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Analysis of the spectrum of a particle on a triangular lattice with two magnetic fluxes by algebraic and numerical methods

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Abstract. We consider an electron on a triangular lattice with two magnetic fluxes. Using a C^*-algebra formalism a perturbation theory around rational fluxes is developed. This semiclassical type of analysis leads to the Wilkinson–Rammal formula for the energy eigenvalues. The analytic result is verified numerically with high accuracy up to second order. Crossing of eigenvalues near band edges is shown analytically as well as numerically.

1. Introduction

Magnetic field effects in solids have been of great conceptual, phenomenological and even technological importance. The Hall effect, discovered a century ago, led to the concept of particles, holes and bands (Hall 1897). The de Haas–van Alphen effect is a formidable approach to get information about the Fermi surface (de Haas and van Alphen 1930, Onsager 1952). More recently it turned out that the spectrum of the Hamiltonian for one particle on a two-dimensional lattice, with constant magnetic field perpendicular to the lattice direction, has an amazing wealth of interesting structure. In his thesis Hofstadter produced beautiful pictures of the spectrum for the case of the square lattice. They were numerically computed. He gave also some rules formalizing the self-similarity in this so-called 'Hofstadter butterfly' (Hofstadter 1976). These rules have been analysed by several authors, in particular by Helffer and Sjöstrand (1988b) and Guillement *et al* (1989), who were able to prove a considerable part of these numerically motivated conjectures.

Consider the Hofstadter Hamiltonian

$$H = T_1 + T_2 + T_1^* + T_2^*. \tag{1}$$

It can be interpreted as the tight binding approximation of a Bloch electron in a given band, submitted to a homogeneous magnetic field. In this sense the band structure of H and some of its generalizations to be discussed below will have to be interpreted as the sub-band structure of the original Bloch Hamiltonian. Otherwise it can interpreted as the finite difference approximation of a particle in a homogeneous magnetic field.

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The Hofstadter Hamiltonian H belongs to the algebra of operators generated by the unit magnetic translations in one and two directions T_1 and T_2. They will be defined explicitly in the following section. Their predominent property is the commutation relation

$$T_1 T_2 = e^{i\varphi} T_2 T_1 \qquad \varphi := 2\pi \frac{\phi}{\phi_0} \qquad \phi_0 := \frac{h}{e} \tag{2}$$

where ϕ denotes the magnetic flux through the unit cell of the square lattice. It can be argued, that this property alone is enough to compute the spectrum of H. From this point of view the analysis of H is an algebraic problem about the so-called rotational algebra $\mathcal{A}_\varphi$ of operators generated by $T_1 T_2$ with the commutation relations (2)

$$\mathcal{A}_\varphi = \text{Norm closure of} \left\{ \sum_{-\infty}^{+\infty} a_{m,n} T_1^n T_2^m \middle| \{a_{m,n}\} \text{ rapidly decreasing} \right\}.$$

The algebra can be analysed easily in the case $\varphi_0 = 2\pi p/q$, where p and q are integers and relative prime. This case of so-called 'rational flux' leads to a problem of matrix valued functions (Bloch's theorem) and to a spectrum of H which can be computed numerically with great accuracy—even on a PC at least as long as q is smaller than 40.

Due to the similarity of (2) with the Heisenberg commutation relations for unit translations in coordinate and momentum space, the limit φ to zero is the semiclassical limit. This is of course well known and at the root of Landau's treatment of an electron in uniform magnetic field (Landau 1930).

This idea can be developed further: the two commutation relations

$$T_1^{(1)} T_2^{(1)} = e^{i\varphi_0} T_2^{(1)} T_1^{(1)} \qquad T_1^{(2)} T_2^{(2)} = e^{i\Delta} T_2^{(2)} T_1^{(2)} \qquad \varphi_0, \Delta \in \mathbb{R}$$

imply for the direct product operators

$$T_k := T_k^{(1)} \otimes T_k^{(2)} \qquad k = 1, 2$$

the commutation relation

$$T_1 T_2 = e^{i(\varphi_0 + \Delta)} T_2 T_1 .$$

Hence the 'semiclassical limit', Δ to zero, permits an analysis of the algebra—and therefore of H—in the vicinity of φ_0.

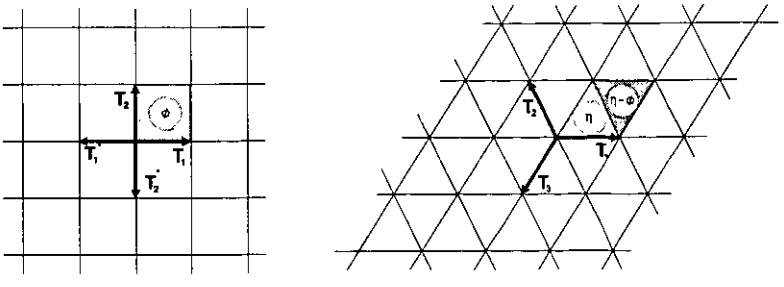

Figure 1. Magnetic translations and fluxes through elementary cells.

The above construction, together with the remark about the case of a rational field, suggests the following strategy for the analysis of the spectrum of Hamiltonians which are elements of the rotation algebra. Choose $\varphi = \varphi_0 + \Delta$, $\varphi_0 = 2\pi p/q$. Then the spectrum of the Hamiltonian for φ close to the rational flux φ_0 is discussed in terms of the semiclassical limit $\Delta \to 0$. This approach, which is of algebraic character, will be illustrated in this paper for a triangular lattice with flux $(\varphi - \eta)$ and η through triangles with one vertex down and one vertex up respectively (figure 1).

In the triangular case the Hamiltonian is again an element of the rotation algebra generated by T_1 and T_2. It is given by

$$H = T_1 + T_2 + T_3 + T_1^* + T_2^* + T_3^* \tag{3}$$

with T_3 defined by

$$T_1 T_2 T_3 = \mathrm{e}^{\mathrm{i}\eta}. \tag{2'}$$

The semiclassical approach leads to a Hamiltonian reminiscent of the Born–Oppenheimer problem (20)

$$H(\Delta, k) = \mathscr{H}(k) + \sqrt{|\Delta|}\left(\frac{\partial}{\partial k_\mu}\mathscr{H}(k)\right)K_\mu + \frac{|\Delta|}{2}\left(\frac{\partial}{\partial k_\mu}\frac{\partial}{\partial k_\nu}\mathscr{H}(k)\right)K_\mu K_\nu$$
$$+ \Delta\partial_\Delta H(0, k) + \mathrm{O}(|\Delta|^{3/2}).$$

$\mathscr{H}(k)$ is a matrix-valued function on the torus and K_1, K_2 are canonical operators. They satisfy Heisenberg commutation relations. In a generic case (no band touching) an extremal eigenvalue E of $\mathscr{H}(k)$ with eigenprojector P generates an effective potential $\mathscr{E}(k)$ and the system is described by the quantum fluctuations around E

$$H(\Delta, k) \sim E + \frac{\Delta}{2}(\partial_\mu\partial_\nu\mathscr{E})K_\mu K_\nu - \frac{|\Delta|}{2}\mathrm{i}\,\mathrm{Trace}(P((\partial\mathscr{H}) \wedge (\partial P)))$$
$$+ \Delta\,\mathrm{Trace}\,P(\partial_\Delta H(0)) + \mathrm{O}(|\Delta|^{3/2}) \qquad (E \text{ extremal of } \mathscr{E}). \tag{25}$$

The spectrum of this effective Hamiltonian is given by the Wilkinson–Rammal formula (26) (Wilkinson 1984, Wang *et al* 1987, Bellissard 1988)

$$E_n(\Delta) = E \pm |\Delta|\sqrt{\det(\partial_\mu\partial_\nu\mathscr{E})}\,(n + \tfrac{1}{2}) - \frac{\Delta}{2}\mathrm{i}\,\mathrm{Trace}(P((\partial\mathscr{H} \wedge (\partial P)))$$
$$+ \Delta\,\mathrm{Trace}\,P(\partial_\Delta H(0)) + \mathrm{O}(|\Delta|^{3/2}).$$

It describes the spectrum of the original system near band edges.

The first term proportional to $|\Delta|$ is related to the curvature of the effective potential $\mathscr{E}$ at its extremal point. The second term originates from the non-commutativity of the canonical operators K_1 and K_2. It is related to the occurrence of a Berry phase (Wilkinson 1984, Berry 1988). The third term is a result of the explicit Δ dependence of the matrix $\mathscr{H}(k, \Delta)$. Note that the overall slope of an asymptotic line is given by the sum of all three terms, while the change of slope between the different asymptotics $\partial E_n/\partial\Delta$ $(n = 1, 2, 3, \ldots)$ belonging to the same extremal is entirely given by the curvature of $\mathscr{E}(k)$ at this extremal, which in terms of Bloch theory is called the effective mass tensor of the Bloch electron.

We should like to stress that the spectral curves $E_n(\Delta)$ exhibit several crossings since they approach several distinct band edges (29) (see figures 4-6 below).

In the generic case—described by the Wilkinson–Rammal formula (26)—the spectral curves approach the minima linearly in Δ. This changes in the case of band touching. The corresponding formula will contain a square root of Δ. We have not analysed this situation in detail (Helffer and Sjöstrand 1988a, Rammal and Bellissard 1990a).

In the present work we have especially investigated the accuracy of the semiclassical expansion in describing the spectrum. We shall illustrate this for the triangular lattice with two fluxes, where band crossing occurs. We have compared the theoretical work with the numerical calculation of the eigenvalues, and we shall see that the agreement is quite good.

We will not consider broadening of Landau levels due to tunnelling. This phenomenon has been analysed by Wilkinson and Austin (1990) for the model with threefold symmetry. They computed a tunnelling Hamiltonian describing the interaction between bottom wells in different unit cells. Furthermore they show numerically that it is sufficient to consider only neighbouring unit cells. This allows us to write the effective tunnelling Hamiltonian as a renormalized version of the original Hamilton operator.

Similar methods as the ones used here have been applied recently in the study of the stability of spectra for an electron submitted to a homogeneous or periodic magnetic field (Rammal and Bellissard 1990b, Barelli *et al* 1990).

The paper is organized as follows. In section 2 we describe the model in the algebraic language. Section 3 is devoted to the calculation of the semiclassical expansion for the band edges near a rational number. In section 4 we describe and discuss the numerical calculations.

2. Definition of the model

In this section we shall first describe in more detail the model considered. Next the semiclassical calculation of energy eigenvalues will be described. Finally the numerical results will be compared with the analytic computation.

2.1. Realizations of the rotation algebra

For the spectral analysis of the Hamiltonians to be considered, it is useful to introduce three different realizations of the rotation algebra. Since the spectrum of elements in the algebra are defined in terms of the trace only and since this trace is unique it does not matter which realization is used.

The elementary constituents of all Hamiltonians considered are the magnetic translations T_1 and T_2 defined below. They obey the commutation relations (2) and hence provide the first realization of the rotation algebra $\mathcal{A}_\varphi$.

The operators T_1, T_2 act on $l^2(\mathbb{Z}^2)$, the space of square integrable functions defined on the lattice $\mathbb{Z}^2$, and are given by the equations in a Landau gauge:

$$(T_1 f)(k, l) = f(k+1, l)$$

$$(T_2 f)(k, l) = e^{i\varphi k} f(k, l+1).$$

In this representation the Hamiltonians (1) is easily interpreted as the finite difference approximation of the one-particle Hamiltonian for an electron moving in the plane submitted to an external and constant magnetic field. The same realization leads to an interpretation of the Hamiltonians (1) and (3) as the tight binding approximation of an electron on a square lattice and a triangular lattice in an external magnetic field respectively.

We shall refer to (1) and (3) together with the commutation relations (2), (2′) as the square lattice Hamiltonian with flux φ and the triangular Hamiltonian with fluxes φ, η respectively. They belong to the rotation algebra $\mathscr{A}_\varphi$. In fact the triangular Hamiltonian is a family of elements in $\mathscr{A}_\varphi$ parametrized by the flux η. Two members of this family are of special importance: The first one has the parameter value $\eta = \varphi/2$ and is the ordinary triangular lattice as discussed by Claro and Wannier (1979); the second one is characterized by $\eta = 0$ and related to the hexagonal lattice (Rammal 1985) (see also section 2.2).

To support physical intuition it is useful to associate with the magnetic translations the diagrammatic representations shown in figure 1.

The second realization of the rotation algebra $\mathscr{A}_\varphi$ is given in terms of the usual Schrödinger representation of the Heisenberg commutation relation. Let K_2 and K_1 be momentum and position operators on the space of square integrable functions $L^2(\mathbb{R}, \mathrm{d}x)$; then

$$T_j = \mathrm{e}^{\mathrm{i}\sqrt{\varphi}K_j} \qquad j = 1, 2, \quad \varphi \geqslant 0 \tag{4}$$

satisfy the commutation relation (2) due to

$$[K_2, K_1] = \mathrm{i}. \tag{5}$$

If $\varphi \leqslant 0$ we choose alternatively

$$T_j = \mathrm{e}^{\mathrm{i}\sqrt{-\varphi}\,K_j} \qquad j = 1, 2 \tag{4′}$$

and exchange the role of K_2 and K_1:

$$[K_1, K_2] = \mathrm{i}. \tag{5′}$$

To see the use of this representation of $\mathscr{A}_\varphi$ note that a formal second order expansion in $\sqrt{\varphi}$ of the square lattice Hamiltonian (1) simply gives a harmonic oscillator:

$$H(\varphi) = 4 - |\varphi|(K_1^2 + K_2^2) + \ldots.$$

Hence this representation is useful for the analysis of the spectrum near $\varphi \approx 0$; more generally one has to expand around an extremal point in the 'classical phase space' as will be shown later.

In the case of rational flux, $\varphi = 2\pi p/q$, where p and q are integers with no common divisor, the elements of the rotation algebra $\mathscr{A}_\varphi$ can be realized as covariant matrix valued functions on the torus $\mathbb{T}^2$. This is the third realization of $\mathscr{A}_\varphi$ which will be used. In particular the triangular Hamiltonian $H(\varphi = 2\pi p/q, \eta)$ is realized by the following matrix valued function on the torus

$$\mathscr{H}(\varphi, \eta; k) = \mathrm{e}^{\mathrm{i}k_1} w_1 + \mathrm{e}^{\mathrm{i}k_2} w_2 + \mathrm{e}^{\mathrm{i}\eta}\,\mathrm{e}^{-\mathrm{i}(k_1+k_2)} w_2^* w_1^* + \ldots + \mathrm{cc}. \tag{6}$$

Here

$$w_1 = \begin{bmatrix} 0 & 1 & & \\ & \ddots & \ddots & \\ & & \ddots & 1 \\ 1 & & & 0 \end{bmatrix} \qquad w_2 = \begin{bmatrix} 1 & & & \\ & \mathrm{e}^{2\pi\mathrm{i}(p/q)l} & & \\ & & \ddots & \\ & & & \mathrm{e}^{2\pi\mathrm{i}(p/q)(q-1)} \end{bmatrix} \qquad l = 0, \ldots, q-1 \tag{7}$$

are 2 independent $q \times q$ matrices. They satisfy the commutation relation (2). This comes about because T_1 and T_2 are the following matrix valued functions:

$$T_l = e^{ik_l} w_l \qquad l = 1, 2 \tag{8}$$

It is going to be useful to think of $\mathcal{H}$ as a classical Hamilton function, which is, however, matrix valued.

The representation of the Hamiltonian for rational flux in terms of matrix valued functions on the torus is the algebraic version of Bloch's theorem. It is applicable here because in the case of a rational flux the magnetic field does not entirely destroy translational symmetry. In fact the three operators $H(\varphi, \eta)$, T_1^q and T_2 commute and can therefore be diagonalized simultaneously.

2.2. The spectrum for rational flux

The spectrum of the Hamiltonian $H(\varphi = 2\pi(p/q), \eta)$ is given by the equation

$$\sigma\left(H\left(\varphi = 2\pi\frac{p}{q}, \eta\right)\right) = \bigcup_{k \in \mathbb{T}^2} \sigma\left(\mathcal{H}\left(\varphi = 2\pi\frac{p}{q}, \eta; k\right)\right). \tag{9}$$

It has been discovered by Chambers (1965) that the secular determinant for the square lattice has a simple structure. It is the sum of two terms, the first one a polynomial in z not depending on k, the second one a trigonometric function not depending on z. At the root of this phenomenon lies the fact that the Hamiltonian is built up by nearest-neighbour terms. This holds also for the triangular Hamiltonian. So it is understandable but still remarkable that the secular determinant of the triangular Hamiltonian has the same structure:

$$\begin{aligned} &\det\left(z - \mathcal{H}\left(\varphi = 2\pi\frac{p}{q}, \eta; k\right)\right) = P(z) - h(k) \\ &P(z) = z^q + a_1 z^{q-1} + \ldots + a_q \\ &\tfrac{1}{2}h(k) = \cos qk_1 + \cos qk_2 + (-1)^{q-1} \cos q(k_1 + k_2 - \eta). \end{aligned} \tag{10}$$

Due to (9) we get for the spectrum of $H(\varphi, \eta)$ the equation

$$\sigma\left(H\left(\varphi = 2\pi\frac{p}{q}, \eta\right)\right) = \{z | P(z) \in \text{Image } h\}. \tag{11}$$

This equation can be interpreted graphically with the help of figure 2.

The image of h is the interval with the boundary points $\{h_{\min}, h_{\max}\}$. Hence the spectrum of $H(\varphi, \eta)$ is the inverse image of the interval $[h_{\min}, h_{\max}]$ by the polynomial map P. The numerical implication of this fact leads to figures 4-8 below. They show the band structure of the spectrum very clearly The number of bands is equal to q up to a few exceptions, where one observes 'band touching'. For the square lattice see for details Bellissard and Simon (1982), van Mouche (1987) and Choi *et al* (1990). Setting the secular determinant of $H(\varphi, \eta)$ equal to zero

$$\det\left(\mathcal{E}_n(k) - \mathcal{H}\left(\varphi = 2\pi\frac{p}{q}, \eta; k\right)\right) = 0$$

defines the band functions

$$z = \mathcal{E}_n(k) \qquad n = 1 \ldots q \qquad k \in \mathbb{T}^2.$$

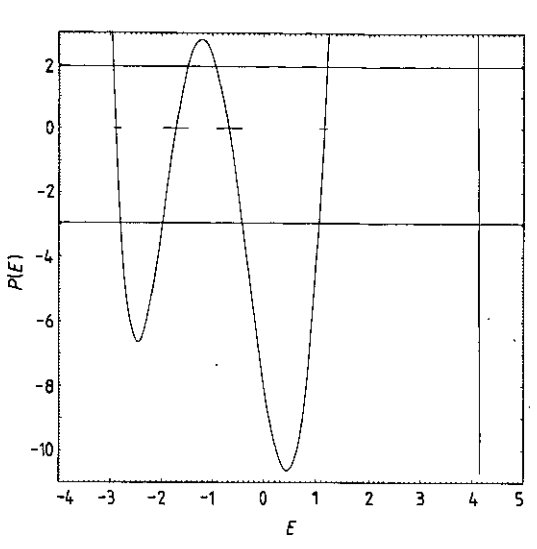

Figure 2. The spectrum of H according to (11).

The band edges are characterized by critical points k_c of $h(\varphi, \eta; k)$;

$$\frac{\partial h}{\partial k}(k_c) = 0.$$

From Chamber's relation (10) it follows that for the nth band

$$\frac{\partial \mathscr{E}_n(k_c)}{\partial k} = 0 \tag{12}$$

provided there is no band touching,

$$\frac{\partial P}{\partial z}(z = \mathscr{E}_n(k_c)) \neq 0.$$

2.3. Spectrum of the honeycomb lattice

The spectrum of the honeycomb or hexagonal lattice is easily related to the triangular lattice with flux zero through one type of triangle.

Consider a triangular lattice Γ. Then the hexagonal lattice Γ_H can be seen as a subset of Γ. Γ_H is not a Bravais lattice and it decomposes into two types of lattice points belonging to triangular lattices Γ_A, $\Gamma_B \subset \Gamma$ with $\Gamma = \Gamma_A \cup \Gamma_B$. Where these sublattices have twice the lattice spacing of the underlaying lattice Γ.

Correspondingly the space of physical states on the hexagonal lattice decomposes into the direct sum

$$l^2(\Gamma) = l^2(\Gamma_A) \oplus l^2(\Gamma_B).$$

The hexagonal Hamiltonian H_6 can now be written as a 2×2 matrix with operator entries. Due to the geometrical structure of the lattice it is off-diagonal,

$$H_6 = \begin{bmatrix} 0 & H_{AB} \\ H_{BA} & 0 \end{bmatrix}$$

with

$$H_{AB} = T_1 + T_2 + T_3 \qquad \text{and} \qquad H_{BA} = T_1^* + T_2^* + T_3^*$$

where the magnetic translations are defined on the underlying triangular lattice such that

$$T_1 T_2 = T_2 T_1 \, e^{i\phi/3} \qquad \text{and} \qquad T_1 T_2 T_3 = e^{i\phi/6}.$$

Then ϕ is the flux through a unit hexagon in Γ_H. The square of H_6 is diagonal and of the form

$$H_6^2 = \begin{bmatrix} H_{AA} & 0 \\ 0 & H_{BB} \end{bmatrix}.$$

where

$$\begin{aligned} H_{AA} &= 3 + T_1 T_2^* + T_2 T_3^* + T_3 T_1^* + \text{CC} \\ &= 3 + T_1^{(A)} + T_2^{(A)} + T_3^{(A)} + \text{CC}. \end{aligned}$$

The translations $T_k^{(A)}$ act on the triangular lattice Γ_A only and fulfil the commutation relations of a triangular lattice with flux ϕ through an up-triangle and flux 0 through a down-triangle. Hence the spectrum of the hexagonal and triangular lattice for rational flux are related by the formula

$$\sigma(H_6^2) = \sigma\left(H\left(\varphi = 2\pi \frac{p}{q}, \eta = 0 \right) \right) + 3.$$

3. Semiclassical analysis near band edges

Before going into details about the spectrum in the vicinity of band edges, we shall introduce Weyl operators replacing magnetic translations:

$$W(m) := T_1^{m_2} T_2^{-m_1} \, e^{(i/2)\varphi m_1 m_2} \qquad m \in \mathbb{Z}^2. \tag{13}$$

They satisfy the multiplication law

$$W(m)\, W(n) = e^{i\varphi/2(m_1 n_2 - m_2 n_1)} W(m+n) \qquad m, n \in \mathbb{Z}^2$$

due to (2). Clearly every element of the rotation algebra $\mathcal{A}_\varphi$ can again be written in terms of the Weyl operators (13),

$$\mathcal{A}_\varphi = \text{closure}\left\{ \sum_{m \in \mathbb{Z}^2} b(m)\, W(m) \,\middle|\, (b(m)) \text{ sequence of rapid decrease} \right\}.$$

In particular the triangular Hamiltonian is of the form

$$H(\varphi, \eta) = \sum_{m \in \mathbb{Z}^2} h(\varphi, \eta; m)\, W(m).$$

The coefficients h are summarized in table 1. It is convenient to introduce the following notation:

$$\begin{aligned}\partial_1 H(\varphi,\eta) &= \sum h(\varphi,\eta;m)(-\mathrm{i}m_2)\,W(m)\\ \partial_2 H(\varphi,\eta) &= \sum h(\varphi,\eta;m)(\mathrm{i}m_1)\,W(m)\\ \partial_\varphi H(\varphi,\eta) &= \sum \frac{\partial h}{\partial\varphi}(\varphi,\eta;m)\,W(m).\end{aligned} \tag{14}$$

Table 1. Coefficients of the triangular Hamiltonian.

m_1	m_2	$h(\varphi,\eta;m_1,m_2)$
0	−1	1
0	1	1
−1	0	1
1	0	1
−1	1	$\exp(\mathrm{i}\eta-\mathrm{i}\varphi/2)$
1	−1	$\exp(-\mathrm{i}\eta+\mathrm{i}\varphi/2)$

It is motivated as follows: in the case of rational flux we have already seen that the magnetic translations and hence the Weyl oeprators are matrix valued functions of $k\in\mathbb{T}^2$ (algebraic Bloch theorem). It is easily verified that in this case we get the identities

$$\partial_l H(\varphi,\eta;k)=\frac{\partial}{\partial k_l}H(\varphi,\eta;k)\qquad l=1,2. \tag{15}$$

Hence definitions (14) are arranged in such a way as to extend the derivatives with respect to k, which is well defined for the rational case, to the case of arbitrary flux.

Now we shall investigate the spectrum of the triangular Hamiltonian at the band edges by combining two realizations of the rotation algebra as follows: the realization by matrix valued functions (rational flux) (7), (8), and by the usual one-particle quantum mechanics (4), (5), where a semiclassical expansion is easy.

Consider the triangular Hamiltonian for flux $\varphi=2\pi(p/q)+\Delta$, with p, q relatively prime. Then $H(\Delta)$ has the structure

$$H(\Delta)=\sum h(\Delta,m)\,W^{(1)}(m)\otimes W^{(2)}(\Delta,m). \tag{16}$$

$W^{(1)}(m)$ is a matrix valued function of $k\in\mathbb{T}^2$. Hence $H(\Delta)$ can be viewed as a $q\times q$ matrix with operator valued entries.

As an introductory example let us consider the case $q=1$. Then the magnetic translations get the simple form

$$\tilde{T}_j=T_j^{(1)}\otimes T_j^{(2)}=\exp(\mathrm{i}\sqrt{\Delta}\,K_j+\mathrm{i}k_j)\qquad j=1,2.$$

A formal expansion in $\sqrt{\Delta}$ around a critical point $k=k_c$ of the triangular Hamiltonian (3) in this representation gives

$$\begin{aligned}H(k_c,\Delta)=\cos(k_{c1})+\cos(k_{c1})+\cos(k_{c1}+k_{c2}-\eta)+|\Delta|\{&\sin(k_{c1})K_1^2+\sin(k_{c2})K_2^2\\&+\sin(k_{c1}+k_{c2}-\eta)(K_1+K_2)^2+\Delta\sin(k_{c1}+k_{c2}-\eta)+O(|\Delta|^{3/2})\}.\end{aligned}$$

Diagonalizing this quadratic form shows that, like in the square lattice case, we have a harmonic oscillator. We will come back to this example in section 4.

To get semiclassical results about the spectrum in the vicinity of the rational flux $2\pi p/q$ we expand $H(\Delta)$ and

$$W^{(2)}(m, \Delta) = e^{i\sqrt{\Delta}\, m_2 K_1}\, e^{-i\sqrt{\Delta}\, m_1 K_2}\, e^{(i/2)\Delta m_1 m_2} \tag{17}$$

in powers of $\sqrt{\Delta}$. Defining $m \wedge K = m_2 K_1 - m_1 K_2$ this leads to

$$W(\Delta, m) = W(0, m)\left\{1 + i\sqrt{|\Delta|}\,(m \wedge K) - \frac{|\Delta|}{2}(m \wedge K)^2 + O(|\Delta|^{3/2})\right\}$$

$$H(\Delta) = H(0) + \sqrt{|\Delta|}\,(\partial_\mu H(0))K_\mu + \frac{|\Delta|}{2}(\partial_\mu \partial_\nu H(0))K_\mu K_\nu + \Delta(\partial_\Delta H(0)) + O(|\Delta|^{3/2}). \tag{18}$$

It is important to note the structure of each term in the above formulae:

$$\begin{aligned} &H(0) = H(0)^{(1)} \otimes 1^{(2)} \\ &\frac{|\Delta|}{2}(\partial_\mu \partial_\nu H(0))K_\mu K_\nu = \frac{|\Delta|}{2}(\partial_\mu \partial_\nu H(0))^{(1)} \otimes K_\mu K_\nu^{(2)} \\ &\Delta(\partial_\Delta H(0)) = \Delta(\partial_\Delta H(0))^{(1)} \otimes 1^{(2)}. \end{aligned} \tag{19}$$

Formula (18) can be rewritten in terms of the matrix valued function $\mathcal{H}(k)$, the 'classical Hamiltonian' for rational flux (see equations (14) and (15)):

$$\begin{aligned} H(\Delta, k_0) = \mathcal{H}(k_0) + \sqrt{|\Delta|}\left(\frac{\partial}{\partial k_\mu}\mathcal{H}(k_0)\right)K_\mu + \frac{|\Delta|}{2}\left(\frac{\partial}{\partial k_\mu}\frac{\partial}{\partial k_\nu}\mathcal{H}(k_0)\right)K_\mu K_\nu \\ + \Delta(\partial_\Delta H(0, k_0)) + O(|\Delta|^{3/2}). \end{aligned} \tag{20}$$

The expansion can be viewed as the quantization of the harmonic approximation of the classical Hamiltonian in a vicinity of k_0

$$\mathcal{H}(k_0 + k) = \mathcal{H}(k_0) + \left(\frac{\partial}{\partial k_\mu}\mathcal{H}(k_0)\right)k_\mu + \left(\frac{\partial}{\partial k_\mu}\frac{\partial}{\partial k_\nu}\mathcal{H}(k_0)\right)k_\mu k_\nu + O(k^3). \tag{21}$$

At this point we continue our investigation of the spectrum close to a band edge $\mathcal{E}(k_c)$ by a kind of phase space localization in the spirit of the Born-Oppenheimer approximation. The band function $\mathcal{E}(k)$ is viewed as a 'potential surface'. The spectrum of $H(\Delta)$ close to the band edge is expected to be dominated by the classical Hamiltonian at the corresponding critical points $k_0 = k_c$. If $q = 1$, the classical Hamiltonian is a real valued function on the torus. For $\eta = 0.3\ \pi$ we have produced a plot of the function (figure 3) that shows well that the levels of constant energy near the extremals are almost elliptical. Also we see the existence of the two distinct extremals leading to the level crossing.

The 'quantum fluctuations' are quadratic in K_1 and K_2 up to corrections of order $|\Delta|^{3/2}$. The spectrum will now be computed by perturbation theory in the parameter

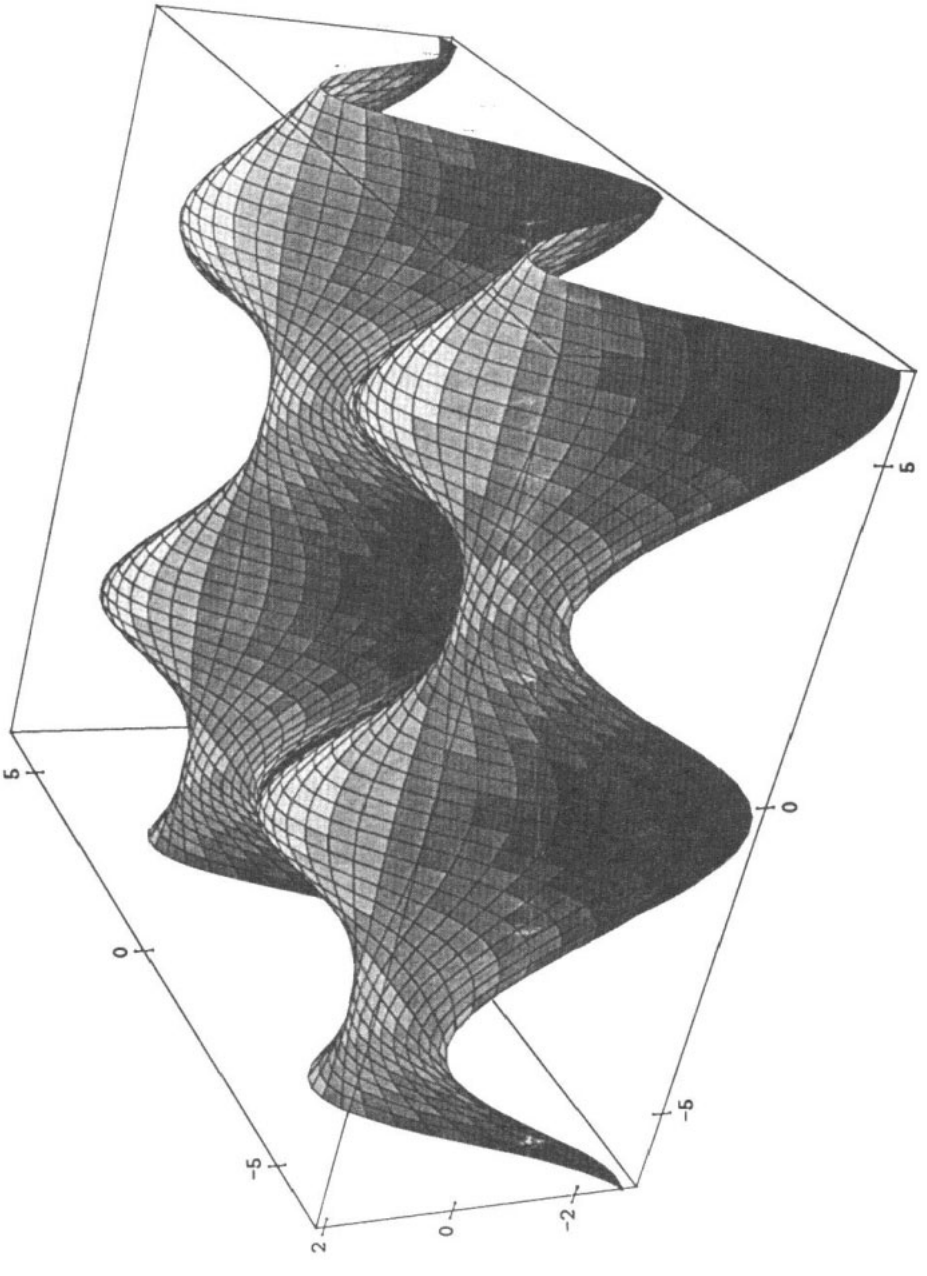

Figure 3. Plot of the classical Hamiltonian $\mathscr{H}(x, y) = \cos(x) + \cos(y) + \cos(x + y - \eta)$ for $\eta = 0.3\pi$.

$\sqrt{\Delta}$ and this is more or less a problem about the harmonic oscillator. Notice that the individual terms in (20) have structures analogous to the ones explained in formulae (19).

To start perturbation theory consider the eigenvalue $\mathscr{E}(k_c)$ of the unperturbed Hamiltonian $\mathscr{H}(k_c)$ (20). It belongs to a band edge for rational flux $2\pi p/q$ and is infinitely degenerate: this comes about because the corresponding eigenprojector has the structure.

$$P(k_c) = P^{(1)}(k_c) \otimes 1. \tag{22}$$

For what follows we shall make the assumption:

$$\dim P^{(1)}(k_c) = 1. \tag{23}$$

This means that there is no band touching at k_c. To simplify notation we shall adopt the following notational convention. If a function $f(k)$ of $k \in \mathbb{R}^2$ is evaluated at $k = k_c$ we drop the variable k_c and write simply f.

The standard formulae of perturbation theory (Messiah 1969, Kato 1966, Hunziker 1988) reduce the computation of the eigenvalues of $H(\Delta)$ to the analysis of an effective Hamiltonian $\mathscr{H}_{\text{eff}}(\Delta)$. This operator lives on the range of P only, i.e. it vanishes on the orthogonal complement of range P:

$$H_{\text{eff}}(\Delta) = P\mathscr{H} + \sqrt{\Delta}\, P(\partial_\mu \mathscr{H}) P\, K_\mu + \frac{|\Delta|}{2} P(\partial_\mu \partial_\nu \mathscr{H}) P\, K_\mu K_\nu$$

$$+ |\Delta| P(\partial_\mu \mathscr{H}) \mathscr{R} (\partial_\nu \mathscr{H}) P\, K_\mu K_\nu + \Delta P(\partial_\Delta H) + O(|\Delta|^{3/2}).$$

$\mathscr{R}$ denotes the reduced resolvent at energy E:

$$\mathscr{R} := (\mathscr{H} - E)^{-1} P^\perp \qquad P^\perp := 1 - P.$$

To start perturbation theory let us apply the above formalism to the 'classical Hamiltonian', the matrix valued function (21) at $k_0 = k_c$. It will lead to a result which is useful for the quantum case. The effective 'classical Hamiltonian', which is computed along the same lines as $H_{\text{eff}}(\Delta)$, is given by the formula

$$\mathscr{H}_{\text{eff}}(k) = P\mathscr{H} + P(\partial_\mu \mathscr{H}) P\, k_\mu + \tfrac{1}{2} P(\partial_\mu \partial_\nu \mathscr{H}) P\, k_\mu k_\nu + P(\partial_\mu \mathscr{H}) \mathscr{R} (\partial_\nu \mathscr{H}) P\, k_\mu k_\nu + O(k^3).$$

To simplify notation we dropped in all terms on the right-hand side of the above formula and of (21) the superscript (1), which refers to the matrix representation defined through (8). To be precise we should have written for instance $P^{(1)}\mathscr{H}^{(1)}$ since $\mathscr{H}(k)$ and $\mathscr{H}_{\text{eff}}(k)$ are both matrix valued functions.

Due to stability of the spectrum under small perturbations and the hypothesis excluding band touching (23) the eigenvalue of $\mathscr{H}(k)$ is given by the formula

$$\mathscr{E}(k) = \text{Trace}\, \mathscr{H}_{\text{eff}}(k) P.$$

This formula can easily be evaluated. One gets the result

$$\mathscr{E}(k) = E + \tfrac{1}{2}(\partial_\mu \partial_\nu \mathscr{E}) k_\mu k_\nu + O(k^3)$$

$$(\partial_\mu \partial_\nu \mathscr{E}) = \text{Trace}\, P(\partial_\mu \partial_\nu \mathscr{H} + (\partial_\mu \mathscr{H}) \mathscr{R} (\partial_\nu \mathscr{H}) + (\partial_\nu \mathscr{H}) R (\partial_\mu \mathscr{H})) P$$

since

$$\text{Trace } P(\partial_\mu \mathscr{H})P = \partial_\mu \mathscr{E} = 0.$$

This equation holds due to the so-called Helman-Feynman theorem and (12).

Now we return to the corresponding calculation for the quantum operator $H(\Delta)$, respectively its effective counterpart $H_{\text{eff}}(\Delta)$. Due to the hypothesis which excludes band touching (23) the eigenvalues of $H_{\text{eff}}(\Delta)$ and of Trace $(H_{\text{eff}}(\Delta))$ are the same. Notice that 'Trace' means the partial trace with respect to the matrix part of the tensor product and should rather be denoted by Trace$^{(1)}$. To simplify notation we drop the index.

Trace $H_{\text{eff}}(\Delta)$ contains terms which are almost the same as the terms in $\mathscr{H}_{\text{eff}}(k)$:

$$\begin{aligned}\text{Trace } H_{\text{eff}}(\Delta) = E &+ \sqrt{\Delta}\,\text{Trace } P(\partial_\mu \mathscr{H})P K_\mu + \frac{|\Delta|}{2}\,\text{Trace } P(\partial_\mu \partial_\nu \mathscr{H})P K_\mu K_\nu \\ &+ \Delta\,\text{Trace } P\partial_\Delta H(0)P + |\Delta|\,\text{Trace } P(\partial_\mu \mathscr{H})\mathscr{R}(\partial_\nu \mathscr{H})P K_\mu K_\nu \\ &+ O(|\Delta|^{3/2}).\end{aligned}$$

To make the close analogy of the formula above and of (24) more transparent we split the term quadratic in K into its symmetric and antisymmetric part. The first one corresponds to the classical counterpart and the second gives a quantum correction due to the non-commutativity of K_1 and K_2:

$$\text{Trace } H_{\text{eff}}(\Delta) = E + \frac{|\Delta|}{2}(\partial_\mu \partial_\nu \mathscr{E})K_\mu K_\nu - \frac{\Delta}{2}B + \Delta\,\text{Trace } P(\partial_\Delta H(0)) + O(|\Delta|^{3/2}). \tag{25}$$

Here B denotes the expression

$$\begin{aligned}B &= \mathrm{i}\,\text{Trace}(P(\partial_1 \mathscr{H})\mathscr{R}(\partial_2 \mathscr{H})P - P(\partial_2 \mathscr{H})\mathscr{R}(\partial_1 \mathscr{H})P) \\ &= \mathrm{i}\,\text{Trace}(P((\partial \mathscr{H}) \wedge (\partial P))).\end{aligned}$$

This is a term reminiscent of Berry's phase. Now the spectrum of $H(\Delta)$ can be read off easily. It is given by the Wilkinson-Rammal formula

$$E_n(\Delta) = E \pm |\Delta|\sqrt{\det(\partial_\mu \partial_\nu \mathscr{E})}\,(n+\tfrac{1}{2}) - \frac{\Delta}{2}B + \Delta\,\text{Trace } P(\partial_\Delta H(0)) + O(|\Delta|^{3/2}) \qquad n \in \mathbb{N}. \tag{26}$$

The sign in front of the second term reflects the maxima and minima in the phase space localization.

4. Numerical computation

In the remainder of this paper we use the above formula to interpret the numerical data presented in tables 2 and 3 and figures 4–8. In order to do that we compute the right-hand side term by term for the two cases $q = 1$ and $q = 2$.

Table 2. Semiclassical against numerically computed coefficients for $\eta = 2\pi \times 0.0175$; (*a*), (*b*) expansion near $p/q = 1$ with $\Delta > 0$; compare with figure 5; (*c*), (*d*) expansion near $p/q = 1/2$ with $\Delta > 0$; compare with figure 6.

(*a*)

q	m	n	$E0_{SC}$	$E0_{num}$	$E1_{SC}$	$E1_{num}$	$E2_{num}$	$E2_{SC}$
1	1	0	−1.594 195 7	−1.594 20	0.883 765 6	0.883 99	−0.247 72	−0.241 58
1	1	1	−1.594 195 7	−1.594 20	1.804 175 0	1.805 14	−1.002 39	−0.976 89
1	1	2	−1.594 195 7	−1.594 20	2.724 584 3	2.727 53	−2.278 14	−2.202 98
1	1	3	−1.594 195 7	−1.594 20	3.644 993 6	3.652 27	−4.099 84	−3.919 83
1	1	4	−1.594 195 7	−1.594 20	4.565 403 0	4.581 07	−6.503 66	−6.127 46
1	1	5	−1.594 195 7	−1.594 20	5.485 812 3	5.516 57	−9.542 87	−8.825 85
1	1	6	−1.594 195 7	−1.594 20	6.406 221 7	6.463 95	−13.312 3	−12.015 0
1	1	7	−1.594 195 7	−1.594 20	7.326 631 0	7.427 23	−17.898 9	−15.694 9
(*b*)								
1	−1	0	−1.403 789 4	−1.403 79	−0.036 643 7	−0.036 628	−0.004 573	−0.004 16
1	−1	1	−1.403 789 4	−1.403 79	0.773 834 5	0.774 302	−0.273 882	−0.261 20
1	−1	2	−1.403 789 4	−1.403 70	1.584 312 7	1.586 51	−1.087 32	−1.030 38
1	−1	3	−1.403 789 4	−1.403 79	2.394 790 9	2.401 64	−2.484 98	−2.311 73
1	−1	4	−1.403 789 4	−1.403 79	3.205 269 1	3.221 91	−4.519 93	−4.105 23
1	−1	5	−1.403 789 4	−1.403 79	4.015 747 4	4.052 86	−7.361 81	−6.410 89
(*c*)								
2	−1	0	−1.530 727 0	−1.536 73	0.576 962 5	0.577 55	−0.554 17	
2	−1	1	−1.530 727 0	−1.539 73	1.212 972 1	1.216 12	−2.244 11	
2	−1	2	−1.530 727 0	−1.530 73	1.848 981 6	1.859 59	−5.224 01	
2	−1	3	−1.530 727 0	−1.530 73	2.484 991 2	2.511 43	−9.690 90	
2	−1	4	−1.530 727 0	−1.530 74	3.121 000 7	3.180 14	−16.043 9	
2	−1	5	−1.530 727 0	−1.530 74	3.757 010 3	3.882 71	−25.024 5	
2	−1	6	−1.530 727 0	−1.530 74	4.393 019 8	4.667 26	−38.537 5	
(*d*)								
2	0	0	−1.467 258 2	−1.467 26	−0.063 186 3	−0.063 101 0	−0.034 050 1	
2	0	1	−1.467 258 2	−1.467 26	0.450 589 9	0.452 678	−0.831 757	
2	0	2	−1.467 258 2	−1.467 26	0.964 366 1	0.976 372	−3.325 28	
2	0	3	−1.467 258 2	−1.467 26	1.478 142 4	1.471 82	−6.638 3	

The first step in this direction is the computation of the local extrema and the second derivative for the energy band function $\mathscr{E}(k)$. From the Chambers relation (10) one gets the formula

$$\mathscr{E}'(k) = \frac{h'(k)}{P'(\mathscr{E}(k))}. \tag{27}$$

Hence it is enough to compute the extremal points for the trigonometric function

$$h(k) = 2\{\cos qk_1 + \cos qk_2 + (-1)^{q-1} \cos q(k_1 + k_2 - \eta)\}$$

Table 3. Semiclassical against numerically computed coefficients for $\eta = \pi/2$ expansion near $p/q = 1/2$ with (*a*) $\Delta > 0$, (*b*) $\Delta < 0$; compare with figure 8.

(*a*)

q	m	n	$E0_{sc}$	$E0_{num}$	$E1_{sc}$	$E1_{num}$	$E2_{num}$
2	1	0	−0.866 025	−0.865 953	−1.0	−0.991 37	0.815 426
2	0	0	−0.866 025	−0.865 917	−1.5	−1.496 10	2.228 40
2	1	1	−0.866 025	−0.865 881	−2.0	−1.990 26	4.328 94
2	0	1	−0.866 025	−0.865 945	−2.5	−2.481 94	7.119 05
2	1	2	−0.866 025	−0.865 912	−3.0	−2.975 10	10.668 8
2	0	2	−0.866 025	−0.865 912	−3.5	−3.476 28	15.161 8

(*b*)

2	1	0	−0.866 025	−0.866 042	−0.5	−0.499 579	−0.163 151
2	0	0	−0.866 025	−0.866 025	0.0	0.001 502 57	−0.354 297
2	1	1	−0.866 025	−0.866 009	0.5	0.503 026	−1.416 56
2	0	1	−0.866 025	−0.865 993	1.0	1.004 61	−3.305 84
2	1	2	−0.866 025	−0.865 978	1.5	1.507 83	−6.040 11
2	0	2	−0.866 025	−0.865 960	2.0	3.017 60	−9.739 06

at least in the case of no band touching ($P'(k) \neq 0$). A straightforward computation leads to the following result for the extremal points of h (up *to* $2\pi/q$ periodicity in both variables):

$$qk_c = \tfrac{1}{3}(q\eta + \pi(q-1) + 2\pi mq,\ q\eta + \pi(q-1) + 2\pi mq) \qquad m \in \mathbb{Z}.$$

The periodicity allows for a reduction to the cases $m \in \{-1, 0, 1\}$.

The corresponding extremal values are given by:

$$h(k_c) = 6\cos(\theta_m) \qquad \theta_m = q/3(\eta + 2\pi m).$$

This triangular symmetry in phase space reflects the triangular structure underlaying the Hamiltonian (Wilkinson and Austin 1990).

For the second derivative (the Hessian) we find at the extremal points

$$h''(k_c) = -2q^2\cos(\theta_m)\begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}. \tag{28}$$

Notice that both eigenvalues of h'' have the same sign as they should since the Hessian is the harmonic approximation at a local extremum.

The second term in the Wilkinson–Rammal formula can now be computed. Differentiating equations (10) and (27) once again and setting $k = k_c$ one gets

$$\mathscr{E}''(k_c) = \frac{h''(k_c)}{P'(\mathscr{E}(k_c))}.$$

Together with (28) this leads to

$$\mathscr{E}''(k_c) = -\frac{2q^2\cos(\theta_m)}{P'(\mathscr{E}(k_c))}\begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}.$$

The harmonic oscillator frequency is given by the square root of the second derivative of $\mathscr{E}_n''(k_c)$ evaluated either at a maximum (+sign) or a minimum (−sign)

$$\pm\sqrt{\det \mathscr{E}''(k_c)} = -2q^2\frac{\cos(\theta_m)}{P'(\mathscr{E}(k_c))}\sqrt{3}. \tag{28'}$$

As mentioned above we restrict our investigation of the Wilkinson-Rammal formula to the cases $q=1$ and $q=2$. Here the polynomial $P(z)$ is computed explicitly.

Using formulae (6) and (7) it is easily seen that the classical Hamiltonians are

$$\mathscr{H}(k)=\begin{cases}2[\cos k_1+\cos(k_1+k_2-\eta)+\cos k_2] & q=1\\ 2[\sigma_1\cos k_1+\sigma_2\sin(k_1+k_2-\eta)+\sigma_3\cos k_2] & q=2\end{cases}$$

where σ_i $(i=1,2,3)$ refer to the Pauli matrices.

Hence one gets for the polynomials

$$P(z)=\begin{cases}z & q=1\\ z^2-6 & q=2.\end{cases}$$

The classical energy can now be expressed in terms of h only:

$$\mathscr{E}(k)=\begin{cases}h(k) & q=1\\ \pm\sqrt{h(k)+6} & q=2.\end{cases}$$

where the $\pm$ refers to the two sub-bands present in the case $q=2$. Evaluated at extremal points it gives the first term in the Wilkinson-Rammal formula.

Inserting the expression for $P'(\mathscr{E}(k_c))$ into formula (28') one gets

$$\pm\sqrt{\det\mathscr{E}''(k_c)}=\begin{cases}-2\sqrt{3}\cos\theta_m & q=1\\ -4\sqrt{3}\dfrac{\cos\theta_m}{\mathscr{E}(k_c)} & q=2.\end{cases}$$

The third term B is only present if $q=2$. For $q=1$ it vanishes, because the projector P is one (there is no reduced resolvent). After a straightforward computation using Pauli matrices one finds

$$B=\frac{1}{2}\frac{\sin\eta+\sin(\theta_m-\eta)}{1+\cos(\theta_m)}.$$

To compute the last term we differentiate formula (16) with respect to Δ, using (17) we find

$$\partial_\Delta(H(\Delta,k)=\frac{\mathrm{i}}{2}\mathrm{e}^{\mathrm{i}(k_1+k_2-\eta)}W_1^{(1)}W_2^{(1)}+\mathrm{cc}.$$

The relevant trace can be computed easily:

$$\text{Trace } P\partial_\Delta H(0,k_c)=\begin{cases}\sin(\theta_m) & q=1\\ \dfrac{\sin(\theta_m)}{\sqrt{6+6\cos\theta_m}} & q=2\end{cases}$$

where P denotes

$$P=\begin{cases}1 & q=1\\ \dfrac{1}{2}\left(1+\dfrac{\mathscr{H}(k_c)}{\mathscr{E}(k_c)}\right) & q=2\end{cases}$$

and projects on the eigenspace characterized by $\mathscr{E}(k_c)$.

Summarizing all the results about the Wilkinson-Rammal formula for the cases $q=1$ and $q=2$, we get the formulae:

$q=1$:

$$E(\Delta)=6\cos(\theta_m)-2\cos(\theta_m)\sqrt{3}\,(n+\tfrac{1}{2})\Delta+\sin(\theta_m)\Delta+O(|\Delta|^2)$$

$q=2$:

$$E(\Delta)=\pm 2\sqrt{6+6\cos(\theta_m)}\mp\Delta\frac{2\sqrt{3}\cos(\theta_m)}{\sqrt{6+6\cos(\theta_m)}}(n+\tfrac{1}{2}) \tag{29}$$

$$\pm\Delta\frac{\sin(\theta_m)}{\sqrt{6+6\cos(\theta_m)}}-\Delta\frac{(\sin\eta-\sin(\theta_m-\eta))}{1+\cos(\theta_m)}+O(|\Delta|^2).$$

where

$$\theta_m=\begin{cases}\dfrac{2\pi m+\eta}{3} & q=1\\[2ex] \dfrac{2\pi(m+1/2)+2\eta}{3} & q=2\end{cases}\qquad m\in\{-1,0,1\}.$$

The above formula allows us to compute the zeroth- and first-order coefficients in the semiclassical expansion of the spectral energy $E(\Delta)=E0+\Delta E1+O(|\Delta|^{3/2})$ around a minimum $E0$ for $q=1$ and $q=2$. Please notice that in the expansion of the energy in powers of Δ there is no fractional powers, unless if there is band touching. So the remainder is of order Δ^2. If necessary we distinguish the three minima by its index m according to (29).

For the case $q=1$ Rammal and Bellissard (1990, section 3.5b) have computed the second-order correction $E2$ to the energy. A slight modification of their result, taking into account the shift of $\varphi/2$ due to the direct φ dependence of the triangular Hamiltonian, gives

$$E2=\frac{1}{8}\cos(\theta_m)(1+(1+2n)^2)+\frac{1}{18}\frac{\sin^2(\theta_m)}{\cos(\theta_m)}\frac{3(2n+1)^2+5}{4}$$

$$-\frac{1}{12}\cos(\theta_m)-\frac{\sqrt{3}}{6}\sin(\theta_m)(2n+1). \tag{30}$$

4.1. Numerical results

On the basis of equation (11) the spectrum for rational flux $\phi=2\pi(p/q)$ could be computed numerically. For some values of the parameter η we present the data in figures 4-8. The horizontal axis shows the energy scaled by 1/2 and the vertical axis shows the flux ϕ through a unit parallelogram scaled by 2π. Note that η represents a fixed flux through the up-triangle. Every picture displays the energy bands for various rational fluxes up to a maximal denominator of $q=40$. Around the $q=1$ and $q=2$ bands we have taken values of q up to 110 to emphasize the asymptotic behaviour. For a small value of $\eta=2\pi$ 0.0175 (figure 4) we observe a crossing of levels near the lowest eigenvalue. Figures 5 and 6 give an enlargement of this effect near $q=1$ and

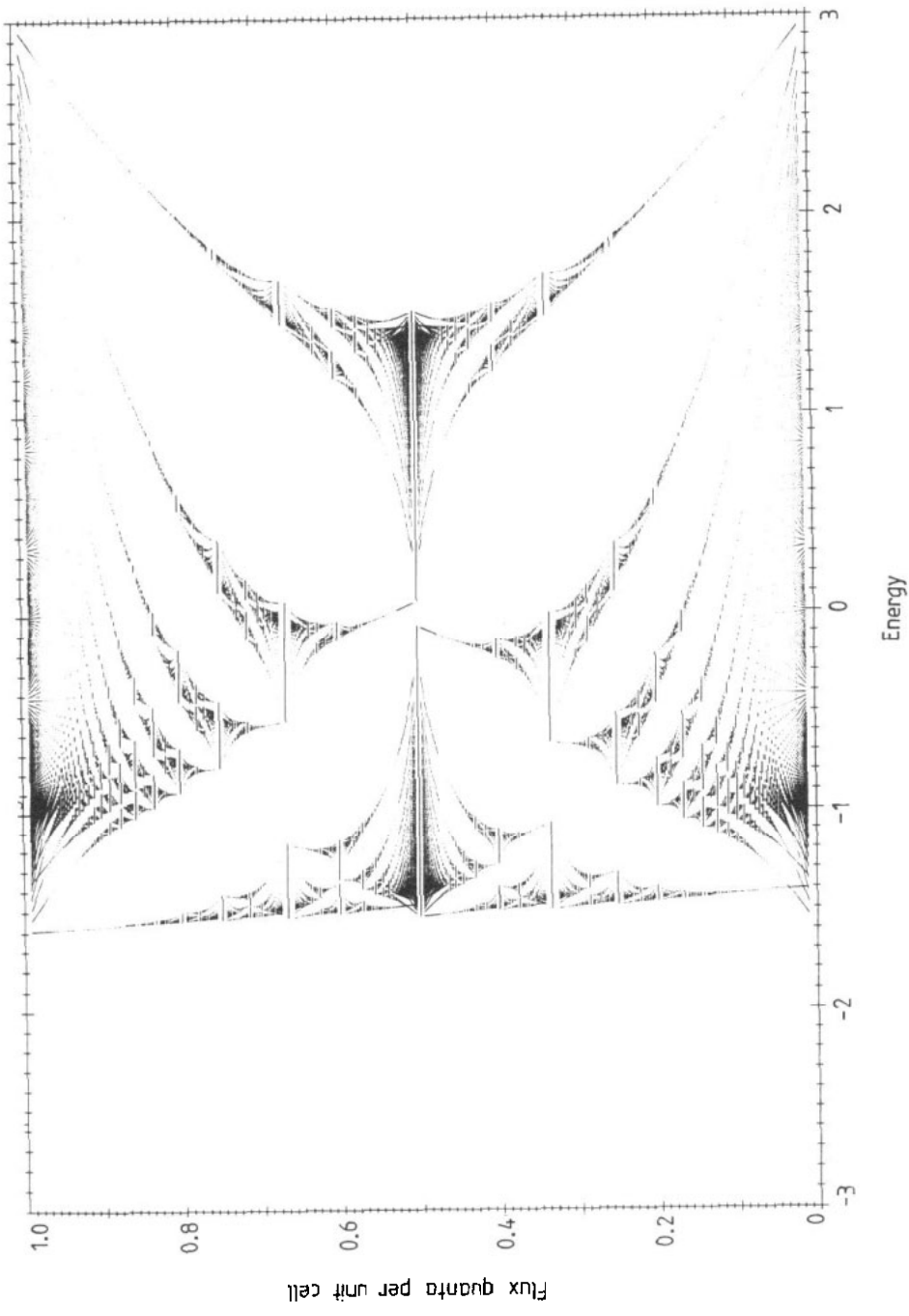

Figure 4. Spectrum of triangular lattice with $\eta = 2\pi\ 0.0175$ and $\varphi \in [0, 2\pi]$

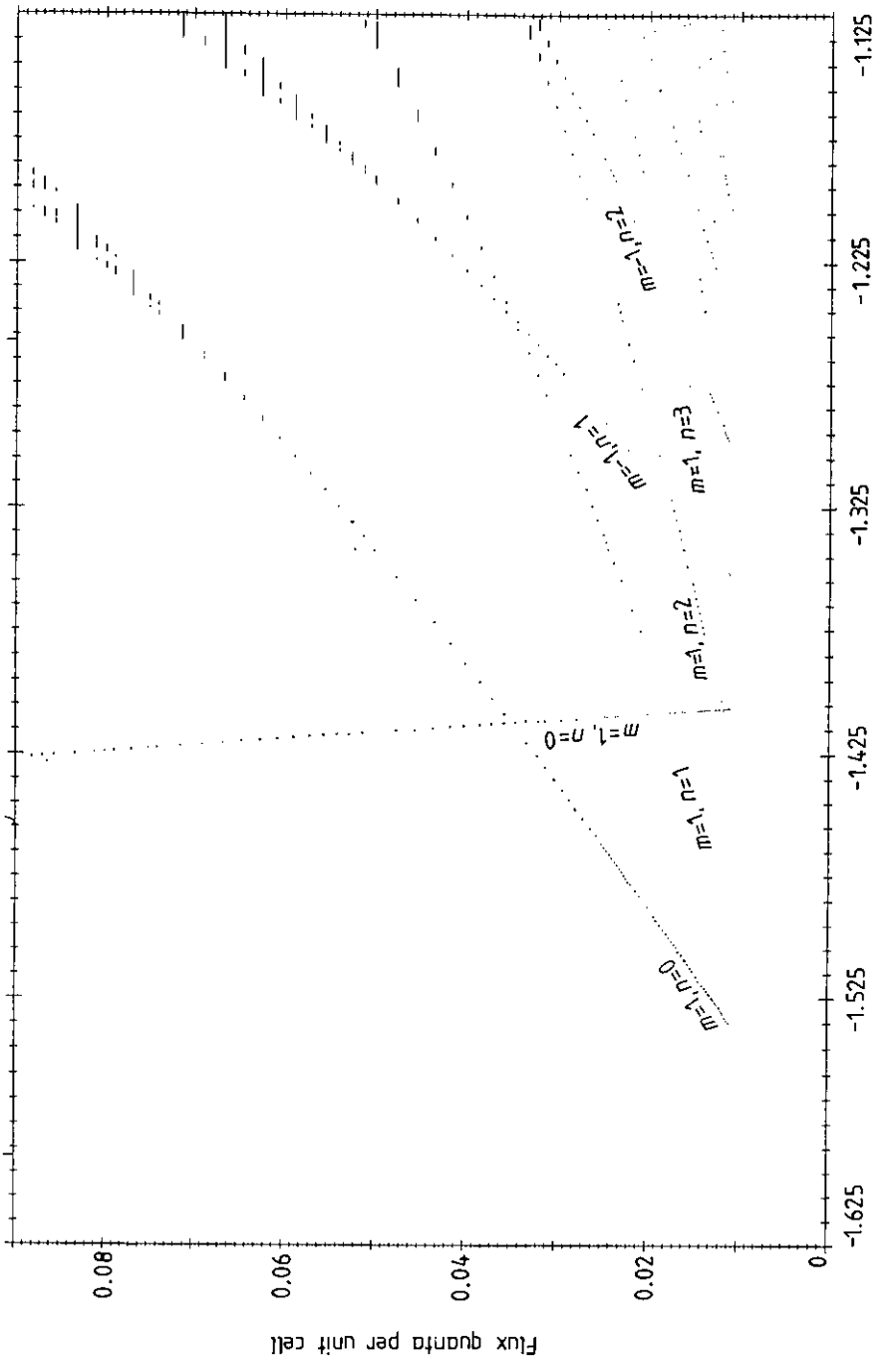

Figure 5. Spectrum of triangular lattice with $\eta = 2\pi\ 0.0175$ and $\varphi \approx 0$.

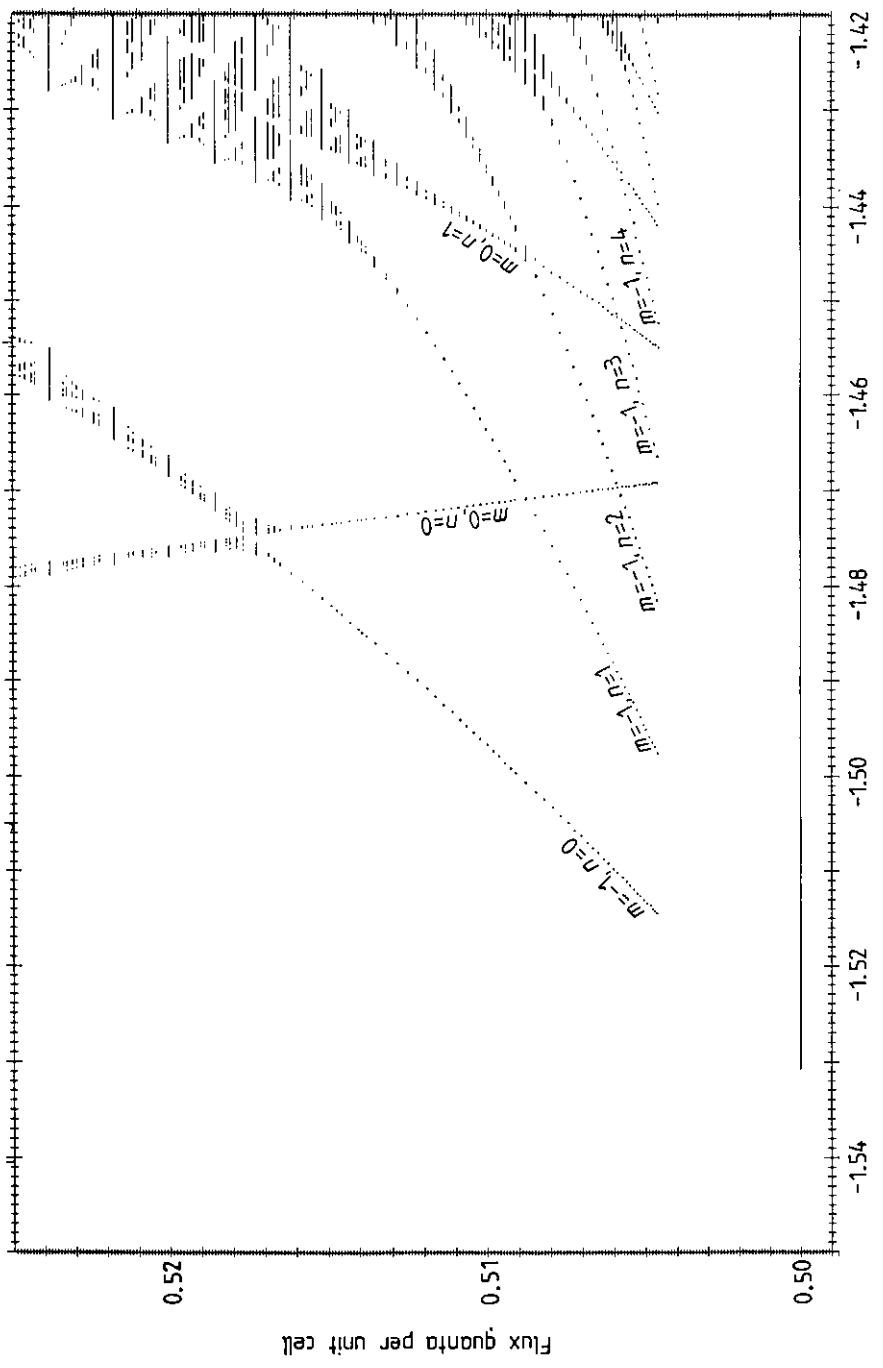

Figure 6. Spectrum of triangular lattice with $\eta = 2\pi\ 0.0175$ and $\varphi \approx 0.5$.

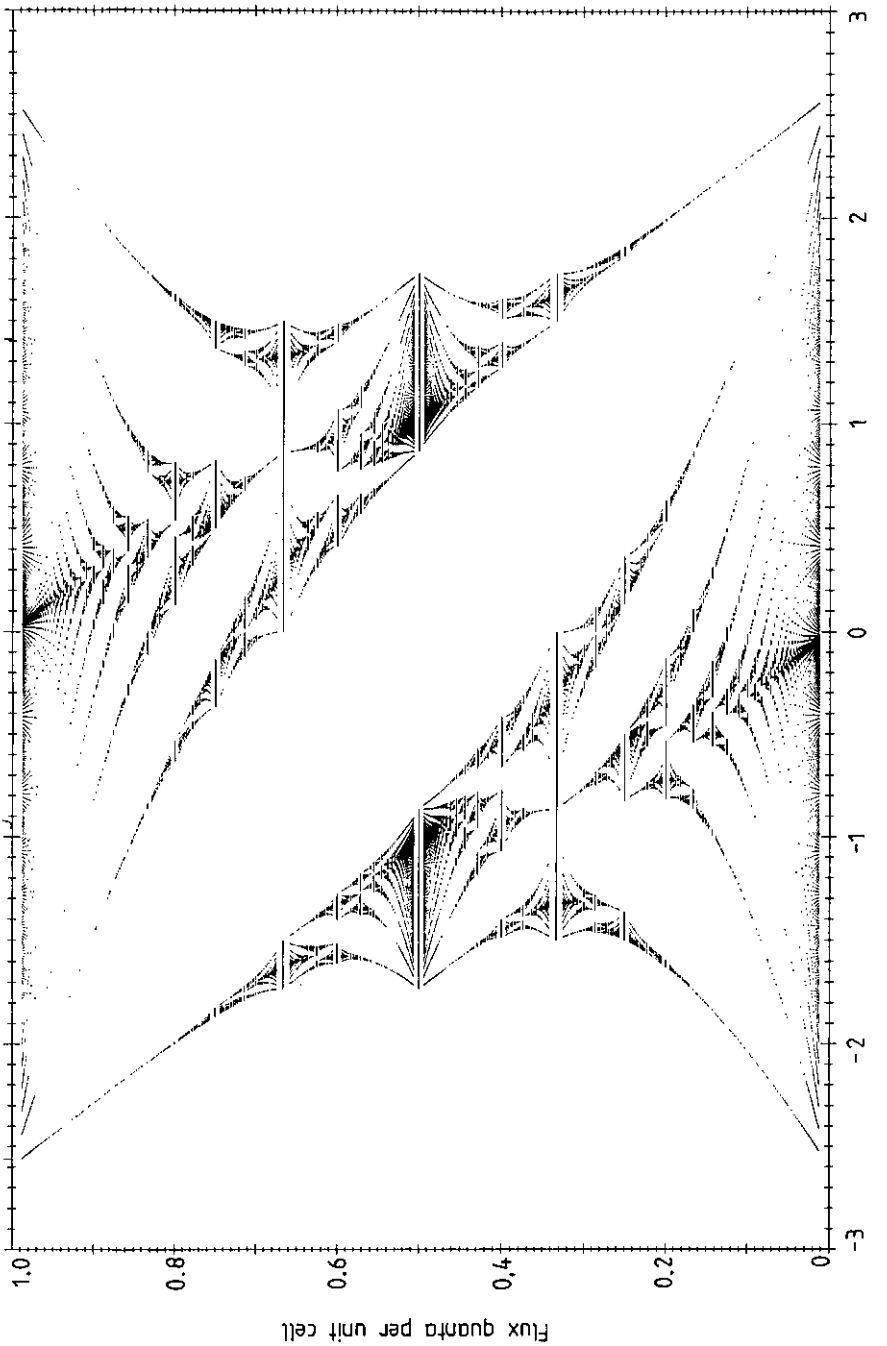

Figure 7. Spectrum of triangular lattice with $\eta = \pi/2$ and $\varphi \in [0, 2\pi]$.

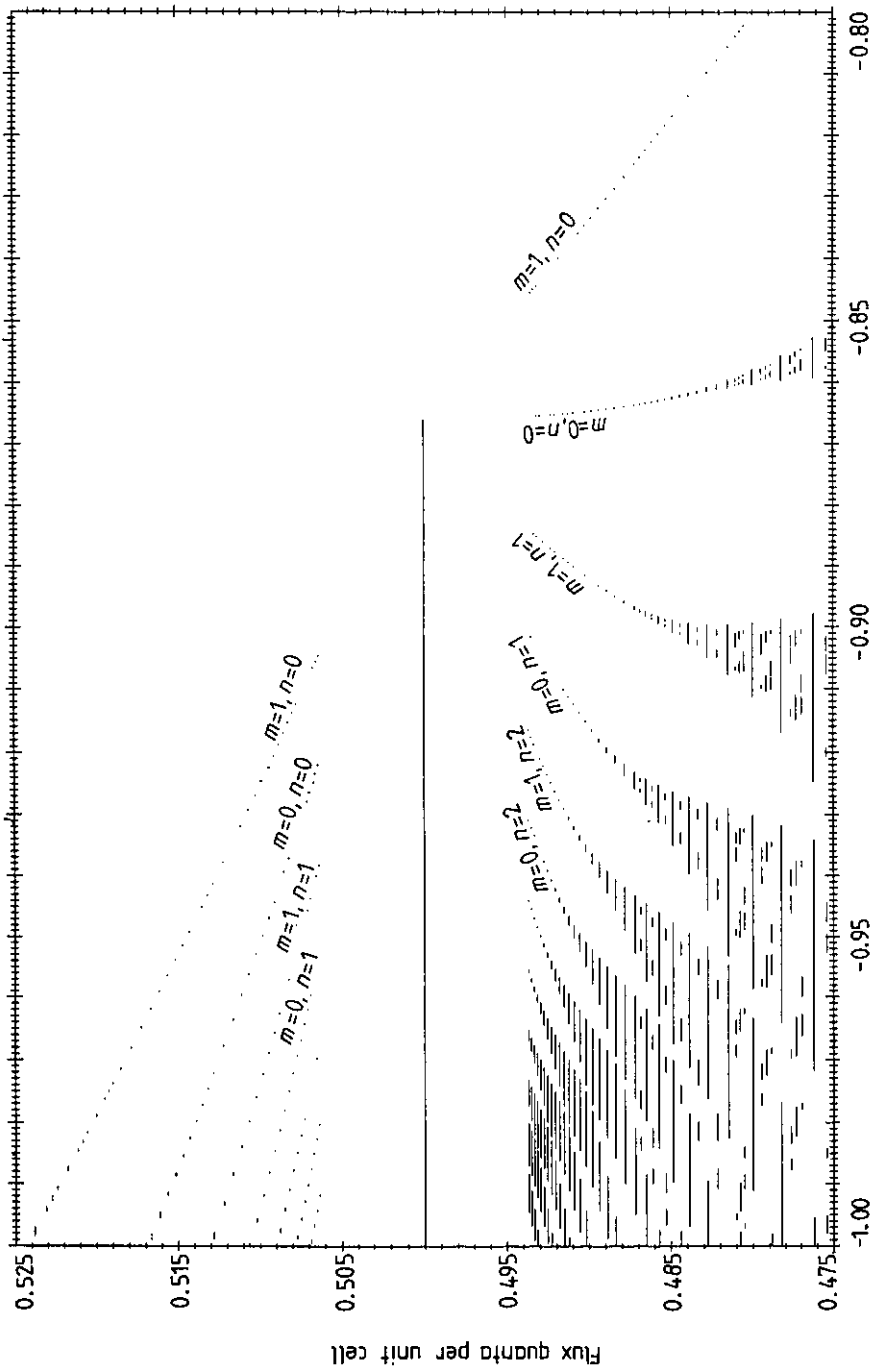

Figure 8. Spectrum of triangular lattice with $\eta = \pi/2$ and $\varphi \approx 0.5$.

$q = 2$, respectively. The pictures show already quite well that the spectral curves (as a function of flux) approach the band edges in general linearly. Exceptions are seen, where bands come close for instance in the centre of figure 4.

For $\eta = \pi/2$ the spectrum shows a symmetry under a reflection $E \to E$ and $\phi \to -\phi$ (figure 7), which can be proven analytically. As a result we find a degeneracy for the two minimal energies $E0$ with index $m = 0$ and $m = 1$ as shown in figure 8.

The numerical work was done on a simple personal computer using the 80-bit floating point format of the coprocessor. To solve the secular equation (10) we used the fact that in the triangular case for some values of k the secular problem gets into the form of a real-tridiagonal-matrix problem. It was solved by a modified Newton–Maehly algorithm (Stoer and Bulirsch 1980).

From the data of figures 5 and 6 we have extracted the spectral points belonging to 'semiclassical' asymptotics near the minima E_m of the energy. We have chosen some cases which show level crossing. That is, for $q = 1$ the minima with index $m = 1$, $m = -1$ and for $q = 2$ the one with $m = 0$, $m = -1$. Through a least-squares fit with a parabola we have adopted coefficients $E_{\text{num}} = E0_{\text{num}} + \Delta E1_{\text{num}} + \Delta^2 E2_{\text{num}}$. In table 2 they are compared with the results of the semiclassical approximation (denoted by the index 'sc') and show a very good agreement up to four digits. For $\eta = 0$ both minima are degenerate and the corresponding asymptotics coincide. For η small, $\neq 0$ the minimal values become different as well as there harmonic approximations. According to the Wilkinson–Rammal formula (26) the terms up to second order enter into the slope of the asymptotic line. This is the origin of the observed level crossing. For the $q = 1$ cases we have computed the second-order term E_{SC} according to formula (30). The results are shown in tables 2(a) and 2(b) and should be compared with the measured values $E2_{\text{num}}$. The agreement is not as good as for the first-order terms, since we fitted with a parabola only.

A similar table is taken from the data of figure 8 around the degenerate minima for $m = 0$ and $m = 1$, both for positive and negative Δ. In table 3 the numerical results are compared with the semiclassical formula. Note that the first-order coefficients take integer values (the tables show half-integers due to the scale in the energy axis). For $\eta = \pi/2$ again we find degeneracy for the extremal energy. While in the case of $\eta = 0$ also the slopes of $E(\Delta)$ show this degeneracy, now the asymptotics coming from the two coinciding extremals are distinct. As a result the level crossing for $\eta \approx \pi/2$ occurs for very small Δ only. With the accuracy of our calculation it cannot be displayed.

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Appendix. Symmetries of the triangular lattice spectra

Let $\sigma(\varphi, \eta)$ denote the spectrum of the triangular lattice Hamiltonian (3) as defined above. Using algebraic homomorphisms we prove the following symmetries of the

spectra:

(i) $\sigma(\varphi, \eta) = (-1)^n \sigma(\varphi, \eta + \pi \cdot n) \qquad n \in \mathbb{Z}$

(ii) $\sigma(\varphi, \eta = \pi/2) = -\sigma(\varphi, \eta = \pi/2).$

To prove (i) consider the map

$$\beta: \mathscr{A}_\varphi \mapsto \mathscr{A}_\varphi$$

defined through

$$\beta(T_1) := -T_1 \qquad \text{and} \qquad \beta(T_2) := -T_2$$

and the extension as a linear $*$-homomorphism (i.e. $\beta(AB) = \beta(A)\beta(B)$, $\beta(B^*) = (\beta(B))^*$, A, $B \in \mathscr{A}_\varphi$). The map is well defined since it preserves the commutation relation (2). It is invertible and therefore an automorphism of the algebra. Hence for the triangular lattice Hamiltonian (3) we have the symmetry

$$\beta(H(\eta + \pi)) = -H(\eta).$$

That is z belongs to the spectrum of $H(\eta + \pi)$ if and only iff-z belongs to the spectrum of $H(\eta)$. To prove (ii) we consider a second $*$-homomorphism

$$\beta': \mathscr{A}_\varphi \mapsto \mathscr{A}_{-\varphi}$$

with

$$\beta'(T_1) := -T_2^* \qquad \text{and} \qquad \beta(T_2) := -T_1^*.$$

Now we get

$$\beta'(H(\varphi, \eta = \pi/2)) = -H(-\varphi, \eta = \pi/2).$$

So z is a spectral point of $H(\varphi, \eta = \pi/2)$ if and only if $-z$ belongs to the spectrum of $H(-\varphi, \eta = \pi/2)$.

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