}_0(0,-qM_\nu k)|B_\nu(k,\delta)\rangle$ is periodic, for any value of M_ν. A set of N_ν generalized Wannier functions $|\phi^{(\nu)}_\mu\rangle$, $\mu = 1,\ldots,N_\nu$ can be obtained from the Bloch states as follows (equation (3.A.4), with a different normalization factor):

$$\begin{aligned}|\phi^{(\nu)}_\mu\rangle &= \frac{1}{\sqrt{p}N_\nu}\sum_{\lambda=1}^{N_\nu}\exp[2\pi{\rm i}\mu\lambda/N_\nu]\,\hat{T}_0(2\pi\lambda/N_\nu,0)\int_0^{2\pi/q}{\rm d}k\int_0^{2\pi p/q}{\rm d}\delta\ \exp[{\rm i}qk\lambda]\ |C_\nu(k,\delta)\rangle \\ |C_\nu(k,\delta)\rangle &= \hat{T}_0(0,-qM_\nu k)\,|B_\nu(k,\delta)\rangle\,.\end{aligned} \tag{6.1}$$

Here the subscript zeros again mean that the $\hat{T}$ operators are evaluated at $\hbar_0 = 2\pi p/q$, and it is assumed that the Bloch waves $|B_\nu(k,\delta)\rangle$ are gauged such that the $\{u_n\}$ are obtained by sampling an analytic function $U_\nu(x;k)$ with period 2π, as in (2.1). The renormalized Hamiltonian is of the form (2.5), and the Fourier coefficients are given by equation (3.5.8):

$$H^{(\nu)}_{nm} = \sum_N\sum_M H_{NM}\ \tau^{NM}_{nm}\,. \tag{6.2}$$

Here the H_{NM} are the Fourier coefficients of the original Hamiltonian, and the coefficients τ_{nm}^{NM} are obtained from the generalized Wannier functions using (3.4.15) and (3.4.18):

$$\tau_{nm}^{NM} = (-1)^{(nN+mM-nmq)p} \sum_{\mu=1}^{N_\nu} \langle \phi_\mu^{(\nu)} | \hat{\tau}_{nm}^{NM} | \phi_\mu^{(\nu)} \rangle$$
$$\hat{\tau}_{nm}^{NM} = \hat{t}(M-nq, N-mq)\, \hat{T}\big((-2\pi m + N\kappa_\nu)/N_\nu, (-2\pi n + M\kappa_\nu)\overline{h}/\kappa_\nu\big)\,. \tag{6.3}$$

In this expression

$$\kappa_\nu = 2\pi M_\nu + N_\nu \overline{h} \tag{6.4}$$

is the period of the Brillouin zone for a set of generalized Bloch functions defined in subsection 2.2 of [3] for irrational β; we have $\kappa_\nu \to 2\pi/q$ in the limit $\overline{h} \to 2\pi p/q$. The operator $\hat{t}(\lambda_1, \lambda_2)$ is defined (for integer values of λ_1, λ_2) by the relation (3.4.16):

$$\hat{t}(\lambda_1, \lambda_2) | \phi_\mu^{(\nu)} \rangle = \exp\left[\frac{2\pi \mathrm{i} M_\nu}{N_\nu} (\mu - \tfrac{1}{2}\lambda_1)\lambda_2 \right] | \phi_{\mu-\lambda_1}^{(\nu)} \rangle\,. \tag{6.5}$$

The $\hat{t}(\lambda_1, \lambda_2)$ operators have a non-commuting algebra analogous to (1.3).

6.2. Zeroth-order term

We will now use these results to calculate the zeroth-order term of the Fourier coefficients. The result has already been given in [1,2,3], but the approach used here, based on (6.2) and (6.3), is different from that of the earlier papers; it will be used as a model for calculating the first-order correction.

First we consider the matrix elements appearing in (6.3); using (6.5), we have

$$\langle \phi_\mu^{(\nu)} | \hat{\tau}_{nm}^{NM} | \phi_\mu^{(\nu)} \rangle = \exp\left[\frac{2\pi \mathrm{i} M_\nu}{N_\nu} \big(\mu - \tfrac{1}{2}(M-nq)\big)(N-mq) \right]$$
$$\times \langle \phi_\mu^{(\nu)} | \hat{T}\big((-2\pi m + N\kappa_\nu)/N_\nu, (-2\pi n + M\kappa_\nu)\overline{h}/\kappa_\nu\big) | \phi_{\mu-(M-nq)}^{(\nu)} \rangle\,. \tag{6.6}$$

If we now substitute for the Wannier functions using (6.1) then we have

$$\tau_{nm}^{NM} = \frac{1}{pN_\nu^2} (-1)^{(nN+mM-nmq)p} \exp\big[-\pi \mathrm{i} M_\nu (M-nq)(N-mq)/N_\nu\big]$$
$$\times \sum_{\lambda=1}^{N_\nu} \sum_{\lambda'=1}^{N_\nu} \sum_{\mu=1}^{N_\nu} \exp\left[\frac{2\pi \mathrm{i}}{N_\nu} \mu \big(M_\nu(N-mq) - \lambda + \lambda'\big) \right] \exp\big[-2\pi \mathrm{i}(M-nq)\lambda'/N_\nu\big]$$
$$\times \int_0^{2\pi/q} \mathrm{d}k \int_0^{2\pi/q} \mathrm{d}k' \int_0^{2\pi p/q} \mathrm{d}\delta \int_0^{2\pi p/q} \mathrm{d}\delta' \, \exp[\mathrm{i}q(k\lambda' - k'\lambda)]$$
$$\times \langle C_\nu(k', \delta') | \hat{T}_0\left(\frac{-2\pi\lambda}{N_\nu}, 0 \right) \hat{T}\left(\frac{-2\pi m + N\kappa_\nu}{N_\nu}, \frac{-2\pi n + M\kappa_\nu}{\kappa_\nu/\overline{h}} \right)$$
$$\times \hat{T}_0\left(\frac{2\pi\lambda'}{N_\nu}, 0 \right) | C_\nu(k, \delta) \rangle \tag{6.7}$$

(note that in this expression, one of the translation operators, $\hat{T}$ is evaluated at $\overline{h}$, while others denoted $\hat{T}_0$ are evaluted at $\overline{h}_0 = 2\pi p/q$). The sum over μ will vanish unless

$$(M_\nu(N - mq) - \lambda + \lambda') \bmod N_\nu = 0 \tag{6.8}$$

so that substituting in (6.2) and performing the sum, we have

$$\begin{aligned} H_{nm}^{(\nu)} = \frac{1}{pN_\nu} \sum_N \sum_M (-1)^{(nN+mM-nmq)p}\, H_{NM} \\ \times \exp\left[-\pi \mathrm{i} M_\nu (M - nq)(N - mq)/N_\nu\right] \sum_{\lambda'=1}^{N_\nu} \exp[-2\pi \mathrm{i}(M - nq)\lambda'/N_\nu] \\ \times \int_0^{2\pi/q} \mathrm{d}k \int_0^{2\pi/q} \mathrm{d}k' \int_0^{2\pi p/q} \mathrm{d}\delta \int_0^{2\pi p/q} \mathrm{d}\delta' \, \exp[\mathrm{i}q(\lambda' k - \lambda k')] \\ \times \langle C_\nu(k', \delta')|\hat{T}_0\left(\frac{-2\pi\lambda}{N_\nu}, 0\right)\hat{T}\left(\frac{-2\pi m + N\kappa_\nu}{N_\nu}, \frac{-2\pi n + M\kappa_\nu}{\kappa_\nu/\overline{h}}\right) \\ \times \hat{T}_0\left(\frac{2\pi\lambda'}{N_\nu}, 0\right)|C_\nu(k, \delta)\rangle \end{aligned} \tag{6.9}$$

where λ is given by (6.8). This result is exact; we now use it to calculate the first two terms of an expansion in $\Delta\overline{h}$.

To calculate the zeroth-order term in $\Delta\overline{h}$ we proceed setting $\overline{h} = 2\pi p/q$ and $\kappa_\nu = 2\pi/q$; applying (1.3), we find after some work that (6.9) reduces to

$$\begin{aligned} H_{nm}^{(\nu)} = (-1)^{nmpq} \frac{1}{pN_\nu} \sum_{\lambda=1}^{N_\nu} \int_0^{2\pi/q} \mathrm{d}k \int_0^{2\pi/q} \mathrm{d}k' \int_0^{2\pi p/q} \mathrm{d}\delta \int_0^{2\pi p/q} \mathrm{d}\delta' \, \exp[\mathrm{i}q\lambda(k - k')] \\ \times \langle B_\nu(k', \delta')|\hat{T}_0(-2\pi mp, -2\pi np)\hat{H}_0\hat{T}_0\big(0, qM_\nu(k' - k)\big)|B_\nu(k, \delta)\rangle + \mathrm{O}(\Delta\overline{h}) . \end{aligned} \tag{6.10}$$

We now define states $|D_\nu(k, \delta)\rangle$ and $|V_\nu(k, \delta)\rangle$ as follows:

$$|D_\nu(k, \delta)\rangle = \frac{1}{\sqrt{p}} \sum_{\mu=1}^{p} |B_\nu(k, \delta + 2\pi\mu/q)\rangle = \exp[\mathrm{i}k\hat{x}/\overline{h}]|V_\nu(k, \delta)\rangle . \tag{6.11}$$

Equation (6.11) will be re-written in terms of matrix elements of the $|D_\nu(k, \delta)\rangle$ states, with the integral over δ restricted to the range from 0 to $2\pi/q$. These matrix elements are

$$\begin{aligned} \langle D_\nu(k', \delta')|\hat{T}_0(-2\pi mp, -2\pi np)\, \hat{H}_0\, \hat{T}_0\big(0, qM_\nu(k' - k)\big)|D_\nu(k, \delta)\rangle \\ = \exp[-\mathrm{i}q(n\delta - mk)]\, \mathcal{E}_\nu(k, \delta)\, \langle V_\nu(k', \delta')|\exp[\mathrm{i}pN_\nu(k - k')\hat{x}]|V_\nu(k, \delta)\rangle \\ = \exp[-\mathrm{i}q(n\delta - mk)]\, \mathcal{E}_\nu(k, \delta) \sum_{J=0}^{N_\nu - 1} \delta(\delta - \delta')\, \delta(k - k' - 2\pi J/qN_\nu)\, I_J(k, \delta) \end{aligned} \tag{6.12}$$

where the last equality defines the coefficients $I_J(k, \delta)$, and the factor $\delta(k - k' - 2\pi J/qN_\nu)$ arises because the states $|V_\nu(k, \delta)\rangle$ are derived by sampling the 2π periodic function $U_\nu(x; k)$

at points separated by $2\pi/q$. Note that normalization of the Bloch states implies that $I_0(k,\delta) = 1$. Re-writing equation (6.10) in terms of these matrix elements, we have

$$
\begin{aligned}
H_{nm}^{(\nu)} = (-1)^{nmpq} \frac{1}{N_\nu} \sum_{\lambda=1}^{N_\nu} \int_0^{2\pi/q} \mathrm{d}k \int_0^{2\pi/q} \mathrm{d}k' \int_0^{2\pi/q} \mathrm{d}\delta \int_0^{2\pi/q} \mathrm{d}\delta' \ \exp[\mathrm{i}q\lambda(k-k')] \\
\times \mathcal{E}_\nu(k,\delta) \ \exp[-\mathrm{i}q(n\delta - mk)] \, \langle D_\nu(k',\delta')|\hat{T}_0(0, qM_\nu(k'-k))|D_\nu(k,\delta)\rangle \\
+ \mathrm{O}(\Delta\overline{h}) \\
= (-1)^{nmpq} \frac{1}{N_\nu} \sum_{\lambda=1}^{N_\nu} \sum_{J=0}^{N_\nu - 1} \exp[2\pi \mathrm{i}\lambda J/N_\nu] \\
\times \int_0^{2\pi/q} \mathrm{d}k \int_0^{2\pi/q} \mathrm{d}\delta \, \mathcal{E}_\nu(k,\delta) \ \exp[-\mathrm{i}q(n\delta - mk)] \, I_J(k,\delta) + \mathrm{O}(\Delta\overline{h}) \, . \qquad (6.13)
\end{aligned}
$$

The sum over λ vanishes unless $J = 0$, in which case we use the fact that $I_0(k,\delta) = 1$ and obtain our final result, that to zeroth order

$$
H_{nm}^{(\nu)} = (-1)^{nmpq} \int_0^{2\pi/q} \mathrm{d}k \int_0^{2\pi/q} \mathrm{d}\delta \, \mathcal{E}_\nu(k,\delta) \exp[-\mathrm{i}q(n\delta - mk)] + \mathrm{O}(\Delta\overline{h}) \qquad (6.14)
$$

as expected.

6.3. First-order correction

Here we calculate the first-order correction to the Hamiltonian in the general case. We only highlight the differences from the case $M_\nu = 0$ considered in section 5; some of the details are therefore omitted.

To calculate the first-order term we must go back to (6.8) and differentiate $\hat{T}((-2\pi m + N\kappa_\nu)/N_\nu, (-2\pi n\overline{h}/\kappa_\nu + M\overline{h}))$ with respect to $\overline{h}$. Remembering that κ_ν and $\overline{h}$ are related by (6.4), we have four terms

$$
\left.\frac{\partial \hat{T}}{\partial \overline{h}}\right|_0 = (2\pi \mathrm{i} n N_\nu/\kappa_\nu^2)\hat{x}\hat{T}_0 - (\mathrm{i}N/\overline{h})\hat{T}_0\hat{p} - \tfrac{1}{2}\mathrm{i}NM\hat{T}_0 + (2\pi^2 \mathrm{i} nm/\kappa_\nu^2)\hat{T}_0 \, . \qquad (6.15)
$$

The required first-order correction to the Hamiltonian is

$$
\begin{aligned}
\Delta H_{nm}^{(\nu)} = \Delta\overline{h} \frac{1}{N_\nu} \sum_N \sum_M (-1)^{p(nN+mM-qnm)} \, H_{NM} \ \exp\bigl[-\pi \mathrm{i} M_\nu(M-nq)(N-mq)/N_\nu\bigr] \\
\times \sum_{\lambda'=1}^{N_\nu} \exp\bigl[-2\pi \mathrm{i}(M-nq)\lambda'/N_\nu\bigr] \\
\times \int_0^{2\pi/q} \mathrm{d}k \int_0^{2\pi/q} \mathrm{d}k' \int_0^{2\pi p/q} \mathrm{d}\delta \int_0^{2\pi p/q} \mathrm{d}\delta' \ \exp[\mathrm{i}q(\lambda' k - \lambda k')] \\
\times \langle C_\nu(k',\delta')|\hat{T}_0\bigl(-2\pi\lambda/N_\nu, 0\bigr) \left.\frac{\partial \hat{T}}{\partial \overline{h}}\right|_0 \hat{T}_0\bigl(2\pi\lambda'/N_\nu, 0\bigr)|C_\nu(k,\delta)\rangle \\
= (I_1 + I_2 + I_3 + I_4)\Delta\overline{h} \qquad (6.16)
\end{aligned}
$$

where the integrals I_1 to I_4 are obtained by substituting the four terms in (6.15), and λ is given by (6.8). The final two integrals are straightforward as they are similar to those calculated earlier for the zeroth-order term. Following similar procedures to those in sections 5 and 6.2, the third term gives us

$$I_3 = -\frac{\mathrm{i}}{2}\int_0^{2\pi/q}\mathrm{d}k\int_0^{2\pi/q}\mathrm{d}\delta\ \exp[-\mathrm{i}q(n\delta - mk)]\left(u_\nu\left|\frac{\partial^2\tilde{H}}{\partial\delta\partial k}\right|u_\nu\right) \tag{6.17}$$

and the fourth term is

$$I_4 = \frac{\mathrm{i}}{2}\int_0^{2\pi/q}\mathrm{d}k\int_0^{2\pi/q}\mathrm{d}\delta\ \exp[-\mathrm{i}q(n\delta - mk)]\frac{\partial^2\mathcal{E}_\nu}{\partial\delta\partial k}(k,\delta)\,. \tag{6.18}$$

The first two terms which involve matrix elements of $\hat{x}$ and $\hat{p}$ require a little more care; the second term reduces to

$$\begin{aligned} I_2 = -\frac{\mathrm{i}}{N_\nu\hbar}\sum_{\lambda=1}^{N_\nu}\int_0^{2\pi/q}\mathrm{d}k\int_0^{2\pi/q}\mathrm{d}k'\int_0^{2\pi p/q}\mathrm{d}\delta\int_0^{2\pi p/q}\mathrm{d}\delta'\ \exp[\mathrm{i}q\lambda(k-k')]\ \exp[-\mathrm{i}q(n\delta - mk)] \\ \times\sum_N\sum_M N\,H_{NM}\langle B_\nu(k',\delta')|\hat{T}(N\hbar, M\hbar) \\ \times\,\hat{T}_0\big(0, qM_\nu(k'-k)\big)[-kqM_\nu + \hat{p}]|B_\nu(k,\delta)\rangle \end{aligned} \tag{6.19}$$

where we have commuted $\hat{p}$ with $\hat{T}_0(0, -qM_\nu k)$; we find

$$I_2 = \int_0^{2\pi/q}\mathrm{d}k\int_0^{2\pi/q}\mathrm{d}\delta\ \exp[-\mathrm{i}q(n\delta - mk)]\left[\frac{kqN_\nu}{2\pi}\frac{\partial\mathcal{E}_\nu}{\partial k}(k,\delta) - \mathrm{i}\left(u_\nu\left|\frac{\partial\hat{H}}{\partial k}\right|\frac{\partial u_\nu}{\partial\delta}\right)\right]. \tag{6.20}$$

The first term requires a lengthy discussion; in appendix D we show that

$$I_1 = \int_0^{2\pi/q}\mathrm{d}k\int_0^{2\pi/q}\mathrm{d}\delta\left[\mathrm{i}\left(u_\nu\left|\frac{\partial u_\nu}{\partial k}\right.\right)\frac{\partial\mathcal{E}_\nu}{\partial\delta} + \mathrm{i}\mathcal{E}_\nu\frac{\partial}{\partial\delta}\left(u_\nu\left|\frac{\partial u_\nu}{\partial k}\right.\right)\right]\exp[-\mathrm{i}q(n\delta - mk)]\,. \tag{6.21)}$$

Combining I_1 to I_4, we find $H_{nm}^{(\nu)}$, and the Fourier coefficients $N_{nm}^{(\nu)}$ are given by replacing $\mathcal{E}_\nu(k,\delta)$ in by unity in these expressions. Therefore following the same argument as in section 5 we finally obtain

$$(\Delta H_1^{(\nu)})_{nm} = \Delta\hbar\int_0^{2\pi/q}\mathrm{d}k\int_0^{2\pi/q}\mathrm{d}\delta\ \exp[-\mathrm{i}q(n\delta - mk)]\ H_1^{(\nu)} \tag{6.22}$$

where

$$H_1^{(\nu)} = H_{1a}^{(\nu)} + \mathrm{i}\left(u_\nu\left|\frac{\partial u_\nu}{\partial k}\right.\right)\frac{\partial\mathcal{E}_\nu}{\partial\delta} - \mathrm{i}\left(u_\nu\left|\frac{\partial u_\nu}{\partial\delta}\right.\right)\frac{\partial\mathcal{E}_\nu}{\partial k} + \frac{kqN_\nu}{2\pi}\frac{\partial\mathcal{E}_\nu}{\partial k}\,. \tag{6.23}$$

This establishes (1.9) in the general case.

7. Effects of gauge transformations

We shall consider the effect on the effective Hamiltonian of making an infinitesimal gauge transformation to the original Bloch states or, equivalently, a gauge transformation on the finite-dimensional vectors $|u_\nu(k,\delta))$:

$$\begin{aligned} |B_\nu(k,\delta)\rangle &\to |B'_\nu(k,\delta)\rangle = \exp[\mathrm{i}\theta(k,\delta)\mathrm{d}\tau]|B_\nu(k,\delta)\rangle \\ |u_\nu(k,\delta)) &\to |u'_\nu(k,\delta)) = \exp[\mathrm{i}\theta(k,\delta)\mathrm{d}\tau]|u_\nu(k,\delta))\,. \end{aligned} \tag{7.1}$$

Any finite gauge transformation can be constructed by integrating over infinitesimal ones. Because we wish to maintain the periodicity (up to a specified phase, when $M_\nu \neq 0$) of the Bloch waves in k and δ, the gauge function $\theta(k,\delta)$ will be periodic on the Brillouin zone, with a Fourier series

$$\theta(k,\delta) = \sum_N \sum_M \theta_{NM}\ \exp[-\mathrm{i}q(N\delta - Mk)]\,. \tag{7.2}$$

We shall find that the effect of this gauge transformation is equivalent to allowing the effective Hamiltonian to evolve for a time $\mathrm{d}\tau$ under the action of a 'gauge Hamiltonian' $\hat{G}$, where

$$\hat{G} = \overline{h}'_\nu\ \theta(\hat{x}'/q, \hat{p}'/q)\,. \tag{7.3}$$

i.e. $\hat{G}$ is related to the gauge function $\theta(k,\delta)$ by the same type of Weyl quantization as that used in (1.6).

Substituting equation (7.1) in (1.9), we find that the effective Hamiltonian is transformed as follows (the band index ν will be omitted):

$$\begin{aligned} H \to H' &= H + \left[\frac{\partial\theta}{\partial\delta}\frac{\partial\mathcal{E}}{\partial k} - \frac{\partial\theta}{\partial k}\frac{\partial\mathcal{E}}{\partial\delta}\right]\Delta\overline{h}\mathrm{d}\tau + \mathrm{O}(\Delta\overline{h}^2) + \mathrm{O}(\mathrm{d}\tau^2) \\ &= H(x',p') + q^2\Delta\overline{h}\left[\frac{\partial H}{\partial x'}\frac{\partial\theta}{\partial p'} - \frac{\partial H}{\partial p'}\frac{\partial\theta}{\partial x'}\right]\mathrm{d}\tau + \mathrm{O}(\Delta\overline{h}^2) + \mathrm{O}(\mathrm{d}\tau^2) \end{aligned} \tag{7.4}$$

where we have used the fact that $x' = qk$, $p' = q\delta$ in (1.6), and $H = \mathcal{E} + \mathrm{O}(\Delta\overline{h})$. The change in the effective Hamiltonian induced by an infinitesimal gauge transformation (7.1) is therefore proportional to the Poisson bracket of the Hamiltonian with a Hamiltonian $G(x',p')$, given by (7.3), which acts as the generator of an infinitesimal canonical transformation:

$$H' = H + \{H,G\}\mathrm{d}\tau + \mathrm{O}(\mathrm{d}\tau^2) + \mathrm{O}(\Delta\overline{h}^2) \qquad G = \overline{h}'\theta \tag{7.5}$$

where $\{A,B\}$ is the Poisson bracket of A and B in the (x',p') phase space. The Moyal identity [22] shows that the commutator $[\hat{A},\hat{B}]$ is equivalent to the Weyl quantization of the Poisson bracket $\mathrm{i}\overline{h}'\{A,B\}$ up to terms $\mathrm{O}(\overline{h}'^3)$. We therefore have

$$\hat{H}' = \hat{H} - \frac{\mathrm{i}}{\overline{h}'}[\hat{H},\hat{G}] + \mathrm{O}(\mathrm{d}\tau^2) + \mathrm{O}(\overline{h}'^2)\,. \tag{7.6}$$

We have shown that, up to correction terms which are $\mathrm{O}(\overline{h}'^2)$ (and therefore beyond the accuracy of our approximations), the change in the Hamiltonian induced by an infinitesimal gauge transformation is equivalent to a unitary evolution under the Hamiltonian $\hat{G}$. We remark that, beyond the zeroth-order approximation, the low field effective Hamiltonian for Bloch electrons in a magnetic field also depends on the gauge of the Bloch basis states [11, 12].

We could arrive at the same conclusion by considering the action of the gauge transformation on the $|B_\nu(k,\delta)\rangle$ state vectors rather than the $|u_\nu(k,\delta)\rangle$ vectors; this leads to a much lengthier calculation. It is of interest however to note how the gauge transformation specified by (7.1) and (7.2) transforms the Wannier functions. In appendix E we show that the effect of the infinitesimal gauge transformation is to induce the following transformation of the Wannier functions:

$$|\phi_\mu^{(\nu)}\rangle \to |\phi'^{(\nu)}_\mu\rangle = |\phi_\mu^{(\nu)}\rangle + \mathrm{i}\mathrm{d}\tau \sum_N \sum_M (-1)^{pqNM}\ \theta_{NM} \times \hat{T}(-2\pi M/N_\nu, -2\pi N\overline{h}/\kappa_\nu)\ \hat{t}(-Nq, -Mq)\,|\phi_\mu^{(\nu)}\rangle\,. \tag{7.7}$$

Apart from the unusual form of the translation operator, this relationship is similar to that found for the effect of an infinitesimal gauge transformation on conventional Wannier functions.

8. Numerical experiments

In this section we describe numerical work which confirms that equations (1.5) to (1.9) do fully describe the spectrum up to order $\Delta\overline{h}$. We present Fourier coefficients of the zeroth- and first-order terms of the effective Hamiltonian (1.5), and we compare the spectrum of the first-order approximation to the effective Hamiltonian with the exact spectrum of the Harper model, for a sequence of high-order rationals p_1/q_1, which approximate p/q. We find that the RMS error in the positions of the band edges scales as $\mathrm{O}(\Delta\overline{h}^2)$, as expected. Because the Fourier coefficients are dependent on the gauge choice of the $|u_\nu(k,\delta)\rangle$, we must first specify the gauge imposed on this vector.

8.1. Choice of gauge

We used the Harper model for our numerical investigations, and obtained the vector $|u_\nu(k,\delta)\rangle$ as the νth eigenvector of a $q\times q$ Hamiltonian for which the non-zero elements are (using (4.7) and the Fourier coefficients quoted below (1.3))

$$H_{nm}(k,\delta) = \begin{cases} 2\cos(n\overline{h}+\delta) & n=m \\ \exp[\pm\mathrm{i}k] & n = m\pm 1 \mod q\,. \end{cases} \tag{8.1}$$

We set up a grid in k–δ space with $0 \leqslant k \leqslant 2\pi/q$ and $0 \leqslant \delta \leqslant 2\pi p/q$, with $\mathcal{N}_k$, $\mathcal{N}_\delta$ equally spaced points, separated by Δk, $\Delta\delta$ respectively. For every point in this grid, the elements of the νth eigenvector of the matrix (8.1) are stored in an array. These vectors are initially gauged such that their first non-zero element is real. Before applying a specific gauge, we first ensure that the vectors are an analytic function of k and δ; this need not be satisfied if the first element of any of the vectors vanishes. We satisfy this requirement by imposing a connection rule along specified paths covering k–δ space. Starting at the origin, we move up the k axis to k_1, gauging the vector $|u_\nu(k+\Delta k,\delta)\rangle$ so that the overlap $\langle u(k,\delta)|u(k+\Delta k,\delta)\rangle$ is real. Then starting from $\delta=0$ and moving along the line $k=k_1$, we gauge the vector $|u(k, \delta + \Delta\delta))$ so that $(u(k, \delta)|u(k, \delta + \Delta\delta))$ is real for all values of δ in the interval $[0, 2\pi p/q]$. We repeat this for different values of k_1 in the interval $[0, 2\pi/q]$.

Having ensured that $|u_\nu(k, \delta))$ is an analytic function, we next adjust the gauge such that the vector $|C_\nu(k, \delta)\rangle$ defined in (6.1) is periodic in k, with period $2\pi/q$. We construct the wavefunction $\langle x|C_\nu(k, \delta)\rangle$, and for each value of δ a comparison is made between $|C(0, \delta)\rangle$ and $|C(2\pi/q, \delta)\rangle$; these vectors are identical up to a phase angle $\theta(\delta)$. The function $\theta(\delta)$ is defined such that $-\pi \leqslant \theta(0) < \pi$, and $\theta(\delta)$ is a smooth function of δ. The $|u_\nu(k, \delta))$ are then multiplied by a phase factor $\exp[\mathrm{i}\chi]$ defined by $\chi(k, \delta) = -\theta(\delta)kq/2\pi$, which makes the state $|C_\nu(k, \delta)\rangle$ periodic in k.

Now it remains for us to make a final gauge transformation to ensure that the function $U_\nu(x; k)$ defined in (2.1) is periodic in x with period 2π. We compare the vectors $|u_\nu(k, 0))$ and $|u_\nu(k, 2\pi/q))$. These are identical up to a phase and a permutation of the elements of one of the vectors: $u_n(k, 0) = \exp[\mathrm{i}\phi(k)]u_m(k, 2\pi/q)$, where $n = m - N_\nu$ (and again the phase is defined so that $\phi(0)$ lies between $-\pi$ and π, and the function is a smooth function of k). We then multiply all the vectors $|u_\nu(k, \delta))$ which have $0 \leqslant \delta \leqslant 2\pi/q$ by $\exp[\mathrm{i}\xi]$, where $\xi(k, \delta) = -\phi(k)\delta q/2\pi$. The vectors which have $\delta > 2\pi/q$ are then defined by the requirement that $u_n(k, \delta) = u_m(k, \delta + 2\pi/q)$ where $m = n - N_\nu$.

8.2. Fourier coefficients and spectrum

Having determined a choice of gauge we can use (1.9) to evaluate the Fourier coefficient defining $\hat{H}_1^{(\nu)}$. We list the first few coefficients in table 1 for one choice of commensurability p/q and band index ν; we used a grid size of $\mathcal{N}_k = \mathcal{N}_\delta = 60$ for these calculations. The Fourier coefficients of the dispersion relation, which define $\hat{H}_0^{(\nu)}$, are also tabulated. The Fourier coefficients $(H_1^{(\nu)})_{nm}$ do not have the symmetry $H_{nm} = H_{m,-n}$ exhibited by the original Hamiltonian, and by the Fourier coefficients of the dispersion relation. This is a consequence of the choice of gauge specified in section subsection 8.1; in [3] it is shown that gauges can be chosen which do respect this symmetry.

We compared the spectrum of a band computed using the first two terms of the Taylor expansion of the effective Hamiltonian with the appropriate subset of the 'exact' spectrum of Harper's equation, computed numerically at some high-order rationals $\beta = p_1/q_1$ which approximate the low-order rational p/q. The renormalized commensurability, given

Table 1. Fourier coefficients of the first two terms of the effective Hamiltonian for the case $p = 2$, $q = 5$, $\nu = 2$, $M_\nu = -1$, $N_\nu = 3$.

(n, m)	$(H_0^{(\nu)})_{nm}$	$\mathrm{Re}(H_1^{(\nu)})_{nm}$	$\mathrm{Im}(H_1^{(\nu)})_{nm}$
(0, 0)	−1.909 961	0.099 091	0.000 000
(0, 1)	−0.053 291	−0.305 237	0.024 538
(0, 2)	−0.002 487	−0.014 164	0.010 928
(1, −2)	−0.001 350	−0.010 963	−0.010 671
(1, −1)	−0.004 348	−0.122 362	−0.013 177
(1, 0)	−0.053 291	−0.408 219	−0.020 010
(1, 1)	−0.004 348	−0.115 926	0.001 398
(1, 2)	−0.001 350	−0.007 481	0.009 351
(2, −2)	−0.000 501	−0.004 753	−0.007 130
(2, −1)	−0.001 350	−0.076 575	−0.013 427
(2, 0)	−0.002 487	−0.099 689	−0.014 807
(2, 1)	−0.001 350	−0.073 020	−0.002 460
(2, 2)	−0.000 501	−0.002 535	0.005 978

Table 2. Root-mean square error S in the spectrum of the effective Hamitonian for different values of $\Delta\beta$; the data for all three cases show that $S = \mathrm{O}(\Delta\beta^2)$.

p_1/q_1	p'/q'	$\Delta\beta$	S
Case (a). $p = 1,\ q = 3,\ \nu = 1,\ M_\nu = 0,\ N_\nu = 1$			
196/571	17/196	9.92×10^{-3}	5.71×10^{-3}
160/473	7/160	4.93×10^{-3}	1.48×10^{-3}
50/149	1/50	2.24×10^{-3}	3.07×10^{-4}
100/299	1/100	1.12×10^{-3}	7.34×10^{-5}
200/599	1/200	5.57×10^{-4}	1.66×10^{-5}
Case (b). $p = 2,\ q = 3,\ \nu = 2,\ M_\nu = -1,\ N_\nu = 2$			
329/487	13/171	8.90×10^{-3}	9.00×10^{-3}
100/151	−2/49	-4.42×10^{-3}	2.81×10^{-3}
200/301	−2/99	-2.22×10^{-3}	7.28×10^{-4}
200/601	−2/199	-1.11×10^{-3}	1.80×10^{-4}
337/505	1/169	6.60×10^{-4}	4.64×10^{-5}
Case (c). $p = 2,\ q = 5,\ \nu = 2,\ M_\nu = -1,\ N_\nu = 3$			
154/371	28/91	1.51×10^{-2}	1.62×10^{-2}
20/51	−2/9	-7.84×10^{-3}	6.72×10^{-3}
40/101	−2/19	-3.96×10^{-3}	1.64×10^{-3}
80/201	−2/39	-1.99×10^{-3}	3.49×10^{-4}
109/273	−1/54	-7.23×10^{-4}	6.04×10^{-5}

by (1.7), is also rational: $\beta'_\nu = p'/q'$. Both spectra consist of a set of q' bands with upper and lower band edges $E_i^{(+,\mathrm{ex})}$ and $E_i^{(-,\mathrm{ex})}$ respectively for the exact spectrum, and $E_i^{(+,\mathrm{eff})}$, $E_i^{(-,\mathrm{eff})}$ for the spectrum of the effective Hamiltonian. In table 2 we show the statistic

$$S = \left[\frac{1}{2q'}\sum_{i=1}^{q'}(E_i^{(+,\mathrm{ex})} - E_i^{(+,\mathrm{eff})})^2 + (E_i^{(-,\mathrm{ex})} - E_i^{(-,\mathrm{eff})})^2\right]^{1/2} \tag{8.2}$$

which is a measure of the RMS difference between the spectra; the results clearly show that $S = \mathrm{O}(\Delta\bar{h}^2)$, as expected. We used Fourier coefficients $(H_1^{(\nu)})_{nm}$ of order up to $|n|, |m| = 18$ to evaluate the effective Hamiltonian.

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Appendix A

Here we derive results quoted in section 4. Firstly we shall consider the overlap $\langle C(k', \delta')|B(k, \delta)\rangle$:

$$\langle C(k', \delta')|B(k, \delta)\rangle = \sum_{n=-\infty}^{\infty}\sum_{m=-\infty}^{\infty} \exp[-\mathrm{i}k'(n\bar{h} + \delta')/\bar{h}]\exp[\mathrm{i}k(m\bar{h} + \delta)/\bar{h}]v_n^*(k', \delta')u_m(k, \delta)$$
$$\times \int_{-\infty}^{\infty}\mathrm{d}x\ \delta(x - n\bar{h} - \delta')\ \delta(x - m\bar{h} - \delta)\,. \tag{A.1}$$

The integral reduces to $\delta_{nm} \times \delta(\delta - \delta')$ where δ_{nm} is the usual Kronecker delta function, so that

$$\langle C(k', \delta')|B(k, \delta)\rangle \sum_{n=-\infty}^{\infty} \exp[\mathrm{i}n(k-k')]\ v_n^*(k', \delta')\, u_n(k, \delta)\ \exp[\mathrm{i}(k\delta - k'\delta')/\overline{h}]\, \delta(\delta - \delta')\,. \tag{A.2}$$

Now since both u_n and v_n are periodic in n with period q, we can write (A.2) as

$$\sum_{n=1}^{q} v_n^*(k', \delta')\, u_n(k, \delta) \exp[\mathrm{i}n(k-k')] \times \sum_{m=-\infty}^{\infty} \exp[\mathrm{i}mq(k-k')]\ \exp[\mathrm{i}(k\delta - k'\delta')/\overline{h}]\, \delta(\delta - \delta')\,. \tag{A.3}$$

The second sum vanishes unless $k = k'$. Normalizing the Bloch states so that $\langle B(k', \delta')|B(k, \delta)\rangle = \delta(\delta - \delta')\delta(k - k')$, we have

$$\langle C(k', \delta')|B(k, \delta)\rangle = \delta(\delta - \delta')\, \delta(k - k')\ (v(k, \delta)|u(k, \delta))\,. \tag{A.4}$$

We will also consider matrix elements of the operators $\hat{x}$, $\hat{p}$: the $\hat{x}$ matrix element is

$$\langle C(k', \delta')|\hat{x}|B(k, \delta)\rangle = \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} \exp[\mathrm{i}(mk - nk')]\ \exp[\mathrm{i}(k\delta - k'\delta')/\overline{h}] \times\ v_n^*(k', \delta')u_n(k, \delta)(m\overline{h} + \delta) \int_{-\infty}^{\infty} \mathrm{d}x\ \delta(x - n\overline{h} - \delta')\ \delta(x - m\overline{h} - \delta) \tag{A.5}$$

which, after writing $m\overline{h} \exp[\mathrm{i}km] = -\mathrm{i}\overline{h} \frac{\partial}{\partial k} \exp[\mathrm{i}km]$ and simplifying gives (4.6).

Similarly

$$\langle C(k', \delta')|\hat{p}|B(k, \delta)\rangle = -\mathrm{i}\overline{h} \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} \exp[\mathrm{i}(mk - nk')]\ \exp[\mathrm{i}(k\delta - k'\delta')/\overline{h}] \times v_n^*(k', \delta')u_n(k, \delta) \int_{-\infty}^{\infty} \mathrm{d}x\ \delta(x - n\overline{h} - \delta') \frac{\partial}{\partial x} \delta(x - m\overline{h} - \delta) \tag{A.6}$$

and the integral gives $-\delta_{nm} \frac{\partial}{\partial \delta} \delta(\delta - \delta')$, so that

$$\langle C(k', \delta')|\hat{p}|B_\nu(k, \delta)\rangle = \mathrm{i}\overline{h}\delta(k - k')\ \exp[\mathrm{i}(k\delta - k'\delta')/\overline{h}]\, (v(k', \delta')|u(k, \delta))\, \frac{\partial}{\partial \delta} \delta(\delta - \delta')\,. \tag{A.7}$$

Alternatively, we can write this in the form (4.5).

Appendix B

Here we relate the operator $\hat{A}$ to a $q \times q$ matrix $\tilde{A}(k, \delta)$ such that if $|C(k', \delta')\rangle = \hat{A}|B(k, \delta)\rangle$, then $v_n = \sum_m A_{nm} u_m$. If $\hat{A}$ is represented by its Fourier expansion (4.2), then

$$\begin{aligned}\langle x|C(k,\delta)\rangle &= \sum_{n=-\infty}^{\infty} \exp[\mathrm{i}k(n\overline{h}+\delta)/\overline{h}]\, v_n(k,\delta)\, \delta(x - n\overline{h} - \delta) \\ &= \sum_{n=-\infty}^{\infty} \exp[\mathrm{i}k(n\overline{h}+\delta)/\overline{h}]\, u_n(k,\delta) \\ &\quad \times \sum_{N=-\infty}^{\infty} \sum_{M=-\infty}^{\infty} A_{NM}\ \hat{T}(N\overline{h}, M\overline{h})\ \delta(x - n\overline{h} - \delta)\,. \end{aligned} \qquad \text{(B.1)}$$

Using the fact that $\hat{T}(N\overline{h}, M\overline{h}) = \exp[-\mathrm{i}NM\overline{h}/2]\exp[-\mathrm{i}M\hat{p}]\exp[\mathrm{i}N\hat{x}]$, the term in (B.1) becomes

$$\hat{T}(N\overline{h}, M\overline{h})\delta(x - n\overline{h} - \delta) = \exp[\mathrm{i}M((n + N/2)\overline{h} + \delta)]\delta\big(x - (n+N)\overline{h} - \delta\big)\,. \qquad \text{(B.2)}$$

Therefore from (B.1) we have

$$\begin{aligned}\langle x|C(k,\delta)\rangle &= \sum_{n=-\infty}^{\infty} \exp[\mathrm{i}k(n\overline{h}+\delta)/\overline{h}] \\ &\quad \times u_n(k,\delta) \sum_{N=-\infty}^{\infty} \sum_{M=-\infty}^{\infty} A_{NM}\ \exp[\mathrm{i}M((n + N/2)\overline{h} + \delta)]\ \delta(x - n\overline{h} - \delta) \\ &= \sum_{n=-\infty}^{\infty} \exp[\mathrm{i}k(n\overline{h}+\delta)/\overline{h}] \sum_{N=-\infty}^{\infty} \sum_{M=-\infty}^{\infty} A_{NM}\ \exp[\mathrm{i}(M\delta - Nk)] \\ &\quad \times \exp[\mathrm{i}M(n - \tfrac{1}{2}N)\overline{h}]\ u_{n-N}(k,\delta)\ \delta(x - n\overline{h} - \delta)\,. \end{aligned} \qquad \text{(B.3)}$$

Comparing with (4.3) we have

$$v_n = \sum_N \sum_M A_{NM}\ \exp[\mathrm{i}(M\delta - Nk)]\ \exp[\mathrm{i}M(n - \tfrac{1}{2}N)\overline{h}]u_{n-N} = \sum_{m=1}^{q} A_{nm}(k,\delta)u_m \qquad \text{(B.4)}$$

from which equation (4.7) follows immediately. This allows us to relate a $q \times q$ matrix to the Fourier coefficients of an operator defined on the real line, so that $\langle B(k', \delta')|\hat{A}|B_\nu(k, \delta)\rangle = (u(k, \delta)|\tilde{A}(k, \delta)|u(k, \delta))$.

Appendix C

Here we consider the Fourier coefficents of a product of operators

$$\begin{aligned}\hat{C} &= \hat{A}\hat{B} = \sum_N \sum_M A_{NM} \exp[\mathrm{i}(N\hat{x}' - M\hat{p}'] \sum_I \sum_J B_{IJ} \exp[\mathrm{i}(I\hat{x}' - J\hat{p}'] \\ \hat{C} &= \sum_n \sum_m C_{nm} \exp[\mathrm{i}(n\hat{x}' - m\hat{p}'] \end{aligned} \qquad \text{(C.1)}$$

with $[\hat{x}', \hat{p}'] = \mathrm{i}\overline{h}'_\nu$. Comparing the two lines of (C.1), and using (1.3), we find

$$C_{NM} = \sum_I \sum_J A_{N-I,M-J}\, B_{IJ}\ \exp[\mathrm{i}\overline{h}'(IM - NJ)/2]\,. \tag{C.2}$$

Now from (2.6) we have $\overline{h}'_\nu \simeq q^2 \Delta\overline{h}$, implying that to leading order in $\Delta\overline{h}$ the phase factor in (C.2) can be neglected. Using the convolution theorem, we then have

$$\begin{aligned} C_{NM} &= \sum_X \sum_Y A_{N-X,M-Y}\, B_{XY} + \mathrm{O}(\Delta\overline{h}) \\ &= \int_0^{2\pi/q} \mathrm{d}k \int_0^{2\pi/q} \mathrm{d}\delta\ \exp[-\mathrm{i}q(N\delta - Mk)]A(k,\delta)B(k,\delta) + \mathrm{O}(\Delta\overline{h})\,. \end{aligned} \tag{C.3}$$

To lowest order the product of operators $\hat{A}\hat{B}$ is therefore obtained by quantizing the product $A(k,\delta)B(k,\delta)$.

Appendix D

The first term in (6.15) gives

$$\begin{aligned} I_1 = \frac{2\pi \mathrm{i} p^2 n}{\overline{h}^2} \sum_{\lambda=1}^{N_\nu} \int_0^{2\pi/q} \mathrm{d}k \int_0^{2\pi/q} \mathrm{d}k' \int_0^{2\pi p/q} \mathrm{d}\delta \int_0^{2\pi p/q} \mathrm{d}\delta'\ \exp[\mathrm{i}q\lambda(k-k')] \\ \times \exp[-\mathrm{i}q(n\delta - mk)]\mathcal{E}_\nu(k,\delta)\langle B_\nu(k',\delta')|[\hat{x} - 2\pi\lambda/N_\nu] \\ \times \hat{T}_0(0, qM_\nu(k'-k))|B_\nu(k,\delta)\rangle\,. \end{aligned} \tag{D.1}$$

We have two terms to calculate, one involving $\hat{x}$ and the other λ; we will consider the latter one first. Consider the expression

$$\begin{aligned} I_{1a} = \frac{1}{N_\nu} \sum_{\lambda=1}^{N_\nu} \lambda \int_0^{2\pi/q} \mathrm{d}k' \int_0^{2\pi p/q} \mathrm{d}\delta'\ \exp[\mathrm{i}q\lambda(k-k')] \\ \times \langle B_\nu(k',\delta')|\hat{T}_0(0, qM_\nu(k'-k))|B_\nu(k,\delta)\rangle\,. \end{aligned} \tag{D.2}$$

Writing $q\lambda\exp[\mathrm{i}q\lambda(k-k')] = -(\partial/\partial k')\exp[\mathrm{i}q\lambda(k-k')]$, and integrating (D.2) by parts we have

$$\begin{aligned} I_{1a} = \frac{1}{qN_\nu} \sum_{\lambda=1}^{N_\nu} \int_0^{2\pi/q} \mathrm{d}k' \int_0^{2\pi p/q} \mathrm{d}\delta'\ \exp[\mathrm{i}q\lambda(k-k')] \\ \times \frac{\partial}{\partial k'}\langle B_\nu(k',\delta')|\hat{T}_0(0, qM_\nu(k'-k))|B_\nu(k,\delta)\rangle\,. \end{aligned} \tag{D.3}$$

Writing $|B_\nu(k,\delta)\rangle = \exp[\mathrm{i}k\hat{x}/\overline{h}]|U(k,\delta)\rangle$,

$$\begin{aligned} I_{1a} &= \frac{1}{N_\nu} \sum_{\lambda=1}^{N_\nu} \int_0^{2\pi/q} \mathrm{d}k' \int_0^{2\pi p/q} \mathrm{d}\delta'\ \exp[\mathrm{i}q\lambda(k-k')] \\ &\quad\times \frac{\partial}{\partial k'}\langle B_\nu(k',\delta')|\exp[\mathrm{i}qM_\nu(k'-k)\hat{x}/\overline{h}]|B_\nu(k,\delta)\rangle \\ &= \frac{1}{N_\nu} \sum_{\lambda=1}^{N_\nu} \int_0^{2\pi/q} \mathrm{d}k' \int_0^{2\pi p/q} \mathrm{d}\delta'\ \exp[\mathrm{i}q\lambda(k-k')] \\ &\quad\times \bigg[\Big\langle\frac{\partial U}{\partial k'}(k',\delta')\Big|\exp[\mathrm{i}pN_\nu(k-k')\hat{x}/\overline{h}]|U(k,\delta)\rangle \\ &\quad - \frac{\mathrm{i}pN_\nu}{\overline{h}}\langle B_\nu(k',\delta')|\hat{T}_0\big(0, qM_\nu(k'-k)\big)\hat{x}|B_\nu(k,\delta)\rangle\bigg]\,. \end{aligned} \tag{D.4}$$

As in section 6 the sum over λ will ensure that the only contributing term from the overlap is $k = k'$: we find

$$\langle B_\nu(k', \delta')|\hat{T}_0\big(0, qM_\nu(k'-k)\big)\hat{x}|B_\nu(k,\delta)\rangle$$
$$= \frac{\mathrm{i}\hbar}{pN_\nu}\frac{\partial}{\partial k'}\left[\delta(\delta-\delta')\delta(k-k')\exp[\mathrm{i}(k\delta - k'\delta')/\hbar](u_\nu(k',\delta')|u_\nu(k,\delta))\right]$$
$$- \frac{\mathrm{i}\hbar}{pN_\nu}\delta(\delta-\delta')\delta(k-k')\left(\frac{\partial u_\nu(k,\delta)}{\partial k'}\middle| u_\nu(k,\delta)\right). \quad \text{(D.5)}$$

It can be seen that on integrating over k' and δ' (D.4) gives no contribution. Thus from (D.1) we have

$$I_1 = \frac{2\pi \mathrm{i} p^2 N_\nu n}{\hbar^2}\sum_{\lambda=1}^{N_\nu}\int_0^{2\pi/q}\mathrm{d}k\int_0^{2\pi/q}\mathrm{d}k'\int_0^{2\pi p/q}\mathrm{d}\delta\int_0^{2\pi p/q}\mathrm{d}\delta'\ \exp[\mathrm{i}q\lambda(k-k')]$$
$$\times \langle B_\nu(k',\delta')|\hat{x}\hat{T}(0, qM_\nu(k'-k))|B_\nu(k,\delta)\rangle\ \mathcal{E}_\nu(k,\delta)\ \exp[-\mathrm{i}q(n\delta - mk)]\,. \quad \text{(D.6)}$$

We have seen in (D.5) the result of placing $\hat{x}$ between two Bloch states, so we can rewrite (D.1) as

$$I_1 = -\int_0^{2\pi/q}\mathrm{d}k\int_0^{2\pi/q}\mathrm{d}\delta\ qn\exp[-\mathrm{i}q(n\delta - mk)]\mathcal{E}_\nu(k,\delta)\left(u_\nu\middle|\frac{\partial u_\nu}{\partial k}\right). \quad \text{(D.7)}$$

Appendix E

The Bloch states can be obtained from the Wannier functions as follows (equation (3.3.15) of [3]):

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

where C is a normalization constant. Consider the effect of one term of the Fourier series (7.2) on the Bloch state $|B_\nu(k,\delta)\rangle$: using (E.1) and replacing n by $n + M$ in the summation

$$\exp[-2\pi\mathrm{i}(Np\delta/\hbar - Mk/\kappa_\nu)]\ |B_\nu(k,\delta)\rangle$$
$$= C\sum_n\sum_m\sum_{\mu=1}^{N_\nu}\exp\left[-\frac{2\pi\mathrm{i}}{\hbar}\left((m+Np)\delta + \frac{(k+\mu\hbar)(n+M)}{N_\nu}\right)\right]$$
$$\times \exp[2\pi\mathrm{i}Mk/\kappa_\nu]\ \hat{T}(0, 2\pi m)\ \hat{T}(-2\pi(n+M)/N_\nu, 0)$$
$$\times \hat{T}(0, 2\pi M_\nu k/\kappa_\nu)\ |\phi_\mu^{(\nu)}\rangle$$
$$= \sum_n\sum_m\sum_{\mu=1}^{N_\nu}\exp\left[-\frac{2\pi\mathrm{i}}{\hbar}\left(m\delta + \frac{(k+\mu\hbar)n}{N_\nu}\right)\right]$$
$$\times \exp[4\pi^2\mathrm{i}Npn/N_\nu\hbar]\ \exp[-2\pi\mathrm{i}\mu M/N_\nu]$$
$$\times \hat{T}(0, 2\pi m)\ \hat{T}(-2\pi n/N_\nu, 0)\ \hat{T}(0, 2\pi M_\nu k/\kappa_\nu)$$
$$\times \hat{T}(-2\pi Np, 0)\ \hat{T}(-2\pi M/N_\nu, 0)\,|\phi_\mu^{(\nu)}\rangle \quad \text{(E.2)}$$

(equations (1.3) and (6.4) have been used to simplify this result). Now in the rational case $\bar{h} = 2\pi p/q$, the phase factor involving n is $\exp[4\pi^2 \mathrm{i} Npn/N_\nu \bar{h}] = \exp[2\pi \mathrm{i} Nqn/N_\nu]$, so that (E.2) can now be written

$$\begin{aligned} &\exp[-2\pi\mathrm{i}(Np\delta/\bar{h} - Mk/\kappa_\nu)]\ |B_\nu(k,\delta)\rangle \\ &\quad = \sum_n \sum_m \sum_{\mu=1}^{N_\nu} \exp\left[-\frac{2\pi\mathrm{i}}{\bar{h}}\left(m\delta + \frac{(k+\mu\bar{h})n}{N_\nu}\right)\right] \exp\left[-2\pi\mathrm{i}(\mu + \tfrac{1}{2}Nq)M/N_\nu\right] \\ &\qquad \times\ \hat{T}(0, 2\pi m)\ \hat{T}(-2\pi n/N_\nu, 0)\ \hat{T}(0, 2\pi M_\nu k/\kappa_\nu) \\ &\qquad \times \hat{T}(-2\pi M/N_\nu, -2\pi Np)\,|\phi^{(\nu)}_{\mu+Nq}\rangle\,. \end{aligned} \tag{E.3}$$

Using equation (1.8), the additional phase factor in (E.3) can be rewritten as follows:

$$\exp\left[-\frac{2\pi\mathrm{i}}{N_\nu}\left(\mu + \tfrac{1}{2}Nq\right)M\right] = (-1)^{pqNM} \exp\left[-\frac{2\pi\mathrm{i}M_\nu}{N_\nu}\left(\mu + \tfrac{1}{2}Nq\right)Mq\right]. \tag{E.4}$$

Inserting this result into (E.3), and using (6.5) gives

$$\begin{aligned} &\exp[-2\pi\mathrm{i}(Np\delta/\bar{h} - Mk/\kappa_\nu)]\ |B_\nu(k,\delta)\rangle \\ &\quad = (-1)^{pqNM} \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} \sum_{\mu=1}^{N_\nu} \exp\left[\frac{2\pi\mathrm{i}}{\bar{h}}\left(m\delta + \frac{(k+\mu\bar{h})n}{N_\nu}\right)\right] \\ &\qquad \times \hat{T}(0, 2\pi m)\ \hat{T}(-2\pi n/N_\nu, 0)\ \hat{T}(0, 2\pi M_\nu k/\kappa_\nu) \\ &\qquad \times \hat{T}(-2\pi M/N_\nu, -2\pi N\bar{h}/\kappa_\nu)\ \hat{t}(-Nq, -Mq)\,|\phi^{(\nu)}_{\mu}\rangle \end{aligned} \tag{E.6}$$

(we used the fact that, in the rational case, $\bar{h}/\kappa_\nu = p$). Equation (7.7) follows directly from this result.

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