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SPLITTING LANDAU LEVELS ON THE 2-D TORUS BY PERIODIC PERTURBATIONS

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We study the spectrum of the Schroedinger operator for a particle constrained on a two dimensional flat torus under the combined action of a transverse magnetic field and a conservative force. A numerical method is presented which allows to compute the spectrum with high accuracy. The method employs a fast Fourier transform to accurately represent the momentum variables and takes into account the twisted boundary conditions required by the presence of the magnetic field. An accuracy of twelve digits is attained even with coarse grids. Landau levels are reproduced in the case of a uniform magnetic field satisfying Dirac's condition. A new fine structure of levels within the single Landau level is formed when the field has a sinusoidal component with period commensurable to the integer magnetic charge. This fact is interpreted in terms of the peculiar symmetry $Z_N \times Z_N$ which holds in the unperturbed case.

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1. Introduction

The quantum mechanics of a charged particle living on a two-dimensional flat torus subject to a uniform magnetic field, orthogonal to the surface, has been solved years ago[1,2,3]. The degeneration of the ground state coincides with the flux of the magnetic field, in units of the elementary flux hc/e (in this paper we shall adopt units such that $\hbar = e/c = 1$). From a mathematical point of view, this is a simple example of the more general theorem about cohomology groups for hermitian line bundles[4], known in the physical literature as Dirac's quantization condition: quantum mechanics requires that the flux of the magnetic field across a closed surface be quantized. This is also known as the Weil-Souriau-Kostant quantization condition.

In general, the problem with a non uniform magnetic field and/or in presence of a scalar potential cannot be solved analytically. There exists a vast literature dealing with Landau levels which attracted much attention in the last thirty years.

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We shall not attempt to position the present paper in the physics literature, our aim being limited to present a simple numerical algorithm which is very accurate in representing the quantum Hamiltonian: key ingredients are the use of Fourier transform to represent momentum variables (spectral method) and the due attention to the constraints posed by differential geometry. The interested reader may find useful information in the literature[5,6].

The algorithm computes the spectrum of the quantum particle on the torus in presence of both a transverse magnetic field and a scalar potential. If the potential vanishes and the magnetic field is uniform then the algorithm reproduces the known spectrum, in terms of eigenvalues and degeneration, to a typical accuracy of twelve digits. The effect of the potential energy is to split the Landau Levels; this fact is at the basis of Klauder's formulation of path integrals in phase space [7] and our algorithm could be used to explore this approach to quantization theory. Also the case of a non-uniform magnetic field and the corresponding splitting pattern of Landau levels can be studied using our algorithm. We consider the case of a sinusoidal contribution to the magnetic field in Sec. 4. A peculiar fine structure emerges, which is made visible by the accuracy of the algorithm. This fine-structure within each Landau level could be dubbed *Landau-Mathieu levels* and it manifests itself when the number of oscillations of the perturbed field is commensurate to the quantized magnetic flux. Finally it will be shown that the degeneracy pattern is due to the breaking of the discrete symmetry $Z_N \times Z_N$ which holds in the case of a uniform magnetic field.

2. Model setup

Quantum mechanics on a compact surface, in the presence of a magnetic field transverse to the surface, requires the introduction of either a singular magnetic potential (Dirac's string) or a collection of local potentials A_α, one for each local chart of a given atlas on the surface. The description in terms of local potentials is preferable for its mathematical rigor[8]. The implementation of the local description within a numerical approach should be easily achieved in terms of finite elements methods. In this paper we take an alternative route, working on a single chart, but imposing the correct (twisted) boundary conditions to the wave function, as we explain in the next section.

2.1. *Local charts and twisted boundary conditions*

Let the torus be identified with the two-dimensional plane $\mathbb{R}^2$ modulo the discrete subgroup of translations generated by $x \to x + L_1, y \to y + L_2$. We cover the torus

with four charts defined as follows

$$
\mathcal{C}_\alpha : \begin{cases} 0 < x < L_1 \\ 0 < y < L_2 \end{cases} \qquad \mathcal{C}_\beta : \begin{cases} \delta_1 < x < L_1 + \delta_1 \\ 0 < y < L_2 \end{cases}
$$
$$
\mathcal{C}_\gamma : \begin{cases} 0 < x < L_1 \\ \delta_2 < y < L_2 + \delta_2 \end{cases} \qquad \mathcal{C}_\delta : \begin{cases} \delta_1 < x < L_1 + \delta_1 \\ \delta_2 < y < L_2 + \delta_2 \end{cases} \tag{1}
$$

In each chart we define a local magnetic potential by

$$
\forall i : \boldsymbol{\mathcal{A}}_i = (-\tfrac{1}{2} B y, \tfrac{1}{2} B x) \tag{2}
$$

(remember that in our units $e/c = 1$). All local potentials are defined in the same way, but their *values* are different. Within the overlaps of the local charts we easily find the transition functions realizing the gauge transformations from one description to another. For instance, the chart β overlaps α in two distinct regions, $\mathcal{I}_{\alpha\beta}^{(1)} = \{\delta_1 < x_\alpha = x_\beta < L_1\}$ and $\mathcal{I}_{\alpha\beta}^{(2)} = \{0 < x_\alpha < \delta_1, L_1 < x_\beta < L_1 + \delta_1\}$. In the overlap $\mathcal{I}_{\alpha\beta}^{(1)}$ the value of the potentials coincide, while in $\mathcal{I}_{\alpha\beta}^{(2)}$ we have

$$
\begin{aligned}
\boldsymbol{\mathcal{A}}_\beta &= \boldsymbol{\mathcal{A}}_\alpha + (0, \tfrac{1}{2} B L_1) \\
&= \boldsymbol{\mathcal{A}}_\alpha + \nabla \chi_{\alpha\beta}
\end{aligned} \tag{3}
$$

with $\chi_{\alpha\beta} = \tfrac{1}{2} B L_1 y$. The other transition functions are determined similarly. For instance in $\mathcal{I}_{\alpha\gamma}^{(2)} = \{0 < y_\alpha < \delta_2, L_2 < y_\gamma < L_2 + \delta_2\}$ it holds

$$
\begin{aligned}
\boldsymbol{\mathcal{A}}_\gamma &= \boldsymbol{\mathcal{A}}_\alpha + (-\tfrac{1}{2} B L_2, 0) \\
&= \boldsymbol{\mathcal{A}}_\alpha + \nabla \chi_{\alpha\gamma}
\end{aligned} \tag{4}
$$

with $\chi_{\alpha\gamma} = -\tfrac{1}{2} B L_2 x$.

Now, to build the Hamiltonian operator, which is *formally* given by the usual minimal coupling, one has to establish the transition functions proper to the local wave functions. As it is well-known, these are obtained by exponentiating the transition functions, i.e.

$$
\psi_\beta(x, y) = e^{i \chi_{\alpha\beta}^{(j)}} \psi_\alpha(x, y) \qquad \text{on } \mathcal{I}_{\alpha\beta}^{(j)} \tag{5}
$$

Now take a sequence of points s_1 converging to (L_1, y) from the left and a second sequence s_2 converging from the right to the same point. On s_1 we have $\psi_\alpha = \psi_\beta \to \psi_\alpha(L_1, y)$; on s_2 we have $\psi_\beta \to \psi_\alpha(0, y) \exp\{\tfrac{1}{2} i B L_1 y\}$. By continuity of ψ_β we get a condition on ψ_α namely

$$
\psi_\alpha(L_1, y) = e^{\frac{1}{2} i B L_1 y} \psi_\alpha(0, y). \tag{6}
$$

By a similar argument we find a second condition

$$
\psi_\alpha(x, L_2) = e^{-\frac{1}{2} i B L_2 x} \psi_\alpha(x, 0). \tag{7}
$$

At this point we are allowed to work on a single local chart (let's choose $\mathcal{C}_\alpha$) and the Hamiltonian is defined by

$$
H = \tfrac{1}{2}(-i\partial_x + \tfrac{1}{2} B y)^2 + \tfrac{1}{2}(-i\partial_y - \tfrac{1}{2} B x)^2 + V(x, y) \tag{8}
$$

on a domain of differentiable functions satisfying Eq.s(6,7) as boundary conditions. Notice that the b.c. are only consistent if Dirac's condition is satisfied. To see this, compute $\psi(L_1, L_2)$ by applying the b.c. in two different orders:

$$\psi(L_1, L_2) = \psi(0, L_2)\, e^{\,\frac{1}{2}iBL_1L_2} = \psi(0,0)\, e^{\,\frac{1}{2}iBL_1L_2} \tag{9}$$

$$\psi(L_1, L_2) = \psi(L_1, 0)\, e^{-\,\frac{1}{2}iBL_1L_2} = \psi(0,0)\, e^{-\,\frac{1}{2}iBL_1L_2} \tag{10}$$

hence $\exp\{i\,B\,L_1\,L_2\} = 1$. All this is well–known, but it was recalled here to introduce the main idea behind the algorithm we describe in the next section.

3. Numerical Algorithms

A simple code, based on a discrete approximation of partial derivatives, is easily produced; the twisted boundary conditions Eq.s (6, 7) are implemented without difficulty. However this method has serious limitations in attaining good accuracies. A test run with $B = 2\pi$, $L_1 = L_2 = 2$ performed with a 64×64 grid in configuration space yields the low energy spectrum (first 20 eigenvalues) with an average error of 1.5%. In particular the first four eigenvalues, which should coincide with π, turn out to be $\pi \times (0.9997, 1.0082, 1.0082, 1.0419)$. With a finer mesh ($128 \times 128$) the error improves (0.5%) but the computing time grows considerably (from 25 sec to ≈ 400 sec). This fact encourages to design an algorithm with a better accuracy on partial derivatives. This is achieved by using a "spectral method" based on the Fourier transform.

3.1. *The spectral method*

A very accurate representation of partial derivatives can be obtained by using Fourier transform. We use the very efficient encoding FFTW[9], which is now included in Matlab. However, Fourier transform assumes a periodic wave-function, which is not the case with our problem. The way out is to apply the transformation separately along x and y; the x transform is applied to the function $\phi = \exp\{-\frac{1}{2}iB\,x\,y\}\,\psi$, which turns out to be periodic in x with period L_1. The minimal coupling is then recovered by realizing that

$$(-i\partial_x + \tfrac{1}{2}B\,y)\,\psi \equiv e^{\frac{1}{2}iBxy}(-i\partial_x\phi) + B\,y\,\psi\,. \tag{11}$$

Now the partial derivative can be computed in $x-$Fourier space. Similarly $\phi = \exp\{\frac{1}{2}iB\,x\,y\}\,\psi$ is periodic in y with the right period, and we may compute

$$(-i\partial_y - \tfrac{1}{2}B\,x)\,\psi \equiv e^{-\frac{1}{2}iBxy}(-i\partial_y\phi) - B\,x\,\psi\,. \tag{12}$$

The idea is used to compute with high accuracy the action of the Hamiltonian on any function satisfying the twisted b.c.; this is then used as the unique piece of information needed by the Arnoldi algorithm to get the spectrum. We should also choose an initial vector as a seed of the Arnoldi algorithm, or else rely on *random* initial vector. A function satisfying the boundary conditions can be constructed as

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follows. Choose any $\psi_0(x, y)$, e.g. a Gaussian centered in the middle of the rectangle of sides L_1, L_2. Let $BL_1L_2 = 2\pi N$; then the following equation defines a "good" wave-function:

$$\psi(x, y) = \sum_{n_1, n_2} (-1)^{n_1 n_2 N} e^{\frac{1}{2}iBL_2 x - \frac{1}{2}iBL_1 y} \psi_0 \left(x + n_1 L_1, y + n_2 L_2 \right)$$

The series can be truncated if ψ_0 is a Gaussian with a width small with respect to L_i.

These are the ingredients which can be used to make a call to Matlab's routine `eigs`[a], which provides a very friendly interface to the Arnoldi package `Arpack`[10]. The result is rather spectacular as we report next.

3.2. *Test runs and error estimates*

We apply the algorithm to a grid $n \times n$, starting with very coarse grids. In Tab.1 we report the average error and the timings to compute the first 20 eigenvalues with the same data as before.

Table 1.   Relative error and timings

n	Relative Error	Time (sec)
8	1.8×10^{-2}	0.15
12	5.3×10^{-7}	0.35
16	1.0×10^{-13}	0.60
24	1.8×10^{-13}	1.35
32	2.4×10^{-13}	2.85
64	6.0×10^{-13}	24.7

As we see, the algorithm reproduces the correct spectrum (including degeneracy) already at very low n. The relative error saturates around 10^{-12} which seems to be inherent to the Arnoldi algorithm as implemented in Matlab (routine `eigs`).
In Fig. 1 we see a typical spectrum obtained with the algorithm. The degeneracy of the eigenvalues is within 10^{-12}, obtained with a 32×32 grid.

Let us notice that if we plug a value of B which does not respect Dirac'c condition, the degeneracy is broken; this fact can be interpreted as due to the fact that there is a spurious singular contribution to the magnetic field at the boundary of the local chart which breaks the original symmetry.

Another check of accuracy can be performed by adding a potential energy $\frac{1}{2}\omega^2(x^2 + y^2)$: in this case the spectrum is known in the limit of large L_1 and L_2 to be given by $E = (n_+ + \frac{1}{2})\omega_+ + (n_- + \frac{1}{2})\omega_-$, $n_\pm \geq 0$, $\omega_\pm = \sqrt{\omega^2 + (B/2)^2} \pm B/2$.

[a]The Matlab code can be found at the author's web site `http://www.fis.unipr.it:`~ `enrico.onofri`.
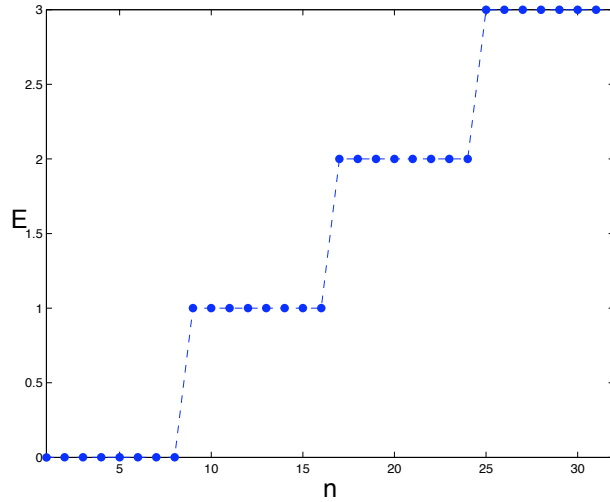
Figure 1.   The Landau levels with $N_\Phi = \frac{1}{2\pi} B L_1 L_2 = 8$, in units of the Larmor frequency.

The program reproduces this spectrum with a relative error of 10^{-13} on a 64×64 grid.

4. Fine Structure of Landau Levels

Having an algorithm which allows for accurate eigenvalue computations is like having a microscope with higher resolution power: you can resolve details which would otherwise be invisible. We started to explore other situations where the spectrum was not known a priori. The first idea was to perturb the magnetic field by adding an undulating term

$$B \rightarrow B + \lambda \, \sin(2\pi\nu x/L_1) + \sigma \, \sin(4\pi\nu x/L_1) + \ldots \tag{13}$$

Whatever the physical agent which may produce such a field, nevertheless the Hamiltonian is mathematically sound. In this case, a structure in Landau levels is revealed, *provided that the number of oscillations is commensurable to the integer flux* $N_\Phi = \frac{1}{2\pi} B L_1 L_2$. Notice that boundary conditions adapted to this choice of gauge fields must be reformulated, along the lines of Sec. 2.1. Figure 2 shows the splitting of the first Landau level which occurs at $\nu = 4$ for a purely harmonic perturbation ($\sigma = 0$). The pattern is reproduced for other choices of parameters and it looks numerically very stable and degeneracy within the fine structure levels is observed numerically at 12 digits precision.(see Fig. 3). There are N_Φ states in the first level; these are subdivided in finer sub-levels if N_Φ is a multiple of ν: degeneracy is given by the greatest common divisor $\gcd(N_\Phi, \nu)$, hence it is destroyed if N_Φ and ν are relatively prime, but it is left unchanged if ν is a multiple of N_Φ.

We also explored the stability of this phenomenon with respect to deformation
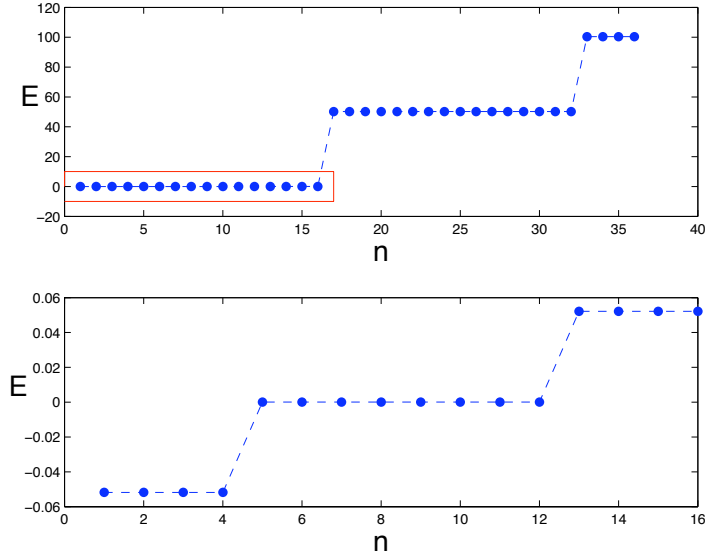
Figure 2.   The fine structure pattern of the first Landau level, $\nu = 4, N_\Phi = 16, \sigma = 0$. The picture below is a blow–up of the portion in the picture above enclosed within the rectangle .

of the magnetic field, by keeping its periodicity on the torus, e.g. by adding a higher harmonic contribution ($\sigma \neq 0$); the pattern of degeneracy stays the same, only the eigenvalues are shifted (see Fig. 4).
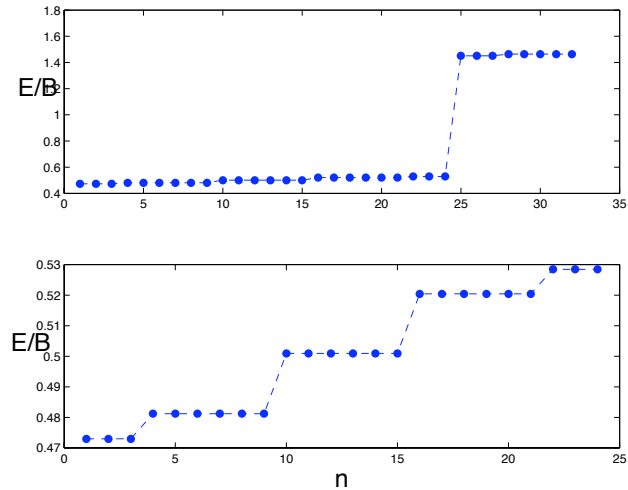

Figure 3.   The fine structure pattern of the first Landau level for $\nu = 3$, $N_\Phi = 24$, $\lambda = 1/10$, $\sigma = 0$.

The finite structure energy gap is not uniform, but a regular pattern emerges looking at sufficiently large N_Φ/ν. The evidence is that the gaps are approximately reproduced by

$$E_{n+1} - E_n \propto \sin(n\pi/N_\Phi), \quad n + \nu/2 \equiv 0 \mod (2\nu), \tag{14}$$

at least when the degeneracy pattern $\{\nu, 2\nu, 2\nu, ..., 2\nu, \nu\}$ is realised. At this level, however, the study is still preliminary.
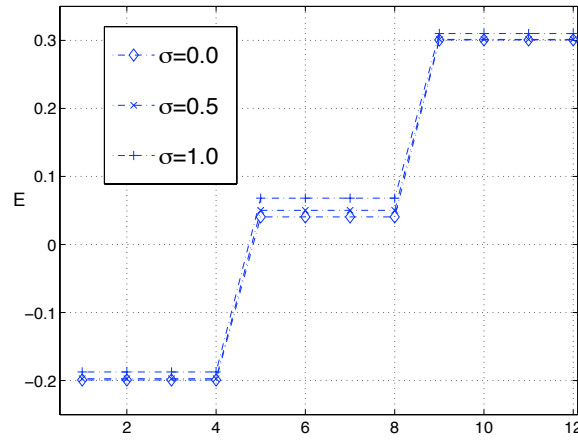

Figure 4.   The gaps in the fine structure of the first Landau level under a periodic deformation of the magnetic field, $\nu = 4, N_\Phi = 12$, σ is the coupling of the higher harmonic.

5. Symmetry Breaking

The numerical accuracy of degeneracy pattern we found numerically under a periodic perturbation of the magnetic field call for a simple explanation in terms of physical symmetry.

We recall that unperturbed Landau levels are understood on the basis of a discrete symmetry $Z_{N_\Phi} \times Z_{N_\Phi}$, the remnant of the classical $U(1) \times U(1)$ which is broken by a quantum anomaly [2] : in the case of Eq. (13) the symmetry is reduced to $Z_r \times Z_r$ with $r = \gcd(N_\Phi, \nu)$. Even if the symmetry group is Abelian, its quantum representation has a *central charge*, which forces the degeneration of Landau levels to be a multiple of r. The same argument applies when the Hamiltonian contains a potential $V(x, y)$ periodic with period commensurable to N_Φ, a fact which can easily be checked using our algorithm. Since our algorithm preserves the bundle structure of the gauge field it also preserves exactly the discrete symmetry, which explains the correct reproduction of the degeneracy pattern. Let us notice that the eigenvalues themselves, however, are computed correctly only at sufficiently fine grids.

Concluding remarks

We presented a spectral algorithm which can compute the energy spectrum for a scalar particle on the 2-D flat torus, subject to a transverse magnetic field and a potential energy. To realize the algorithm, it is crucial to implement the correct boundary conditions in a way compatible with adopting a spectral method based on the Fourier transform. The spectrum is typically obtained to a relative error of 10^{-12} even on rather coarse meshes. When the field deviates from uniformity in a sinusoidal way, we find a fine structure in the splitting of Landau levels with a regular degeneracy pattern. The problem we considered here originated from the formulation of the Hamiltonian path integral introduced long ago by J.R. Klauder[7,11].

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