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Diophantine equation for the 3D transport coefficients of Bloch electrons in a strong tilted magnetic field with quantum Hall effect

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Abstract

We study the 3D integer transport coefficients of the electron gas in a tilted magnetic field with the model of Bloch electrons. Calculations without any approximation of the relevant basis functions and matrix elements yield the topologically invariant conductances and their Diophantine equation.

Introduction

Equations for integers, named Diophantine after Diophantus of Alexandria (about AD 250), are an important topic in the theory of numbers (Fermat, Euler etc) [1]. In the theoretical physics of condensed matter, they appear as a result of magnetic translational symmetry in studies of Bloch electrons in a magnetic field exhibiting a quantum Hall effect in two and three dimensions. For reviews and books see for instance Thouless [2], Sokoloff [3], Prange and Girvin [4], MacDonald [5], Das Sarma and Pinczuk [6], Thouless [7], Girvin [8].

For two dimensions, such an equation was written for the first time by Wannier [9] in a study of the location of energy gaps upon splitting of a Bloch band into subbands, then it was used by Streda [10] in the discussion of the quantum Hall effect in the 'tight binding' limit.

Hall conductance calculations in the seminal paper by Thouless *et al* (TKNN) [11] on Bloch electrons in a uniform perpendicular magnetic field were based on the Kubo formula, they also yield such an equation connecting the 'quantum numbers' which appear.

More generally, similar equations were shown to yield a labelling of gaps in the energy spectra of a Schrödinger equation with an (almost) periodic potential. (See, for instance, [12] and [13].)

Dana, Avron and Zak [14] were the first to show them to be a consequence of magnetic translational invariance: when the number of flux quanta per unit cell is $\varphi = p/q$ with p and

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q relatively prime, an isolated magnetic subband carries an integer Hall conductance $\sigma_{\rm H}$ and an integer adiabatic transport coefficient $\sigma_{\rm V}$ such that

$$p\sigma_{\rm H} + q\sigma_{\rm V} = 1$$

with $\sigma_{\rm H}$ and $\sigma_{\rm V}$ Chern numbers.

Kunz [15] was the first to give the physical significance of the 'second' topological invariant $\sigma_{\rm V}$: it measures, in convenient units, charge transport when the (lattice) periodic potential is adiabatically displaced.

In previous work [16] (in the following TAH), following Zak [17, 18] and Kunz [15], the basis functions, matrix element, Hall conductance and adiabatic charge transport coefficient for the 2D problem and the relevant Diophantine equations were explicitly calculated by one of us.

A wealth of new phenomena have been observed in experimental studies of 2D Bloch electrons where the magnetic field is no longer perpendicular to the plane where the electron motion is confined, originating in an important literature [19–25]. Among the most noteworthy:

- the collapse of the even-denominator fractional quantum Hall effect upon tilting the magnetic field;
- the appearance of states of the 2DEG in high Landau levels ($N > 2$) showing a high anisotropy that is also sensitive to the magnetic field direction.

All of them evidence the importance of the 3D character in the electron gas behaviour and have prompted a variety of theoretical studies.

Halperin [26] has first derived, as a generalization of the arguments of Thouless *et al*, an abstract formula for the 3D quantized Hall conductivity, using the Kubo–Greenwood formula, in terms of the eigenfunctions of the Hamiltonian of 3D non-interacting Bloch electrons in a magnetic field.

Montambaux and Kohmoto [27] started from a 3D tight binding Hamiltonian in a specific geometry where the magnetic field is perpendicular to the Bravais lattice a–b plane and the vector c tilted at an angle θ with respect to the field. They derived the Hall conductance in 3D as 'a set of three integers' found as solutions to a Diophantine equation.

Kohmoto *et al* [28] then expressed the Hall conductance of 3D electrons in a periodic potential in a topologically invariant form with a set of three integers in a more general case.

None of these authors discuss the possible physical significance of these invariants.

We work with the model of independent Bloch electrons in a magnetic field tilted at an angle θ with respect to the z axis perpendicular to the motion. Our calculations are performed without any approximation.

Part 1 deals with the framework: the concepts and the methods involved in the 'pure' 2D case are first briefly summarized for the benefit of non-specialist readers; then the 3D Hamiltonian, the construction of new magnetic translation operators adapted to the problem using Schellnhuber's [29] method, the new basis functions and eigenvalue equations are presented. In part 2 and appendix A, the 3D Hamiltonian matrix elements are calculated analytically. In part 3, after, again, a 2D 'reminder', the relevant conductances and the Diophantine equations are derived and interpreted in terms of transport in the electron gas.

1. The framework

1.1. A short trip back to the 'pure' 2D case

Bloch electrons in a magnetic field are two-dimensional independent electrons in a periodic potential and a uniform magnetic field B perpendicular to their xOy plane, to which, in the following, we assume them to be confined by some confining potential. For more details, the reader is referred to [2–13]. Details on the possible form and the effects of such a confining potential will be presented subsequently.

The Landau Hamiltonian is

$$H_0 = \frac{p_x^2 + (p_y + eBx)^2}{2m} \tag{1}$$

with the vector potential in the Landau gauge

$$\vec{A} = (0, Bx) \tag{2}$$

with energy levels $E = (n + \frac{1}{2})\hbar\omega_c$, where $\omega_c = \frac{eB}{m}$. The orbit centre operators

$$X = -\frac{p_y}{eB} \qquad \text{and} \qquad Y = \frac{p_x}{eB} + y \tag{3}$$

commute with H_0, but not with each other; they are conjugate variables: $[X, Y] = \mathrm{i}\ell^2$ with $\ell^2 = \frac{\hbar}{eB}$ the square magnetic length. The Landau eigenfunctions of H_0 are

$$\Phi_{q_y,n}(x, y) = \mathrm{e}^{\mathrm{i}yq_y} f_n\left(\frac{x + q_y\ell^2}{\ell}\right) \tag{4}$$

with f_n the oscillator eigenfunction for the nth Landau level and q_y the quasi-impulsion along y.

The periodic potential can be considered either as the mean field of two- and four-body interactions between electrons [16] or as an external potential, often a crystal potential or, for example, due to density modulations:

$$V(x, y) = V_x \cos\left(\frac{2\pi}{a}x\right) + V_y \cos\left(\frac{2\pi}{b}y\right). \tag{5}$$

Although the system as described is translation invariant,

$$H = H_0 + V(x, y) \tag{6}$$

no longer commutes with the usual translation operators

$$T_a = \mathrm{e}^{\mathrm{i}\frac{ap_x}{\hbar}} \qquad T_b = \mathrm{e}^{\mathrm{i}\frac{bp_y}{\hbar}}. \tag{7}$$

This is due to the potential vector term, linear in x, and is a purely quantum effect. Other translation operators must then be defined that can describe translational invariance in the presence of a magnetic field. The first to understand the form to be given to those operators was Joshua Zak [17].

The operators

$$S_a = \mathrm{e}^{\mathrm{i}\frac{a(p_x+eBy)}{\hbar}} \qquad \text{and} \qquad S_b = \mathrm{e}^{\mathrm{i}\frac{bp_y}{\hbar}} \tag{8}$$

commute with H_0 and H. We can also write

$$S_a = \mathrm{e}^{\mathrm{i}\frac{a\Pi_{Cx}}{\hbar}} \qquad S_b = \mathrm{e}^{\mathrm{i}\frac{b\Pi_{Cy}}{\hbar}} \tag{9}$$

where

$$\Pi_{Cx} = p_x + eBx \qquad \Pi_{Cy} = p_y. \tag{10}$$

The action of these operators on the wavefunctions is no more only just to effect a translation, but also now to multiply them by a position dependent phase factor. Furthermore, they do not commute with each other:

$$S_a S_b = S_b S_a \mathrm{e}^{-\mathrm{i}\frac{abeB}{\hbar}} \tag{11}$$

where

$$\frac{abeB}{\hbar} = 2\pi \frac{abB}{h/e} = 2\pi \frac{\phi}{\phi_0} = 2\pi\varphi. \tag{12}$$

This phase is the number of magnetic flux quanta through a unit cell, multiplied by 2π. One can write

$$S_a S_b S_a^{-1} S_b^{-1} = \mathrm{e}^{-\mathrm{i}2\pi\phi/\phi_0} \tag{13}$$

which expresses the following property: a translation of the wavefunction around a rectangle of sides a and b results in the multiplication of this wavefunction by a phase factor with phase equal to, in convenient units, the number of flux quanta through the rectangle area. This is the Aharonov–Bohm effect [30].

If we want to define a complete set of commuting observables (CSCO) so as to be able to write down a complete orthonormal basis of eigenfunctions adapted to the problem symmetries, we need translation operators which commute with each other. To this end [17], we impose the following condition: $\frac{abeB}{\hbar} = 2\pi\frac{p}{q}$ or $\frac{abB}{h/e} = \frac{p}{q}$—the number of flux quanta per unit cell is a rational number.

When this condition is fulfilled, operators S_a and S_{qb} commute with each other. They are defined on a cell which is q times the unit cell and therefore contains p flux quanta. Such a condition is not very restrictive, since the group of rationals is dense in the group of reals.

Now the Landau Hamiltonian H_0 and the two magnetic translation operators S_a and S_{qb} can define a CSCO. It is therefore possible to define a basis of complete orthonormal eigenfunctions for these operators, which will enable us to diagonalize our problem.

The magnetic translation operators are unitary; they obey

$$S_{a(qb)}^{-1} = S_{a(qb)}^{+}. \tag{14}$$

Their eigenvalue equation is

$$\begin{aligned} S_a\phi_{nj}^{\vec{q}}(x, y) &= \mathrm{e}^{\mathrm{i}aq_x}\phi_{nj}^{\vec{q}}(x, y) \\ S_{qb}\phi_{nj}^{\vec{q}}(x, y) &= \mathrm{e}^{\mathrm{i}qbq_y}\phi_{nj}^{\vec{q}}(x, y) \end{aligned} \tag{15}$$

where $\vec{q} = (q_x, q_y)$ characterizes the eigenvalue and the associated eigenvector. This quantity plays the same role as the wavevector of the usual Bloch electron problem; it is called the 'quasi-impulsion' of the eigenstate ϕ. It is defined, by analogy with the case without a magnetic field, in the following Brillouin zone:

$$-\frac{\pi}{a} \leqslant q_x < \frac{\pi}{a} \qquad \text{and} \qquad -\frac{\pi}{qb} \leqslant q_y < \frac{\pi}{qb}. \tag{16}$$

By construction of magnetic translation operators, the quasi-impulsion is connected to the position of the cyclotron orbit centre.

It can then be shown, using Zak's k–q representation theory [31], that the eigenfunctions for the operators which enclose one single flux quantum

$$S_{a/p} = \mathrm{e}^{\mathrm{i}\frac{aP}{p\hbar}} \qquad \text{and} \qquad S_{qb} = \mathrm{e}^{\mathrm{i}\frac{qbX}{\ell^2}} = \mathrm{e}^{-\mathrm{i}p\frac{2\pi X}{a}} \tag{17}$$

can be written as a function of one of the orbit centre operators, X, alone ('X representation'):

$$g_{q'_x q_y}(X) = \sqrt{\frac{2\pi}{a}p}\sum_{\mu} \mathrm{e}^{\mathrm{i}\mu q'_x a/p}\delta\left(X - q_y\ell^2 - \mu\frac{a}{p}\right) \qquad \text{with } \mu \in Z \tag{18}$$

and, as such, they form a complete orthonormal basis [31].

The $g_{q'_x q_y}(X)$ period as a function of q'_x is $2\pi p/a$ while, the potential period in x being a, its Fourier components are a function of $2\pi/a$. This means that the periodic potential will mix the q'_x components of $g_{q'_x q_y}(X)$ which differ by $2\pi/a$, and the matrix element calculated using these functions will not be diagonal in q'_x: this is a direct consequence of the property $[V(x, y), S_{a/p}] \neq 0$. To resolve this difficulty [18], we define q_x such that $q'_x = q_x + 2\pi \frac{j}{a}$ with $j = 1, \ldots, p$ where the eigenvalue q_x of S_a varies in the Brillouin zone defined in the previous section. Now the periodic potential will mix the js but not the q_xs; therefore the matrix element will be diagonal in q_x and q_y:

$$g_{q_x q_y j}(X) = \sqrt{\frac{2\pi}{a} p} \sum_\mu \mathrm{e}^{\mathrm{i}\left(q_x + \frac{2\pi}{a} j\right)\frac{a}{p}\mu} \delta\left(X - q_y \ell^2 - \mu \frac{a}{p}\right) \tag{19}$$

with $\mu \in Z, \vec{q} = (q_x, q_y)$. For more detailed properties of the g functions, and more details in general, the interested reader is referred to [14, 16–18].

To build a basis of eigenfunctions depending on x and y, complete and orthonormal, which be eigenfunctions of the Landau Hamiltonian H_0 as well, we have to sum the product of the $g_{q_x q_y j}(X)$ with $\Phi_{\vec{q},n}(x, y)$ over all the possible orbit centres, with X varying between $-\infty$ and $+\infty$, and the final form is

$$\begin{aligned} \phi^{\vec{q}}_{nj}(x, y) &= \sqrt{\frac{2\pi}{a} p} \sum_\mu \int \mathrm{d}X\, \mathrm{e}^{-\mathrm{i}y\frac{X}{\ell^2}} f_n\left(\frac{x - X}{\ell^2}\right) \mathrm{e}^{-\mathrm{i}\frac{\mu a}{p}(q_x + \frac{2\pi}{a} j)} \delta\left(X - q_y \ell^2 - \frac{\mu a}{p}\right) \\ &= \sqrt{\frac{2\pi}{a} p} \sum_\mu \mathrm{e}^{-\mathrm{i}\frac{\mu a}{p}(q_x + \frac{2\pi}{a} j)} \mathrm{e}^{-\mathrm{i}y(q_y + \frac{2\pi}{qb}\mu)} f_n\left(\frac{x - \left(q_y + \frac{2\pi}{qb}\mu\right)\ell^2}{\ell^2}\right). \end{aligned} \tag{20}$$

In order to give a slightly more concrete view of its behaviour, in (21) we give a few examples of the translation (periodicity) properties of this basis in direct and reciprocal space:

$$\begin{aligned} &\phi^{\vec{q}}_{nj}(x + a, y) = \mathrm{e}^{\mathrm{i}aq_x} \mathrm{e}^{-\mathrm{i}y\frac{aeB}{\hbar}} \phi^{\vec{q}}_{nj}(x, y) \\ &\phi^{\vec{q}}_{nj}\left(x + \frac{a}{p}, y\right) = \mathrm{e}^{\mathrm{i}\frac{a}{p}(q_x + \frac{2\pi}{a} j)} \mathrm{e}^{-\mathrm{i}y\frac{aeB}{p\hbar}} \phi^{\vec{q}}_{nj}(x, y) \\ &\phi^{\vec{q}}_{nj}(x, y + qb) = \mathrm{e}^{\mathrm{i}qbq_y} \phi^{\vec{q}}_{nj}(x, y) \\ &\phi^{q_x + \frac{2\pi}{a}, q_y}_{nj}(x, y) = \phi^{\vec{q}}_{nj+1}(x, y) \\ &\phi^{q_x + \frac{2\pi}{a} p, q_y}_{nj}(x, y) = \phi^{\vec{q}}_{nj}(x, y) \\ &\phi^{q_x, q_y + \frac{2\pi}{qb}}_{nj}(x, y) = \mathrm{e}^{\mathrm{i}\frac{a}{p}(q_x + \frac{2\pi}{a} j)} \phi^{\vec{q}}_{nj}(x, y) \\ &\phi^{q_x, q_y + \frac{2\pi}{qb} p}_{nj}(x, y) = \mathrm{e}^{\mathrm{i}aq_x} \phi^{\vec{q}}_{nj}(x, y). \end{aligned} \tag{21}$$

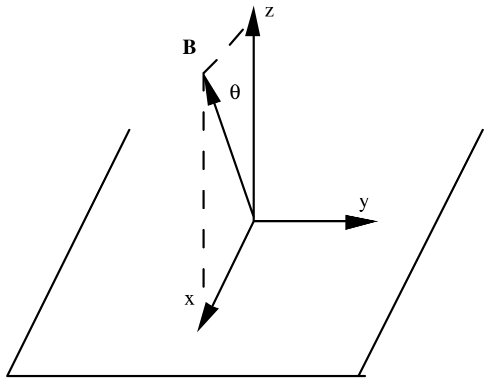
The matrix element $h^{\vec{q}\vec{q}'}_{nn' jj'}$ for the operator H can now be calculated:

$$h^{\vec{q}\vec{q}'}_{\substack{nn' \\ jj'}} = \int \mathrm{d}x\, \mathrm{d}y\, \phi^{*\vec{q}'}_{n'j'}(x, y) H \phi^{\vec{q}'}_{nj}(x, y) \tag{22}$$

with n and n' relative integers varying from $-\infty$ to $+\infty$, j and j' integers from 1 to p, and the wavevector $\vec{q}$ in the Brillouin zone as previously defined:

$$-\frac{\pi}{a} \leqslant q_x, q'_x < \frac{\pi}{a} \qquad -\frac{\pi}{qb} \leqslant q_y, q'_y < \frac{\pi}{qb}. \tag{23}$$

When the field B is no longer perpendicular to the $x\mathrm{O}y$ plane, it may, without loss of generality, be chosen to be in the $x\mathrm{O}z$ plane (see the figure below). The scheme outlined above is now adapted to this new configuration.



1.2. The Hamiltonian in 3D

In the Landau gauge, the vector potential now reads

$$\vec{A} = (0, Bx\cos\theta - Bz\sin\theta, 0). \tag{24}$$

The Hamiltonian then reads

$$H = \frac{p_x^2 + (p_y^2 + eBx\cos\theta - eBz\sin\theta)^2 + p_z^2}{2m} + V(x, y, z) = H_0 + V(x, y, z) \tag{25}$$

with

$$V(x, y, z) = V_x \cos\left(\frac{2\pi}{a}x\right) + V_y \cos\left(\frac{2\pi}{b}y\right) + V_z \cos\left(\frac{2\pi}{c}z\right). \tag{26}$$

1.3. Calculation of the magnetic translation operators

The quantities

$$\Pi_{Cx} = p_x + eBy\cos\theta \qquad \Pi_{Cy} = p_y \qquad \Pi_{Cz} = p_z - eBy\sin\theta \tag{27}$$

are the conserved quantities of the problem in the absence of a periodic potential [32], the operators which are their quantum equivalent commute with the Hamiltonian H_0 and allow us to define new magnetic translation operators:

$$S_a^\theta = \mathrm{e}^{\mathrm{i}\frac{a(p_x+eBy\cos\theta)}{\hbar}} \qquad S_b^\theta = \mathrm{e}^{\mathrm{i}\frac{bp_y}{\hbar}} \qquad S_c^\theta = \mathrm{e}^{\mathrm{i}\frac{c(p_z-eBy\sin\theta)}{\hbar}} \tag{28}$$

with

$$S_a^\theta S_b^\theta = \mathrm{e}^{\mathrm{i}2\pi\varphi_c} S_b^\theta S_a^\theta \qquad S_b^\theta S_c^\theta = \mathrm{e}^{\mathrm{i}2\pi\varphi_a} S_c^\theta S_b^\theta \qquad S_a^\theta S_c^\theta = S_c^\theta S_a^\theta \tag{29}$$

where now

$$\varphi_a = \frac{bcB\sin\theta}{h/e} = \frac{bc\sin\theta}{2\pi\ell^2} \qquad \varphi_c = \frac{abB\cos\theta}{h/e} = \frac{ab\cos\theta}{2\pi\ell^2}. \tag{30}$$

If, by analogy with the 2D case, one sets

$$\varphi_a = \frac{bc\sin\theta}{2\pi\ell^2} = \frac{r}{s} \qquad \varphi_c = \frac{ab\cos\theta}{2\pi\ell^2} = \frac{p}{q} \tag{31}$$

where r and s, on the one hand, and p and q, on the other, are relatively prime, one gets the compatibility condition

$$\frac{c\sin\theta}{a\cos\theta} = \frac{rq}{sp} \tag{32}$$

which is in some sense the transposition to the tilted field case of what is usually called the 'rationality condition for the magnetic field' [9]. This implies

$$\begin{aligned}
\vec{B} &= (B\sin\theta)\hat{x} + (B\cos\theta)\hat{z} \\
\vec{B} &= \left(\frac{h}{ebc}\frac{r}{s}\right)\hat{x} + \left(\frac{h}{eba}\frac{p}{q}\right)\hat{z} \\
&= \left(\frac{h}{eabc}\frac{r}{s}\right)\vec{a} + \left(\frac{h}{ecba}\frac{p}{q}\right)\vec{c} \\
&= \left(\frac{h}{eabc}\right)\left[\frac{r}{s}\vec{a} + \frac{p}{q}\vec{c}\right] \\
\vec{B} &= \frac{\phi_0}{v_0}\left[\frac{r}{s}\vec{a} + \frac{p}{q}\vec{c}\right]
\end{aligned} \tag{33}$$

where $v_0 = abc$ is the volume of the unit cell of the Bravais lattice and ϕ_0 the magnetic flux quantum.

We now try to choose for operators of our CSCO S_a^θ, S_{qsb}^θ and S_c^θ and build their eigenfunctions. But this is hampered by the following facts. When θ is zero, among the three operators in 3D, two do not commute with each other; S_c does commute with S_a and S_b. From these new operators, we can build our basis functions. Now for non-zero θ, S_c^θ no longer commutes with S_a^θ. This prevents us from building the basis of functions using the k–q method [31] as had been done in the 2D case.

To solve this difficulty, we use a variant of Schellnhuber's method [29], which consists in using translation operators which are built not on the lattice defined by $\vec{a}$, $\vec{b}$ and $\vec{c}$, but on one defined by other vectors $\vec{a}_1$, $\vec{a}_2$ and $\vec{a}_3$, which result in a Bravais lattice equivalent to the previous one, but on which the new translation operators S_1, S_2 and S_3 that we get have the following adequate commutation relations, identical to those of the former translation operators when the angle θ is zero:

$$[S_1, S_2] \neq 0 \qquad [S_1, S_3] = 0 \qquad [S_2, S_3] = 0. \tag{34}$$

1.4. Schellnhuber's framework for the problem and a new Brillouin zone

The criteria for defining the new Bravais lattice are twofold:

(a) In order for the magnetic translation operator to commute with the two others, it must 'translate' along the direction of the magnetic field $\vec{B}$:

$$\vec{B} = \left(\frac{h}{eabc}\right)\left[\frac{r}{s}\vec{a} + \frac{p}{q}\vec{c}\right]. \tag{35a}$$

(b) The number of states in the associated Brillouin zone must be unchanged.

Let t be the smallest common multiple of s and q, and L the largest common factor of r and p, we may rewrite $\vec{B}$ in the following way:

$$\vec{B} = \left(\frac{h}{eabc}\right)\frac{L}{t}\left[n_1\vec{a} + n_2\vec{c}\right] \tag{35b}$$

where n_1 and n_2 are relatively prime integers and so are L and t. Then,

$$\frac{Ln_1}{t} = \frac{r}{s} \qquad \text{and} \qquad \frac{Ln_2}{t} = \frac{p}{q} \tag{36a}$$

and

$$\frac{c\sin\theta}{a\cos\theta}=\frac{n_1}{n_2} \tag{36b}$$

which yields

$$n_2 c\sin\theta - n_1 a\cos\theta = 0. \tag{36c}$$

Let us take for the first vector $\vec{a}_3$ of the new Bravais lattice

$$\vec{a}_3 = n_1\vec{a} + n_2\vec{c} \tag{37a}$$

which will be used to build the first new magnetic translation operator and keep

$$\vec{a}_2 = \vec{b} \tag{37b}$$

since in the y direction nothing is changed, and define

$$\vec{a}_1 = \tilde{n}_1\vec{a} + \tilde{n}_2\vec{c} \tag{37c}$$

where $\tilde{n}_1$ and $\tilde{n}_2$ are integers to be determined so as to fulfil the second condition—that is, that the unit cell volume of the new lattice be identical to the previous one ($V_0 = abc$), so as to ensure the conservation of the number of states:

$$\begin{aligned}\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3) &= \vec{a}_1\cdot[b\hat{y}\times(n_1 a\hat{x} + n_2 c\hat{z})]\\ &= \vec{a}_1\cdot[-n_1 ab\hat{z} + n_2 bc\hat{x}]\\ &= (\tilde{n}_1 a\hat{x} + \tilde{n}_2 c\hat{z})\cdot[-n_1 ab\hat{z} + n_2 bc\hat{x}]\\ &= abc(\tilde{n}_1 n_2 - \tilde{n}_2 n_1).\end{aligned} \tag{38}$$

This leads to the condition

$$(\tilde{n}_1 n_2 - \tilde{n}_2 n_1) = 1 \tag{39}$$

which allows the determination of $\tilde{n}_1$ and $\tilde{n}_2$ by

$$\tilde{n}_1 a\cos\theta - \tilde{n}_2 c\sin\theta = \frac{a\cos\theta}{n_2}. \tag{40}$$

When θ is zero,

$$n_1 = 0 \qquad n_2 = 1 \qquad L = p \qquad t = q \qquad \tilde{n}_1 = 1 \qquad \tilde{n}_2 = 0.$$

On the new Bravais lattice a new Brillouin zone is defined as usual:

$$\begin{aligned}\vec{G}_i &= \varepsilon_{ijk} 2\pi\frac{\vec{a}_j\times\vec{a}_k}{v_0}\\ \vec{G}_1 &= \frac{2\pi}{a}n_2\hat{x} - \frac{2\pi}{c}n_1\hat{z}\\ \vec{G}_2 &= \frac{2\pi}{b}\hat{y}\\ \vec{G}_3 &= -\frac{2\pi}{a}\tilde{n}_2\hat{x} + \frac{2\pi}{c}\tilde{n}_1\hat{z}.\end{aligned} \tag{41}$$

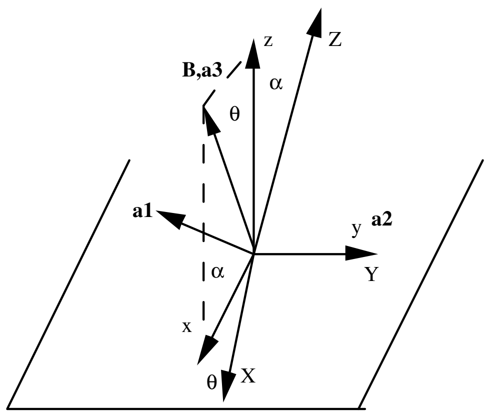
If we denote by

$$\vec{g}_1 = \frac{2\pi}{a}\hat{x} \qquad \vec{g}_2 = \frac{2\pi}{b}\hat{y} \qquad \vec{g}_3 = \frac{2\pi}{c}\hat{z} \tag{42}$$

the vectors of the former Brillouin zone, then the new Brillouin zone has

$$\vec{G}_1 = n_2\vec{g}_1 - n_1\vec{g}_3 \qquad \vec{G}_2 = \vec{g}_2 \qquad \vec{G}_3 = -\tilde{n}_2\vec{g}_1 + \tilde{n}_1\vec{g}_3 \tag{43}$$

and the angle α appears in the figure below. The volume and hence the number of states are the same.



Then the translation operators read

$$S_1 = e^{i\vec{\Pi}_c\cdot\vec{a}_1/\hbar} \qquad S_2 = e^{i\vec{\Pi}_c\cdot\vec{a}_2/\hbar} \qquad S_3 = e^{i\vec{\Pi}_c\cdot\vec{a}_3/\hbar} \tag{44}$$

where

$$\begin{aligned}\vec{\Pi}_C\cdot\vec{a}_1 &= (p_x + eBy\cos\theta)\tilde{n}_1 a + (p_z - eBy\sin\theta)\tilde{n}_2 c \\ &= \tilde{n}_1 a p_x + \tilde{n}_2 c p_z + eBy(\tilde{n}_1 a\cos\theta - \tilde{n}_2 c\sin\theta)\end{aligned}$$

$$\vec{\Pi}_C\cdot\vec{a}_1 = \tilde{n}_1 a p_x + \tilde{n}_2 c p_z + eBy\frac{a\cos\theta}{n_2} \tag{45a}$$

$$\vec{\Pi}_C\cdot\vec{a}_2 = b p_y \tag{45b}$$

$$\begin{aligned}\vec{\Pi}_C\cdot\vec{a}_3 &= (p_x + eBy\cos\theta)n_1 a + (p_z - eBy\sin\theta)n_2 c \\ &= n_1 a p_x + n_2 c p_z + eBy(n_1 a\cos\theta - n_2 c\sin\theta)\end{aligned}$$

$$\vec{\Pi}_C\cdot\vec{a}_3 = n_1 a p_x + n_2 c p_z. \tag{45c}$$

Then,

$$\begin{aligned}&S_1 S_2 = e^{i2\pi\varphi_{3d}} S_2 S_1 \\ &[S_2, S_3] = 0 \qquad [S_1, S_3] = 0\end{aligned} \tag{46}$$

with

$$\varphi_{3d} = \frac{ab\cos\theta}{2\pi\ell^2 n_2} = \frac{L}{t} \tag{47}$$

$$S_1 S_2 = e^{i2\pi\varphi_{3d}} S_2 S_1 \Rightarrow S_1 S_2 S_1^{-1} S_2^{-1} = e^{i2\pi\varphi_{3d}}.$$

This equation means that when we translate the wavefunction around a surface defined by $\vec{a}_1$ and $\vec{a}_2$, it is multiplied by a phase factor $e^{i2\pi\varphi_{3d}}$, which is again nothing but the Aharonov–Bohm effect [30]. This phase must therefore be equal to the number of flux quanta φ through this surface multiplied by 2π:

$$2\pi\varphi = \frac{\vec{B}\cdot(\vec{a}_1\times\vec{a}_2)}{h/e} = 2\pi\frac{h/e}{v_0}\frac{L}{t}\frac{\vec{a}_3\cdot(\vec{a}_1\times\vec{a}_2)}{h/e} = 2\pi\frac{L}{t} \tag{48}$$

and φ_{3d} is indeed the number of flux quanta through the unit cell defined by $\vec{a}_1$ and $\vec{a}_2$.

The quantity φ_{3d} then plays the same role in the theory as $\varphi = p/q$ in 2D; similarly L plays the same role as p, t the same as q.

1.5. New basis functions

To build the complete orthonormal basis of functions from these operators, we choose, by analogy with what is currently being done in 2D, S_1, $(S_2)^t$ and S_3, which are defined on the cell enclosing L flux quanta.

S_3 commutes with S_1, $(S_2)^t$. We begin by constructing a basis on a cell enclosing one flux quantum using $S_1^{1/L}$ and S_2^t using the k–q representation. The conjugate operators are now

$$\tilde{X} = -\frac{p_y}{eB} \qquad \text{and} \qquad \tilde{P} = n_2 \frac{\tilde{n}_1 a p_x + \tilde{n}_2 c p_z}{a\cos\theta} + eBy \tag{49}$$

and from these we obtain the translation operators

$$S_1^{1/L} = \mathrm{e}^{\mathrm{i}\frac{a\cos\theta}{n_2 L\hbar}\tilde{P}} \qquad S_2^t = \mathrm{e}^{-\mathrm{i}\frac{2\pi L n_2}{a\cos\theta}\tilde{X}}. \tag{50}$$

Their eigenfunctions are [31]

$$g_{q_X q_Y}(X) = \sqrt{\frac{2\pi L n_2}{a\cos\theta}} \sum_\mu \mathrm{e}^{\mathrm{i}\mu\frac{a\cos\theta}{Ln_2}q_X} \delta\left(X - q_Y \ell^2 - \frac{a\cos\theta}{Ln_2}\mu\right). \tag{51}$$

The question of other possible choices (e.g. Wannier functions, [33]) will not be discussed here. As before, to get eigenfunctions of S_1 and S_2^t, we define the index j as varying between 1 and L:

$$g_{q_X q_Y j}(X) = \sqrt{\frac{2\pi L n_2}{a\cos\theta}} \sum_\mu \mathrm{e}^{\mathrm{i}\mu\frac{a\cos\theta}{Ln_2}\left(q_X + \frac{2\pi n_2}{a\cos\theta} j\right)} \delta\left(X - q_Y \ell^2 - \frac{a\cos\theta}{Ln_2}\mu\right) \tag{52a}$$

with

$$-\frac{\pi n_2}{a\cos\theta} \leqslant q_X < \frac{\pi n_2}{a\cos\theta} \qquad \text{and} \qquad -\frac{\pi}{tb} \leqslant q_Y < \frac{\pi}{tb}. \tag{52b}$$

What will the eigenfunction for S_3 be? It is a 'usual' translation operator in the direction of the magnetic field:

$$S_3 = \exp\left(\mathrm{i}\frac{n_1 a p_x + n_2 c p_z}{\hbar}\right) = \exp\left(\mathrm{i}\left(\frac{n_2 c}{\cos\theta}\right)\right)\frac{\sin\theta p_x + \cos\theta p_z}{\hbar}. \tag{53}$$

S_2 is also a translation operator in real space, with a multiplication by a y-dependent phase factor:

$$\begin{aligned} S_2 &= \exp\left(\mathrm{i}\frac{\tilde{n}_1 a p_x + \tilde{n}_2 c p_z + eBy\frac{a\cos\theta}{n_2}}{\hbar}\right) \\ &= \exp\left(\mathrm{i}\left(\frac{\tilde{n}_1 a}{\cos\alpha}\right)\frac{\cos\alpha p_x + \sin\alpha p_z}{\hbar}\right)\exp\left(\mathrm{i}eBy\frac{a\cos\theta}{\hbar n_2}\right) \end{aligned} \tag{54}$$

where α is the angle between $\vec{a}_1$ and the x axis (see figure above):

$$\frac{\tilde{n}_2 c}{\tilde{n}_1 a} = \frac{\sin\alpha}{\cos\alpha}.$$

We are therefore looking for an eigenfunction of S_3 on which S_2 does not act; we may choose

$$\frac{1}{\sqrt{2\pi}}\mathrm{e}^{\mathrm{i}q_Z(-x\sin\alpha + z\cos\alpha)}.$$

The effect of S_2 on this function is a translation in x and a translation in z:

$$-\tilde{n}_1 a\sin\alpha + \tilde{n}_2 c\cos\alpha = 0 \tag{55}$$

where we used the relationship between $\tilde{n}_1$ and $\tilde{n}_2$ and the angle α. (Note that $\alpha = 0$ when $\theta = 0$.) Therefore S_2 has no effect on this function. S_3 induces a translation in x and a translation in z, so

$$-n_1 a\sin\alpha + n_2 c\cos\alpha = \frac{-n_1\tilde{n}_2 ac + n_2\tilde{n}_1 ca}{a_1} = \frac{ca}{a_1} \tag{56}$$

and we get

$$S_3\left\{\frac{1}{\sqrt{2\pi}}\mathrm{e}^{\mathrm{i}q_Z(-x\sin\alpha+z\cos\alpha)}\right\} = \mathrm{e}^{\mathrm{i}q_Z\frac{ac}{a_1}}\left\{\frac{1}{\sqrt{2\pi}}\mathrm{e}^{\mathrm{i}q_Z(-x\sin\alpha+z\cos\alpha)}\right\}. \tag{57}$$

In view of the presence of the periodic potential, we rewrite the function as

$$\frac{1}{\sqrt{2\pi}}\exp(\mathrm{i}(q_Z + kG_3)(-x\sin\alpha + z\cos\alpha))$$

where k is an integer and G_3 is the norm of the third vector of the Brillouin zone:

$$G_3 = 2\pi\frac{a_1}{ac}.$$

We are now able to build out of these elements an eigenfunction basis, in a way very much analogous to the 'pure' 2D case when the field is perpendicular [31], using the eigenfunctions of the Landau Hamiltonian, which will make the calculation of the matrix element simpler. Now that the field is tilted, they are of the form

$$\Phi_{q_y,n}(x, y) = \mathrm{e}^{\mathrm{i}yq_Y} f_n\left(\frac{x\cos\theta - z\sin\theta + q_Y\ell^2}{\ell}\right) \tag{58}$$

with f_n the eigenfunction of the 1D harmonic oscillator. A standard calculation then yields

$$\begin{aligned}\Phi_{njk}^{q_Xq_Yq_Z}(x, y, z) &= \sqrt{\frac{Ln_2}{(2\pi)^2 a\cos\theta}}\exp(\mathrm{i}(q_Z + kG_3)(-x\sin\alpha + z\cos\alpha))\\ &\times \sum_\mu \exp\left(-\mathrm{i}\mu\frac{a\cos\theta}{Ln_2}\left(q_X + \frac{2\pi n_2}{a\cos\theta}j\right)\right)\\ &\times \exp\left(\mathrm{i}y\left(q_Y + \frac{2\pi}{tb}\mu\right)\right) f_n\left(\frac{x\cos\theta - z\sin\theta + \left(q_Y + \frac{2\pi}{tb}\mu\right)\ell^2}{\ell}\right)\end{aligned} \tag{59a}$$

with

$$-\frac{\pi n_2}{a\cos\theta} \leqslant q_X < \frac{\pi n_2}{a\cos\theta} \qquad -\frac{\pi}{tb} \leqslant q_Y < \frac{\pi}{tb} \qquad -\frac{\pi a_1}{ac} \leqslant q_Z < \frac{\pi a_1}{ac}. \tag{59b}$$

1.6. The eigenvalue equation

We study the action of S_1, S_2 and S_3, then of S_a^θ, S_{tb}^θ and S_c^θ, then write the transform which connects the two sets of operators and (q_X, q_Y, q_Z) to (q_x, q_y, q_z). The eigenvalues can be shown to be

$$\text{for } S_1: \quad \exp\left(\mathrm{i}\frac{La\cos\theta}{n_2L}\left(q_X + \frac{2\pi n_2}{a\cos\theta}j\right)\right) = \exp\left(\mathrm{i}\frac{a\cos\theta}{n_2}q_X\right) \tag{60a}$$

$$\text{for } S_2: \quad \mathrm{e}^{\mathrm{i}tbq_Y} \tag{60b}$$

$$\text{and for } S_3: \quad \mathrm{e}^{\mathrm{i}q_Z\frac{ac}{a_1}} = \mathrm{e}^{\mathrm{i}q_Z\frac{2\pi}{G_3}}. \tag{60c}$$

Therefore

$$\begin{aligned}S_1\Phi_{njk}^{q_Xq_Yq_Z} &= \mathrm{e}^{\mathrm{i}\frac{a\cos\theta}{n_2}q_X}\Phi_{njk}^{q_Xq_Yq_Z}\\ S_2\Phi_{njk}^{q_Xq_Yq_Z} &= \mathrm{e}^{\mathrm{i}tbq_Y}\Phi_{njk}^{q_Xq_Yq_Z}\\ S_3\Phi_{njk}^{q_Xq_Yq_Z} &= \mathrm{e}^{\mathrm{i}\frac{2\pi}{G_3}q_Z}\Phi_{njk}^{q_Xq_Yq_Z}.\end{aligned} \tag{61}$$

Similarly, one gets, for S_a^θ, S_b^θ and S_c^θ,

$$\begin{aligned} S_a^\theta \Phi_{njk}^{q_X q_Y q_Z} &= \mathrm{e}^{\mathrm{i}a(q_X \cos\theta - q_Z \sin\alpha)} \Phi_{njk}^{q_X q_Y q_Z} \\ S_{tb}^\theta \Phi_{njk}^{q_X q_Y q_Z} &= \mathrm{e}^{\mathrm{i}tbq_Y} \Phi_{njk}^{q_X q_Y q_Z} \\ S_c^\theta \Phi_{njk}^{q_X q_Y q_Z} &= \mathrm{e}^{\mathrm{i}c(-q_X \sin\theta + q_Z \cos\alpha)} \Phi_{njk}^{q_X q_Y q_Z}. \end{aligned} \tag{62}$$

And we can write

$$\begin{aligned} q_x &= q_X \cos\theta - q_Z \sin\alpha \\ q_y &= q_Y \\ q_z &= -q_X \sin\theta + q_Z \cos\alpha \end{aligned} \tag{63}$$

together with the inverse

$$\begin{aligned} q_X &= \frac{1}{\cos(\theta+\alpha)} \{q_x \cos\alpha + q_z \sin\alpha\} \\ q_Y &= q_y \\ q_Z &= \frac{1}{\cos(\theta+\alpha)} \{q_x \sin\theta + q_z \cos\theta\}. \end{aligned} \tag{64}$$

The completeness and orthogonality relationships read

$$\int_{\mathrm{BZ}} \mathrm{d}q_x \, \mathrm{d}q_y \, \mathrm{d}q_z \, \Phi_{njk}^{*\vec{q}}(\vec{r}\,') \Phi_{njk}^{\vec{q}}(\vec{r}) = \delta(\vec{r}\,' - \vec{r})$$

and

$$\int \mathrm{d}x \, \mathrm{d}y \, \mathrm{d}z \, \Phi_{n'j'k'}^{*\vec{q}\,'}(\vec{r}) \Phi_{njk}^{\vec{q}}(\vec{r}) = \delta(\vec{q}\,' - \vec{q}) \delta_{n'n} \delta_{k'k} \delta_{j'j}.$$

2. The matrix element of the 3D Hamiltonian

The calculation of the matrix element of the Hamiltonian

$$H = \frac{p_x^2 + (p_y^2 + eBx\cos\theta - eBz\sin\theta)^2 + p_z^2}{2m} + V(x, y, z) = H_0 + V(x, y, z) \tag{65}$$

with

$$V(x, y, z) = V_x \cos\left(\frac{2\pi}{a} x\right) + V_y \cos\left(\frac{2\pi}{b} y\right) + V_z \cos\left(\frac{2\pi}{c} z\right) \tag{66}$$

on the complete orthonormal basis defined above is described in appendix A. For the sake of simplicity, let M_{01} and M_{02} be the two terms of the matrix element of H_0, M_1 and M_2, M_3 and M_4, M_5 and M_6 the matrix elements of, respectively, the x, y and z terms of the periodic potential. One has

$$\begin{aligned} M_{01} &= \delta(q_x' - q_x)\delta(q_y' - q_y)\delta(q_z' - q_z)\delta_{k'k}\delta_{n'n}\delta_{j'j} \\ &\quad \times \left[\left(n + \frac{1}{2}\right)\hbar\omega_C + \frac{\hbar^2}{2m} \left(\frac{q_x \cos\alpha + q_z \sin\alpha}{\cos(\theta+\alpha)} + kG_3 \right)^2 \right] \end{aligned} \tag{A.12}$$

$$\begin{aligned} M_{02} &= -\frac{\delta(q_X' - q_X)\delta(q_Y' - q_Y)\delta(q_Z' - q_Z)}{\cos(\theta+\alpha)} \frac{\sin(\theta+\alpha)}{m} \hbar(q_Z + kG_3)\delta_{k'k}\delta_{j'j} \\ &\quad \times \int \mathrm{d}\tilde{X} \, f_{n'}\left(\frac{\tilde{X}}{\ell}\right) P_X f_n\left(\frac{\tilde{X}}{\ell}\right) \end{aligned} \tag{A.13}$$

which is obtained using the known formula

$$\int \mathrm{d}\tilde{X}\, f_{n'}\left(\frac{\tilde{X}}{\ell}\right) P_X\, f_n\left(\frac{\tilde{X}}{\ell}\right) = -\frac{\mathrm{i}\hbar}{\ell\sqrt{2}}\delta_{n',n-1}\sqrt{n} + \frac{\mathrm{i}\hbar}{\ell\sqrt{2}}\delta_{n',n+1}\sqrt{n+1}. \quad \text{(A.14)}$$

The matrix element $\int \mathrm{d}x\, \mathrm{d}y\, \mathrm{d}z\, \phi^{*\vec{q}'}_{n'j'k'} V(x) \phi^{q'}_{njk}$ of the 3D periodic potential yields for the term in x

$$\begin{aligned} M_1 + M_2 = {} & \delta(q'_x - q_x)\delta(q'_y - q_y)\delta(q'_z - q_z)\Bigg\{\delta(k' - k + n_1)\delta(j' - j + \tilde{n}_1)\mathrm{e}^{\mathrm{i}\tilde{n}_1 \frac{tb}{L} q_Y} \\ & \times \int \mathrm{d}\tilde{X}\, \phi_{n'}\left(\frac{\tilde{X}}{\ell}\right)\mathrm{e}^{-\mathrm{i}\frac{2\pi}{a}\frac{n_2\tilde{n}_1}{\cos\theta}\tilde{X}} f_n\left(\frac{\tilde{X}}{\ell}\right) + \delta(k' - k - n_1)\delta(j' - j - \tilde{n}_1)\mathrm{e}^{-\mathrm{i}\tilde{n}_1 \frac{tb}{L} q_Y} \\ & \times \int \mathrm{d}\tilde{X}\, \phi_{n'}\left(\frac{\tilde{X}}{\ell}\right)\mathrm{e}^{\mathrm{i}\frac{2\pi}{a}\frac{n_2\tilde{n}_1}{\cos\theta}\tilde{X}} f_n\left(\frac{\tilde{X}}{\ell}\right)\Bigg\}\frac{V_x}{2} \end{aligned} \quad \text{(A.9)}$$

and for the term in y

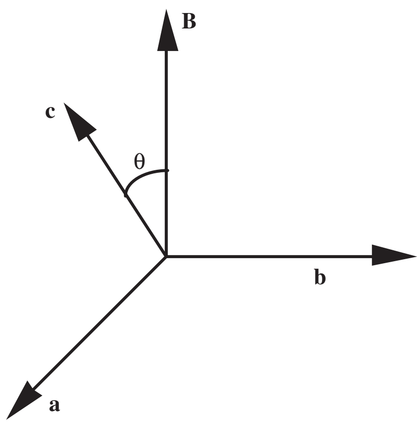
$$\begin{aligned} M_3 + M_4 = {} & \frac{V_y}{2}\delta(\vec{q}' - \vec{q})\delta_{j'j}\delta_{k'k}\Bigg\{\mathrm{e}^{\mathrm{i}t\frac{a\cos\theta}{Ln_2}\left(\frac{\{q_x\cos\alpha + q_z\sin\alpha\}}{\cos(\theta+\alpha)} + \frac{2\pi n_2}{a\cos\theta}j\right)} \int \mathrm{d}\tilde{X}\, f_{n'}\left(\frac{\tilde{X} + 2\pi\ell^2/b}{\ell}\right) f_n\left(\frac{\tilde{X}}{\ell}\right) \\ & + \mathrm{e}^{-\mathrm{i}t\frac{a\cos\theta}{Ln_2}\left(\frac{\{q_x\cos\alpha + q_z\sin\alpha\}}{\cos(\theta+\alpha)} + \frac{2\pi n_2}{a\cos\theta}j\right)} \int \mathrm{d}\tilde{X}\, f_{n'}\left(\frac{\tilde{X} - 2\pi\ell^2/b}{\ell}\right) f_n\left(\frac{\tilde{X}}{\ell}\right)\Bigg\} \end{aligned} \quad \text{(A.10)}$$

and for the term in z

$$\begin{aligned} M_5 + M_6 = {} & \delta(q'_x - q_x)\delta(q'_y - q_y)\delta(q'_z - q_z)\frac{V_z}{2}\Bigg\{\delta(j' - j - \tilde{n}_2)\delta(k' - k - n_2)\mathrm{e}^{-\mathrm{i}\tilde{n}_2 t b q_y} \\ & \times \int \mathrm{d}\tilde{X}\, f_{n'}\left(\frac{\tilde{X}}{\ell}\right)\mathrm{e}^{\mathrm{i}\frac{2\pi}{a}\frac{n_2\tilde{n}_2}{\cos\theta}\tilde{X}} f_n\left(\frac{\tilde{X}}{\ell}\right) + \delta(j' - j + \tilde{n}_2)\delta(k' - k + n_2)\mathrm{e}^{\mathrm{i}\tilde{n}_2 t b q_y} \\ & \times \int \mathrm{d}\tilde{X}\, f_{n'}\left(\frac{\tilde{X}}{\ell}\right)\mathrm{e}^{-\mathrm{i}\frac{2p}{a}\frac{n_2\tilde{n}_2}{\cos\theta}\tilde{X}} f_n\left(\frac{\tilde{X}}{\ell}\right)\Bigg\}. \end{aligned} \quad \text{(A.11)}$$

As in the 2D case [16, 18], these formulae lend themselves to simple band structure and transport coefficient numerical calculations without approximations. The results will be presented elsewhere.

We now compare this result with Montambaux and Kohmoto's finding [27]. In their article, the geometry was different (see below) and, using the tight binding approximation, they studied the spectrum of a Harper equation in 3D.



Here, the magnetic field remains perpendicular to the xy plane determined by the vectors $\vec{a}$ and $\vec{b}$, but not aligned with the third vector $\vec{c}$ of the Bravais lattice. In this geometry, Harper's equation depends on the two fluxes of the problem

$$\varphi_a = \frac{bc\sin\theta}{2\pi\ell^2} = \frac{p'}{q'} \qquad \text{and} \qquad \varphi_c = \frac{ab}{2\pi\ell^2} = \frac{p}{q}. \tag{67}$$

This case can also be dealt with using Schellnhuber's method. The conclusions are close to those reached and explained above: the spectrum is found to have qq' subbands if q and q' are mutually prime; otherwise it will have t subbands, with t the greatest common multiple of q and q'. For a comparison with the 2D matrix elements, see e.g. Zak [18] and TAH [16].

3. Transport coefficients and Diophantine equation

3.1. Back again to the 2D case

As was done in the first part, we return to the 2D case in order to present the main relevant concepts and the theoretical framework.

The Hall conductance calculation is generally based on the Kubo formula [11]. In the following, we use indifferently for the level or band indexes α or β as do as well well as for instance m.

$$\sigma_{\mathrm{H}} = \frac{\mathrm{i}e^2\hbar}{A}\sum_{E_\alpha<E_{\mathrm{F}}}\sum_{E_\beta>E_{\mathrm{F}}}\frac{v_x^{\alpha\beta}v_y^{\beta\alpha} - v_y^{\alpha\beta}v_x^{\beta\alpha}}{(E_\alpha - E_\beta)^2} \tag{68}$$

with

$$v_x^{\alpha\beta} = \langle\Psi_{\vec{q}}^{\alpha}|v_x|\Psi_{\vec{q}}^{\beta}\rangle$$

where A is the area of the sample, a and b label two non-degenerate energy levels. It is a velocity–velocity correlation function. It is rewritten using the 2D Hamiltonian, with the functions $u_{\vec{q}}^{\alpha}(\vec{r})$ such that $\Psi_{\vec{q}}^{\alpha}(\vec{r}) = \mathrm{e}^{\mathrm{i}\vec{q}\cdot r}u_{\vec{q}}^{\alpha}(\vec{r})$ with the Ψ eigenfunctions of the energy operator and the $u_{\vec{q}}^{\alpha}(\vec{r})$ verify the translation properties

$$\begin{aligned} u_{\vec{q}}^{\alpha}(x+a, y) &= \mathrm{e}^{-\mathrm{i}ya/\ell^2}u_{\vec{q}}^{\alpha}(x, y) \\ u_{\vec{q}}^{\alpha}(x, y+b) &= u_{\vec{q}}^{\alpha}(x, y). \end{aligned} \tag{69}$$

The Schrödinger equation then reads

$$\left[\frac{1}{2m}\left(-\mathrm{i}\hbar\frac{\partial}{\partial x} - \hbar q_x\right)^2 + \frac{1}{2m}\left(-\mathrm{i}\hbar\frac{\partial}{\partial y} - \hbar q_y + eBx\right)^2 + V(x, y)\right]u_{\vec{q}}^{\alpha}(\vec{r}) = E^{\alpha}(\vec{q})u_{\vec{q}}^{\alpha}(\vec{r}) \tag{70}$$

and the velocity operators appearing in the Kubo formula

$$v_x = \frac{1}{\hbar}\frac{\partial H(q_x, q_y)}{\partial q_x} \qquad \text{and} \qquad v_y = \frac{1}{\hbar}\frac{\partial H(q_x, q_y)}{\partial q_y}$$

are rewritten as

$$\begin{aligned} \hbar v_x^{\alpha\beta} = \langle u_{\vec{q}}^{\alpha}|\frac{\partial H(q_x, q_y)}{\partial q_x}|u_{\vec{q}}^{\beta}\rangle = \frac{\partial}{\partial q_x}\langle u_{\vec{q}}^{\alpha}|H(q_x, q_y)|u_{\vec{q}}^{\beta}\rangle - \left\langle\frac{\partial u_{\vec{q}}^{\alpha}}{\partial q_x}\right| H(q_x, q_y)|u_{\vec{q}}^{\beta}\rangle \\ - \langle u_{\vec{q}}^{\alpha}|H(q_x, q_y)\left|\frac{\partial u_{\vec{q}}^{\beta}}{\partial q_x}\right\rangle. \end{aligned}$$

Then the Hall conductance is

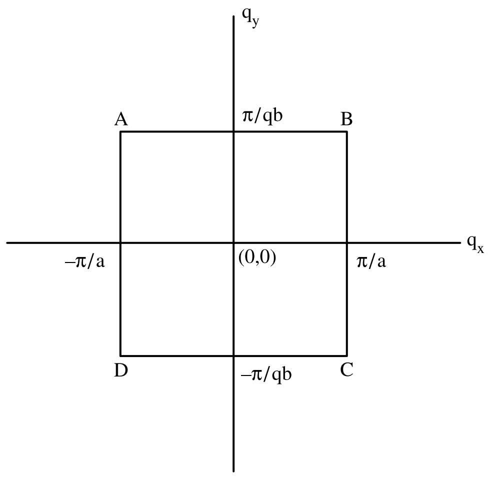
$$\sigma_{\mathrm{H}} = -\frac{\mathrm{i}e^2}{(2\pi)^2\hbar}\int \mathrm{d}q_x\,\mathrm{d}q_y\left[\left\langle\frac{\partial u^\alpha_{\vec q}}{\partial q_x}\middle|\frac{\partial u^\alpha_{\vec q}}{\partial q_y}\right\rangle - \left\langle\frac{\partial u^\alpha_{\vec q}}{\partial q_y}\middle|\frac{\partial u^\alpha_{\vec q}}{\partial q_x}\right\rangle\right]$$

$$\sigma_{\mathrm{H}} = -\frac{\mathrm{i}e^2}{(2\pi)h}\oint \mathrm{d}\vec q\cdot\left\langle u^\alpha_{\vec q}\middle|\frac{\partial u^\alpha_{\vec q}}{\partial \vec q}\right\rangle \tag{71}$$

where the integration path is along the edge of the Brillouin zone. This integral is precisely the change of phase when we move the wavefunction along the contour ABCD around the Brillouin zone as shown in the figure below.

Finally,

$$\sigma_{\mathrm{H}} = \frac{e^2}{h}n_{\mathrm{H}} \tag{72}$$



where n_{H} is the integer associated to the Hall conductance, which, in this formalism, is calculated as the phase change of the eigenfunction of the Hamiltonian.

The Hall conductance verifies a Diophantine equation [14, 16, 18] which is easily deduced from the magnetic translational symmetry of the system. This equation also connects the Hall conductance to another topological invariant of the system, the adiabatic charge transport coefficient σ_{V}. Both quantities (σ_{H} and σ_{V}) are integers that enable us to label the gap where we compute them, in the sense that a combination of the two yields the electronic density of this gap.

To establish the Diophantine equation, we refer to Dana and Zak [18] and consider a filled band, placing ourselves above it in a gap. The energy is periodic in q_x and q_y, and this periodicity coincides with the Brillouin zone. Let $\vec{Q}_n$ be a vector in the Brillouin zone and let $\Psi_{\vec q+\vec Q}$ and $\Psi_{\vec q}$ have the same energies and the same eigenvalues for the magnetic translation operators. They can be said to be the same state to within a phase, which depends of the wavevector: $\Psi_{\vec q+\vec Q} = \mathrm{e}^{\mathrm{i}\alpha(\vec q)}\Psi_{\vec q}$. When the magnetic field is zero, we know [35] that it is possible to build eigenfunctions of the Bloch Hamiltonian the phase of which is also periodic in q_x and q_y; but the conditions allowing this property no longer exists in the presence of a magnetic field, because the Hamiltonian then depends on x, and Weinreich's reasoning is no longer valid.

Because of the gauge choice, the Hamiltonian in y is the same as that for Bloch electrons when $B = 0$, the translation operators along y are the usual translation operators and we can therefore build Bloch functions in q_y:

$$\Psi_{q_x,q_y+\frac{2\pi}{qb}} = \Psi_{q_x,q_y} \tag{73a}$$

while

$$\Psi_{q_x+\frac{2\pi}{a},q_y} = \mathrm{e}^{\mathrm{i}\zeta(q_x,q_y)}\Psi_{q_x,q_y}. \tag{73b}$$

What form can we take for the phase? It must obey, for any Landau level or band, the periodicity properties

$$\Psi_{q_x+\frac{2\pi}{a},q_y+\frac{2\pi}{qb}} = \Psi_{q_x+\frac{2\pi}{a},q_y} = \mathrm{e}^{\mathrm{i}\zeta(q_x,q_y)}\Psi_{q_x,q_y} \tag{74a}$$

$$\Psi_{q_x+\frac{2\pi}{a},q_y+\frac{2\pi}{qb}} = \mathrm{e}^{\mathrm{i}\zeta(q_x,q_y+\frac{2\pi}{qb})}\Psi_{q_x,q_y+\frac{2\pi}{qb}} = \mathrm{e}^{\mathrm{i}\zeta(q_x,q_y+\frac{2\pi}{qb})}\Psi_{q_x,q_y} \tag{74b}$$

and therefore

$$\zeta\left(q_x, q_y + \frac{2\pi}{qb}\right) = \zeta(q_x, q_y) + 2\pi\sigma \tag{75}$$

where σ is an integer.

This allows us to choose the expression for the phase as follows [35]:

$$\zeta(q_x, q_y) = \sigma q_y qb. \tag{76a}$$

This expression obeys condition (75).

What is the integer σ? The Hall conductance is (phase)/i2π which appears when we move the wavefunction around the Brillouin zone. But, from the expression for the boundary conditions, going around the Brillouin zone corresponds to multiplying the wavefunction by $\mathrm{e}^{\mathrm{i}2\pi\sigma}$, so σ is indeed the Hall conductance. If we continue to make use of the magnetic translation invariance properties of the problem, the operator $S_b = \mathrm{e}^{\mathrm{i}\frac{bp_y}{\hbar}}$ commutes with the Hamiltonian; also, $\Psi_{\vec{q}}$ and $S_b\Psi_{\vec{q}}$ have the same energies. But also

$$S_a S_b \Psi_{\vec{q}} = \mathrm{e}^{\mathrm{i}\frac{2\pi p}{q}} S_b S_a \Psi_{\vec{q}} = \mathrm{e}^{\mathrm{i}\frac{2\pi p}{q}} \mathrm{e}^{\mathrm{i}aq_x} S_b \Psi_{\vec{q}} = \mathrm{e}^{\mathrm{i}a(q_x+\frac{2\pi p}{qa})} S_b \Psi_{\vec{q}}. \tag{77}$$

Consequently $S_b\Psi_{\vec{q}}$ and $\Psi_{q_x+\frac{2\pi p}{qa},q_y}$ are also the same state with identical energies and wavevectors to within a phase:

$$S_b\Psi_{\vec{q}} = \mathrm{e}^{\mathrm{i}\eta(q_x,q_y)}\Psi_{q_x+\frac{2\pi p}{qa},q_y}. \tag{78}$$

How can we choose the phase? The condition that we gave implies

$$S_b\Psi_{q_x,q_y+\frac{2\pi}{qb}} = \mathrm{e}^{\mathrm{i}\eta(q_x,q_y+\frac{2\pi}{qb})}\Psi_{q_x+\frac{2\pi p}{qa},q_y+\frac{2\pi}{qb}}$$

but since

$$\Psi_{q_x,q_y+\frac{2\pi}{qb}} = \Psi_{q_x,q_y}$$

this means that

$$\eta\left(q_x, q_y + \frac{2\pi}{qb}\right) = \eta(q_x, q_y) + 2\pi m \qquad \text{with } m \text{ integer.}$$

Therefore we can take [35]

$$\eta(q_x, q_y) = mq_y qb. \tag{76b}$$

We are now able to derive the Diophantine equation, since

$$S_{qb}\Psi_{q_x,q_y} = \mathrm{e}^{\mathrm{i}q_y qb(qm)}\Psi_{q_x+\frac{2\pi}{a}p,q_y} = \mathrm{e}^{\mathrm{i}q_y qb(qm+p\sigma)}\Psi_{q_x,q_y} = \mathrm{e}^{\mathrm{i}q_y qb}\Psi_{q_x,q_y}$$

must be true for any value of the wavevector; therefore,

$$p\sigma + qm = 1. \tag{79}$$

We showed the equation for a given band, but it can be easily seen that, when we place ourselves in the gap above n_b bands,

$$p\sigma_{\mathrm{H}} + qm_{n_b} = n_b. \tag{80}$$

The first to have understood the physical meaning of the second topological invariant m_{n_b} is Hervé Kunz [15]. By construction, σ is the Hall conductance. What does m represent? Kunz has shown that in a system subjected to a periodic potential

$$V_x \cos\left(\frac{2\pi}{a}x\right) + V_y \cos\left(\frac{2\pi}{b}y + \gamma\right). \tag{5}$$

If we vary γ adiabatically up to the completion of a period, which corresponds to moving the lattice along the y direction, a charge displacement along y can take place; we can calculate it in the following fashion. The quantity

$$e(\vec{v} \cdot \mathrm{d}\vec{s})\rho(t)\,\mathrm{d}t$$

is the charge going through the surface element pointing in the y direction at a given point r and during the time interval $(t, t + \mathrm{d}t)$. We are interested in spatial averages and the quantity that we are looking for is

$$\sigma_{\mathrm{V}} = \lim_{T\to\infty} e \int_0^T \mathrm{d}t \left\{M(v_y\rho(t)) - M(v_y\rho(0))\right\} \tag{81}$$

where M represents the spatial average of the operator in parentheses:

$$M(\text{operator}) = \lim_{V\to\infty} \frac{1}{V}\int_V (\text{operator})\,\mathrm{d}\vec{r}.$$

Kunz has shown that this expression can be rewritten as

$$\sigma_{\mathrm{V}} = \frac{e}{\hbar(2\pi)^2}\int_0^{2\pi/a} \mathrm{d}q_x \int_0^{2\pi/qb} \mathrm{d}q_y \left[\left\langle \frac{\partial \Psi_{\vec{q}}^{\gamma}}{\partial q_y} \middle| \frac{\partial \Psi_{\vec{q}}^{\gamma}}{\partial \gamma} \right\rangle - \left\langle \frac{\partial \Psi_{\vec{q}}^{\gamma}}{\partial \gamma} \middle| \frac{\partial \Psi_{\vec{q}}^{\gamma}}{\partial q_y} \right\rangle\right] \tag{82}$$

where a is the period in x. This expression resembles very closely the expression from which TKNN started. To calculate it, we follow a reasoning inspired by [16]: when we add a phase to the potential, the basis of functions chosen above remains a good basis for diagonalizing the problem since the phase has not modified the translation properties of the system. Thus we may write

$$\Psi_{\vec{q}}^{m,\gamma}(x, y) = \sum_{nj} C_{nj}^m(\vec{q}, \gamma)\phi_{nj}^{\vec{q}}(x, y). \tag{83}$$

All the dependence in γ is therefore in the coefficients of the development and we may write

$$\sigma_{\mathrm{V}} = \frac{e}{\hbar(2\pi)^2}\int_0^{2\pi/a} \mathrm{d}q_x \int_0^{2\pi/qb} \mathrm{d}q_y \sum_{nj}\left[\left\langle \frac{\partial \Psi_{\vec{q}}^{m,\gamma}}{\partial q_y} \middle| \frac{\partial C_{nj}^m}{\partial \gamma} \right\rangle \phi_{nj}^{\vec{q}} - \left\langle \frac{\partial C_{nj}^m}{\partial \gamma} \middle| \frac{\partial \Psi_{\vec{q}}^{\gamma}}{\partial q_y} \right\rangle \phi_{nj}^{*\vec{q}}\right]. \tag{84}$$

The important remark here is that the matrix element with a phase γ added to the potential in y has the same expression as the matrix element in $(q_x + \frac{b\gamma}{2\pi\ell^2}, q_y)$. We can therefore replace $\frac{\partial}{\partial\gamma}$ by $\frac{b}{2\pi\ell^2}\frac{\partial}{\partial q_x}$. It can be shown that

$$\sigma_{\mathrm{V}} = \frac{e}{q\hbar(2\pi)^2 a}\int_0^{2\pi p/a} \mathrm{d}q_x \int_0^{2\pi/qb} \mathrm{d}q_y \sum_{nj}\left[\left(\frac{\partial C_{nj}^{*m}}{\partial q_y}.\frac{\partial C_{nj}^m}{\partial q_x}\right) - \left(\frac{\partial C_{nj}^{*m}}{\partial q_x}.\frac{\partial C_{nj}^m}{\partial q_y}\right)\right]. \tag{85}$$

And from Stokes's theorem,

$$\sigma_{\mathrm{V}} = \frac{e}{q\hbar(2\pi)^2 a} \sum_{nj} \int_{Z\mathrm{d}B} \mathrm{d}\vec{q}.\left\langle C_{nj}^m \middle| \frac{\partial C_{nj}^m}{\partial \vec{q}} \right\rangle. \tag{86}$$

Following a reasoning similar to that in the Hall conductance case we again call ABCD the Brillouin zone rectangle and if

$$C_{nj}^m(CD) = C_{nj}^m(AB)\mathrm{e}^{\mathrm{i}\vartheta(\vec{q})}$$

one can show that the expression is indeed the change of phase of the C_{nj}^m coefficients when we translate them along and around the extended Brillouin zone. Therefore,

$$\sigma_{\mathrm{V}} = \frac{e}{ha}\frac{pn_h - 1}{q} = \frac{e}{ha}m,$$

where we have just shown that m is the integer characterizing the adiabatic charge transport coefficient. This Diophantine equation can also be written [15] as

$$B^{-1}\sigma_h + a^{-1}\sigma_{\mathrm{V}} = \rho \tag{87}$$

where ρ is the electronic density and we have changed m into σ_{V}.

In the present situation, a change of phase γ along y in the periodic potential is equivalent to a translation of $b\gamma/2\pi$ along y. Therefore, we define

$$H_\gamma = S_{b\gamma/2\pi}^{-1} H S_{b\gamma/2\pi}. \tag{88}$$

In particular, a change of phase of one period corresponds to a transformation of the Hamiltonian by S_b. But we just showed that this translation corresponds to a certain displacement in the Brillouin zone. This is how charge transport can also be understood as a Berry phase, the Diophantine equation then being nothing but a coherence equation between two displacements in the Brillouin zone. Results on the adiabatic charge transport in zero magnetic field appear in [13].

3.2. The Hall conductance in 3D

The expression for the Hall conductance in 3D when the Fermi energy is in a gap is, after Kubo's formula [11]

$$\sigma_{ij}^m = \frac{e^2}{(2\pi)^2 h} \int \mathrm{d}q^3 \sum_{m' \leqslant m} \int \mathrm{d}r^3 \left(\frac{\partial u_{\vec{q},m'}^*}{\partial q_i} \frac{\partial u_{\vec{q},m'}}{\partial q_j} - \frac{\partial u_{\vec{q},m'}^*}{\partial q_j} \frac{\partial u_{\vec{q},m'}}{\partial q_i} \right) \tag{89}$$

where i and j are x, y or z, since we want to compute the transport properties in the plane where the electrons move in reality, m here is the band index and, as usual,

$$u_{\vec{q},m}(x, y, z) = \mathrm{e}^{-\mathrm{i}\vec{q}\cdot\vec{r}} \Psi_{\vec{q},m}(x, y, z). \tag{90}$$

3.2.1. Computation of σ_{xy}^m

$$\sigma_{xy}^m = \frac{e^2}{(2\pi)^2 h} \int \mathrm{d}q^3 \sum_{m' \leqslant m} \int \mathrm{d}r^3 \left(\frac{\partial u_{\vec{q},m'}^*}{\partial q_x} \frac{\partial u_{\vec{q},m'}}{\partial q_y} - \frac{\partial u_{\vec{q},m'}^*}{\partial q_y} \frac{\partial u_{\vec{q},m'}}{\partial q_x} \right) \tag{90}$$

with m the band index.

We rewrite this equation as a function of the components of the rotated Brillouin zone as above, recalling that

$$\begin{aligned} q_x &= q_X \cos\theta - q_Z \sin\alpha \\ q_y &= q_Y \\ q_z &= -q_X \sin\theta + q_Z \cos\alpha \end{aligned}$$

and

$$\begin{aligned} q_X &= \frac{1}{\cos(\theta+\alpha)} \{q_x \cos\alpha + q_z \sin\alpha\} \\ q_Y &= q_y \\ q_Z &= \frac{1}{\cos(\theta+\alpha)} \{q_x \sin\theta + q_z \cos\theta\}. \end{aligned} \tag{91}$$

Let

$$\begin{aligned} \frac{\partial}{\partial q_x} &= \frac{1}{\cos(\theta+\alpha)} \left\{\cos\alpha \frac{\partial}{\partial q_X} + \sin\theta \frac{\partial}{\partial q_Z}\right\} \\ \frac{\partial}{\partial q_y} &= \frac{\partial}{\partial q_Y} \\ \frac{\partial}{\partial q_z} &= \frac{1}{\cos(\theta+\alpha)} \left\{\sin\alpha \frac{\partial}{\partial q_X} + \cos\theta \frac{\partial}{\partial q_Z}\right\}. \end{aligned} \tag{92}$$

Then

$$\begin{aligned} \sigma_{xy}^m = \frac{e^2}{(2\pi)^2 h} \int \mathrm{d}q_X\, \mathrm{d}q_Y\, \mathrm{d}q_Z \sum_{m' \leqslant m} \int \mathrm{d}r^3\, \cos\alpha \left(\frac{\partial u^*_{\vec{q},m'}}{\partial q_X} \frac{\partial u_{\vec{q},m'}}{\partial q_Y} - \frac{\partial u^*_{\vec{q},m'}}{\partial q_Y} \frac{\partial u_{\vec{q},m'}}{\partial q_X} \right) \\ +\ \sin\theta \left(\frac{\partial u^*_{\vec{q},m'}}{\partial q_Z} \frac{\partial u_{\vec{q},m'}}{\partial q_Y} - \frac{\partial u^*_{\vec{q},m'}}{\partial q_Y} \frac{\partial u_{\vec{q},m'}}{\partial q_Z} \right). \end{aligned}$$

For the complete calculation, we begin with

$$\int \mathrm{d}q_X\, \mathrm{d}q_Y\, \mathrm{d}q_Z \int \mathrm{d}r^3 \left(\frac{\partial u^*_{\vec{q},m'}}{\partial q_X} \frac{\partial u_{\vec{q},m'}}{\partial q_Y} - \frac{\partial u^*_{\vec{q},m'}}{\partial q_Y} \frac{\partial u_{\vec{q},m'}}{\partial q_X} \right)$$

which equals the phase change of the wavefunction when we transport it on a closed circuit around a section of the Brillouin zone parallel to the (q_X, q_Y) plane, that is $2\pi \times$ integer.

The article by Avron, Seiler and Simon [34] proves that this integer does not depend on the section of the Brillouin zone chosen; that is, here it does not depend on q_Z. Therefore we may write

$$\begin{aligned} \int \mathrm{d}q_X\, \mathrm{d}q_Y\, \mathrm{d}q_Z \sum_{m \leqslant m'} \int \mathrm{d}r^3 \left(\frac{\partial u^*_{\vec{q},m'}}{\partial q_X} \frac{\partial u_{\vec{q},m'}}{\partial q_Y} - \frac{\partial u^*_{\vec{q},m'}}{\partial q_Y} \frac{\partial u_{\vec{q},m'}}{\partial q_X} \right) \\ = 2\pi m_1 \int \mathrm{d}q_Z = 2\pi m_1 G_3 = (2\pi)^2 m_1 \frac{a_1}{ac}. \end{aligned} \tag{93}$$

Similarly,

$$\begin{aligned} \int \mathrm{d}q_X\, \mathrm{d}q_Y\, \mathrm{d}q_Z \sum_{m' \leqslant m} \int \mathrm{d}r^3 \left(\frac{\partial u^*_{\vec{q},m'}}{\partial q_Z} \frac{\partial u_{\vec{q},m'}}{\partial q_Y} - \frac{\partial u^*_{\vec{q},m'}}{\partial q_Y} \frac{\partial u_{\vec{q},m'}}{\partial q_Z} \right) \\ = 2\pi m_2 \int \mathrm{d}q_X = 2\pi m_2 \frac{2\pi n_2}{a\cos\theta} = (2\pi)^2 m_2 \frac{n_2}{a\cos\theta} \end{aligned}$$

where m_1 and m_2 are integers which result from the calculation followed by the addition of all results for bands under the Fermi level. Finally,

$$\sigma_{xy} = \frac{e^2}{h}\left\{\frac{m_1 a_1}{ac}\cos\alpha + \frac{m_2 n_2}{a\cos\theta}\sin\theta\right\} = \frac{e^2}{h}\left\{\frac{m_1 a_1}{ac}\frac{\tilde{n}_1 a}{a_1} + \frac{m_2 n_1}{c}\right\}$$

$$\sigma_{xy} = \frac{e^2}{h}\frac{m_1\tilde{n}_1 + m_2 n_1}{c}. \qquad (94a)$$

This 3D conductance appears to be the sum of two terms. When $\theta = 0$, the integer n_1 is also equal to 0 and the second term disappears. We see here explicitly how the conductance changes upon tilting the magnetic field, keeping its intensity constant.

3.2.2. Computation of σ^m_{yz}

$$\sigma^m_{yz} = \frac{e^2}{(2\pi)^2 h}\int \mathrm{d}q_x\,\mathrm{d}q_y\,\mathrm{d}q_z \sum_{m'\leqslant m}\int \mathrm{d}r^3\left(\frac{\partial u^*_{\vec{q},m'}}{\partial q_y}\frac{\partial u_{\vec{q},m'}}{\partial q_z} - \frac{\partial u^*_{\vec{q},m'}}{\partial q_z}\frac{\partial u_{\vec{q},m'}}{\partial q_y}\right)$$

and, after performing the coordinate change, one has, using notation similar to that for the previous calculation,

$$\sigma^m_{yz} = \frac{e^2}{h}\left\{\sin\alpha\frac{-m_1 a_1}{ac} + \cos\theta\frac{-m_2 n_2}{a\cos\theta}\right\}$$

$$= \frac{e^2}{h}\left\{\frac{\tilde{n}_2 c}{a_1}\frac{(-m_1 a_1)}{ac} + \cos\theta\frac{(-m_2 n_2)}{a\cos\theta}\right\}$$

$$\sigma^m_{yz} = -\frac{e^2}{h}\frac{m_1\tilde{n}_2 + m_2 n_2}{a}. \qquad (94b)$$

3.2.3. Computation of σ^m_{xz}

$$\sigma^m_{xz} = \frac{e^2}{(2\pi)^2 h}\int \mathrm{d}q_x\,\mathrm{d}q_y\,\mathrm{d}q_z \sum_{m'\leqslant m}\int \mathrm{d}r^3\left(\frac{\partial u^*_{\vec{q},m'}}{\partial q_x}\frac{\partial u_{\vec{q},m'}}{\partial q_z} - \frac{\partial u^*_{\vec{q},m'}}{\partial q_z}\frac{\partial u_{\vec{q},m'}}{\partial q_x}\right).$$

Then, it is easy to show that

$$\sigma^m_{xz} = \frac{e^2}{(2\pi)^2 h}\int \mathrm{d}q_X\,\mathrm{d}q_Y\,\mathrm{d}q_Z \sum_{m'\leqslant m}\int \mathrm{d}r^3\left(\frac{\partial u^*_{\vec{q},m'}}{\partial q_X}\frac{\partial u_{\vec{q},m'}}{\partial q_Z} - \frac{\partial u^*_{\vec{q},m'}}{\partial q_Z}\frac{\partial u_{\vec{q},m'}}{\partial q_X}\right)$$

$$\sigma^m_{xz} = \frac{e^2}{h}\frac{m_3}{tb} \qquad (94c)$$

where m_3 is equal, in appropriate units, to the phase which appears when the wavefunction is transported around a circuit around the Brillouin zone in q_X and $q_Z/2\pi$. We show later that this quantity is identically zero.

$$\sigma^m_{xy} = \frac{e^2}{h}\frac{m_1\tilde{n}_1 + m_2 n_1}{c} \qquad \sigma^m_{yz} = -\frac{e^2}{h}\frac{m_1\tilde{n}_2 + m_2 n_2}{a} \qquad \sigma^m_{xz} = \frac{e^2}{h}\frac{m_3}{tb}. \qquad (94)$$

The three independent components of the conductivity tensor when the Fermi level is in a gap now appear, in appropriate units, as the sums of two terms, depending on a sum of integers. Among these integers, m_1, m_2 and m_3 are the 'Berry phases' appearing upon displacements around the Brillouin zone, called 'TKNN integers' by Avron, Seiler and Simon [34]. They are topological quantities related to the geometry of the fibre bundle with as the basis the Brillouin zone seen as a 3D torus. In 3D, there exist only three independent such integers since one can build only three 2D sections of the 3D torus.

To pursue the analogy with the case where the magnetic field is perpendicular to the plane of the electron motion, we now calculate the Diophantine equation relating the conductances. To this end, we first study adiabatic charge transport along y.

3.3. Adiabatic charge transport along y

In the quantity

$$\sigma_{\mathrm{V}y} = -e\hbar \int \mathrm{d}q_x\,\mathrm{d}q_y\,\mathrm{d}q_z \left[\left\langle \frac{\partial u^{\gamma}_{\vec{q}}}{\partial q_y}\middle|\frac{\partial u^{\gamma}_{\vec{q}}}{\partial \gamma}\right\rangle - \left\langle \frac{\partial u^{\gamma}_{\vec{q}}}{\partial \gamma}\middle|\frac{\partial u^{\gamma}_{\vec{q}}}{\partial q_y}\right\rangle\right] \tag{95}$$

the phase γ_y appears in the potential defined by

$$2\cos\left(\frac{2\pi}{b}y + \gamma_y\right) = \mathrm{e}^{\mathrm{i}\frac{2\pi}{b}y}\mathrm{e}^{\mathrm{i}\gamma_y} + \mathrm{e}^{-\mathrm{i}\frac{2\pi}{b}y}\mathrm{e}^{-\mathrm{i}\gamma_y}.$$

This phase does not modify the translation properties of the Hamiltonian, our 'usual' basis can still be used and we may write

$$u^m_{\vec{q}}(\vec{r}) = \mathrm{e}^{-\mathrm{i}\vec{q}\cdot\vec{r}} \sum_n \sum_k \sum_{j=1}^{L} c^m_{njk}(\vec{q}, \gamma_y)\phi^{\vec{q}}_{njk}(\vec{r}) \tag{96}$$

where the dependence on γ_y lies in the coefficients c^m_{njk}. This phase is 'equivalent' to the translation

$$q_X \to q_X + \gamma_y \frac{n_2 L}{ta\cos\theta}.$$

Therefore,

$$\frac{\partial}{\partial \gamma_y} = \frac{n_2 L}{ta\cos\theta}\frac{\partial}{\partial q_X}$$

$$\sigma_{\mathrm{V}y} = e\hbar \frac{n_2 L}{Lta\cos\theta} \int_{-\pi n_2 L/a\cos\theta}^{\pi n_2 L/a\cos\theta} \mathrm{d}q_x \int \mathrm{d}q_Y \int \mathrm{d}q_Z \sum_{nj} \cos(\theta+\alpha)$$
$$\times \left[\frac{\partial c^{m*}_{nj}(\vec{q})}{\partial q_X}\frac{\partial c^{m}_{nj}(\vec{q})}{\partial q_Y} - \frac{\partial c^{m*}_{nj}(\vec{q})}{\partial q_Y}\frac{\partial c^{m}_{nj}(\vec{q})}{\partial q_X}\right].$$

We know that the change of phase of the total wavefunction when it is displaced around this 'enlarged' Brillouin zone is equal to Lm_1, and the change of phase of the c^m_{njk} will therefore be $Lm_1 - 1$. The expression for the adiabatic transport coefficient therefore becomes

$$\sigma_{\mathrm{V}y} = \frac{e}{h}\frac{n_2 L}{Lta\cos\theta} G_3 \cos(\theta+\alpha)[Lm_1 - 1].$$

Hence,

$$\sigma_{\mathrm{V}y} = \frac{e}{h}\frac{n_2 L}{Lta\cos\theta}\frac{a_1}{ac}\frac{a\cos\theta}{a_1 n_2}[Lm_1 - 1] = \frac{e}{h}\frac{2\pi}{ac}\frac{[Lm_1 - 1]}{N}$$

so

$$n_{\mathrm{v}y} = \frac{[Lm_1 - 1]}{t} \qquad \text{or} \qquad \sigma_{\mathrm{V}y} = \frac{e}{hac} n_{\mathrm{v}y} \tag{97}$$

and since

$$m_1 = n_2\tilde{\sigma}_{xy} + n_1\tilde{\sigma}_{yz}$$

with $\tilde{\sigma}$ in convenient units, one gets the final formula

$$1 = t\tilde{\sigma}_{\mathrm{V}y} + Ln_2\tilde{\sigma}_{xy} + Ln_1\tilde{\sigma}_{yz}. \tag{98}$$

3.4. Diophantine equation and boundary conditions on the Brillouin zone

We have shown that in the present case adiabatic transport along the y direction is connected with two Hall conductances, we have not yet proved that it is an integer.

To do so, we follow a reasoning close to what has been presented above, where the magnetic field is perpendicular to the plane of the electrons [18]. We may write in 3D, using the translation properties of the basis functions in the Brillouin zone,

$$\Psi^{q_x+\frac{2\pi}{a},q_y,q_z} = \mathrm{e}^{\mathrm{i}\zeta(q_x,q_y,q_z)}\Psi^{\vec{q}} \qquad \Psi^{q_x,q_y+\frac{2\pi}{tb},q_z} = \Psi^{\vec{q}} \qquad \Psi^{q_x,q_y,q_z+\frac{2\pi}{c}} = \mathrm{e}^{\mathrm{i}\eta(q_x,q_y,q_z)}\Psi^{\vec{q}} \tag{99}$$

with its edges identified as usual, since two nodes of the Brillouin zone correspond to equivalent states, having the same energies and the same eigenvalues under the translation operators. Therefore,

$$\begin{aligned}
&\zeta\left(q_x, q_y + \frac{2\pi}{tb}, q_z\right) = \zeta(q_x, q_y, q_z)\\
&\eta\left(q_x, q_y + \frac{2\pi}{tb}, q_z\right) = \eta(q_x, q_y, q_z)\\
&\zeta\left(q_x, q_y, q_z + \frac{2\pi}{c}\right) + \eta(\vec{q}) = \zeta(\vec{q}) + \eta\left(q_x + \frac{2\pi}{a}, q_y, q_z\right).
\end{aligned} \tag{100}$$

We may choose the phases as follows:

$$\zeta(\vec{q}) = \sigma_1 tbq_y + \zeta_1(q_x, q_z) \qquad \eta(\vec{q}) = \sigma_2 tbq_y + \eta_1(q_x, q_z) \tag{101}$$

with

$$\zeta_1\left(q_x, q_z + \frac{2\pi}{c}\right) + \eta_1(q_x, q_z) = \zeta_1(q_x, q_z) + \eta_1\left(q_x + \frac{2\pi}{a}, q_z\right)$$

remembering that

$$S_b\Psi^{\vec{q}} = \mathrm{e}^{\mathrm{i}m'q_y(tb)}\Psi^{q_x+\frac{2\pi}{ta}Ln_1,q_y,q_z+\frac{2\pi}{tc}Ln_2}.$$

$S_b\Psi^{\vec{q}}$ and $\Psi^{\vec{q}}$ have the same energy, but not the same eigenvalue under the magnetic translation operators because of the commutation properties of the operators S_a, S_{tb}, S_c. In this expression, m' is an integer and we again follow the reasoning by Weinreich [35]. For these two equations to be compatible, one must have for each Landau level (or band)

$$1 = Ln_2\sigma_1 + Ln_1\sigma_2 + tm' \qquad L \text{ integer} \tag{102}$$

and

$$\zeta_1(q_x, q_z) = \eta_1(q_x, q_z) = 0.$$

We showed that adiabatic charge transport is quantized, and note that the conditions on the edges of the Brillouin zone impose $m_3 = 0$.

Our results coincide with those previously obtained by Montambaux and Kohmoto [27] who started from Halperin's [26] results for the 3D conductance using a particular geometry and in the tight binding approximation, and also with those of Kohmoto *et al* [28], who calculated a Diophantine equation for the quantum Hall effect in 3D using Streda's method.

Our approach has the advantage of calculating the matrix element without approximation and deducing from it the transport properties and the Diophantine equation. It also allows the rigorous numerical calculation of the energy spectra and of the conductances associated with the gaps.

3.5. Other transport coefficients

Tesanovic *et al* (TAH) [16] have shown that adiabatic charge transport can be calculated using an expression which takes into account the derivative in γ_x and the derivative in γ_y, where γ_x and γ_y are phases added to the potential, in a way similar to what we presented for the y direction. This method allows, on also adding a phase in z, the definition of the two other relevant quantities, one with phases in y and z, another with phases in x and z. Adding a phase in x is equivalent to the following change:

$$q_y \to q_y + \gamma_x \frac{L}{tb\tilde{n}_1}$$

and adding a phase in z is equivalent to

$$q_y \to q_y + \gamma_z \frac{1}{tb\tilde{n}_1}.$$

Then,

$$\frac{\partial}{\partial\gamma_x} = \frac{L}{tbn_1}\frac{\partial}{\partial q_y} \qquad \text{and} \qquad \frac{\partial}{\partial\gamma_z} = \frac{1}{tbn_1}\frac{\partial}{\partial q_y}.$$

This means that, among the three quantities that we can calculate using the TAH method, one depending on γ_x and γ_z will be identically zero, since it has only derivatives with respect to q_y; the remaining two will be proportional to each other, since the derivatives are. Therefore,

$$\sigma_{\mathrm{V}xy} = L\sigma_{\mathrm{V}zy}. \tag{103}$$

4. Concluding remarks

The appropriate basis functions, the matrix element and the topologically invariant transport coefficients for the 3D electron gas in a strong tilted magnetic field and a general 3D periodic potential have been calculated without any approximation. This original result is a very powerful tool for investigating the transport properties of the three-dimensional electron gas.

Since high resolution measurements of the longitudinal and Hall resistances for a 2D electron gas in a weak superlattice potential [35] have provided evidence for the existence of a fractal structure of the Hofstadter type in the energy spectrum, this is now a topic of particular interest.

Recently, various authors [36–39] have studied and tried to label the gaps of such energy diagrams for the 3D electron gas by means of calculations based on tight binding models.

Our work allows not only the description but also the rigorous prediction of such gaps. Numerical studies will be published elsewhere.

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Appendix A. Calculation of the 3D Hamiltonian matrix element

We present the calculation of the matrix element of the Hamiltonian

$$H = \frac{p_x^2 + (p_y^2 + eBx\cos\theta - eBz\sin\theta)^2 + p_z^2}{2m} + V(x, y, z) = H_0 + V(x, y, z) \qquad (65)$$

with

$$V(x, y, z) = V_x \cos\left(\frac{2\pi}{a}x\right) + V_y \cos\left(\frac{2\pi}{b}y\right) + V_z \cos\left(\frac{2\pi}{c}z\right) \qquad (66)$$

with the complete basis defined above. For simplicity, let M_{01} and M_{01} be the two terms of the matrix element of H_0, M_1 and M_2, M_3 and M_4, M_5 and M_6 the matrix elements of respectively the x, y and z terms of the periodic potential.

A.1. Periodic potential: term in x

M_1 is the term with $\exp\left(\mathrm{i}\frac{2\pi}{a}x\right)$:

$$\begin{aligned} M_1 = \frac{Ln_2}{(2\pi)^3 a\cos\theta} &\int \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\, \exp(-\mathrm{i}(q'_Z + k'G_3)(-x\sin\alpha + z\cos\alpha)) \\ &\times \sum_{\mu'} \exp\left(\mathrm{i}\mu' \frac{a\cos\theta}{Ln_2}\left(q'_X + \frac{2\pi n_2}{a\cos\theta}j'\right)\right) \exp\left(-\mathrm{i}y\left(q'_Y + \frac{2\pi}{tb}\mu'\right)\right) \\ &\times f_{n'}\left(\frac{x\cos\theta - z\sin\theta + (q'_Y + 2\pi\mu'/tb)\ell^2}{\ell}\right) \exp\left(\mathrm{i}\frac{2\pi}{a}x\right) \\ &\times \exp(\mathrm{i}(q_Z + kG_3)(-x\sin\alpha + z\cos\alpha)) \sum_{\mu} \exp\left(-\mathrm{i}\mu \frac{a\cos\theta}{Ln_2}\left(q_X + \frac{2\pi n_2}{a\cos\theta}j\right)\right) \\ &\times \exp\left(\mathrm{i}y\left(q_Y + \frac{2\pi}{tb}\mu\right)\right) f_n\left(\frac{x\cos\theta - z\sin\theta + (q_Y + 2\pi\mu/tb)\ell^2}{\ell}\right). \end{aligned} \qquad (A.1)$$

Calculating the integral over y,

$$\begin{aligned} M_1 = \frac{Ln_2\delta(q'_Y - q_Y)}{(2\pi)^2 a\cos\theta} &\int \mathrm{d}x\,\mathrm{d}z\, \exp(-\mathrm{i}(q'_Z + k'G_3)(-x\sin\alpha + z\cos\alpha)) \\ &\times \sum_{\mu} \exp\left(\mathrm{i}\mu \frac{a\cos\theta}{Ln_2}\left(q'_X + \frac{2\pi n_2}{a\cos\theta}j'\right)\right) \\ &\times f_{n'}\left(\frac{x\cos\theta - z\sin\theta + (q_Y + 2\pi\mu/tb)\ell^2}{\ell}\right) \exp\left(\mathrm{i}\frac{2\pi}{a}x\right) \\ &\times \exp(\mathrm{i}(q_Z + kG_3)(-x\sin\alpha + z\cos\alpha)) \\ &\times \exp\left(-\mathrm{i}\mu \frac{a\cos\theta}{Ln_2}\left(q_X + \frac{2\pi n_2}{a\cos\theta}j\right)\right) \\ &\times f_n\left(\frac{x\cos\theta - z\sin\theta + (q_Y + 2\pi\mu/tb)\ell^2}{\ell}\right). \end{aligned} \qquad (A.2)$$

With the changes

$$\begin{aligned} X &= x\cos\theta - z\sin\theta \\ Z &= -x\sin\alpha + z\cos\alpha \\ x &= \frac{1}{\cos(\theta+\alpha)}(X\cos\alpha + Z\sin\theta) \\ z &= \frac{1}{\cos(\theta+\alpha)}(X\sin\alpha + Z\cos\theta) \\ \mathrm{d}x\,\mathrm{d}z &= \frac{1}{\cos(\theta+\alpha)}\,\mathrm{d}X\,\mathrm{d}Z \end{aligned} \tag{A.3}$$

we get

$$\begin{aligned} M_1 = {}& \frac{Ln_2\delta(q'_Y - q_Y)}{(2\pi)^2 a\cos\theta\cos(\theta+\alpha)} \int \mathrm{d}X\,\mathrm{d}Z\ \exp(-\mathrm{i}(q'_Z + k'G_3)Z) \\ & \times \sum_\mu \exp\left(\mathrm{i}\mu\frac{a\cos\theta}{Ln_2}\left(q'_X + \frac{2\pi n_2}{a\cos\theta}j'\right)\right) f_{n'}\left(\frac{X + (q_Y + 2\pi\mu/tb)\ell^2}{\ell}\right) \\ & \times \exp\left(\mathrm{i}\frac{2\pi}{a}\frac{X\cos\alpha + Z\sin\theta}{\cos(\theta+\alpha)}\right)\exp(\mathrm{i}(q_Z + kG_3)Z) \\ & \times \exp\left(-\mathrm{i}\mu\frac{a\cos\theta}{Ln_2}\left(q_X + \frac{2\pi n_2}{a\cos\theta}j\right)\right) f_n\left(\frac{X + (q_Y + 2\pi\mu/tb)\ell^2}{\ell}\right) \end{aligned} \tag{A.4}$$

and since

$$\begin{aligned} \cos(\theta+\alpha) &= \cos\theta\frac{\tilde{n}_1 a}{a_1} - \frac{\tilde{n}_2 c}{a_1}\sin\theta = \frac{a\cos\theta}{a_1}\left(\tilde{n}_1 - \tilde{n}_2\frac{c\sin\theta}{a\cos\theta}\right) = \frac{a\cos\theta}{a_1}\left(\tilde{n}_1 - \tilde{n}_2\frac{n_1}{n_2}\right) \\ &= \frac{a\cos\theta}{n_2 a_1} \end{aligned} \tag{A.5}$$

and

$$\begin{aligned} &\frac{\cos\alpha}{\cos(\theta+\alpha)} = \frac{\tilde{n}_1 a}{a_1}\frac{n_2 a_1}{a\cos\theta} = \frac{n_2\tilde{n}_1}{\cos\theta} \qquad \frac{\cos\theta}{\cos(\theta+\alpha)} = \frac{n_2 a_1}{a} \\ &\frac{\sin\alpha}{\cos(\theta+\alpha)} = \frac{\tilde{n}_2 c}{a_1}\frac{n_2 a_1}{a\cos\theta} = \frac{c}{a}\frac{n_2\tilde{n}_2}{\cos\theta} = \frac{n_1\tilde{n}_2}{\sin\theta} \qquad \frac{\sin\theta}{\cos(\theta+\alpha)} = \frac{n_2 a_1\sin\theta}{a\cos\theta} = \frac{n_1 a_1}{c} \end{aligned} \tag{A.6}$$

the integral over Z equals

$$\begin{aligned} &\int \mathrm{d}Z\ \exp(-\mathrm{i}(q'_Z + k'G_3)Z)\exp\left(\mathrm{i}\frac{2\pi}{a}\frac{Z\sin\theta}{\cos(\theta+\alpha)}\right)\exp(\mathrm{i}(q_Z + kG_3)Z) \\ &\quad = \int \mathrm{d}Z\ \exp(-\mathrm{i}[(q'_Z - q_Z) + (k'-k)G_3]Z)\exp\left(\mathrm{i}2\pi n_1\frac{a_1}{ac}Z\right) \\ &\quad = \int \mathrm{d}Z\ \exp(-\mathrm{i}[(q'_Z - q_Z) + (k'-k)G_3]Z)\exp(\mathrm{i}n_1 G_3 Z) \\ &\quad = 2\pi\delta[(q'_Z - q_Z) + (k' - k - n_1)G_3] = 2\pi\delta(q'_Z - q_Z)\delta(k' - k - n_1). \end{aligned}$$

The expression now reads

$$\begin{aligned} M_1 = {}& \frac{Ln_2\delta(q'_Y - q_Y)\delta(q'_Z - q_Z)\delta(k'-k-n_1)}{(2\pi)a\cos\theta\cos(\theta+\alpha)} \int \mathrm{d}X \sum_\mu \exp\left(\mathrm{i}\mu\frac{a\cos\theta}{Ln_2}\left(q'_X + \frac{2\pi n_2}{a\cos\theta}j'\right)\right) \\ & \times f_{n'}\left(\frac{X + (q_Y + 2\pi\mu/tb)\ell^2}{\ell}\right)\exp\left(\mathrm{i}\frac{2\pi}{a}\frac{X\cos\alpha}{\cos(\theta+\alpha)}\right) \\ & \times \exp\left(-\mathrm{i}\mu\frac{a\cos\theta}{Ln_2}\left(q_X + \frac{2\pi n_2}{a\cos\theta}j\right)\right) f_n\left(\frac{X + (q_Y + 2\pi\mu/tb)\ell^2}{\ell}\right). \end{aligned} \tag{A.7}$$

With the change of variable

$$\tilde{X} = X + (q_Y + 2\pi\mu/tb)\ell^2 \tag{A.8}$$

we get

$$M_1 = \frac{Ln_2\delta(q'_Y - q_Y)\delta(q'_Z - q_Z)\delta(k' - k - n_1)}{(2\pi)a\cos\theta\cos(\theta+\alpha)}$$
$$\times \int \mathrm{d}\tilde{X} \sum_{\mu} \exp\left(\mathrm{i}\mu\frac{a\cos\theta}{Ln_2}\left[(q'_X - q_X) + \frac{2\pi n_2}{a\cos\theta}(j - j')\right]\right)$$
$$\times f_{n'}\left(\frac{\tilde{X}}{\ell}\right)\exp\left(\mathrm{i}\frac{2\pi}{a}\frac{\cos\alpha}{\cos(\theta+\alpha)}(\tilde{X} - (q_Y + 2\pi\mu/tb)\ell^2)\right) f_n\left(\frac{\tilde{X}}{\ell}\right).$$

Rewriting the second exponential:

$$\exp\left(\mathrm{i}\frac{2\pi}{a}\frac{\cos\alpha}{\cos(\theta+\alpha)}(\tilde{X} - (q_Y + 2\pi\mu/tb)\ell^2)\right)$$
$$= \exp\left(\mathrm{i}\frac{2\pi}{a}\frac{n_2\tilde{n}_1}{\cos\theta}\tilde{X}\right)\exp\left(-\mathrm{i}\frac{2\pi}{a}\frac{n_2\tilde{n}_1}{\cos\theta}\ell^2 q_Y\right)\exp\left(\mathrm{i}\frac{2\pi}{a}\frac{n_2\tilde{n}_1}{\cos\theta}\frac{2\pi\ell^2}{tb}\mu\right)$$

and using the rationality properties of the magnetic field (32), this expression becomes

$$\exp\left(\mathrm{i}\frac{2\pi}{a}\frac{\cos\alpha}{\cos(\theta+\alpha)}(\tilde{X} - (q_Y + 2\pi\mu/tb)\ell^2)\right)$$
$$= \exp\left(\mathrm{i}\frac{2\pi}{a}\frac{n_2\tilde{n}_1}{\cos\theta}\tilde{X}\right)\exp\left(-\mathrm{i}\tilde{n}_1\frac{tb}{L}q_Y\right)\exp\left(-\mathrm{i}2\pi\frac{\tilde{n}_1}{L}\mu\right).$$

Therefore,

$$M_1 = \frac{Ln_2\delta(q'_Y - q_Y)\delta(q'_Z - q_Z)\delta(k' - k - n_1)}{(2\pi)a\cos\theta\cos(\theta+\alpha)}\exp\left(-\mathrm{i}\tilde{n}_1\frac{tb}{L}q_Y\right)$$
$$\times \sum_{\mu}\exp\left(\mathrm{i}\mu\frac{a\cos\theta}{Ln_2}\left[(q'_X - q_X) + \frac{2\pi n_2}{a\cos\theta}(j - j' - \tilde{n}_1)\right]\right)$$
$$\times \int \mathrm{d}\tilde{X}\, f_{n'}\left(\frac{\tilde{X}}{\ell}\right)\exp\left(\mathrm{i}\frac{2\pi}{a}\frac{n_2\tilde{n}_1}{\cos\theta}\tilde{X}\right) f_n\left(\frac{\tilde{X}}{\ell}\right)$$

and since

$$\sum_{\mu}\exp\left(\mathrm{i}\mu\frac{a\cos\theta}{Ln_2}\left[(q'_X - q_X) + \frac{2\pi n_2}{a\cos\theta}(j' - j - \tilde{n}_1)\right]\right)$$
$$= \frac{2\pi Ln_2}{a\cos\theta}\sum_{\nu}\delta\left((q_X - q'_X) + \frac{2\pi n_2}{a\cos\theta}(j - j' - \tilde{n}_1 + L\nu)\right)$$

this equals

$$\delta(q_X - q'_X)\delta(j - j' - \tilde{n}_1) \qquad (\mathrm{mod}\ L).$$

We finally get

$$= \frac{\delta(q'_X - q_X)\delta(q'_Y - q_Y)\delta(q'_Z - q_Z)}{\cos(\theta+\alpha)}\delta(k' - k - n_1)\delta(j' - j - \tilde{n}_1)\exp\left(-\mathrm{i}\tilde{n}_1\frac{tb}{L}q_Y\right)$$
$$\times \int \mathrm{d}\tilde{X}\, f_{n'}\left(\frac{\tilde{X}}{\ell}\right)\exp\left(\mathrm{i}\frac{2\pi}{a}\frac{n_2\tilde{n}_1}{\cos\theta}\tilde{X}\right) f_n\left(\frac{\tilde{X}}{\ell}\right)$$

and

$$M_1 = \delta(q_x' - q_x)\delta(q_y' - q_y)\delta(q_z' - q_z)\delta(k' - k - n_1)\delta(j' - j - \tilde{n}_1)\exp\left(-\mathrm{i}\tilde{n}_1\frac{tb}{L}q_Y\right)$$
$$\times \int \mathrm{d}\tilde{X}\, f_{n'}\left(\frac{\tilde{X}}{\ell}\right)\exp\left(\mathrm{i}\frac{2\pi}{a}\frac{n_2\tilde{n}_1}{\cos\theta}\tilde{X}\right)f_n\left(\frac{\tilde{X}}{\ell}\right).$$

It is easy to see that the second term is

$$M_2 = \delta(q_x' - q_x)\delta(q_y' - q_y)\delta(q_z' - q_z)\delta(k' - k + n_1)\delta(j' - j + \tilde{n}_1)\exp\left(\mathrm{i}\tilde{n}_1\frac{tb}{L}q_Y\right)$$
$$\times \int \mathrm{d}\tilde{X}\, f_{n'}\left(\frac{\tilde{X}}{\ell}\right)\exp\left(-\mathrm{i}\frac{2\pi}{a}\frac{n_2\tilde{n}_1}{\cos\theta}\tilde{X}\right)f_n\left(\frac{\tilde{X}}{\ell}\right)$$

and the sum is

$$M_1 + M_2 = \delta(q_x' - q_x)\delta(q_y' - q_y)\delta(q_z' - q_z)\left\{\delta(k' - k + n_1)\delta(j' - j + \tilde{n}_1)\exp\left(\mathrm{i}\tilde{n}_1\frac{tb}{L}q_Y\right)\right.$$
$$\times \int \mathrm{d}\tilde{X}\, \phi_{n'}\left(\frac{\tilde{X}}{\ell}\right)\exp\left(-\mathrm{i}\frac{2\pi}{a}\frac{n_2\tilde{n}_1}{\cos\theta}\tilde{X}\right)f_n\left(\frac{\tilde{X}}{\ell}\right)$$
$$+\,\delta(k' - k - n_1)\delta(j' - j - \tilde{n}_1)\exp\left(-\mathrm{i}\tilde{n}_1\frac{tb}{L}q_Y\right)$$
$$\left.\times \int \mathrm{d}\tilde{X}\, \phi_{n'}\left(\frac{\tilde{X}}{\ell}\right)\exp\left(\mathrm{i}\frac{2\pi}{a}\frac{n_2\tilde{n}_1}{\cos\theta}\tilde{X}\right)f_n\left(\frac{\tilde{X}}{\ell}\right)\right\}\frac{V_x}{2}. \qquad \text{(A.9)}$$

A.2. Periodic potential: term in y

For the y term of the potential we calculate

$$M_3 = \frac{Ln_2}{(2\pi)^3 a\cos\theta}\int \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\ \exp(-\mathrm{i}(q_Z' + k'G_3)(-x\sin\alpha + z\cos\alpha))$$
$$\times \sum_{\mu'}\exp\left(\mathrm{i}\mu'\frac{a\cos\theta}{Ln_2}\left(q_X' + \frac{2\pi n_2}{a\cos\theta}j'\right)\right)\exp\left(-\mathrm{i}y\left(q_Y' + \frac{2\pi}{tb}\mu'\right)\right)$$
$$\times\ f_{n'}\left(\frac{x\cos\theta - z\sin\theta + (q_Y' + 2\pi\mu'/tb)\ell^2}{\ell}\right)\exp\left(\mathrm{i}\frac{2\pi}{b}y\right)$$
$$\times \exp(\mathrm{i}(q_Z + kG_3)(-x\sin\alpha + z\cos\alpha))\sum_{\mu}\exp\left(-\mathrm{i}\mu\frac{a\cos\theta}{Ln_2}\left(q_X + \frac{2\pi n_2}{a\cos\theta}j\right)\right)$$
$$\times\ \exp\left(\mathrm{i}y\left(q_Y + \frac{2\pi}{tb}\mu\right)\right)f_n\left(\frac{x\cos\theta - z\sin\theta + (q_Y + 2\pi\mu/tb)\ell^2}{\ell}\right).$$

The integral over y is directly calculated as

$$\int \mathrm{d}y\ \exp\left(-\mathrm{i}y\left[(q_Y' - q_Y) + \frac{2\pi}{tb}(\mu' - \mu - t)\right]\right) = 2\pi\delta(q_Y' - q_Y)\delta(\mu' - \mu - t)$$

and therefore the matrix element is

$$M_3 = \frac{Ln_2}{(2\pi)^2 a\cos\theta}\int \mathrm{d}x\,\mathrm{d}z\ \exp(-\mathrm{i}(q_Z' + k'G_3)(-x\sin\alpha + z\cos\alpha))$$
$$\times \sum_{\mu}\exp\left(\mathrm{i}(\mu + t)\frac{a\cos\theta}{Ln_2}\left(q_X' + \frac{2\pi n_2}{a\cos\theta}j'\right)\right)$$

$$\times\ f_{n'}\left(\frac{x\cos\theta - z\sin\theta + (q_Y + 2\pi(\mu+t)/tb)\ell^2}{\ell}\right)$$
$$\times\ \exp(\mathrm{i}(q_Z + kG_3)(-x\sin\alpha + z\cos\alpha))\exp\left(-\mathrm{i}\mu\frac{a\cos\theta}{Ln_2}\left(q_X + \frac{2\pi n_2}{a\cos\theta}j\right)\right)$$
$$\times\ f_n\left(\frac{x\cos\theta - z\sin\theta + (q_Y + 2\pi\mu/tb)\ell^2}{\ell}\right).$$

The very same change of coordinates (A.3) as in the previous paragraph, yields

$$M_3 = \frac{Ln_2\delta(q'_Y - q_Y)}{(2\pi)^2 a\cos\theta\cos(\theta+\alpha)}\exp\left(\mathrm{i}t\frac{a\cos\theta}{Ln_2}\left(q'_X + \frac{2\pi n_2}{a\cos\theta}j'\right)\right)$$
$$\times\int \mathrm{d}X\,\mathrm{d}Z\ \exp(-\mathrm{i}(q'_Z + k'G_3)Z)\sum_\mu \exp\left(\mathrm{i}\mu\frac{a\cos\theta}{Ln_2}\left(q'_X + \frac{2\pi n_2}{a\cos\theta}j'\right)\right)$$
$$\times\ f_{n'}\left(\frac{X + (q_Y + 2\pi\mu/tb)\ell^2 + 2\pi\ell^2/b}{\ell}\right)\exp(\mathrm{i}(q_Z + kG_3)Z)$$
$$\times\ \exp\left(-\mathrm{i}\mu\frac{a\cos\theta}{Ln_2}\left(q_X + \frac{2\pi n_2}{a\cos\theta}j\right)\right)f_n\left(\frac{X + (q_Y + 2\pi\mu/tb)\ell^2}{\ell}\right)$$

with the second change (A.8)

$$\tilde{X} = X + \left(q_Y + \frac{2\pi\mu}{tb}\right)\ell^2$$

$$M_3 = \frac{Ln_2\delta(q'_Y - q_Y)}{(2\pi)^2 a\cos\theta\cos(\theta+\alpha)}\exp\left(\mathrm{i}t\frac{a\cos\theta}{Ln_2}\left(q'_X + \frac{2\pi n_2}{a\cos\theta}j'\right)\right)$$
$$\times\int \mathrm{d}\tilde{X}\,\mathrm{d}Z\ \exp(-\mathrm{i}[(q'_Z - q_Z) + (k'-k)G_3]Z)$$
$$\times\sum_\mu \exp\left(\mathrm{i}\mu\frac{a\cos\theta}{Ln_2}\left[(q'_X - q_X) + \frac{2\pi n_2}{a\cos\theta}(j'-j)\right]\right)$$
$$\times\ f_{n'}\left(\frac{\tilde{X} + 2\pi\ell^2/b}{\ell}\right)f_n\left(\frac{\tilde{X}}{\ell}\right)$$

which equals

$$M_3 = \frac{Ln_2\delta(q'_Y - q_Y)\delta(q'_Z - q_Z)}{(2\pi)^2 a\cos\theta\cos(\theta+\alpha)}\delta_{k'k}\exp\left(\mathrm{i}t\frac{a\cos\theta}{Ln_2}\left(q'_X + \frac{2\pi n_2}{a\cos\theta}j'\right)\right)$$
$$\times\int \mathrm{d}\tilde{X}\ f_{n'}\left(\frac{\tilde{X} + 2\pi\ell^2/b}{\ell}\right)f_n\left(\frac{\tilde{X}}{\ell}\right)$$
$$\times\sum_\mu \exp\left(\mathrm{i}\mu\frac{a\cos\theta}{Ln_2}\left[(q'_X - q_X) + \frac{2\pi n_2}{a\cos\theta}(j'-j)\right]\right),$$

that is,

$$M_3 = \frac{\delta(q'_X - q_X)\delta(q'_Y - q_Y)\delta(q'_Z - q_Z)}{\cos(\theta+\alpha)}\delta_{j'j}\delta_{k'k}\exp\left(\mathrm{i}t\frac{a\cos\theta}{Ln_2}\left(q_X + \frac{2\pi n_2}{a\cos\theta}j\right)\right)$$
$$\times\int \mathrm{d}\tilde{X}\ f_{n'}\left(\frac{\tilde{X} + 2\pi\ell^2/b}{\ell}\right)f_n\left(\frac{\tilde{X}}{\ell}\right)$$

$$M_3 = \delta(\vec{q}' - \vec{q})\delta_{j'j}\delta_{k'k} \exp\left(\mathrm{i}t\frac{a\cos\theta}{Ln_2}\left(\frac{\{q_x\cos\alpha + q_z\sin\alpha\}}{\cos(\theta+\alpha)} + \frac{2\pi n_2}{a\cos\theta}j\right)\right)$$
$$\times \int \mathrm{d}\tilde{X}\, f_{n'}\left(\frac{\tilde{X} + 2\pi\ell^2/b}{\ell}\right) f_n\left(\frac{\tilde{X}}{\ell}\right).$$

The other term is obviously

$$M_4 = \delta(\vec{q}' - \vec{q})\delta_{j'j}\delta_{k'k} \exp\left(-\mathrm{i}t\frac{a\cos\theta}{Ln_2}\left(\frac{\{q_x\cos\alpha + q_z\sin\alpha\}}{\cos(\theta+\alpha)} + \frac{2\pi n_2}{a\cos\theta}j\right)\right)$$
$$\times \int \mathrm{d}\tilde{X}\, f_{n'}\left(\frac{\tilde{X} - 2\pi\ell^2/b}{\ell}\right) f_n\left(\frac{\tilde{X}}{\ell}\right)$$

yielding (A.10)

$$M_3 + M_4 = \frac{V_y}{2}\delta(\vec{q}' - \vec{q})\delta_{j'j}\delta_{k'k}\Bigg\{\exp\left(\mathrm{i}t\frac{a\cos\theta}{Ln_2}\left(\frac{\{q_x\cos\alpha + q_z\sin\alpha\}}{\cos(\theta+\alpha)} + \frac{2\pi n_2}{a\cos\theta}j\right)\right)$$
$$\times \int \mathrm{d}\tilde{X}\, f_{n'}\left(\frac{\tilde{X} + 2\pi\ell^2/b}{\ell}\right) f_n\left(\frac{\tilde{X}}{\ell}\right)$$
$$+ \exp\left(-\mathrm{i}t\frac{a\cos\theta}{Ln_2}\left(\frac{\{q_x\cos\alpha + q_z\sin\alpha\}}{\cos(\theta+\alpha)} + \frac{2\pi n_2}{a\cos\theta}j\right)\right)$$
$$\times \int \mathrm{d}\tilde{X}\, f_{n'}\left(\frac{\tilde{X} - 2\pi\ell^2/b}{\ell}\right) f_n\left(\frac{\tilde{X}}{\ell}\right)\Bigg\}.$$

A.3. Periodic potential: term in z

We start with the term in $\exp\left(\mathrm{i}\frac{2\pi}{c}z\right)$:

$$M_5 = \frac{Ln_2}{(2\pi)^3 a\cos\theta}\int \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\, \exp(-\mathrm{i}(q'_Z + k'G_3)(-x\sin\alpha + z\cos\alpha))$$
$$\times \sum_{\mu'}\exp\left(\mathrm{i}\mu'\frac{a\cos\theta}{Ln_2}\left(q'_X + \frac{2\pi n_2}{a\cos\theta}j'\right)\right)\exp\left(-\mathrm{i}y\left(q'_Y + \frac{2\pi}{tb}\mu'\right)\right)$$
$$\times f_{n'}\left(\frac{x\cos\theta - z\sin\theta + (q'_Y + 2\pi\mu'/tb)\ell^2}{\ell}\right)$$
$$\times \exp\left(\mathrm{i}\frac{2\pi}{c}z\right)\exp(\mathrm{i}(q_Z + kG_3)(-x\sin\alpha + z\cos\alpha))$$
$$\times \sum_{\mu}\exp\left(-\mathrm{i}\mu\frac{a\cos\theta}{Ln_2}\left(q_X + \frac{2\pi n_2}{a\cos\theta}j\right)\right)\exp\left(\mathrm{i}y\left(q_Y + \frac{2\pi}{tb}\mu\right)\right)$$
$$\times f_n\left(\frac{x\cos\theta - z\sin\theta + (q_Y + 2\pi\mu/tb)\ell^2}{\ell}\right).$$

With the very same steps as for the previous terms, starting with the integral over y,

$$M_5 = \frac{Ln_2\delta(q'_Y - q_Y)}{(2\pi)^2 a\cos\theta}\int \mathrm{d}x\,\mathrm{d}z\, \exp(-\mathrm{i}(q'_Z + k'G_3)(-x\sin\alpha + z\cos\alpha))$$
$$\times \sum_{\mu}\exp\left(\mathrm{i}\mu\frac{a\cos\theta}{Ln_2}\left(q'_X + \frac{2\pi n_2}{a\cos\theta}j'\right)\right)$$
$$\times f'_n\left(\frac{x\cos\theta - z\sin\theta + (q_Y + 2\pi\mu/tb)\ell^2}{\ell}\right)\exp\left(\mathrm{i}\frac{2\pi}{c}z\right)$$

$$\times\ \exp(\mathrm{i}(q_Z + kG_3)(-x\sin\alpha + z\cos\alpha))\exp\left(-\mathrm{i}\mu\frac{a\cos\theta}{Ln_2}\left(q_X + \frac{2\pi n_2}{a\cos\theta}j\right)\right)$$
$$\times\ f_n\left(\frac{x\cos\theta - z\sin\theta + (q_Y + 2\pi\mu/tb)\ell^2}{\ell}\right).$$

We effect the first change of variables (A.3) $(x, z) \to (X, Z)$:

$$M_5 = \frac{Ln_2\delta(q'_Y - q_Y)}{(2\pi)^2 a\cos\theta\cos(\theta+\alpha)}\int \mathrm{d}X\,\mathrm{d}Z\ \exp(-\mathrm{i}[(q'_Z - q_Z) + (k'-k)G_3]Z)$$
$$\times\ \sum_\mu \exp\left(\mathrm{i}\mu\frac{a\cos\theta}{Ln_2}\left[(q'_X - q_X) + \frac{2\pi n_2}{a\cos\theta}(j'-j)\right]\right)$$
$$\times\ f_{n'}\left(\frac{X + (q_Y + 2\pi\mu/tb)\ell^2}{\ell}\right)\exp\left(\mathrm{i}\frac{2\pi}{c}\frac{(X\sin\alpha + Z\cos\theta)}{\cos(\theta+\alpha)}\right)$$
$$\times\ f_n\left(\frac{X + (q_Y + 2\pi\mu/tb)\ell^2}{\ell}\right).$$

Recalling (A.5) and (A.6), we get

$$\exp\left(\mathrm{i}\frac{2\pi}{c}\frac{(X\sin\alpha + Z\cos\theta)}{\cos(\theta+\alpha)}\right) = \exp\left(\mathrm{i}\frac{2\pi}{c}\frac{cn_2\tilde{n}_2}{a\cos\theta}X\right)\exp\left(\mathrm{i}\frac{2\pi}{c}\frac{n_2a_1}{a}Z\right)$$
$$= \exp\left(\mathrm{i}\frac{2\pi}{a}\frac{n_2\tilde{n}_2}{\cos\theta}X\right)\exp(\mathrm{i}G_3n_2Z),$$

that is,

$$M_5 = \frac{Ln_2\delta(q'_Y - q_Y)}{(2\pi)^2 a\cos\theta\cos(\theta+\alpha)}\int \mathrm{d}X\,\mathrm{d}Z\ \exp(-\mathrm{i}[(q'_Z - q_Z) + (k'-k-n_2)G_3]Z)$$
$$\times\ \sum_\mu \exp\left(\mathrm{i}\mu\frac{a\cos\theta}{Ln_2}\left[(q'_X - q_X) + \frac{2\pi n_2}{a\cos\theta}(j'-j)\right]\right)$$
$$\times\ f_{n'}\left(\frac{X + (q_Y + 2\pi\mu/tb)\ell^2}{\ell}\right)\exp\left(\mathrm{i}\frac{2\pi}{a}\frac{n_2\tilde{n}_2}{\cos\theta}X\right)f_n\left(\frac{X + (q_Y + 2\pi\mu/tb)\ell^2}{\ell}\right).$$

We can therefore also calculate the integral over Z:

$$= \frac{Ln_2\delta(q'_Y - q_Y)\delta(q'_Z - q_Z)}{(2\pi)a\cos\theta\cos(\theta+\alpha)}\delta(k'-k-n_2)$$
$$\times\ \int \mathrm{d}X \sum_\mu \exp\left(\mathrm{i}\mu\frac{a\cos\theta}{Ln_2}\left[(q'_X - q_X) + \frac{2\pi n_2}{a\cos\theta}(j'-j)\right]\right)$$
$$\times\ f_{n'}\left(\frac{X + (q_Y + 2\pi\mu/tb)\ell^2}{\ell}\right)\exp\left(\mathrm{i}\frac{2\pi}{a}\frac{n_2\tilde{n}_2}{\cos\theta}X\right)f_n\left(\frac{X + (q_Y + 2\pi\mu/tb)\ell^2}{\ell}\right).$$

With the change (A.8):

$$\tilde{X} = X + (q_Y + 2\pi\mu/tb)\ell^2$$

the integral becomes

$$M_5 = \frac{Ln_2\delta(q'_Y - q_Y)\delta(q'_Z - q_Z)}{(2\pi)a\cos\theta\cos(\theta+\alpha)}\delta(k'-k-n_2)$$
$$\times\ \int \mathrm{d}\tilde{X} \sum_\mu \exp\left(\mathrm{i}\mu\frac{a\cos\theta}{Ln_2}\left[(q'_X - q_X) + \frac{2\pi n_2}{a\cos\theta}(j'-j)\right]\right)$$
$$\times\ f_{n'}\left(\frac{\tilde{X}}{\ell}\right)\exp\left(\mathrm{i}\frac{2\pi}{a}\frac{n_2\tilde{n}_2}{\cos\theta}(\tilde{X} - (q_Y + 2\pi\mu/tb)\ell^2)\right)f_n\left(\frac{\tilde{X}}{\ell}\right),$$

the second exponential is rewritten as

$$\exp\left(\mathrm{i}\frac{2\pi}{a}\frac{n_2\tilde{n}_2}{\cos\theta}(\tilde{X}-(q_Y+2\pi\mu/tb)\ell^2)\right)$$
$$=\exp\left(\mathrm{i}\frac{2\pi}{a}\frac{n_2\tilde{n}_2}{\cos\theta}\tilde{X}\right)\exp\left(-\mathrm{i}\frac{2\pi\ell^2}{a}\frac{n_2\tilde{n}_2}{\cos\theta}q_Y\right)\exp\left(-\mathrm{i}\frac{2\pi}{a}\frac{n_2\tilde{n}_2}{\cos\theta}\frac{2\pi\mu\ell^2}{tb}\right)$$
$$=\exp\left(\mathrm{i}\frac{2\pi}{a}\frac{n_2\tilde{n}_2}{\cos\theta}\tilde{X}\right)\exp(-\mathrm{i}\tilde{n}_2tbq_Y)\exp\left(-\mathrm{i}\frac{2\pi\tilde{n}_2\mu}{L}\right)$$

and

$$M_5=\frac{Ln_2\delta(q'_Y-q_Y)\delta(q'_Z-q_Z)}{(2\pi)a\cos\theta\cos(\theta+\alpha)}\delta(k'-k-n_2)\int\mathrm{d}\tilde{X}\,\exp(-\mathrm{i}\tilde{n}_2tbq_Y)$$
$$\times\sum_\mu\exp\left(\mathrm{i}\mu\frac{a\cos\theta}{Ln_2}\left[(q'_X-q_X)+\frac{2\pi n_2}{a\cos\theta}(j'-j-\tilde{n}_2)\right]\right)$$
$$\times f_{n'}\left(\frac{\tilde{X}}{\ell}\right)\exp\left(\mathrm{i}\frac{2\pi}{a}\frac{n_2\tilde{n}_2}{\cos\theta}\tilde{X}\right)f_n\left(\frac{\tilde{X}}{\ell}\right).$$

As in the previous case,

$$\sum_\mu\exp\left(\mathrm{i}\mu\frac{a\cos\theta}{Ln_2}\left[(q'_X-q_X)+\frac{2\pi n_2}{a\cos\theta}(j'-j-\tilde{n}_2)\right]\right)$$
$$=\frac{2\pi Ln_2}{a\cos\theta}\sum_\nu\delta\left((q_X-q'_X)+\frac{2\pi n_2}{a\cos\theta}(j-j'-\tilde{n}_2+L\nu)\right)$$
$$=\delta(q_X-q'_X)\delta(j-j'-\tilde{n}_2)\qquad(\mathrm{mod}\,L)$$

which yields

$$M_5=\frac{\delta(q'_X-q_X)\delta(q'_Y-q_Y)\delta(q'_Z-q_Z)}{\cos(\theta+\alpha)}\delta(j'-j-\tilde{n}_2)\delta(k'-k-n_2)\exp(-\mathrm{i}\tilde{n}_2tbq_Y)$$
$$\times\int\mathrm{d}\tilde{X}\,f_{n'}\left(\frac{\tilde{X}}{\ell}\right)\exp\left(\mathrm{i}\frac{2\pi}{a}\frac{n_2\tilde{n}_2}{\cos\theta}\tilde{X}\right)f_n\left(\frac{\tilde{X}}{\ell}\right),$$

that is,

$$=\delta(q'_x-q_x)\delta(q'_y-q_y)\delta(q'_z-q_z)\delta(j'-j-\tilde{n}_2)\delta(k'-k-n_2)\exp(-\mathrm{i}\tilde{n}_2tbq_y)$$
$$\times\int\mathrm{d}\tilde{X}\,f_{n'}\left(\frac{\tilde{X}}{\ell}\right)\exp\left(\mathrm{i}\frac{2\pi}{a}\frac{n_2\tilde{n}_2}{\cos\theta}\tilde{X}\right)f_n\left(\frac{\tilde{X}}{\ell}\right).$$

With the term in $\exp\left(-\mathrm{i}\frac{2\pi}{c}z\right)$

$$M_6=\delta(q'_x-q_x)\delta(q'_y-q_y)\delta(q'_z-q_z)\delta(j'-j+\tilde{n}_2)\delta(k'-k+n_2)\exp(\mathrm{i}\tilde{n}_2tbq_y)$$
$$\times\int\mathrm{d}\tilde{X}\,f_{n'}\left(\frac{\tilde{X}}{\ell}\right)\exp\left(-\mathrm{i}\frac{2\pi}{a}\frac{n_2\tilde{n}_2}{\cos\theta}\tilde{X}\right)f_n\left(\frac{\tilde{X}}{\ell}\right)$$

the sum is

$$M_5+M_6=\delta(q'_x-q_x)\delta(q'_y-q_y)\delta(q'_z-q_z)\frac{V_z}{2}\Bigg\{\delta(j'-j-\tilde{n}_2)\delta(k'-k-n_2)\exp(-\mathrm{i}\tilde{n}_2tbq_y)$$
$$\times\int\mathrm{d}\tilde{X}\,f_{n'}\left(\frac{\tilde{X}}{\ell}\right)\exp\left(\mathrm{i}\frac{2\pi}{a}\frac{n_2\tilde{n}_2}{\cos\theta}\tilde{X}\right)f_n\left(\frac{\tilde{X}}{\ell}\right)$$
$$+\delta(j'-j+\tilde{n}_2)\delta(k'-k+n_2)\exp(\mathrm{i}\tilde{n}_2tbq_y)$$
$$\times\int\mathrm{d}\tilde{X}\,f_{n'}\left(\frac{\tilde{X}}{\ell}\right)\exp\left(-\mathrm{i}\frac{2\pi}{a}\frac{n_2\tilde{n}_2}{\cos\theta}\tilde{X}\right)f_n\left(\frac{\tilde{X}}{\ell}\right)\Bigg\}.\qquad\text{(A.11)}$$

We now have the analytic expressions for the terms in x, y and z of the periodic potential.

A.4. The H_0 matrix element

We calculate

$$M_0 = \frac{Ln_2}{(2\pi)^3 a\cos\theta}\int \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\ \exp(-\mathrm{i}(q'_Z + k'G_3)(-x\sin\alpha + z\cos\alpha))$$
$$\times \sum_{\mu'}\exp\left(\mathrm{i}\mu'\frac{a\cos\theta}{Ln_2}\left(q'_X + \frac{2\pi n_2}{a\cos\theta}j'\right)\right)\exp\left(-\mathrm{i}y\left(q'_Y + \frac{2\pi}{tb}\mu'\right)\right)$$
$$\times f_{n'}\left(\frac{x\cos\theta - z\sin\theta + (q'_Y + 2\pi\mu'/tb)\ell^2}{\ell}\right)$$
$$\times H_0\exp(\mathrm{i}(q_Z + kG_3)(-x\sin\alpha + z\cos\alpha))$$
$$\times \sum_{\mu}\exp\left(-\mathrm{i}\mu\frac{a\cos\theta}{Ln_2}\left(q_X + \frac{2\pi n_2}{a\cos\theta}j\right)\right)\exp\left(\mathrm{i}y\left(q_Y + \frac{2\pi}{tb}\mu\right)\right)$$
$$\times f_n\left(\frac{x\cos\theta - z\sin\theta + (q_Y + 2\pi\mu/tb)\ell^2}{\ell}\right).$$

Note the following property:

$$H_0\exp\left(\mathrm{i}y\left(q_Y + \frac{2\pi}{tb}\mu\right)\right) = \frac{p_x^2 + [(q_Y + \frac{2\pi}{tb}\mu)^2 + eBx\cos\theta - eBz\sin\theta]^2 + p_z^2}{2m}$$
$$\times\ \exp\left(\mathrm{i}y\left(q_Y + \frac{2\pi}{tb}\mu\right)\right)$$

which allows the calculation of the integral over y:

$$M_0 = \frac{Ln_2\delta(q'_Y - q_Y)}{(2\pi)^2 a\cos\theta}\int \mathrm{d}x\,\mathrm{d}z\ \exp(-\mathrm{i}(q'_Z + k'G_3)(-x\sin\alpha + z\cos\alpha))$$
$$\times \sum_{\mu}\exp\left(\mathrm{i}\mu\frac{a\cos\theta}{Ln_2}\left(q'_X + \frac{2\pi n_2}{a\cos\theta}j'\right)\right)$$
$$\times f_{n'}\left(\frac{x\cos\theta - z\sin\theta + (q_Y + 2\pi\mu/tb)\ell^2}{\ell}\right)$$
$$\times \frac{p_x^2 + [(q_Y + \frac{2\pi}{tb}\mu)^2 + eBx\cos\theta - eBz\sin\theta]^2 + p_z^2}{2m}$$
$$\times\ \exp(\mathrm{i}(q_Z + kG_3)(-x\sin\alpha + z\cos\alpha))$$
$$\times\ \exp\left(-\mathrm{i}\mu\frac{a\cos\theta}{Ln_2}\left(q_X + \frac{2\pi n_2}{a\cos\theta}j\right)\right)$$
$$\times f_n\left(\frac{x\cos\theta - z\sin\theta + (q_Y + 2\pi\mu/tb)\ell^2}{\ell}\right).$$

As has been done previously, we go from (x, z) to (X, Z) and therefore also change the impulsion components:

$$X = x\cos\theta - z\sin\theta \qquad p_x = P_X\cos\theta - P_Z\sin\alpha$$
$$Z = -x\sin\alpha + z\cos\alpha \qquad p_z = -P_X\sin\theta + P_Z\cos\alpha$$

and

$$x = \frac{1}{\cos(\theta+\alpha)}(X\cos\alpha + Z\sin\theta) \qquad P_X = \frac{1}{\cos(\theta+\alpha)}(p_x\cos\alpha + p_z\sin\alpha)$$

$$z = \frac{1}{\cos(\theta+\alpha)}(X\sin\alpha + Z\cos\theta) \qquad P_Z = \frac{1}{\cos(\theta+\alpha)}(p_x\sin\theta + p_z\cos\theta),$$

that is,

$$\begin{aligned} p_x^2 + p_z^2 &= (P_X\cos\theta - P_Z\sin\alpha)^2 + (-P_X\sin\theta + P_Z\cos\alpha)^2 \\ &= P_X^2 + P_Z^2 - 2\cos\theta\sin\alpha P_X^2 P_Z^2 - 2\sin\theta\cos\alpha P_X^2 P_Z^2 \\ &= P_X^2 + P_Z^2 - 2\sin(\theta+\alpha) P_X P_Z \end{aligned}$$

which, in the new coordinates, reads

$$\begin{aligned} M_0 = {} & \frac{Ln_2\delta(q'_Y - q_Y)}{(2\pi)^2 a\cos\theta\cos(\theta+\alpha)} \int \mathrm{d}X\,\mathrm{d}Z\, \exp(-\mathrm{i}(q'_Z + k'G_3)Z) \\ & \sum_{\mu'} \exp\left(\mathrm{i}\mu\frac{a\cos\theta}{Ln_2}\left(q'_X + \frac{2\pi n_2}{a\cos\theta}j'\right)\right) f_{n'}\left(\frac{X + (q_Y + 2\pi\mu/tb)\ell^2}{\ell}\right) \\ & \times \frac{P_X^2 + [(q_Y + \frac{2\pi}{tb}\mu)^2 + eBX]^2 + P_Z^2 - 2\sin(\theta+\alpha)P_X P_Z}{2m} \\ & \times \exp(\mathrm{i}(q_Z + kG_3)Z)\exp\left(-\mathrm{i}\mu\frac{a\cos\theta}{Ln_2}\left(q_X + \frac{2\pi n_2}{a\cos\theta}j\right)\right) \\ & \times f_n\left(\frac{X + (q_Y + 2\pi\mu/tb)\ell^2}{\ell}\right) = M_{01} + M_{02}. \end{aligned}$$

We start by calculating the term M_{01} with

$$\frac{P_X^2 + [(q_Y + \frac{2\pi}{tb}\mu)^2 + eBX]^2 + P_Z^2}{2m}$$

using

$$P_Z^2\exp(\mathrm{i}(q_Z + kG_3)Z) = \hbar^2(q_Z + kG_3)^2\exp(\mathrm{i}(q_Z + kG_3)Z)$$

which becomes

$$\begin{aligned} M_{01} = {} & \frac{Ln_2\delta(q'_Y - q_Y)}{(2\pi)^2 a\cos\theta\cos(\theta+\alpha)} \int \mathrm{d}X\,\mathrm{d}Z\, \exp(-\mathrm{i}[(q'_Z - q_Z) + (k'-k)G_3]Z) \\ & \times \sum_{\mu} \exp\left(\mathrm{i}\mu\frac{a\cos\theta}{Ln_2}\left(q'_X + \frac{2\pi n_2}{a\cos\theta}j'\right)\right) f_{n'}\left(\frac{X + (q_Y + 2\pi\mu/tb)\ell^2}{\ell}\right) \\ & \times \frac{P_X^2 + [(q_Y + \frac{2\pi}{tb}\mu)^2 + eBX]^2 + \hbar^2(q'_Z + k'G_3)^2}{2m} \\ & \times \exp\left(-\mathrm{i}\mu\frac{a\cos\theta}{Ln_2}\left(q_X + \frac{2\pi n_2}{a\cos\theta}j\right)\right) f_n\left(\frac{X + (q_Y + 2\pi\mu/tb)\ell^2}{\ell}\right). \end{aligned}$$

Since the f_n are harmonic oscillator eigenfunctions,

$$\begin{aligned} & \frac{P_X^2 + [(q_Y + \frac{2\pi}{tb}\mu)^2 + eBX]^2 + \hbar^2(q'_Z + k'G_3)^2}{2m} f_n\left(\frac{X + (q_Y + 2\pi\mu/tb)\ell^2}{\ell}\right) \\ & \quad = \left[\left(n + \frac{1}{2}\right)\hbar\omega_C + \frac{\hbar^2(q'_Z + k'G_3)^2}{2m}\right] f_n\left(\frac{X + (q_Y + 2\pi\mu/tb)\ell^2}{\ell}\right). \end{aligned}$$

Therefore,

$$M_{01} = \frac{Ln_2\delta(q'_Y - q_Y)}{(2\pi)^2 a\cos\theta\cos(\theta+\alpha)}\left[\left(n+\frac{1}{2}\right)\hbar\omega_C + \frac{\hbar^2(q'_Z + k'G_3)^2}{2m}\right]$$
$$\times \int \mathrm{d}X\,\mathrm{d}Z\,\exp(-\mathrm{i}[(q'_Z - q_Z) + (k'-k)G_3]Z)$$
$$\times \sum_\mu \exp\left(\mathrm{i}\mu\frac{a\cos\theta}{Ln_2}\left[(q'_X - q_X) + \frac{2\pi n_2}{a\cos\theta}(j'-j)\right]\right)$$
$$\times f_{n'}\left(\frac{X + (q_Y + 2\pi\mu/tb)\ell^2}{\ell}\right) f_n\left(\frac{X + (q_Y + 2\pi\mu/tb)\ell^2}{\ell}\right)$$

and after calculating the integral over Z

$$M_{01} = \frac{Ln_2\delta(q'_Y - q_Y)\delta(q'_Z - q_Z)}{(2\pi)a\cos\theta\cos(\theta+\alpha)}\delta_{k'k}\left[\left(n+\frac{1}{2}\right)\hbar\omega_C + \frac{\hbar^2(q_Z + kG_3)^2}{2m}\right]$$
$$\times \int \mathrm{d}X \sum_\mu \exp\left(\mathrm{i}\mu\frac{a\cos\theta}{Ln_2}\left[(q'_X - q_X) + \frac{2\pi n_2}{a\cos\theta}(j'-j)\right]\right)$$
$$\times f_{n'}\left(\frac{X + (q_Y + 2\pi\mu/tb)\ell^2}{\ell}\right) f_n\left(\frac{X + (q_Y + 2\pi\mu/tb)\ell^2}{\ell}\right)$$

the integral over X can be obtained using the orthonormality properties of the oscillator eigenfunction:

$$M_{01} = \frac{Ln_2\delta(q'_Y - q_Y)\delta(q'_Z - q_Z)}{(2\pi)a\cos\theta\cos(\theta+\alpha)}\delta_{k'k}\delta_{n'n}\left[\left(n+\frac{1}{2}\right)\hbar\omega_C + \frac{\hbar^2(q_Z + kG_3)^2}{2m}\right]$$
$$\times \sum_\mu \exp\left(\mathrm{i}\mu\frac{a\cos\theta}{Ln_2}\left[(q'_X - q_X) + \frac{2\pi n_2}{a\cos\theta}(j'-j)\right]\right),$$

that is,

$$M_{01} = \frac{\delta(q'_X - q_X)\delta(q'_Y - q_Y)\delta(q'_Z - q_Z)}{\cos(\theta+\alpha)}\delta_{k'k}\delta_{n'n}\delta_{j'j}\left[\left(n+\frac{1}{2}\right)\hbar\omega_C + \frac{\hbar^2(q_Z + kG_3)^2}{2m}\right]$$

$$M_{01} = \delta(q'_x - q_x)\delta(q'_y - q_y)\delta(q'_z - q_z)\delta_{k'k}\delta_{n'n}\delta_{j'j}\left[(n+\tfrac{1}{2})\hbar\omega_C + \frac{\hbar^2}{2m}\left(\frac{q_x\cos\alpha + q_z\sin\alpha}{\cos(\theta+\alpha)} + kG_3\right)^2\right]. \quad \text{(A.12)}$$

The second term is

$$M_{02} = \frac{Ln_2\delta(q'_Y - q_Y)}{(2\pi)^2 a\cos\theta\cos(\theta+\alpha)}\int \mathrm{d}X\,\mathrm{d}Z\,\exp(-\mathrm{i}(q'_Z + k'G_3)Z)$$
$$\times \sum_\mu \exp\left(\mathrm{i}\mu\frac{a\cos\theta}{Ln_2}\left(q'_X + \frac{2\pi n_2}{a\cos\theta}j'\right)\right)$$
$$\times f_{n'}\left(\frac{X + (q_Y + 2\pi\mu/tb)\ell^2}{\ell}\right)\frac{-\sin(\theta+\alpha)}{m}P_X P_Z \exp(\mathrm{i}(q_Z + kG_3)Z)$$
$$\times \exp\left(-\mathrm{i}\mu\frac{a\cos\theta}{Ln_2}\left(q_X + \frac{2\pi n_2}{a\cos\theta}j\right)\right) f_n\left(\frac{X + (q_Y + 2\pi\mu/tb)\ell^2}{\ell}\right)$$

$$
\begin{aligned}
M_{02} = -\frac{Ln_2\delta(q'_Y - q_Y)}{(2\pi)^2 a\cos\theta\cos(\theta+\alpha)}\frac{\sin(\theta+\alpha)}{m}\hbar(q_Z + kG_3) \\
\times \int \mathrm{d}X\,\mathrm{d}Z\ \exp(-\mathrm{i}[(q'_Z - q_Z) + (k'-k)G_3]Z) \\
\times \sum_{\mu'} \exp\left(\mathrm{i}\mu\frac{a\cos\theta}{Ln_2}\left(q'_X + \frac{2\pi n_2}{a\cos\theta}j'\right)\right) f_{n'}\left(\frac{X + (q_Y + 2\pi\mu/tb)\ell^2}{\ell}\right) \\
\times P_X \exp\left(-\mathrm{i}\mu\frac{a\cos\theta}{Ln_2}\left(q_X + \frac{2\pi n_2}{a\cos\theta}j\right)\right) f_n\left(\frac{X + (q_Y + 2\pi\mu/tb)\ell^2}{\ell}\right),
\end{aligned}
$$

the integral over Z is

$$
\begin{aligned}
M_{02} = -\frac{Ln_2\delta(q'_Y - q_Y)\delta(q'_Z - q_Z)}{(2\pi)a\cos\theta\cos(\theta+\alpha)}\frac{\sin(\theta+\alpha)}{m}\delta_{k'k}\hbar(q_Z + kG_3) \\
\times \int \mathrm{d}X \sum_{\mu} \exp\left(\mathrm{i}\mu\frac{a\cos\theta}{Ln_2}\left[(q'_X - q_X) + \frac{2\pi n_2}{a\cos\theta}(j'-j)\right]\right) \\
\times f_{n'}\left(\frac{X + (q_Y + 2\pi\mu/tb)\ell^2}{\ell}\right) P_X f_n\left(\frac{X + (q_Y + 2\pi\mu/tb)\ell^2}{\ell}\right),
\end{aligned}
$$

that is, with $\tilde{X} = X + (q_Y + 2\pi\mu/tb)\ell^2$,

$$
\begin{aligned}
M_{02} = -\frac{Ln_2\delta(q'_Y - q_Y)\delta(q'_Z - q_Z)}{(2\pi)a\cos\theta\cos(\theta+\alpha)}\frac{\sin(\theta+\alpha)}{m}\delta_{k'k}\hbar(q_Z + kG_3) \\
\times \sum_{\mu} \exp\left(\mathrm{i}\mu\frac{a\cos\theta}{Ln_2}\left[(q'_X - q_X) + \frac{2\pi n_2}{a\cos\theta}(j'-j)\right]\right) \\
\times \int \mathrm{d}\tilde{X}\ f_{n'}\left(\frac{\tilde{X}}{\ell}\right) P_X f_n\left(\frac{\tilde{X}}{\ell}\right)
\end{aligned}
$$

$$
\begin{aligned}
M_{02} = -\frac{\delta(q'_X - q_X)\delta(q'_Y - q_Y)\delta(q'_Z - q_Z)}{\cos(\theta+\alpha)}\frac{\sin(\theta+\alpha)}{m}\hbar(q_Z + kG_3)\delta_{k'k}\delta_{j'j}\int \mathrm{d}\tilde{X}\ f_{n'}\left(\frac{\tilde{X}}{\ell}\right) \\
\times P_X f_n\left(\frac{\tilde{X}}{\ell}\right) \qquad \text{(A.13)}
\end{aligned}
$$

with

$$
\int \mathrm{d}\tilde{X}\ f_{n'}\left(\frac{\tilde{X}}{\ell}\right) P_X f_n\left(\frac{\tilde{X}}{\ell}\right) = -\frac{\mathrm{i}\hbar}{\ell\sqrt{2}}\delta_{n',n-1}\sqrt{n} + \frac{\mathrm{i}\hbar}{\ell\sqrt{2}}\delta_{n',n+1}\sqrt{n+1} \qquad \text{(A.14)}
$$

where the properties of the harmonic oscillator functions have been applied.

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