On Harper's equation : historics and new questions

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Abstract:
If the first mathematical results were obtained more than 30 years ago with the interpretation of the celebrated Hofstadter butterfly, more recent experiments in Bose-Einstein theory suggest new questions. I will present a survey on sometime old results (Helffer-Sjöstrand, Puig, Avila-Jitomirskaya-Krikorian,...) and also discuss more recent questions with generalized butterflys (Dalibard and coauthors, Hou, Royo-Letelier ... and many authors in this conference). Our historics is focused on the mathematical results and we refer to [DalGerJuzOhb] for a survey on the Physics literature adding perhaps the names of Wilkinson, Bellissard in the list..

The spectral properties of a charged particle in a two-dimensional system submitted to a periodic electric potential and a uniform magnetic field crucially depend on the arithmetic properties of the number θ representing the magnetic flux quanta through the elementary cell of periods, see e.g. [Bel] for a description of various models.

Since the works by Azbel [Az] and Hofstadter [Hof] it is generally believed that for irrational α the spectrum is a Cantor set, that is a now-where dense (the interior of the closure is empty) and perfect set (closed + no isolated point), and the graphical presentation of the dependence of the spectrum on θ shows a fractal behavior known as the Hofstadter butterfly.

After intensive efforts this was rigorously proved recently (Ten Martinis conjecture) for all irrational values of α for the discrete Hofstadter model, i.e. the discrete magnetic Laplacian admitting a reduction to the almost Mathieu equation, see [AvJi] and references therein.

Only few results are available for other models. Traditionally, a couple of semiclassical methods plays an important role in the analysis of the two-dimensional magnetic Schrödinger operators with periodic potentials, see e.g. [BDP] for a review. In particular, the bottom part of the spectrum for strong magnetic fields can be described up to some extent using the tunnelling asymptotics. As this meeting shows, physicists have no problems to use these results without to come back to the initial problem.

Coming back to mathematics, a more detailed analysis (Helffer and Sjöstrand [HS1, HS2, HS3]) shows that the study of some parts of the spectrum for the Schrödinger operator with a magnetic field and a periodic electric potentials reduces to the spectral problem for an operator pencil of one-dimensional quasiperiodic pseudodifferential operators.

Under some symmetry conditions for the electric potentials, the operator pencil reduces to the study of small perturbation of the continuous analog of the almost-Mathieu (=Harper) operator, which allowed one to carry out a rather detailed iterative analysis for special values of α.
In particular, in several asymptotic regimes a Cantor structure of the spectrum was proved.
This involved a pseudo-differential calculus, whose relevance in this context was predicted by the physicist Wilkinson (from england).

Pseudo-differential operators

In [HS1, HS2, HS3] (1988-1990) a machinery was developed for an iterative semiclassical analysis of a special class of pseudodifferential operators. One was concerned with the non-linear spectral problem (or, in other words, with the spectral problem for an operator pencil). Namely, for a family of self-adjoint operators $A(\mu)$ depending $\mu \in \mathbb{R}$ the μ-spectrum $\mu\text{-spec}\, A(\mu)$ denotes the set of all μ such that $0 \in \mathrm{Spec}\, A(\mu)$. The simplest case being the family $A - \mu$.

Quantization

Let $L : \mathbb{R}^2 \to \mathbb{R}$ be a periodic smooth function, $L(x, \xi + 2\pi; \mu, h) = L(x + 2\pi, \xi; \mu, h) = L(x, \xi; \mu, h)$. Here μ and h are real parameters. By the Weyl quantization procedure one can assign to L an operator $\hat{L}_h(\mu)$ in $L^2(\mathbb{R})$ by

$$\hat{L}_h(\mu) f(x) = \frac{1}{2\pi h} \int_{\mathbb{R}} \int_{\mathbb{R}} e^{i\xi(x-y)/h} L(\frac{x+y}{2}, \xi; \mu, h) f(y) d\xi\, dy. \quad (1)$$

The operator $\hat{L}_h$ obtained is referred to as the Weyl h-quantization of L, and quantum Hamiltonians resulting from periodic symbols are often called Harper-like operators.

In particular, the symbol $L(x, \xi) := \cos x + \cos \xi$ produces the Harper operator on the real line,

$$\hat{L}_h f(x) = \frac{f(x+h) + f(x-h)}{2} + \cos x \, f(x). \tag{2}$$

In [HS3], in order to treat the Harper operator and perturbations of it occuring in a renormalization procedure, the following notion was introduced.

Definition

A symbol $L(x, \xi; \mu, h)$ will be called of strong type I if the following conditions are satisfied for all $h \in (0, h_0)$ with some $h_0 > 0$:

(a) L depends analytically on $\mu \in [-4, 4]$.

(b) There exists $\varepsilon > 0$ such that

  (b1) $L(x, \xi; \mu, h)$ is holomorphic in

$$D_\varepsilon = \left\{(\mu, x, \xi) \in \mathbb{C} \times \mathbb{C} \times \mathbb{C} : |\mu| \leq 4, |\Im x| < \frac{1}{\varepsilon}, |\Im \xi| < \frac{1}{\varepsilon}, \right\},$$

  (b2) for $(\mu, x, \xi) \in D_\varepsilon$, there holds

$$\left| L(x, \xi; \mu, h) - (\cos x + \cos \xi - \mu) \right| \leq \varepsilon.$$

Continuation of the definition

(c) The following symmetry conditions hold:

$$L(x, \xi; \mu, h) = L(\xi, x; \mu, h) = L(x, -\xi; \mu, h)$$
$$L(x, \xi; \mu, h) = L(x + 2\pi, \xi; \mu, h) = L(x, \xi + 2\pi; \mu, h).$$

By $\varepsilon(L)$ we will denote the minimal value of ε for which the above conditions hold.

In [HS1, HS2, HS3] a detailed analysis was performed for pseudodifferential operators associated with strong type I symbols. One of the results was

Theorem 1

Let $L(\mu, h)$ be a strong type I symbol. There exist ϵ_0 , C s. t. if $\varepsilon(L) \leq \epsilon_0$ and if $(2\pi)^{-1}h$ is an irrational admitting a representation as a continuous fraction

$$\frac{h}{2\pi} = \cfrac{1}{n_1 + \cfrac{1}{n_2 + \cfrac{1}{n_3 + \ldots}}}$$

with $n_j \geq C$, then the μ-spectrum of the associated operators $\hat{L}_h(\mu)$ is a zero measure Cantor set.

In particular, this applies to the spectrum of the Harper's model. But the theorem says also that this is stable by perturbations respecting all the symmetries.

Schrödinger operators with magnetic potentials

For operators $H = \sum_{j=1}^{2}(hD_{x_j} - A_j)^2 + V$ with periodic potentials V,

$$V(x_1 + 2\pi, x_2) \equiv V(x_1, x_2 + 2\pi) \equiv V(x_1, x_2)\ ,$$

and constant (or periodic) magnetic fields

$$\mathrm{Curl}\,\vec{A} = B\ ,$$

it was shown in several asymptotic regimes that the study of some parts of the spectrum reduces to a non-linear spectral problem of the above type.

This is for example the case when

- B^{-1}-pseudodifferential operators with symbols close to $V(x, \xi)$ (see for example [HS4] which treats the strong magnetic case)
- for B-pseudodifferential operators with symbols to the first Floquet eigenvalue of the Schrödinger operator without magnetic field (Peierls substitution) (corresponding to the case of the weak magnetic field, see [HS1], [HS3] and [HS4] and earlier contribution by physicists (see in [Bel] and references therein).

Hence, strong type I operators appear for strong magnetic field when considering potentials V close to $\cos x_1 + \cos x_2$.
Moreover in the semi-classical limit or in the tight binding situation, it can be shown (case of a square lattice) that—up to the multiplication by an exponentially small term corresponding to the tunneling— the lowest Floquet eigenvalue is close to $(\cos \theta_1 + \cos \theta_2)$.
Here it is important to assume the symmetry for V $V(-x_2, x_1) = V(x_1, x_2)$, an assumption of non degenerate minima for V (one for each cell) and a geometric assumption on the geodesics for neighboring wells (the geometry is the Agmon metric $(V - \min V)dx^2$).

Symbols associated with some discrete operators

It is well known that the spectrum of the operator (2) as a set coincides with the spectrum of the discrete magnetic Laplacian acting on $\ell^2(\mathbb{Z}^2)$, see e.g. [HS1],

$$C_h f(m,n) = e^{ihn} f(m+1,n) + e^{-ihn} f(m-1,n) + f(m,n-1) + f(m,n+1).$$

More generaly consider a bounded linear operator C_h acting on $\ell^2(\mathbb{Z}^2)$ given by an infinite matrix $\big(C(p,q)\big)$, $p,q \in \mathbb{Z}^2$, satisfying

$$C(p+k, q+k) = e^{-ihk_2(p_1-q_1)} C(p,q), \quad p,q,k \in \mathbb{Z}^2, \qquad (3)$$

with some $h > 0$.

Proposition A

Let C_h be a bounded self-adjoint operator in $\ell^2(\mathbb{Z}^2)$ with the property (3) and satisfying $|C(p,q)| \leq ae^{-b|p-q|}$ for some $a, b > 0$ and all $p, q \in \mathbb{Z}^2$. Then the spectrum of C_h coincides with the spectrum of the Weyl h-quantization of the symbol T given by

$$T(x,\xi) = \sum_{m,n\in\mathbb{Z}} c(m,n)e^{-imnh/2}e^{i(mx+n\xi)}, \tag{4}$$

where $c(m,n) = C\big((0,0),(m,n)\big)$, $m, n \in \mathbb{Z}$.

A third point of view

Let us return to the initial operator C_h. By assumption, $C(p,q) = \exp\big(ihp_2(q_1 - p_1)\big)c(q-p)$ for any $p, q \in \mathbb{Z}^2$, hence

$$\begin{aligned} C_h f(p) &= \textstyle\sum_{q\in\mathbb{Z}^2} e^{ihp_2(q_1-p_1)} c(q-p) f(q) \\ &= \textstyle\sum_{q\in\mathbb{Z}^2} e^{ihp_2 q_1} c(q) f(p+q). \end{aligned}$$

Therefore, C_h commutes with the shift $f(p_1,p_2) \mapsto f(p_1+1,p_2)$, and the Floquet-Bloch theory is applicable.

Let us introduce the functions

$$\mathbb{R} \ni \varphi \mapsto b_n(\varphi) = \sum_{k\in\mathbb{Z}} c(k,n)e^{ik\varphi}, \quad n \in \mathbb{Z}, \quad \varphi \in \mathbb{R}.$$

All these functions are 2π-periodic and analytic in a complex neighborhood of $\mathbb{R}$. Consider a family of operators acting in $\ell^2(\mathbb{Z})$,

$$C_h(\theta)g(m) = \sum_{n\in\mathbb{Z}} b_n(mh+\theta)g(m+n), \quad m \in \mathbb{Z}, \quad \theta \in \mathbb{R}\,,$$

which satisfies

$$C_h(\theta) = C_h(\theta + 2\pi)\,.$$

Therefore, by the Floquet-Bloch theory, one has

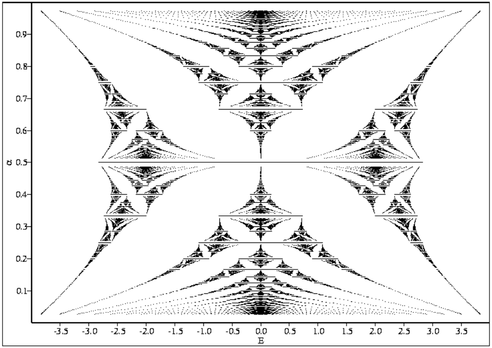
$$\mathrm{Spec}\, C_h = \bigcup_{\theta\in[0,2\pi)} \mathrm{Spec}\, C_h(\theta)\,.$$

Furthermore, for any θ the operators $C_h(\theta)$ and $C_h(\theta+h)$ are unitarily equivalent, $C_h(\theta+h) = SC_h(\theta)S^{-1}$, where S is the shift in $\ell^2(\mathbb{Z})$, $Sf(n) = f(n+1)$, which implies $\mathrm{Spec}\, C_h = \bigcup_{\theta\in[0,h)} \mathrm{Spec}\, C_h(\theta)$.
This coincides with the spectrum of the following operator T_h acting in $L^2\big(\mathbb{Z}\times[0,h)\big)$

$$T_h u(m,\theta) = C_h(\theta)u_\theta(m), \quad u_\theta(m) = u(m,\theta), \quad m\in\mathbb{Z}.$$

In the case of the symbol $(x,\xi) \mapsto \cos x + \cos \xi$ we get the **Hofstadter's butterfly**

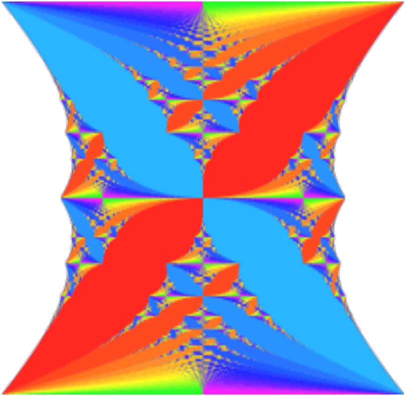
On the vertical axis the parameter proportional to the flux $\alpha = \frac{h}{2\pi} \in [0,1]$. On the horizontal line $y = \alpha$ the union over θ of the spectra of the family $C_h(\theta)$. The picture results of computations for rational α's.



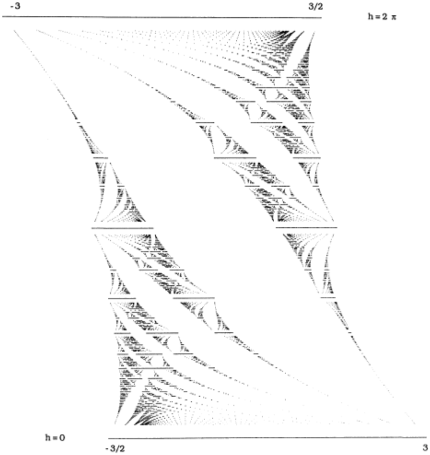
The hamiltonian point of view permits to explain the behavior of the spectrum as $\alpha \mapsto 0$ or more generally as $\alpha \to \frac{p}{q}$.

The gaps in the spectrum.

This is the "colored" butterfly realized in 2003 by Y. Avron and his team.



One can consider other lattices: the hexagonal Hofstadter's butterfly (after Kerdelhue, Kreft-Seiler, Claro,....)



Let us consider more generally the family of operators on $\ell^2(\mathbb{Z})$

$$(H_{\lambda,\alpha}u)_n = u_{n+1} + u_{n-1} + 2\lambda \cos 2\pi(\theta + n\alpha)u_n\,.$$

Different names for this operator are given including Harper or Almost-Mathieu.
If $\alpha = \frac{p}{q}$ is rational the spectrum consists of the union of q intervals possibly touching at the end point. If α is irrational the spectrum is independent of θ and:

Ten Martini Theorem

The spectrum of the almost Mathieu operator $H_{\lambda,\alpha}$ is a Cantor set for all irrational α and for all $\lambda \neq 0$.

Previously, we were discussing the case $\lambda = 1$. Ten Martini conjectures was popularized by B. Simon in reference to some offer of M. Kac.
Computations for $\lambda \neq 1$ are proposed in a "numerical" paper of Guillement-Helffer-Treton [GHT].

Historics

Azbel (1964), Bellissard-Simon (1982), Van Mouche (1989), Helffer-Sjöstrand (1989), Puig (2004), Avila-Krikorian (2008), Avila-Jitomirskaya (2009).
Unfortunately Mark Kac is not here for offering the ten Martini.

About the proof

- The proof is more related to dynamical systems.
- It involves different arguments for different families of irrationals (diophantine, Liouville).
- This result cannot be applied to the magnetic Schrödinger operator.
- The result is unknown for the hexagonal case (see however the semi-classical results by P. Kerdelhue [Kerd]).

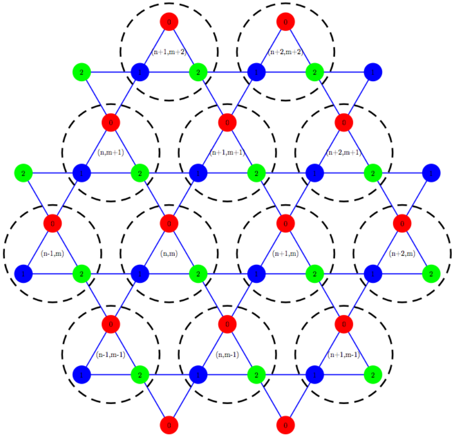
Recent developments

Using lasers one can produce potentials which are related to various lattices. Hence there are new experiments permitting to recover Harper's like spectrum.

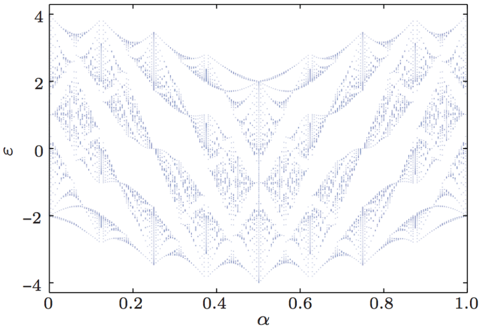
As soon as I understand, one is extremely far of seeing some Cantor spectrum. But one can see, for example if the flux through a cell is close to $2\pi \times \frac{1}{3}$ two "big" gaps in the spectrum.

Other examples

J. Royo-Leteller has started (see [Hou]) to analyze rigorously the case of a Kagome lattice.



The Kagome butterfly



We recall that the Harper model was $\tau_1 + \tau_1^* + \lambda(\tau_2 + \tau_2^*)$, which corresponds to the $h-$ quantification of $2\cos\xi + 2\lambda\cos x$, with $h = 2\pi\alpha$.
Here we take $\tau_1 = e^{ix}$ and $\tau_2 = e^{ihD_x}$, with h proportional to some flux.
$\widehat{\mathcal{K}}$ is isospectral to the h-pseudodifferential system on the line :

$$\begin{pmatrix} 0 & 1+\tau_2^* & 1+e^{i\frac{h}{2}}\tau_1\tau_2^* \\ 1+\tau_2 & 0 & e^{-i\frac{h}{8}}+e^{i\frac{3h}{8}}\tau_1 \\ 1+e^{-i\frac{h}{2}}\tau_2\tau_1^* & e^{i\frac{h}{8}}+e^{-i\frac{3h}{8}}\tau_1^* & 0 \end{pmatrix} \quad (5)$$

The h-principal symbol is

$$\begin{pmatrix} 0 & 1+e^{-i\xi} & 1+e^{-i\xi+ix} \\ 1+e^{i\xi} & 0 & 1+e^{ix} \\ 1+e^{-ix+i\xi} & 1+e^{-ix} & 0 \end{pmatrix} \tag{6}$$

The characteristic polynomial is

$$\begin{aligned}\Delta(\lambda, x, \xi) &= -\lambda^3 + 2\lambda(3 + \cos\xi + \cos(\xi - x) + \cos x) \\ &\quad +4(1 + \cos\xi + \cos x + \cos(\xi - x))\,.\end{aligned}$$

It has three roots :

$$\lambda_1 = -2\,,\; \lambda_\pm(x,\xi) = 1 \pm \sqrt{3 + 2\cos\xi + 2\cos(\xi - x) + 2\cos x}\,.$$

The range is $[-1, 4]$ as confirmed by the numerical computations in [Hou].

This seems to have the triangular symmetry. This characteristic polynomial seems to have a nice structure like for the Harper's model.

In [Kerd], one meets the matrix

$$\begin{pmatrix} 0 & 1+e^{ix}+e^{i\xi} \\ 1+e^{-ix}+e^{-i\xi} & 0 \end{pmatrix}$$

whose characteristic polynomial is

$$\Delta(\lambda) = \lambda^2 - (3 + 2\cos x + 2\cos(x-\xi) + 2\cos\xi)\,.$$

with roots

$$\lambda_\pm(x,\xi) = \pm\sqrt{3 + 2\cos x + 2\cos(x-\xi) + 2\cos\xi}\,.$$

Artificial magnetic flux

We follow the colloquium paper of Dalibard, Gerbier, and co [DalGerJuzOhb] (Colloquium: Artificial gauge potentials for neutral atoms) but just described what is mathematically done. The starting point is a Schrödinger operator on $L^2(\mathbb{R}^2;\mathbb{C}^2)$:

$$S_h := (-h^2\Delta + V(x)) \otimes I + hU(x)\,,$$

where $U(x)$ is the 2×2 matrix:

$$U(x) = \frac{\Omega}{2}\begin{pmatrix} \cos\theta & e^{-i\phi}\sin\theta \\ e^{i\phi}\sin\theta & -\cos\theta \end{pmatrix}\,,$$

ϕ and θ are C^∞ functions, and $\Omega > 0$.

U has two eigenvalues $\pm\frac{\Omega}{2}$ and we would like to see the effect of the term $hU(x)$ on the spectrum.
For each x, the eigenvectors of $U(x)$ are given by

$$\chi_1(x) = \left(\begin{array}{c} \cos\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2} \end{array} \right) , \ \chi_2(x) = \left(\begin{array}{c} -\sin\frac{\theta}{2} e^{-i\phi} \\ \cos\frac{\theta}{2} \end{array} \right) .$$

In some regime (to be determined, and which is called adiabatic in the above mentioned paper) it is natural to look (neglecting the interactions in the two particles) to look at the two operators:

$$L^2(\mathbb{R}^2,\mathbb{C}) \ni u \mapsto H_j^{eff} u := \langle \chi_j(x) \, , S_h(u\chi_j)(x)\rangle_{\mathbb{C}^2} \, ,$$

where $\langle \cdot \, , \, \cdot \rangle_{\mathbb{C}^2}$ denotes the scalar product in $\mathbb{C}^2$ (with the choice that it is antilinear with the second variable).

Let us concentrate on the case $j = 1$ and let us make explicit the effective Hamiltonian H_1^{eff} relative to χ_1.

$$H_1^{eff} := (hD_x - hA)^2 + \frac{h}{2}\Omega + V(x) + \frac{h^2}{4}\left(|\nabla\theta|^2 + \sin^2(\theta)|\nabla\phi|^2\right)$$

where

$$A = -(\sin\frac{\theta}{2})^2\nabla\phi = -\frac{1}{2}(1 - \cos\theta)\nabla\phi\,.$$

The first interesting point to observe is that A is not exact. That is we can compute the corresponding magnetic field and we get

$$B(x) = -\frac{1}{2}\sin\theta(x)\ (\nabla\theta(x) \times \nabla\phi(x))\ , \tag{7}$$

where $\times$ denotes the interior product of two vectors in $\mathbb{R}^2$.

Remarks and naive questions

As observed in [DalGerJuzOhb], if we work with χ_2, we will get an opposite flux.

The semi-classical analysis of the initial model seems to be OK if we assume that V has non degenerate minima and if Ω is small enough. We have indeed to avoid some resonance between the spectra of H_1^{eff} and H_2^{eff}, which can be read on the harmonic approximation at the minima. W does not change anything ! May be ϕ should be h-dependent ?

Question : can we obtain with suitable ϕ and θ a non trivial constant (periodic) magnetic field on $\mathbb{R}^2$? Easy to do it locally (take $\phi(x) = x_2$ and $\theta(x) = \arccos x_1$) but may be impossible globally.

Vector valued magnetic potential.

One can also diagonalize $U(x)$ using the matrix :

$$P(x) = \begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} e^{-i\phi} \\ e^{i\phi}\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix}$$

Our initial operator is unitarily equivalent to a matrix-valued Schrödinger operator

$$(hD - hA)^2 + \mathcal{V}$$

with electric potential

$$\mathcal{V} := V \otimes I + h\Omega \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

and a magnetic potential which can be computed as $A_j = -iP^*(x)\,(\partial_j P)(x)$.
Hence

$$A_j = \begin{pmatrix} \frac{1}{2}(1 - \cos\theta)(\partial_j\phi) & \frac{i}{2}e^{-i\phi}\partial_j\theta \\ -\frac{i}{2}e^{i\phi}\partial_j\theta & \frac{1}{2}(\cos\theta - 1)\partial_j\phi \end{pmatrix}.$$

Finally the magnetic field is given by

$$B_{jk} := \partial_k A_j - \partial_j A_k + i[A_j, A_k]\,,$$

and after computation (?)

$$B_{jk} = \begin{pmatrix} \frac{1}{2}\sin\theta & -\frac{1}{4}(3+\cos\theta)e^{-i\phi} \\ -\frac{1}{4}(3+\cos\theta)e^{i\phi} & -\frac{1}{2}\sin\theta \end{pmatrix} (\partial_k\theta\,\partial_j\phi - \partial_j\theta\,\partial_k\phi)\,.$$

We recover may be in a more natural way the "effective" magnetic field we have found in the effective Hamiltonian H_1^{eff}.

The computations have to be controlled but we can do the semi-classical analysis in the usual way. Starting at the minimum of V with the standard semi-classical analysis.

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