

Spectral/electronic properties of the Octogonal tiling

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The electronic properties of the Octogonal tiling, a quasiperiodic tiling of codimension 2, are studied numerically and theoretically. The energy spectrum as a function of the magnetic flux through the system (the Hofstadter butterfly) displays a rich gap structure, which is being analysed. A relevant parameter of the system, the effective mass, is identified and studied numerically. The magnetic susceptibility is studied.

Introduction

Definition of quasicrystals ; remarquable physical properties¹. Studied a lot during the 80's², with a revival of interest today : new experimental and numerical tools, which allow to study the still ill understood magnetic and electronic properties of quasiperiodic structures. Moreover, quasiperiodic tilings of codimension 2, such as the Octogonal tiling, have not been studied much.

The model

Construction of the Octogonal tiling

The Octogonal tiling is obtained by the cut and project method. Periodic approximants are constructed with the same method, using the Octonacci sequence :

$$\begin{cases} O_1 = 1 \\ O_2 = 2 \\ O_{k+1} = 2O_k + O_{k-1} \end{cases}$$

The Octonacci sequence verifies : $\lim_{n \rightarrow \infty} \frac{O_{n+1}}{O_n} = 1 + \sqrt{2}$.

Note that the Octogonal tiling is composed of square and diamond tiles, of identical edge lengths and of relative surfaces $\sqrt{2}$. By slightly modifying the projection direction, one can obtain a similar tiling, constituted of three types of tiles (small squares, big squares and diamonds), s.t. the big square and diamond tiles have same surface, and that the ratio r_s of the surfaces of the big square and small square tiles is rational. This transformation is essential in order to obtain the complete spectral picture in the presence of a magnetic field, as it will be detailed later. Fig. 1 show the approximant of order three, with $r_s = 2$.

Tight-binding model

Tight-binding Hamiltonian :

$$H = \sum_{\langle i,j \rangle} t_{i,j} |i\rangle \langle j| \quad (1)$$

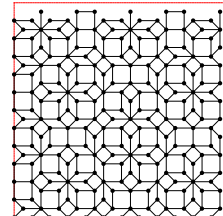


FIG. 1: Approximant of order 3

where $\langle i, j \rangle$ denotes a couple of sites, $|i\rangle$, $|j\rangle$, closest neighbours (e.g. connected by an edge), and $t_{i,j}$ is the coupling amplitude. We set $t_{i,j} = -1$.

In the presence of a magnetic field, one must add a Peierls phase term³ to the coupling amplitude :

$$t_{i,j} \rightarrow t e^{-i\theta_{i \rightarrow j}} = t e^{-i2\pi \int_i^j \mathbf{d}\mathbf{l} \cdot \mathbf{A}}$$

where \mathbf{A} is a potential vector associated to the magnetic field $\mathbf{B} = \nabla \times \mathbf{A}$.

Spectral properties

In this section, we study the spectral property of the Octogonal tiling. We use a tiling with tiles of rational relative surfaces ; in this case, the energy spectrum becomes a periodic function of the flux, and we obtain a complete Hofstadter butterfly by scanning over one period of the flux.

Hofstadter butterfly

In the presence of a uniform magnetic field, perpendicular to the plane of the tiling, gaps appear in the energy spectrum. In the case of the square lattice, the graph of the spectrum as a function of the magnetic flux is called the Hofstadter butterfly⁴. By analogy, we shall use the term Hofstadter butterfly for the Octogonal tiling.

In open boundary conditions, fig. 2, any value of the magnetic flux is permitted. However, the spectrum is polluted by the energies associated to edge modes ; to avoid this, we shall now focus on the periodic boundary conditions case.

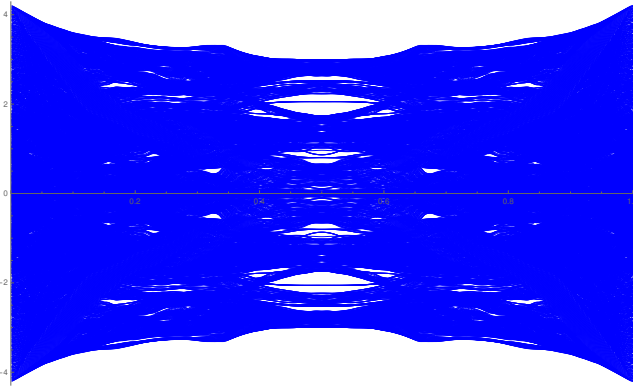


FIG. 2: Hofstadter butterfly for the order 5 approximant, open boundary conditions.

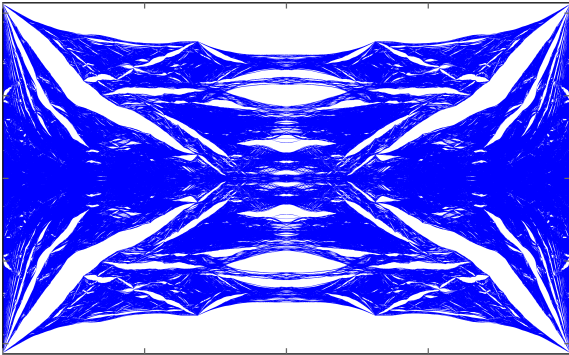


FIG. 3: Hofstadter butterfly for the order 5 approximant, periodic boundary conditions.

In the case of periodic boundary conditions (fig. 3), we need to add a phase term to the coupling coefficients in the Hamiltonian (1), in order to take into account the effect of the magnetic translation operator (see appendices for details).

Note that the butterflies have the symmetry $E \rightarrow -E$ (bipartite tiling), and $f \rightarrow 1 - f$ (time-reversal symmetry).

Discuss quantitatively the level crossing by the edge modes.

The butterflies display a rich gap structure, which we shall now describe and discuss.

Gap labeling

To characterize and quantify the gaps in the Hofstadter butterfly, we turn to the Wannier diagram, fig. 4. It displays reveals gaps of three different types : some associated to the quantum hall effect (integer slopes), some associated to the quasiperiodic order (zero slope), and

some a combination of the two. Only the gaps of the first type resist disorder.

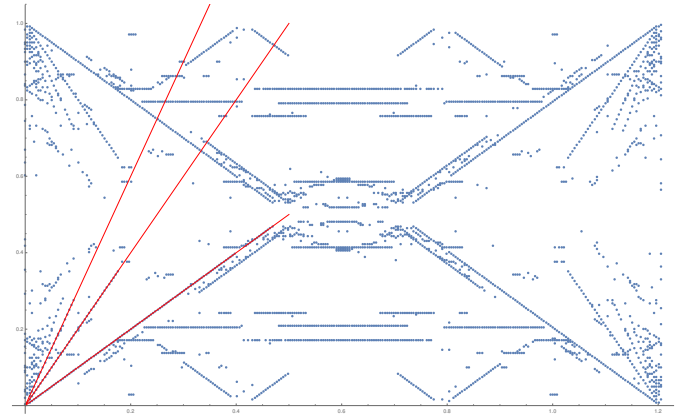


FIG. 4: Wannier diagram for the approximant d'ordre 3, PBC ; the red lines correspond to the Landau levels. X-axis : average flux per tile $\bar{f} = \frac{P_k + 2G_k}{N_k}$; Y-axis : fraction of the number of modes under the successive gaps of the spectrum $N'(\bar{f}, g) = \frac{N_{\bar{f}}(g)}{N_{tot}}$.

Connection with the Octonacci sequence

At some particular values of the flux, the Hofstadter butterfly displays extra Landau levels. Those particular values are related to the Octonacci sequence.

Landau levels broadening

The Landau levels near $f = 0$ resist disorder, and are due purely to the magnetic field.

Broadening of the Landau levels :

- thickness goes to zero fast for square lattice ;
- idem for Rauzy tiling (ref. letter by Jean Noël and Julien) : $\sim e^{-\frac{1}{f}}$;
- Octonacci : $\sim f$;

Ground state localization properties

Effective mass

We wish to identify relevant parameters of the problem. The presence of Landau levels suggests an effective mass ; remind that the energy levels of an electron in vacuum are, in the presence of a uniform magnetic field B :

$$E_n = \hbar \frac{eB}{m_L} \left(n + \frac{1}{2} \right), \quad n \in \mathbb{N}$$

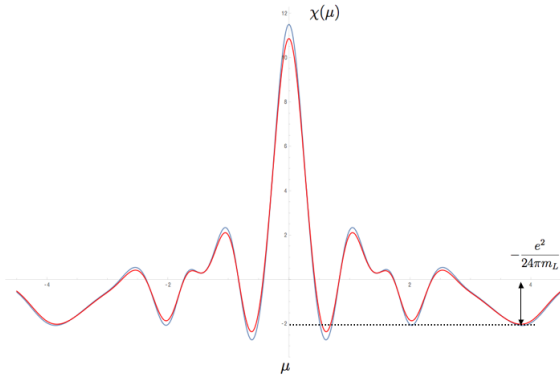


FIG. 5: Orbital magnetic susceptibility $\chi(\mu)$ at $T = 0.2$, in units of $\frac{t}{\phi_0^2}$, as a function of the chemical potential μ (units of t), for the approximant of order 5 ; blue : PBC ; red : OBC.

However, due to the slow narrowing of the Landau levels, it is unclear whether this picture still holds. Numerically, if we chose to measure the slope of the line passing through the middle of the levels, we observe that the numerical values seem to converge to zero as the size of the approximant goes to infinity.

Another approach : the effective mass derived from the effective mass tensor. This quantity is field independant, as it is derived from Bloch's Hamiltonian :

$$H_0(\mathbf{k}) = e^{i\mathbf{k}\cdot\mathbf{r}} H_0 e^{-i\mathbf{k}\cdot\mathbf{r}}$$

where H_0 is the Hamiltonian of the periodic boundary conditions problem, at zero magnetic field.

Magnetic susceptibility

To study the magnetic properties of the system, we study the magnetic susceptibility (fig. 5):

$$\begin{aligned} \chi &= -\frac{1}{V} \left. \frac{\partial^2 \Omega}{\partial B^2} \right|_{B \rightarrow 0} \\ &= -\frac{1}{V} \sum_n \left. \frac{\partial^2 E_n(B)}{\partial B^2} \right|_{B=0} n_F(E_n - \mu) \\ &\quad + \left[\left. \frac{\partial E_n(B)}{\partial B} \right|_{B=0} \right]^2 n'_F(E_n(B) - \mu) \end{aligned}$$

with

$$\Omega(T, \mu, B) = -\frac{1}{\beta} \sum_n \ln \left(1 + e^{-\beta(E_n(B) - \mu)} \right) \quad (2)$$

the grand potential in the grand ensemble formalism.

¹ C. Janot. *Quasicrystals, a primer*. Clarendon Press, Oxford, 1994.

² J. C. Lasjaunias G. Fourcaudot F. Cyrot-Lackmann C. Berger, A. Gozlan. Electronic properties of quasicrystals. *Physica Scripta*, T35:90–4, 1991.

³ R. E. Peierls. Aperiodic tiles. *Z. Phys.*, 80:763, 1933.

⁴ D. R. Hofstadter. Energy levels and wave functions of Bloch electrons in rational and irrational magnetic fields. *Phys. Rev. B*, 14:2239, 1976.