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Generic description of the degeneracies in Harper-like models

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Abstract. We consider quantum Hamiltonians with one degree of freedom, periodic both in position and in momentum (Harper-like Hamiltonians). With the use of the Chern index which topologically characterizes each spectral band and by a semi-classical description of the tunnelling effect, we establish conditions under which spectral degeneracies may occur. For a generic family of Harper-like Hamiltonians $H_{(\gamma_1,\gamma_2)}$, we obtain that degeneracies are localized on small ellipses aligned in one direction, in the space of external parameters γ_1, γ_2.

1. Introduction

We will consider models of quantum mechanics on the torus T^2, where the torus is the phase space. These kind of models include the Harper model, and are mostly studied in solid state physics, for example, in relation with the integer quantum Hall effect [1], or with superconductivity [2].

On the other hand, the simplicity of these models due to the compacity of the toroidal phase space and the finite-dimensionality of the Hilbert space, makes them good models for the study of the semi-classical limit and quantum chaos [3, 4].

We will focus the study on possible degeneracies in the spectrum. Existence of degeneracies is expected by a theorem of Von Neumann [5]: for Hermitian matrices (Hamiltonian without time-reversal symmetry), degeneracies occur with co-dimension three. This means that generically three external parameters have to be varied to find a degeneracy.

Degeneracies have been of special interest in physics since the discovery of Berry's phase [6, 7]. For example, if a stationary state is adiabatically carried along a closed path in a parameter space, the phase gained can be decomposed into a well known dynamical part and a geometrical part. Degeneracies have a direct influence on this geometric phase which can become apparent in interference effects [8]. In this way, degeneracies play a major role where adiabatic transport is involved: in the Aharonov–Bohm effect, in molecular physics beyond the Bohr–Oppenheimer approximation [10], in solid state physics with the Hall effect [1].

For the Harper-like models considered in this study, the spectrum has a finite band structure. To each band n, $n = 1 \to N$, is associated a topological integer Chern index C_n. For a given classical Hamiltonian $H(q, p)$ on the torus (a function of two conjugate dynamical variables (q, p)), the quantum one $\hat{H}$ depends on two quantal parameters (θ_1, θ_2) related to the periodicity conditions of the wavefunction. Degeneracies are of co-dimension three so with one external classical parameter, say γ, degeneracies may occur in the spectrum. Avron *et al* [11] have shown that for a one-parameter-dependent Harper-like model, an integer variation of the Chern index reveals the presence of a degeneracy.

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We look for a description of the Chern index values (and so of the degeneracies locus), for $\hbar \to 0$ in terms of classical dynamics. This paper uses this description and then places it within the general study of semi-classical analysis. The classical limit $\hbar \to 0$ is equivalent to $N \to \infty$. This will be explained in section 2. Note that the classical dynamics has one degree of freedom, so it is integrable. The semi-classical analysis which follows is based on the existence of quasi-modes. Roughly speaking, a quasi-mode is a quantum state which seems stationary for quite long times (over $\Delta t \sim \hbar^{-n}, n \in \mathbb{N}$). A method to construct them has been proposed in [18].

To study the degeneracy phenomenon, in general, we are led to consider a generic family of Hamiltonians depending on a finite number of parameters $H_{(\gamma_1,\gamma_2,\ldots,\gamma_P)}$. Degeneracies form a hypersurface of dimension $P-1$ in the P-dimensional space of external parameters. So they delimit domains with a constant Chern index. Simon has shown that the generic variation is ± 1 for two neighbourhood domains [9].

We look for rules which would give us the location of the degeneracies in the space of the parameters. For Harper-like models, it is already known that generically (over the space $(\gamma_1, \gamma_2, \ldots \gamma_P)$ and over the bands $n = 1 \to N$, for $N \to +\infty$) the Chern index of a given energy band is zero. This result has been obtained numerically by Huo and Bhatt [12]. The non-generic exceptions are due to a possible tunnelling effect between different trajectories. For example Thouless *et al* [1] have obtained non-zero values for the Chern indices in a particular Harper model with trajectories symmetric under translation. But when this symmetry is broken, the Chern indices get zero values, and correspondingly, some degeneracies occur in the spectrum [13].

We will restrict the study to a two-dimensional generic family of Hamiltonians $H_{(\gamma_1,\gamma_2)}$ which possess two different families of trajectories in the extrema of the energy spectrum, just like a double well potential. More precisely, the Chern indices will be calculated for the bands whose energy is between the extremum of the spectrum (the top or the bottom) and the energy of the nearest non-contractible separatrix. In this range of energy, the classical trajectories on the torus are contractible.

We will then obtain that in the two-dimensional space of classical parameters (γ_1, γ_2), degeneracies are generically localized on loops (of exponentially small width) and those loops are aligned in one direction, see figure 5.

In the next section, we precis the formalism of quantum mechanics on the torus. Then in section 3, we calculate the Chern index of a given energy band when there is a possible tunnelling effect between two trajectories. We then obtain two necessary conditions for the Chern index to be non-zero.

Using these results in section 4, we describe the shape of the degeneracies location for a generic family of Hamiltonians. Section 5 is devoted to a numerical illustration.

The following study uses mostly qualitative semi-classical arguments. The results could probably be expressed more quantitatively by using the extensive studies performed by Helffer and Sjöstrand concerning the semi-classical analysis of the Harper equation [14].

2. Quantum mechanics on the torus

We consider a one-degree-of-freedom classical Hamiltonian on the plane, periodic, with periods Q in position, and P in momentum:

$$H(q, p) = H(q + Q, p) = H(q, p + P). \tag{1}$$

This planar phase space will be denoted $\mathcal{P}_{qp}$. By identifying all the domains of sides (Q, P) in $\mathcal{P}_{qp}$, the classical mechanics can be restricted to a torus. This toroidal phase space will

be denoted ny $\mathcal{T}_{qp}$.

Quantum mechanically, (1) reads as

$$[\hat{T}_Q, \hat{H}] = [\hat{T}_P, \hat{H}] = 0$$

where $(\hat{T}_Q, \hat{T}_P)$ are the translations operators in position and momentum, respectively:

$$\hat{T}_Q = \exp(-\mathrm{i}Q\hat{p}/\hbar) \qquad \hat{T}_P = \exp(iP\hat{q}/\hbar)\,.$$

The three operators $\hat{H}, \hat{T}_Q, \hat{T}_P$ commute if in addition $[\hat{T}_Q, \hat{T}_P] = 0$, which is equivalent to $QP = Nh$ with $N \in \mathbb{N}$. The classical limit ($\hbar \to 0$) is then obtained when $N \to +\infty$.

The total Hilbert space $\mathcal{H} = \mathcal{L}^2(\mathbb{R})$ can be decomposed as the direct sum of the eigenspaces of operators $\hat{T}_Q$ and $\hat{T}_P$:

$$\mathcal{H} = \int\int \mathcal{H}_N(\theta_1, \theta_2)\, \mathrm{d}\theta_1\, \mathrm{d}\theta_2$$

$$\mathcal{H}_N(\theta_1, \theta_2) = \left\{ |\Psi\rangle \quad \text{st} \quad \left\{ \begin{array}{l} \hat{T}_Q|\Psi\rangle = \exp(\mathrm{i}\theta_1)|\Psi\rangle \\ \hat{T}_P|\Psi\rangle = \exp(\mathrm{i}\theta_2)|\Psi\rangle \end{array} \right. \right\}$$

with $(\theta_1, \theta_2) \in [0; 2\pi[^2$ related to the periodicity of the wavefunction under translations by an elementary cell. This parameter space also has the topology of a torus and will be denoted $\mathcal{T}_\theta = [0; 2\pi[^2$. This decomposition forms, in fact, a non-trivial vector bundle [15].

Each space $\mathcal{H}_N(\theta_1, \theta_2)$ is finite-dimensional: $\dim_{\mathbb{C}} \mathcal{H}_N(\theta_1, \theta_2) = N$. So in each space $\mathcal{H}_N(\theta_1, \theta_2)$, the spectrum is discrete:

$$\hat{H}|\Psi_n(\theta_1, \theta_2)\rangle = E_n(\theta_1, \theta_2)|\Psi_n(\theta_1, \theta_2)\rangle \qquad n = 1 \to N\,.$$

But for n fixed, as (θ_1, θ_2) are varied in $[0, 2\pi[^2$, the energy level $E_n(\theta_1, \theta_2)$ form a band energy, and the eigenvectors $|\Psi_n(\theta_1, \theta_2)\rangle$ form a 2D surface in the projective space. This surface is the base space of a complex-line-fibre-bundle whose topology is characterized by an integer C_n, the Chern index. It has been shown that C_n characterizes the sensitivity of eigenfunctions to changes of the boundary conditions (θ_1, θ_2) [16, 4, 17].

For what follows, we introduce the operator of orthogonal 'projection' $\hat{P}_{(\theta_1,\theta_2)}$ on the space $\mathcal{H}_N(\theta_1, \theta_2)$.

$$\hat{P}_{(\theta_1,\theta_2)} = \lim_{N\to+\infty} \left(\frac{1}{(2N+1)^2} \sum_{(n_1,n_2)\in[-N,N]^2} \exp(-\mathrm{i}n_1\theta_1 - \mathrm{i}n_2\theta_2)\hat{T}_Q^{n_1}\hat{T}_P^{n_2} \right). \tag{2}$$

Its action on a state $|\Psi\rangle$ is to produce a Bloch state, periodic both in position and momentum up to a phase (θ_1 or θ_2).

3. Resonances between two contractible trajectories

Suppose that at a given energy E, the constant energy lines in phase space $\mathcal{T}_{qp}$ are made of two contractible trajectories denoted by Γ_1 and Γ_2. These trajectories belong to two different families of contractible trajectories on the torus. We note $|1\rangle$ and $|2\rangle$, two semi-classical stationary states (quasi-modes), localized respectively on each family, in the planar phase space $\mathcal{P}_{qp}$, in the fundamental domain $[0, Q] \times [0, P]$. These quasi-modes are independant of (θ_1, θ_2) and can be constructed for example by a method proposed by Paul and Uribe [18]. A quantum state can be represented in the phase space $\mathcal{P}_{qp}$ or $\mathcal{T}_{qp}$ via the Husimi distribution which is a positive function in phase space [19]. Saying that a quantum state is localized on a trajectory means that its normalized Husimi distribution tends point-wise to zero outside the trajectory, for $\hbar \to 0$. The energies of the quasi-modes $|1\rangle$ and $|2\rangle$ are determined by Bohr–Sommerfeld quantization rule.

For fixed values of (θ_1, θ_2), we can construct semi-classical states of the torus $\mathcal{T}_{qp}$ (periodic on the plane) in the space $\mathcal{H}_N(\theta_1, \theta_2)$:

$$|\Psi_1(\theta)\rangle \equiv \hat{P}_{(\theta_1,\theta_2)}|1\rangle \qquad |\Psi_2(\theta)\rangle \equiv \hat{P}_{(\theta_1,\theta_2)}|2\rangle\,.$$

If the two quasi-modes have nearby energy, evaluations of the exact stationary states $|\Psi_+(\theta)\rangle$ and $|\Psi_-(\theta)\rangle$, with energy $E_+(\theta) \geqslant E_-(\theta)$ are obtained by diagonalizing the matrix of the restriction of the Hamiltonian in the subspace generated by $|\Psi_1(\theta)\rangle, |\Psi_2(\theta)\rangle$

$$\tilde{H}(\theta) = \begin{pmatrix} E_1(\theta) & \epsilon(\theta) \\ \bar{\epsilon}(\theta) & E_2(\theta) \end{pmatrix}$$

with $E_i(\theta) = \langle\Psi_i(\theta)|\hat{H}|\Psi_i(\theta)\rangle$, $i = 1, 2$ and $\epsilon(\theta) = \langle\Psi_1(\theta)|\hat{H}|\Psi_2(\theta)\rangle$.

3.1. Algebraic expression of the Chern index

We now wish to calculate the Chern index C_+ (respectively C_-) of the family of states $|\Psi_+(\theta)\rangle$, $\theta \in \mathcal{T}_\theta = [0, 2\pi]^2$ (respectively $|\Psi_-(\theta)\rangle$).

From their definition, the family of states $|\Psi_1(\theta)\rangle$ and $|\Psi_2(\theta)\rangle$ are localized on the trajectories Γ_1 and Γ_2 in the torus $\mathcal{T}_{qp}$, for every value of θ. It follows from an argument exposed in [29] or in [16] that their Chern index C_1 and C_2 are zero. Then because the total Chern index is conserved [11] $C_+ + C_- = C_1 + C_2 = 0$, we deduce that $C_- = -C_+$.

To calculate the Chern index C_+, we will use an algebraic characterization, see [20, ch 1]: C_+ is the algebraic number of intersection of the surface generated by $|\Psi_+(\theta)\rangle$ with a hyperplan $\mathcal{N}$, in the complex projective space of the Hilbert space. Here $\mathcal{N}$ will be the space orthogonal to the state $|\Psi_1\rangle$. So C_+ is the sum of the indices ($\iota = \pm 1$) of the zeros of the locally defined complex function $f_+(\theta) = \langle\Psi_1|\Psi_+(\theta)\rangle$. $\iota = +1$ if the Jacobian of f_+ is positive, $\iota = -1$ otherwise. Note that $f_+(\theta)$ is only locally defined because after diagonalization, $|\Psi_+(\theta)\rangle$ is defined only within a phase that we can fix only locally. For a more detailed discussion, see [17].

To overcome this obstacle, we consider the following complex function, globally defined on the torus $(\theta_1, \theta_2) \in \mathcal{T}_\theta$:

$$F_+(\theta) = \frac{\langle\Psi_1|\Psi_+(\theta)\rangle}{\langle\Psi_2|\Psi_+(\theta)\rangle}\,.$$

C_+ is then given by the sum of the indices ($\iota = \pm 1$) of the zeros of the complex function $F_+(\theta)$, $\theta \in \mathcal{T}_\theta = [0, 2\pi]^2$.

Diagonalization of the matrix $\tilde{H}(\theta)$ gives for θ such that $\epsilon(\theta) \neq 0$:

$$F_+(\theta) = \frac{\epsilon}{E + \left(E^2 + |\epsilon|^2\right)^{1/2}} = \frac{-E + \left(E^2 + |\epsilon|^2\right)^{1/2}}{\bar{\epsilon}}$$

with $E(\theta) = (E_2(\theta) - E_1(\theta))/2$.

Now suppose that $\epsilon(\theta^*) = 0$.

If $E(\theta^*) > 0$ we have for $\theta \to \theta^*$

$$F_+(\theta) = \frac{\epsilon}{E(1 + \left(1 + |\epsilon|^2/E^2\right)^{1/2})} \to 0\,.$$

So θ^* is a zero of F_+.

If $E(\theta^*) < 0$ we have for $\theta \to \theta^*$.

$$|F_+(\theta)| = \left|\frac{-E(1 + (1 + |\epsilon|^2/E^2)^{1/2})}{\epsilon b}\right| \to +\infty$$

θ^* is a pole of F_+.

We have obtained the following result.

Consider the domain $\mathcal{T}^+$ (respectively $\mathcal{T}^0, \mathcal{T}^-$):

$$\mathcal{T}^+ = \{\theta \in \mathcal{T}_\theta \text{st} E(\theta) > 0\}$$

(respectively $E(\theta) = 0$, $E(\theta) < 0$). Moreover, we denote θ^* the zeros of $\epsilon(\theta)$ and $\iota(\theta^*) = \pm 1$ their index. Then

$$C_+ = \sum_{\theta^* \in \mathcal{T}^+} \iota(\theta^*) . \tag{3}$$

This last result is valid, in general, for computing the Chern index of eigenvectors of a two-dimensional family of Hermitian matrices. Moreover, it is an obvious result from topological reasons, because a change of the Chern index occurs in a degeneracy. This happens when a zero θ^* crosses the border $\mathcal{T}^0$ (when $\epsilon(\theta^*) = 0$ and $E_2(\theta^*) - E_1(\theta^*) = 0$).

To calculate the Chern index C_+ there are now three steps: first we have to study the sign of the function $E(\theta)$, then to find the zeros of $\epsilon(\theta)$, and finally to calculate C_+ with (3).

3.2. Sign of $E(\theta)$

Let us write $|1\rangle_{(n_1,n_2)} = \hat{T}_Q^{n_1} \hat{T}_P^{n_2} |1\rangle$ which is the translation of the quasi-mode $|1\rangle$ localized on the trajectory $\Gamma_{1,(n_1,n_2)}$, translated of the trajectory Γ_1 in the cell (n_1, n_2). We similarly define $|2\rangle_{(n_1,n_2)} = \hat{T}_Q^{n_1} \hat{T}_P^{n_2} |2\rangle$ and the trajectory $\Gamma_{2,(n_1,n_2)}$.

From the definition of $E(\theta)$ and (2), we obtain

$$E(\theta) = (E_2 - E_1)/2 \propto (\langle 2|\hat{H}|2\rangle - \langle 1|\hat{H}|1\rangle)/2 + \sum_{(n_1,n_2)\in D_n} \text{Re}\{\exp(-in_1\theta_1 - in_2\theta_2)(\langle 2|\hat{H}|2\rangle_{(n_1,n_2)} - \langle 1|\hat{H}|1\rangle_{(n_1,n_2)})\} \tag{4}$$

with $D_n = \{(\mathbb{Z} \times \mathbb{N}) \setminus (-\mathbb{N} \times \{0\})\}$ being the half-plane of cells.

The term $\langle 1|\hat{H}|1\rangle_{(n_1,n_2)}$ (respectively $\langle 2|\hat{H}|2\rangle_{(n_1,n_2)}$) is exponentially small because it corresponds to the tunnelling interaction between the quasi-mode $|1\rangle$ localized in the cell $(0, 0)$ and the quasi-mode $|1\rangle_{(n_1,n_2)}$ localized in the cell $(n_1, n_2) \neq (0, 0)$. (respectively for $|2\rangle$ and $|2\rangle_{(n_1,n_2)}$). We write such an interaction term as

$$\langle 1|\hat{H}|1\rangle_{(n_1,n_2)} = m_E \exp(i\Phi_E) .$$

There exists semi-classical expression for tunnelling interaction term $m \exp(i\Phi)$ between two trajectories given in [21, 22, 14]

$$m \sim \hbar(\omega_1\omega_2)^{1/2} \exp(-|\text{Im } S|/\hbar) \qquad \Phi \sim \frac{\text{Re } S}{2\pi\hbar} \tag{5}$$

where ω_1 and ω_2 are the classical frequencies of the trajectories and S is the classical complex action between them. The main property we will use is that the modulus m decreases exponentially fast with the distance and with the energy barrier between the trajectories in phase space. $d = |\text{Im } S|$ defines an effective tunnelling distance between the two trajectories like the Agmon distance [23, 24]. Precisely the Agmon distance has been defined in configuration space but not in phase space.

So generically, the moduli of the term in (4) can be ordered, and decrease exponentially: $1 \gg m_{Ea} \gg m_{Eb} \gg m_{Ec} \ldots$. The dominant term in the sum of (4) corresponds to a tunnelling interaction $\langle 1|\hat{H}|1\rangle_{n_{Ea}}$ or $\langle 2|\hat{H}|2\rangle_{n_{Ea}}$ with $n_{Ea} = (n_1, n_2) \in \mathbb{Z}^2$, see figure 1. Then (4) can be written approximately as

$$E(\theta) \approx E_{(0,0)} + s_E m_{Ea} \cos(n_{Ea}\theta - \Phi_{Ea}) \tag{6}$$

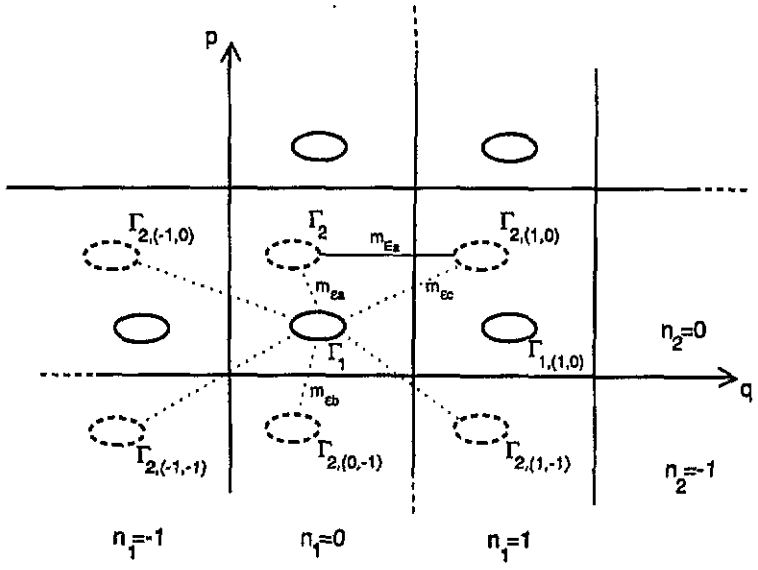

Figure 1. Schematic example of trajectories $\Gamma_{1,(n_1,n_2)}$ and $\Gamma_{2,(n_1,n_2)}$ on the periodic planar phase space $\mathcal{P}_{qp}$ decomposed in cells $(n_1, n_2) \in \mathbb{Z}^2$. Here, the full line between trajectories Γ_2 and $\Gamma_{2,(1,0)}$ means that the dominant term of 'auto-tunnelling-interaction' in (4) is obtained by $\langle 2|\hat{H}|2\rangle_{(1,0)}$ with modulus m_{Ea}. So $n_{Ea} = (1, 0)$. The dotted lines between trajectories Γ_1 and $\Gamma_{2,(n_1,n_2)}$ represent the tunnelling interaction terms in (7). The first three dominant terms of moduli $m_{\epsilon a}, m_{\epsilon b}, m_{\epsilon c}$ are obtained with the cells $n_{\epsilon a} = (0, 0)$, $n_{\epsilon b} = (0, -1)$, $n_{\epsilon c} = (1, 0)$.

with the constant term $E_{(0,0)} = (\langle 2|\hat{H}|2\rangle - \langle 1|\hat{H}|1\rangle)/2$ and the sign $s_E = \pm 1$ corresponds respectively to a dominant term $\langle 2|\hat{H}|2\rangle_{n_{Ea}}$ or $\langle 1|\hat{H}|1\rangle_{n_{Ea}}$.

3.3. Zeros of $\epsilon(\theta)$

$\epsilon(\theta)$ is given by

$$\epsilon(\theta) = \langle \Psi_1|\hat{H}|\Psi_2\rangle \propto \sum_{(n_1,n_2)\in\mathbb{Z}^2} \langle 1|\hat{H}|2\rangle_{(n_1,n_2)} \exp(-in_1\theta_1 - in_2\theta_2)\,. \tag{7}$$

Each term of interaction can be written in the form: $\langle 1|\hat{H}|2\rangle_{(n_1,n_2)} = m_\epsilon \exp(i\Phi_\epsilon)$. The moduli m_ϵ of the terms in the sum can be ordered and generically they decrease exponentially fast: $1 \gg m_{\epsilon a} \gg m_{\epsilon b} \gg m_{\epsilon c} \ldots$. Keeping only the first three dominant terms, $\epsilon(\theta)$ can be written approximatively as

$$\epsilon(\theta) \approx m_{\epsilon a} \exp(-in_{\epsilon a}\theta + i\Phi_{\epsilon a}) + m_{\epsilon b} \exp(-in_{\epsilon b}\theta + i\Phi_{\epsilon b}) + m_{\epsilon c} \exp(-in_{\epsilon c}\theta + i\Phi_{\epsilon c})$$

with $n_{\epsilon a}, n_{\epsilon b}, n_{\epsilon c} \in \mathbb{Z}^2$ being the cells of the first three closer trajectories $\Gamma_{2,(n_1,n_2)}$ from the trajectory Γ_1 in cell $(0, 0)$, with respect to the Agmon distance (cf figure 1).

To pursue the calculation, we now suppose that $\delta = \det((n_{\epsilon a} - n_{\epsilon b}), (n_{\epsilon a} - n_{\epsilon c})) = \pm 1$. This means that the three cell $n_{\epsilon a}, n_{\epsilon b}, n_{\epsilon c}$ are not aligned in the phase space $\mathcal{P}_{qp}$ and that they enclose an area of one cell. For example, figure 1 gives $\delta = +1$.

We now consider the following bijective mapping: $\theta = (\theta_1, \theta_2) \in [0, 2\pi[^2 \rightarrow \phi = (\phi_1, \phi_2) \in [0, 2\pi[^2$ modulus 2π given by

$$\phi \equiv N\theta + \phi \quad [2\pi] \tag{8}$$

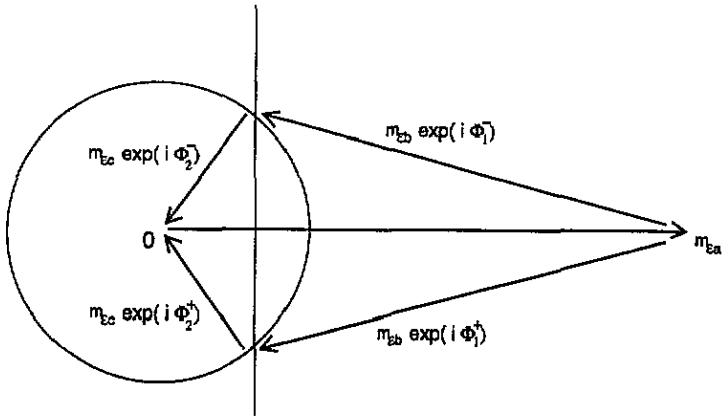

Figure 2. This diagram on the complex plane $\mathbb{C}$ shows the two solutions $(\phi_1^{\pm}, \phi_2^{\pm})$ of $\tilde{\epsilon}(\phi_1, \phi_2) = m_{\epsilon a} + m_{\epsilon b}\exp(i\phi_1) + m_{\epsilon c}\exp(i\phi_2) = 0$ with the assumption that $m_{\epsilon c} \ll m_{\epsilon a}, m_{\epsilon b}$.

with $N = ((n_{\epsilon a} - n_{\epsilon b}); (n_{\epsilon a} - n_{\epsilon c})) \in SL(2, \mathbb{Z})$ and $\phi = (\Phi_1; \Phi_2) = (\Phi_{\epsilon b} - \Phi_{\epsilon a};\ \Phi_{\epsilon c} - \Phi_{\epsilon a}) \in \mathbb{R}^2$.

Note that $|2\rangle$ is defined with an arbitrary choice of phase. $\Phi_{\epsilon a}, \Phi_{\epsilon b}, \Phi_{\epsilon c}$ depend on this phase, but Φ_1, Φ_2 do not.

We have

$$\epsilon(\theta) \approx \exp(-in_{\epsilon a}\theta + i\Phi_{\epsilon a})\,\tilde{\epsilon}(\phi_1, \phi_2)$$

with $\tilde{\epsilon}(\phi_1, \phi_2) = m_{\epsilon a} + m_{\epsilon b}\exp(i\phi_1) + m_{\epsilon c}\exp(i\phi_2)$.

The zeros of $\epsilon(\theta)$ are obtained from those of $\tilde{\epsilon}(\phi_1, \phi_2)$ with the inverse mapping of (8). From figure 2 it is easy to see that $\tilde{\epsilon}(\phi_1, \phi_2) = 0$ has two solutions $(\phi_1^{\pm}, \phi_2^{\pm})$ provided that $m_{\epsilon b} \in [m_{\epsilon a} - m_{\epsilon c}; m_{\epsilon a} + m_{\epsilon c}]$ and $m_{\epsilon c} \ll m_{\epsilon a}, m_{\epsilon b}$:

$$\begin{aligned}(\phi_1^-, \phi_2^-) &\approx \left(\pi, \cos^{-1}\left(\frac{m_{\epsilon b} - m_{\epsilon a}}{m_{\epsilon c}}\right)\right) \qquad \text{with index} \quad \iota = -1 \\ (\phi_1^+, \phi_2^+) &\approx \left(\pi, -\cos^{-1}\left(\frac{m_{\epsilon b} - m_{\epsilon a}}{m_{\epsilon c}}\right)\right) \qquad \text{with index} \quad \iota = +1\,.\end{aligned} \tag{9}$$

3.4. Two necessary conditions to have a non-zero Chern index

First let us remark that the function $\epsilon(\theta)$ has values in $\mathbb{C}$, which is a contractible space. The sum of the indices over all its zeros is therefore equal to zero: $\sum_{\theta^* \in \mathcal{T}_\theta} \iota(\theta^*) = 0$. Mathematically, the Brouwer degree of $\epsilon(\theta)$ is zero [25]. From (3) we deduce that if the sign of $E(\theta)$ is constant ($\mathcal{T}^+ = \mathcal{T}_\theta$ or $\mathcal{T}^+ = \emptyset$) then $C_+ = 0$. Therefore, in order that $C_+ \neq 0$, it is necessary for $E(\theta)$ to change sign. From (6), $E_{(0,0)}$ must be in an exponentially small neighbourhood of zero: $|E_{(0,0)}| < m_{Ea}$. It is, in fact, the well known 'resonance condition' between the two quasi-modes $|\Psi_1\rangle$ and $|\Psi_2\rangle$: $\langle 2|\hat{H}|2\rangle \approx \langle 1|\hat{H}|1\rangle(\pm m_{Ea})$.

Secondly, in order to make $\epsilon(\theta)$ vanish, we found that we must have $m_{\epsilon a} \approx m_{\epsilon b}\ (\pm m_{\epsilon c})$. This means that the two nearest representative, of trajectory Γ_2 on the plane $\mathcal{P}_{qp}$ must be at equal (Agmon) distance from the trajectory Γ_1. This is an 'equidistance condition' (see figure 3).

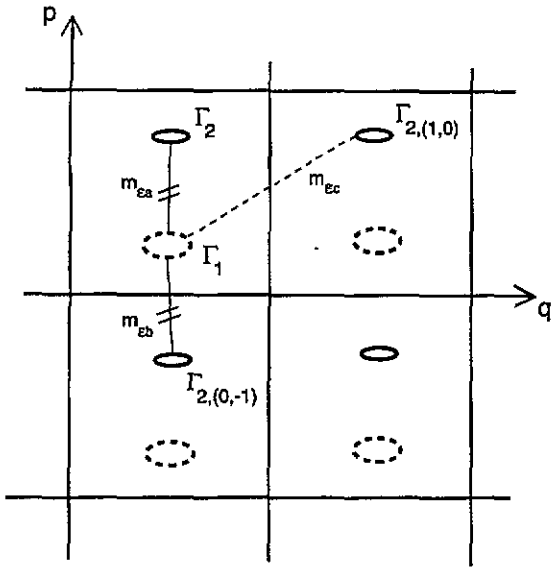

Figure 3. Illustration of the second necessary 'equidistance' condition to have a non-zero Chern index: $m_{\epsilon b} \in [m_{\epsilon a} - m_{\epsilon c}; m_{\epsilon a} + m_{\epsilon c}]$ if $m_{\epsilon c} \ll m_{\epsilon a}, m_{\epsilon b}$. The two nearest representatives of trajectory Γ_2 on the plane $\mathcal{P}_{qp}$ (here Γ_2 and $\Gamma_{2,(0,-1)}$) must be at equal tunnelling distance from the trajectory Γ_1.

4. Qualitative aspect of the degeneracy lines

If we consider $E_{(0,0)}$ and $m_{\epsilon b}$ as independant parameters, from the previous paragraph we deduce that in the two-dimensional space $(E_{(0,0)}, m_{\epsilon b})$, the Chern index C_+ is zero outside a small neighbourhood of the point $(E_{(0,0)}, m_{\epsilon b}) = (0, m_{\epsilon a})$. The degeneracy line which surrounds the domain $C_+ \neq 0$ form a compact curve in this neighbourhood. We find this degeneracy line by solving the system $\{E(\theta) = 0; \epsilon(\theta) = 0\}$ using the above expressions (6), (8) and (9).

Let $X = (m_{\epsilon b} - m_{\epsilon a})/(m_{\epsilon c})$ and $Y = (-s_E E_{(0,0)})/(m_{Ea})$. The system is equivalent to

$$\phi \equiv N\theta + \phi \quad [2\pi] \qquad \phi = (\pi, \pm\cos^{-1}(X)) \qquad Y = \cos(n_{Ea}\theta - \Phi_{Ea}) \tag{10}$$

and gives

$$X = \cos(t + \Phi_2) \qquad Y = \cos(rt + \Psi) \tag{11}$$

with $t \in \mathbb{R}$, $r = \delta \det(n_{\epsilon a} - n_{\epsilon b}; n_{Ea}) \in \mathbb{Z}$ and $\Psi = (\delta \det(n_{Ea}; n_{\epsilon a} - n_{\epsilon c})(\pi - \Phi_1) - \Phi_{Ea}) \in \mathbb{R}$.

If $|\delta| > 1$, the system (10) can be solved and instead of (11), we obtain parametric equations for a finite number of Lissajou curves. But we have not found examples of Hamiltonians where $|r| > 1$ nor $|\delta| > 1$ may be realized.

So we now suppose that $r = \pm 1$. The degeneracy line is therefore an ellipse. As we have said, outside the ellipse the Chern index is $C_+ = 0$. Inside, the Chern index is obviously $C_+ = \pm 1$. From (3) we calculate: $C_+ = \text{sign}(s_E \delta \sin(\Psi - \Phi_2))$.

Up to now, we have emphasized the direct link there is between the Chern index value and the degeneracies. But from its own definition the Chern index informs us on the stationary states $|\Psi_+(\theta)\rangle$, $|\Psi_-(\theta)\rangle$, especially on their density on the phase space $\mathcal{T}_{qp}$, depending on $\theta = (\theta_1, \theta_2)$. If the Chern index is non-zero, we have seen that for a special value θ^*, $\langle\Psi_1(\theta^*)|\Psi_+(\theta^*)\rangle = 0$. It means that the stationary wavefunction of $|\Psi_+(\theta^*)\rangle$ (more exactly its Husimi distribution on phase space [13]) is totally localized on the trajectory Γ_2. Respectively, the stationary wavefunction of $|\Psi_-(\theta^*)\rangle$ is totally localized on the trajectory Γ_1. For this special value θ^* and concerning quantum mechanics in the

Hilbert space $\mathcal{H}_N(\theta_1, \theta_2)$ (and not $\mathcal{L}^2(\mathbb{R})$), we deduce that there is no tunnelling effect between the two trajectories. Conversely, for another value θ^{**}, the state $|\Psi_+(\theta^{**})\rangle$ is localized on the trajectory Γ_1. So for intermediate values of θ, the Husimi distribution of the stationary states on phase space are equally distributed on trajectories Γ_1 and Γ_2, and tunnelling effect occurs. Such a relation between the Chern index value and localization of the wavefunction on the phase space has been put forward by Khomoto [17] in terms of the zeros of the wavefunction in phase space.

Now we discuss the qualitative aspect of the degeneracy lines in the space of external parameters of the classical Hamiltonian. Let us consider a generic two-dimensional family of classical Hamiltonians $H_{(\gamma_1,\gamma_2)}$ having two different families of contractible trajectories. This means that we are assuming that the set $\{(q, p)/H(q, p) = E\}$ has two contractible connected components Γ_1 and Γ_2.

The degeneracy equations (11) depend on the parameters X, Y, Φ_2, Ψ where various tunnelling interaction terms $m\exp(i\Phi)$ are involved. From the semi-classical expressions of these terms, (5), we deduce that a classical parameter γ may have an influence of order

$$(\partial m/\partial\gamma) \sim (m/\hbar) \qquad \text{and} \qquad (\partial\Phi/\partial\gamma) \sim (1/\hbar)\,.$$

Then for the parameters of (11):

$$(\partial X/\partial\gamma) \sim (m_{\epsilon a})/(\hbar m_{\epsilon c}) \qquad (\partial Y/\partial\gamma) \sim (1/(\hbar m_{Ea}))$$

$$(\partial\Phi_2/\partial\gamma) \sim (1/\hbar) \qquad (\partial\Psi/\partial\gamma) \sim (1/\hbar)\,.$$

Thus if γ is varied on a scale $\Delta\gamma \ll \hbar$, Φ_2 and Ψ can be considered as constant. On that scale, (γ_1, γ_2) are then generically mapped on (X, Y). From the previous section, we deduce that in the space (γ_1, γ_2), the degeneracy line is an ellipse inscribed in a rectangle centered in $(\gamma_1, \gamma_2) = (\gamma_1^*, \gamma_2^*)$ with sides exponentially small. If γ_1 is associated with X and γ_2 with Y, these two sides can be calculated from the previous evaluations

$$\Delta\gamma_1 \approx \left|\frac{\partial\gamma_1}{\partial X}\right|\Delta X \sim (\hbar m_{\epsilon c})/(m_{\epsilon b}) \sim h\exp(-(d_c - d_b)/h)$$

$$\Delta\gamma_2 \approx \left|\frac{\partial\gamma_2}{\partial Y}\right|\Delta Y \sim \hbar m_{Ea} \sim h\exp(-d_E/h)$$

where d_E, d_b and d_c are the Agmon distances corresponding to the tunnelling interaction terms $m_{Ea}, m_{\epsilon b}$ and $m_{\epsilon c}$, respectively (see figure 1).

More intuitively, we found, in the previous section, that in order to have a non-zero Chern index, two necessary conditions must be fulfilled. Each of these two conditions are of co-dimension one. For example, the 'resonance condition' can be realized by varying the action of the trajectories of the second well (the phase space surface of the trajectory), here γ_2. The second 'equidistance condition' can be realized by varying the mutual distance between the two trajectories, here γ_1. The particular value of these two parameters, $(\gamma_1, \gamma_2) = (\gamma_1^*, \gamma_2^*)$, corresponds to the case where the two conditions are both satisfied, see figure 4.

Moreover, the energy spacing is of order $\Delta E \sim \hbar$. If γ_2 is varied, the resonance condition will be fulfilled again between two different quantum levels. In this way, we expect a series of degeneracy ellipses, aligned in one direction, with a mutual distance of order $\Delta'\gamma_2 \sim \Delta E/(\partial E/\partial\gamma_2) \sim \hbar$, see figure 5. These ellipses may be non-equivalent because on a scale $\Delta'\gamma_2 \sim \hbar$, Φ_2 and Ψ may have changed.

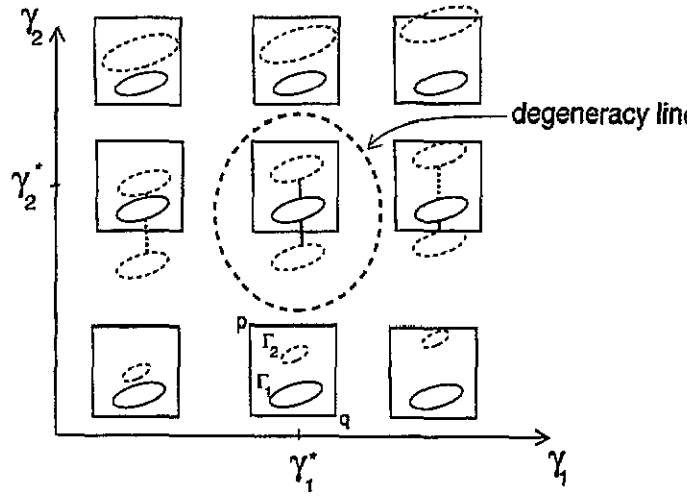

Figure 4. Two families of contractible trajectories Γ_1, Γ_2 (in the neighbourhood of $E = H(q, p)$), *for a two parameters dependant Hamiltonian* $H_{(\gamma_1,\gamma_2)}$. *Here* γ_1 *is the mutual distance* between the two trajectories and γ_2 is the action of the trajectory Γ_2. The equidistance condition is satisfied for $\gamma_1 \approx \gamma_1^*$. The resonance condition (same action of the two trajectories) is satisfied for $\gamma_2 \approx \gamma_2^*$. Then the Chern index of a given band is $C_n = \pm 1$ in a neighbourhood of (γ_1^*, γ_2^*) limited by a closed degeneracy line, outside of which $C_n = 0$.

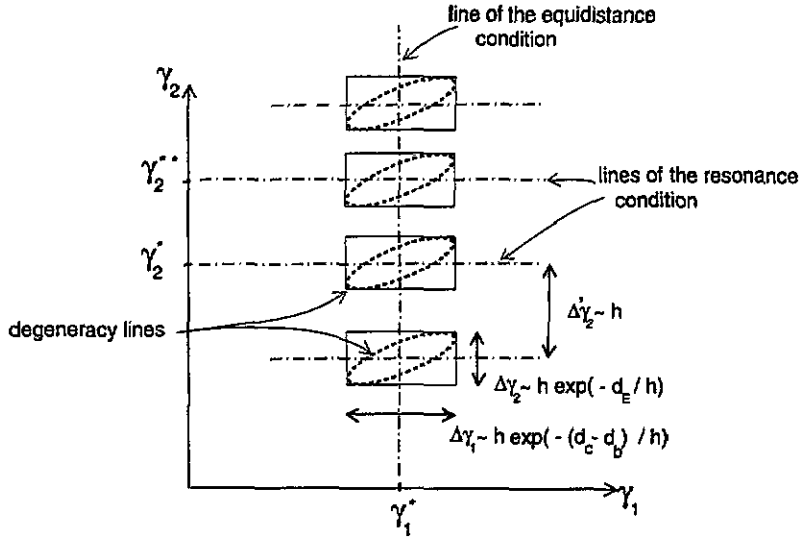

Figure 5. Schematic representation of the degeneracy lines for a given level of a generic family of Harper-like Hamiltonian, with two wells. Each degeneracy line is an exponentially small ellipse. These ellipses take place at the intersection of the line corresponding to the equidistance condition, with the transverse lines corresponding to the resonance condition. Inside the small ellipses, the Chern index is ± 1 and outside it vanishes.

5. Numerical illustration

In order to illustrate the previous analytical result, let us consider the following Hamiltonian dependent on one parameter $\gamma \in [0, 2]$ which has a double well. We take $Q = P = 1$,

$$H_\gamma(q, p) = -\cos(2\pi q) - \cos(4\pi p) - \tfrac{1}{4}\cos\left(4\pi q + \tfrac{1}{4}\pi\right) - \gamma\cos(2\pi p)\,. \tag{12}$$

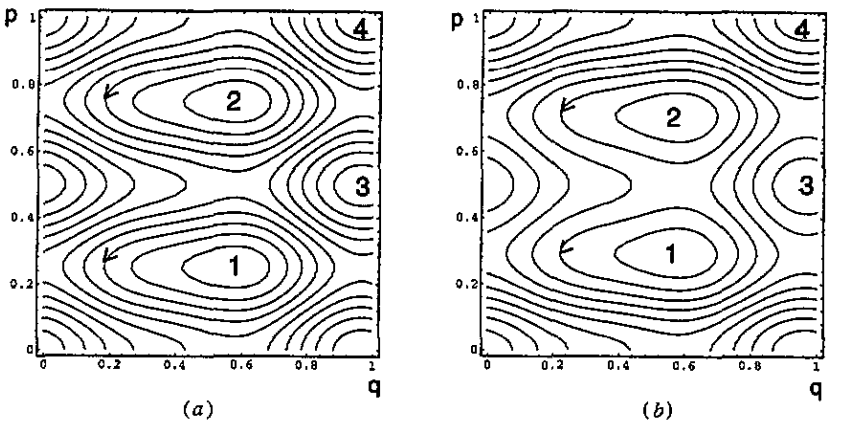

Figure 6. Energy levels of the classical Hamiltonian H, (12). Families of trajectories 1 and 2 are in the upper part of the spectrum and families 3 and 4 in the lower part. (*a*) $\gamma = 0$. Trajectories Γ_1 and Γ_2 encircling the points 1 and 2, respectively, are symmetric under a translation in momentum. (*b*) $\gamma = 1$. The symmetry under translation is broken. Trajectories Γ_1 and Γ_2 get closer to each other, like on figure 4 for the schema corresponding to $\gamma_1 < \gamma_1^*$, $\gamma_2 = \gamma_2^*$. For a given energy, the action of trajectories Γ_4 increases, like on figure 4 for the schema corresponding to $\gamma_1 = \gamma_1^*$, $\gamma_2 > \gamma_2^*$.

The constant energy curves in the torus $\mathcal{T}_{qp}$ are displayed in figure 6. We denote by Γ_1 and Γ_2 the two families of trajectories with positive energy, encircling the points 1 and 2, and by Γ_3 and Γ_4 the two families of trajectories with negative energy.

The Hamiltonian (12) is quantized by replacing the dynamical variables (q, p) by the operators of position and momentum $\hat{q}$, $\hat{p}$, respectively.

From figure 6, we guess that the dominant term of tunnelling interaction comes from the cells pictured in figure 1: $n_{Ea} = (1, 0)$, $n_{\epsilon a} = (0, 0)$, $n_{\epsilon b} = (0, -1)$, $n_{\epsilon c} = (1, 0)$. This numerical example therefore corresponds to the case treated in all the previous figures. There is, however, a slight difference: the numerical example presented here does not satisfy the generic conditions: because of the translation symmetry, for $\gamma = 0$, the dominant term in (4) comes equally from $\langle 1|\hat{H}|1\rangle_{(1,0)}$ and $\langle 2|\hat{H}|2\rangle_{(1,0)}$. But this does not modify qualitatively the results because $|2\rangle = \hat{T}_{P/2}|1\rangle$, and we have $\langle 1|\hat{H}|1\rangle_{(1,0)} = \exp(i\pi N)\langle 2|\hat{H}|2\rangle_{(1,0)}$. If N is odd, in (6) and everywhere, m_{Ea} is changed by $2m_{Ea}$.

For $\gamma = 0$, the trajectories Γ_1 and Γ_2 are symmetric under the translation $\hat{T}_{P/2}$. So the conditions of resonance and equidistance are both fulfilled. We therefore expect the Chern indices to be non-zero. The same statement can be made for the trajectories Γ_3 and Γ_4. As concerns the corresponding bands, we can say that in the parameter space diagram, figure 5, their representative point lies inside the little loop, on the point (γ_1^*, γ_2^*), surrounded by a degeneracy line.

For $\gamma \neq 0$, the symmetry under translation is broken.

The family of trajectories Γ_1 and Γ_2, however, conserve a symmetry by reflexion with respect to the line $p = \frac{1}{2}$. Therefore the resonance condition is still satisfied. But the trajectories Γ_1 and Γ_2 get closer in the phase space, so the second condition of 'equidistance' is not fulfilled. In agreement with the schematic representation of figure 5, where γ acts as γ_1, the representative point in the parameter space gets out of the small ellipse and lies on the half line $\gamma_1 < \gamma_1^*$; $\gamma_2 = \gamma_2^*$ when γ increases. So a degeneracy occurs and the Chern indices change to zero.

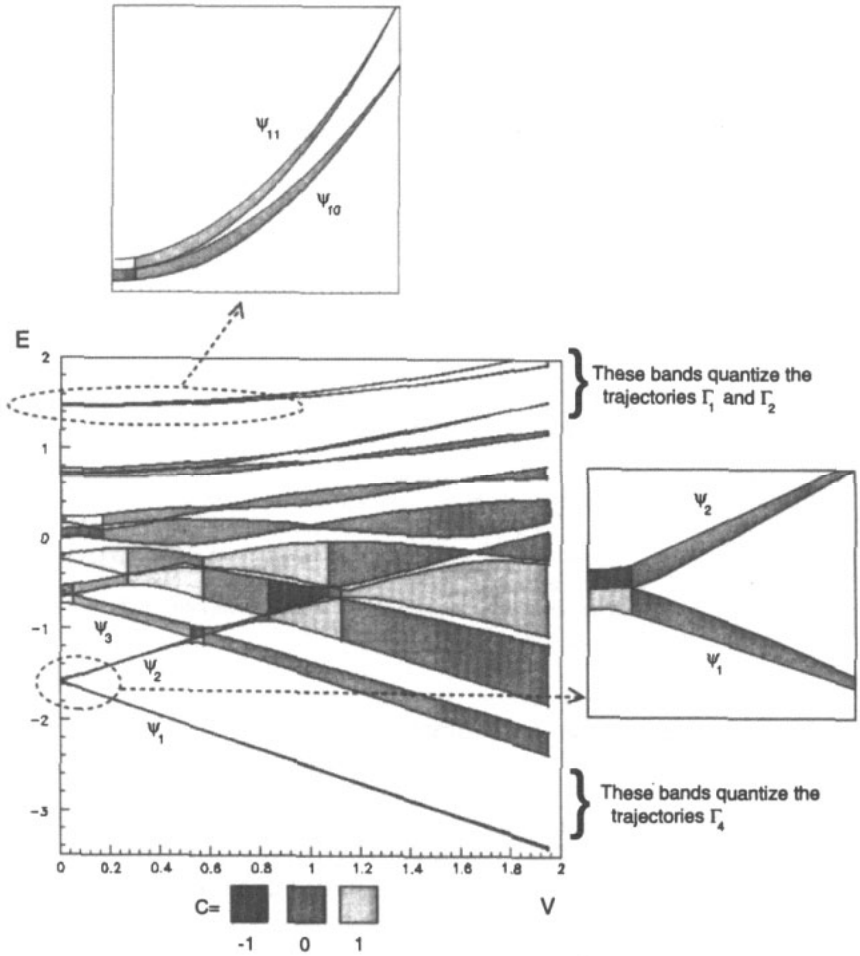

Figure 7. Numerical calculation of the energy bands and Chern indices of H (12), for $N = 11$ bands. For $\gamma = 0$, all the Chern indices are $C = \pm 1$. A variation of the Chern index is marked by a vertical line which indicates a degeneracy. Remark on the details that there are degeneracies in $\gamma \neq 0$.

Figure 7 shows the energy bands and Chern indices of the spectrum of H obtained by a numerical calculation. We observe the phenomenon we are discussing in the upper part of the spectrum, for the states Ψ_{10} and Ψ_{11}. The two bands remain close to each other because the resonance condition is always satisfied.

Concerning the families of trajectories Γ_3 and Γ_4, a quite analoguous description can be made. This time, the equidistance condition is always fulfilled, but the resonance condition is not satisfied when $\gamma \neq 0$. Now the parameter γ plays the same role as the parameter γ_2 of figure 5. As γ increases, the representative point gets out the ellipse on figure 5, and lies on the line $\gamma_1 = \gamma_1^*$. So a degeneracy occurs, the Chern indices change to zero before crossing an other ellipse at the position $\gamma_2 = \gamma_2^{**}$.

Indeed, in figure 7 we observe that the two levels Ψ_1 and Ψ_2 get away from each over in agreement with the Bohr–Sommerfeld semi-classical quantization rule for each family of trajectory. At the very beginning $\gamma \sim 0.01$ there is a degeneracy which makes the Chern

index change to zero. For $\gamma \sim 0.6$, the ground state Ψ_2 of the family of trajectories Γ_3 crosses the first excited state Ψ_3 of the family of trajectories Γ_4. At that point, there is a resonance, accompanied by degeneracies which change the Chern indices. It corresponds to the crossing of a second small ellipse of figure 5 at the value γ_2^{**}.

6. Conclusion

We have obtained a semi-classical description of the degeneracies occurring far away from the first non-contractible separatrix in the spectrum of Harper-like models with two wells. The present description could be generalized for arbitrary Hamiltonians with an arbitrary number of wells and to the whole spectrum, even for non-contractible trajectories, with non-trivial expected results. In [1], Thouless *et al* have shown that for a particular Hamiltonian with trajectories symmetric under translation, the Chern indices are the solution of a diophantine equation.

The results presented here are similar to those obtained by Colin de Verdière [24], and in the same spirit of studying a generic family of Hamiltonians instead of a fixed Hamiltonian. He has studied degeneracies occurring in the bottom of the spectrum with the tunnelling effect, for an arbitrary potential but without magnetic field.

Two-dimensional Bloch electrons in a strong and uniform magnetic field are described by an effective one-dimensional Harper-like Hamiltonian $H(q, p)$. Thouless *et al* [1] have shown that the quantum hall conductivity σ_{xy} is related to the Chern index. Figure 5 then describes the σ_{xy} Hall conductivity for different potential shapes. The Hall conductivity of a given electronic band is then non-zero inside a small ellipse. There is some hope to observe such phenomena in experiments related to mesoscopic physics (quantum dots) [27, 28].

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References

[1] Thouless D J, Khomoto M, Nightingale M P and den Nijs M 1982 *Phys. Rev. Lett.* **49** 405
[2] Doucot B and Rammal R 1985 *Phys. Rev. Lett.* **55** 1148–51
[3] Saraceno M 1989 *Preprint* NSF-FTP-89-129i
[4] Lebœuf P, Kurchan J, Feingold M and Arovas D P 1990 *Phys. Rev. Lett.* **65** 3076; 1992 *Chaos* **2** 125
[5] von Neumann J and Wigner E 1929 *Phys. Z.* **30** 467
[6] Berry M V and Wilkinson M 1984 *Proc. R. Soc.* A **392** 15–43
[7] Berry M V 1984 *Proc. R. Soc.* **392** 45
[8] Shapere A and Wilczek F *Geometric Phases in Physics* (*Advanced Series in Mathematical Physics 5*)
[9] Simon B 1983 *Phys. Rev. Lett.* 51 2167
[10] Hagedorn G A 1990 *Theor. Chimica Acta* 77 163–90
[11] Avron J E, Seiler R and Simon B 1983 *Phys. Rev. Lett.* **51** 51
[12] Huo Y and Bhatt R N 1992 *Phys. Rev. Lett.* **68** 1375
[13] Faure F and Leboeuf P 1993 *Classical to Quantum Chaos Conf. Proc. SIF (Bologna)* vol 41, ed G F Dell'Antonio, S Fantoni and V R Manfredi
[14] Helffer B and Sjöstrand J *Lecture Notes in Physics 345* ed A Jensen and H Holden pp 118–98
[15] Colin de Verdière Y 1993 Fibrés en droites et valeurs propes multiples *Seminar of spectral geometry 11* Institut Fourier Grenoble
[16] Arovas D P, Bhatt P N, Haldane F D M, Littlewood P B and Rammal R 1988 *Phys. Rev. Lett.* **60** 619
[17] Khomoto M 1985 *Ann. Phys., NY* **160** 343

[18] Paul T and Uribe A A construction of quasi-modes using coherent states *Ann. Inst. Poincaré–Phys. Théor* to appear
[19] Takahashi K 1989 *Prog. Theor. Phys.* **98** 109
[20] Griffiths P and Harris J *Principles of Algebraic geometry* (New York: Wiley)
[21] Barelli A and Kreft C 1991 *J. Physique I.* **1** 1229
[22] Wilkinson M and Austin E J *J. Phys. A: Math. Gen.* **23** 2529 1990
[23] Helffer B and Sjöstrand J 1985 *Commun. PDE* **10** 245–340
[24] Colin de Verdière Y *Semi-classical analysis* (Doctoral school course) University Joseph Fourier (1993–94)
[25] Milnor J W 1965 *Topology from the Differential Viewpoint* (Virginia University Press)
[26] Faure F 1993 *Thesis* University Joseph Fourier (Grenoble) pp 93–112
[27] Petschel G and Geisel T 1993 *Phys. Rev. Lett.* **71** 239
[28] Weiss D, Zhang C, Gerhardts R R and v Klitzing K 1989 *Phys. Rev.* B **39** 13 020
[29] Wilkinson M 1986 *Proc. R. Soc.* A **403** 135