

Electronic properties of the Octagonal tiling in a magnetic field

Authors

address

(Dated: October 26, 2016)

The electronic properties of the Octagonal 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.

I. INTRODUCTION

Definition of quasicrystals ; remarkable 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 Octagonal tiling, have not been studied much.

II. THE MODEL

A. Construction of the Octagonal tiling

The Octagonal tiling (or the Amman-Beenker tiling, discovered by Amman²) is a two-dimensional quasiperiodic tiling, whose diffraction pattern has an 8-fold symmetry. It is composed of two types of square and diamond tiles, of identical edge lengths $\sqrt{2}$ (see fig. (1.a)). It can be obtained by the cut and project method³ : a subset of the \mathbf{Z}_4 lattice (points and edges between nearest neighbors) is projected on a two dimensional plane of \mathbf{R}_4 directed by irrational vectors ; since we project a four-dimensional set on a two-dimensional plane, we say that the tiling is of codimension two. The Octagonal tiling is infinite, but one can build a series of so called periodic approximants (periodic tilings) which converge asymptotically to the quasiperiodic structure. To simplify, we will call periodic approximant the unit cell of such a periodic tiling. We choose here the family of approximants described in³ ; however other families are available in the literature (see for example⁴). The approximants are constructed by using rational planes for the projection space. Their properties (number of tiles and size) are related to the Octonacci sequence :

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

Solving the recurrence relation, one finds : $O_k = \frac{1}{2\sqrt{2}}(\lambda^k - \lambda'^k)$, with $\lambda = 1 + \sqrt{2}$ (called the silver mean) and $\lambda' = 1 - \sqrt{2}$; the Octonacci sequence thus verifies : $\lim_{n \rightarrow \infty} \frac{O_{k+1}}{O_k} = 1 + \sqrt{2}$, . The approximant of order k contains $N_k = O_{2k+1} + O_{2k}$ vertices.

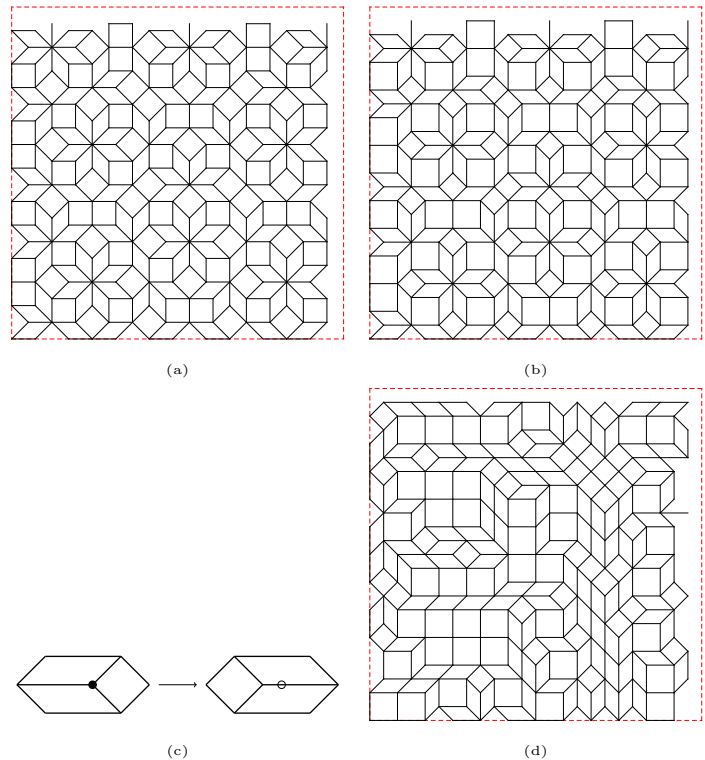


FIG. 1: Approximant of order 3 of the octagonal tiling, (a) in its original form and (b) after a deformation of the edges, with $r_s = 2$. (c) Single phason flip, (d) tiling after $\frac{N^2}{2}$ flips.

Note that the Octagonal tiling is composed of tiles of relative surfaces $\sqrt{2}$, which is an issue for the problem we wish to study, namely the spectral properties of the quasicrystal in the presence of a uniform magnetic field perpendicular to the tiling (see details in the next section). Irrational areas of tiles mean that the energy spectrum is not periodic with the magnetic flux, and we would have to scan the tiling for all values of the flux $f \in \mathbf{R}_+$ in order to obtain the full description of the energy spectrum. To bypass this difficulty, we slightly modify the projection direction, and obtain a tiling with the same connectivity, constituted of three types of tiles (small squares, big squares and rhombi), s.t. the big square and rhombus tiles have the same surface, and that the ratio r_s of the surfaces of the big square and small square tiles is ra-

tionnal (see fig. (1.b)). This transformation does not change the connectivity between the sites nor the symmetries and patterns of the lattice.

In order to study the influence of structural disorder on the spectral properties of the quasicrystal, we also construct random tilings obtained from the Octagonal tiling by flipping tiles at random (see fig. (1.c), (1.d)). In order to reach maximum disorder for a tiling of N sites, one needs to perform $\frac{N^2}{2}$ flips⁵.

B. Tight-binding model

We now wish to study the electronic properties of the quasicrystal. We consider a spinless electron evolving on the lattice, in a quasiperiodic potential. For simplicity, we choose the tight-binding model : the particle is allowed to hop between nearest neighbor sites. In the absence of magnetic field, the corresponding Hamiltonian is

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

where $\langle i,j \rangle$ denotes a couple of sites, $|i\rangle$, $|j\rangle$, closest neighbours, and $t_{i,j}$ the hopping amplitude.

The energy spectrum of such a system has been studied in⁶. Here, we study the effect of an external uniform magnetic field \mathbf{B} , perpendicular to the tiling. In this case, one must add a Peierls phase term⁷ to the hopping amplitude :

$$t_{i,j} \rightarrow te^{-i\theta_{i \rightarrow j}} = te^{-\frac{i2\pi}{\phi_0} \int_i^j \mathbf{d}\mathbf{l} \cdot \mathbf{A}}$$

where ϕ_0 is the flux quantum and \mathbf{A} is a potential vector associated to the magnetic field : $\mathbf{B} = \nabla \times \mathbf{A}$. Due to the magnetic field, 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 butterfly⁸. By analogy, we shall use the term Hofstadter butterfly or butterfly for the Octagonal tiling. We aim at understanding, theoretically, the spectral properties of the (infinite size) Octagonal tiling. However, numerically, we can only study finite size systems ; we will thus use approximants with periodic boundary conditions for the numerics.

In the following, we set $t_{i,j} = -1$, $\hbar = 1$, $e = -2\pi$ so that the elementary flux $\phi_0 = \frac{h}{|e|} = 1$, and $a = 1$ the length of the smallest distance between nearest neighbors. Small tiles have an area $a^2 = 1$, and big tiles have an area $2a^2 = 2$. We call $f = \frac{a^2 B}{\phi_0} = B$ the magnetic flux through a small tile, $2f$ the flux through a big tile, and the average flux through a tile $\bar{f} = \frac{B\bar{A}}{\phi_0} = \frac{1+\sqrt{2}}{2}B \approx 1.2f$, with $\bar{A} = \lim_{k \rightarrow \infty} \frac{A_k}{N_k}$; the value of \bar{A} can be easily calculated by using the relation $A_k = 2O_{k+1}^2$.

In open boundary conditions, any value of the magnetic flux is permitted. However, the spectrum is polluted by the edge modes ; to avoid this, we choose periodic boundary conditions.

In this case, one needs to insure that the Peierls phases match the periodic boundary condition ; unfortunately, only a restricted set of values for the magnetic flux fulfill this requirement. However, one can try to add a gradient term in the vector potential \mathbf{A} , which does not change the physics of the system, and s.t. more values for f are allowed. To derive this gauge transformation we use the following fact : in the presence of a magnetic field, the Hamiltonian is no longer invariant under translational symmetry, because \mathbf{A} is not ; however, H commutes with the magnetic translation operators⁹ : $\mathcal{T}_{\mathbf{a}_i} = e^{2i\pi\chi(\hat{\mathbf{r}})} T_{\mathbf{a}_i}$, $i \in \{1, 2\}$, where \mathbf{a}_i are two vectors along which the sample is translated to obtain a periodic tiling (see fig. 1.a) and $\chi_{\mathbf{a}_i}(\mathbf{r}) = \int_0^{\mathbf{r}} \mathbf{d}\mathbf{l} \cdot (\mathbf{A}(\mathbf{l} - \mathbf{a}_i) - \mathbf{A}(\mathbf{l}))$. Now, the Hamiltonian defined by : $H'_i = e^{-2i\pi\chi_{\mathbf{a}_i}(\hat{\mathbf{r}})} H e^{2i\pi\chi_{\mathbf{a}_i}(\hat{\mathbf{r}})}$, $i \in \{1, 2\}$, describes the same system, and commutes with $T_{\mathbf{a}_1}$, $T_{\mathbf{a}_2}$ respectively. However, magnetic translation operators along different vectors \mathbf{a}_1 , \mathbf{a}_2 do not commute in general. They do when the flux through the entire sample is an integer multiple of ϕ_0 . To insure this, we set :

RETROUVER EXPRESSION EXPLICITE DES TERMES DE SAUT DU HAMILTONIEN.

III. HOFSTADTER BUTTERFLY, WANNIER DIAGRAM AND GAP LABELING

In this section, we present numerical results and discuss the gap structure of the energy spectrum.

A. Hofstadter butterfly

As discussed in the previous section, in periodic boundary conditions, we can restrict our study of the energy spectrum to $f \in [0, 1]$. The butterfly obtained (fig. 2) has the symmetries predicted from the symmetries of the system (symmetry of the spectrum w.r.t. 0, and $f \rightarrow 1 - f$ symmetry due to both the invariance of the spectrum under $f \rightarrow -f$ and the 1-periodicity). It displays a very rich gap structure, which could not be observed in open boundary conditions. Furthermore, we observe the same gaps for all the approximants numerically accessible (up to image resolution), and we predict that the butterfly of the infinite tiling has the same gap structure.

As expected from the presence of magnetic field, we observe Landau levels near $f = 0$, which broaden due to the lattice potential, both in the ordered (fig. 2) and disordered (fig. 3) cases (we will discuss the broadening quantitatively in the next section). Note that the Landau levels are the only gaps which survive the structural disorder (fig. 3), and are not wiped out by it ; therefore, the structural disorder induced by the flips is a weak disorder.

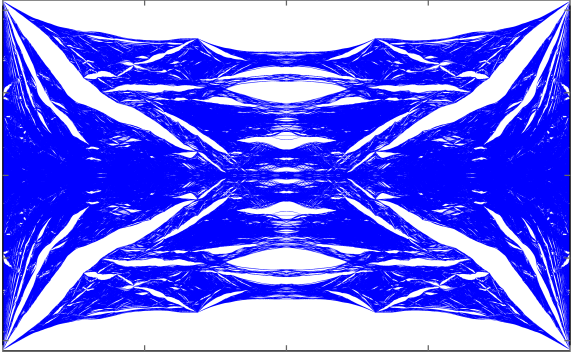


FIG. 2: Hofstadter butterfly for the order 5 approximant, periodic boundary conditions.

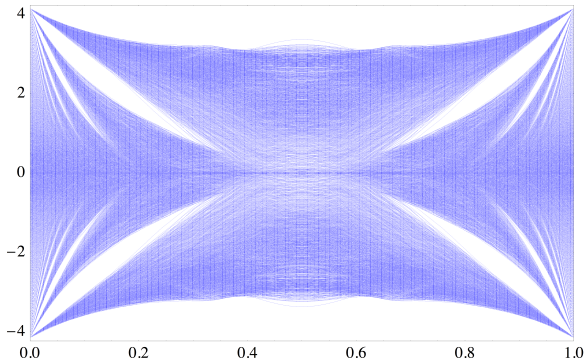


FIG. 3: Hofstadter butterfly for the disordered order 4 approximant, periodic boundary conditions.

B. Gap labeling and Wannier diagram

To characterize the gaps in the Hofstadter butterfly, we turn to the Wannier diagram (fig. 4), namely the normalized integrated density of states $\mathcal{N}(E, \bar{f})$ (NIDoS) in the gaps as a function of the average magnetic flux through one tile \bar{f} : if a gap opens at the energy E , it corresponds to a point $(\bar{f}, \mathcal{N}(E, \bar{f}))$ in the Wannier diagram.

It is well known that the slopes of the lines of the Wannier diagram are connected to the Hall conductivity inside a gap, as given by the Widom-Streda formula^{10, 11}: $\sigma_H = e \frac{\partial \mathcal{N}(E, \bar{f})}{\partial \bar{f}} = \frac{e^2}{h} \nu$, where ν is a topological invariant integer, called the Chern number. Integrating this formula, one finds:

$$\mathcal{N}(E, \bar{f}) = \nu \bar{f} + \mathcal{N}_0$$

where \mathcal{N}_0 is a constant which depends on the gap. As argued by¹² and¹³, the gap labeling theorem implies that the gaps can be labelled using two integers (p, q) in the thermodynamic limit, and that $\mathcal{N}_0 = \frac{p+q\sqrt{2}}{8}$. We argue that, for finite size approximants, one needs three integers to label a gap, but that only two remain at the

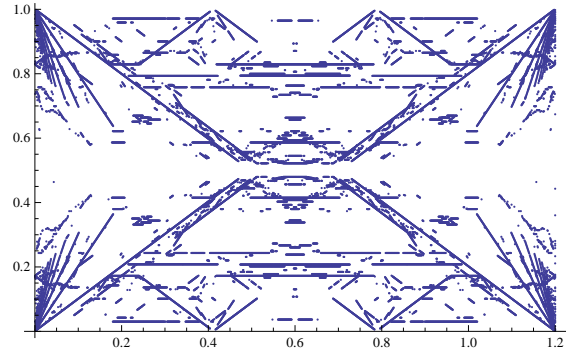


FIG. 4: Wannier diagram for the approximant of order 4, PBC. X-axis: average flux per tile $\bar{f} = \frac{A_k}{N_k} f$; Y-axis: normalized integrated density of states $\mathcal{N}(E, \bar{f})$.

thermodynamic limit. In fact, adapting the argument of¹⁴ and using the Octonacci instead of the Tribonacci sequence, we find that, for an approximant of order k , \mathcal{N}_0 is of the form:

$$\mathcal{N}_0 = \frac{pA_k + qA_{k-1} + r(-1)^k}{N_k}$$

with $(p, q, r) \in \mathbf{Z}$ independent of k ; in the thermodynamical limit, only two integers (p, q) remain and we predict:

$$\mathcal{N}_0 = \frac{p + q\sqrt{2}}{2}$$

i.e. the integers required to label the gaps correspond to those of the labeling of^{12,13} which are multiples of four.

COMMENTER FILAMENTS - 3 ENTIERS - CODIM

This labeling allows us to classify the gaps, according to ν , which is related to the response to an applied magnetic field, and q , which accounts for the quasiperiodic order. The integer p insure that the IDoS is well normalized ($\mathcal{N}(E, \bar{f}) \in [0, 1]$). First, gaps labelled by $\nu \neq 0, q = 0$, which correspond to the main IQHE gaps and are the only gaps to survive disorder (cf. previous section and fig.2, 3). Second, gaps labelled by $\nu \neq 0, q \neq 0$, which form fans reminding the IQHE gaps and are separated by Landau levels; they appear at some specific values of \bar{f} , related to the Octonacci sequence, similarly to what happens at rational fluxes of the Hofstadter butterflies of periodic tilings^{15,8}. Finally, gaps labelled by $\nu = 0, q \neq 0$, which also disappear with disorder and are therefore also associated to the quasiperiodic order. Although it is expected, at $f = \frac{1}{2}$, to find gaps with a nul Chern ν number because of the time-reversal symmetry, the remarkable point here is to find such gaps at other values of f . Such gaps seldom appear and have so far only been observed in the Lieb tiling¹⁶, the dice tiling¹⁷ and the Rauzy tiling¹⁴. The condition of existence and the physics of these gaps are still open questions.

IV. LANDAU LEVELS AT BAND EDGES

We focus here on the Landau levels which appear at band edges. Remind that the energy levels of an electron evolving in a two-dimension plane of surface \mathcal{A} are, in the presence of a uniform magnetic field B :

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

where $\omega = \frac{eB}{m}$ and m is the effective mass of the electron ; each level has a degeneracy $\frac{|B|\mathcal{A}}{\phi_0}$. In the presence of a lattice potential, the levels broaden as the flux increases^{18,19}; however, in the case of the Octagonal tiling, the barycentre of the levels in the butterfly can be fitted by a family of lines expressed by :

$$E_n = \frac{2\pi f}{m} \left(n + \frac{1}{2} \right)$$

with $\frac{1}{m} = 2.9(1)$, a value stable for approximants up to $k = 8$ (1607521 sites) ; we predict that this value remains stable in the thermodynamic limit, which defines an effective mass for the Octagonal tiling.

It is known that, in the presence of a periodic potential, the energy levels tend to broaden slowly^{18,19}. A similar slow broadening, e.g. $\frac{\Delta E_n}{\hbar\omega} \propto e^{-\frac{1}{f}}$ with ΔE_n the width of the n -th level and $\hbar\omega$ the energy difference between two levels) has been observed for quasicrystals as well¹⁴. Here, we observe a much more important broadening : $\lim_{f \rightarrow 0} \frac{\Delta E_n}{\hbar\omega} = C$ where C is a constant, $C \in [0.1, 0.2]$. In the disordered case, it has been observed for the Rauzy tiling that the broadening diverges to infinity⁷.

V. EFFECTIVE MASS IN ZERO FIELD

As discussed in the previous section, in the zero field limit, the effective mass of an electron submitted to the quasiperiodic potential is given by the average slope of the Landau levels.

We aim here at indentifying an effective mass in zero field. There exist several ways to define such a quantity (see complementary material in¹⁴). A first approach consists in measuring the density of state (DoS) at the band edge. At zero temperature, the DoS is : $\rho_{T=0}(E) = \sum_n \delta(E - E_n)$, with $\{E_n\}$ the energy spectrum, which is not analytical ; at finite temperature T however, the DoS is given by : $\rho_T(\mu) = -\sum_n n'_F(E_n - \mu)$ with $n_F(E) = \frac{1}{1+e^{\beta E}}$ the Fermi distribution function at chemical potential $\mu = 0$. The DoS at finite temperature is thus smooth at the band edge, and can be approximated by the DoS associated to a parabolic dispersion relation in 2D, a constant equal to $\frac{m_\rho}{2\pi}$. We find for the Octagonal tiling : $\frac{1}{m_\rho} = 2.9(1)$, as for the effective mass calculated with the Landau levels : $m = m_\rho$.

Another approach uses the so called effective mass tensor²⁰. In the case of another quasiperiodic tiling¹⁴, both the Landau levels slope and the effective mass tensor gave consistent values of the effective mass.

The idea is to calculate the effective mass of an electron of energy $\epsilon(\mathbf{k})$ close to the energy minimum. If the minimum is reached at $\mathbf{k} = \mathbf{k}_0$, then the linear term in $\mathbf{k} - \mathbf{k}_0$ vanishes when we expand $\epsilon(\mathbf{k})$:

$$\epsilon(\mathbf{k}) = \epsilon(\mathbf{k}_0) - \alpha(\mathbf{k} - \mathbf{k}_0)^2 + \mathcal{O}((\mathbf{k} - \mathbf{k}_0)^3)$$

and we define an effective mass m_T s.t. : $\alpha = \frac{\hbar^2}{2m_T}$. The electron thus responds to a driving fields as if it had a mass m_T . To derive the effective mass, we calculate the effective mass tensor, derived from Bloch's Hamiltonian :

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

where H_0 is the Hamiltonian of the periodic boundary conditions problem, at zero magnetic field. To obtain the effective mass tensor, we develop the dispersion relation around the center of the first Brillouin, for the first energy subband :

$$E_1(\mathbf{k}) = E_1(\mathbf{0}) + \frac{1}{2}\alpha_{i,j}k_i k_j + \mathcal{O}(k^2)$$

where the $\alpha_{i,j}$ define the effective mass tensor :

$$\boldsymbol{\alpha} = \begin{pmatrix} \alpha_{x,x} & \alpha_{x,y} \\ \alpha_{x,y} & \alpha_{y,y} \end{pmatrix}$$

and the effective mass m_T is given by :

$$\frac{1}{m_T} = \sqrt{\det \boldsymbol{\alpha}}$$

Up to a constant, it can be shown that m_T is equal to the Thouless condulance²¹, which measures the stiffness of the ground state energy when one modifies the boundary conditions. More precisely, we wish to quantify how the energy spectrum changes when we pass from periodic boundary conditions, with a system invariant under the translation along the vector $\mathbf{L} = L\hat{\mathbf{x}}$: $\psi(\mathbf{r} + \mathbf{L}) = \psi(\mathbf{r})$, to a more general problem where the phase is shifted from a factor $\mathbf{K} \cdot \mathbf{L}$: $\psi(\mathbf{r} + \mathbf{L}) = e^{i\mathbf{K}\cdot\mathbf{L}}\psi(\mathbf{r})$. Formally, this amounts to study the spectrum of the operator $e^{i\mathbf{K}\cdot\mathbf{r}} H e^{-i\mathbf{K}\cdot\mathbf{r}}$. If $\frac{1}{m_T}$ is close to zero, then the groundstate energy does not change a lot when we vary the boundary conditions ; if it is large, then the groundstate energy is less stiff. The stiffness of the groundstate energy can be used as a criteria for localization ; indeed, if the groundstate wave function is very localized, then we expect that it won't be much affected by a twist of the boundary conditions, unlike an extended groundstate. This has been discussed quantitatively in²¹.

For the Octagonal tiling, unlike m and m_ρ , m_T does not converge to a finite value as we increase the size of the approximant ; instead, m_T goes to zero with the size

N_k	239	1 393	8 119	47 321	275 807	1 607 521
$\frac{1}{m_T}$	2.9465	2.9173	2.8861	2.8530	2.8225	2.7891

TABLE I: Inverse effective masses $\frac{1}{m_T}$ obtained with the effective mass tensor, for approximants of orders k going from 3 to 8

of approximant, as can be intuited from the numerical results in table 1.

More precisely, we find that, for the k -th approximant : $\ln\left(\frac{1}{m_T}\right) = c - 0.00624 \ln(N_k)$, with c a constant. This is consistent with the nature of the ground state of the system, which we find to be extended algebraically as shown by the inverse participation ratio I : for an approximant of N_k sites, $I \propto \frac{1}{N_k^\beta}$ with $\beta = 0.987$.

VI. CONCLUSION

-
- 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 C. Oguey M. Duneau, R. Mosseri. Approximants of quasiperiodic structures generated by the inflation mapping. *J. Phys. A*, 22:4549–4564, 1989.
- ⁴ A. Katz P. Kalugin. Electrons in deterministic quasicrystalline potentials and hidden conserved quantities. *J. Phys. A*, 47:315206, 2014.
- ⁵ N. Destainville. Flip Dynamics in Octagonal Rhombus Tiling Sets. *Phys. Rev. Lett.*, 88:6068–74, 2002.
- ⁶ E.S. Zijlstra. Electronic structure of the octagonal tiling. *J. of Non-Crystalline Solids*, 334:126–129, 2004.
- ⁷ R. E. Peierls. Aperiodic tiles. *Z. Phys.*, 80:763, 1933.
- ⁸ D. R. Hofstadter. Energy levels and wave functions of Bloch electrons in rational and irrational magnetic fields. *Phys. Rev. B*, 14:2239, 1976.
- ⁹ E. M. Lifshitz L. D. Landau. *Statistical Physics, part 2, Vol. 9*. Pergamon Press, 1980.
- ¹⁰ P. Streda. Quantised Hall effect in a two-dimensional periodic potential. *J. Phys. C*, 15:1299, 1982.
- ¹¹ A. Widom. doi:10.1016/0375-9601(82)90401-7. *Phys. Lett. A*, 90:474, 1982.
- ¹² I.F. Putnam J. Kellendonk. Electrons in deterministic quasicrystalline potentials and hidden conserved quantities. *CRM Monographs series*, 13:177–206, 2000.
- ¹³ M. Zarrouati J. Bellissard, D. Herrmann. Hull of Aperiodic Solids and Gap Labelling Theorems, in Directions in Mathematical Quasicrystals. *CRM Monographs series*, 13:207–259, 2000.
- ¹⁴ J. Vidal J.-N. Fuchs.
- ¹⁵ I. I. Satija. *Butterfly in the Quantum World*. IOP Concise Physics, 2016.
- ¹⁶ D. Bercioux N. Goldman, D. F. Urban. Topological phases for fermionic cold atoms on the Lieb lattice. *Phys. Rev. A*, 83:063601, 2011.
- ¹⁷ B. Douçot J. Vidal, R. Mosseri. Aharonov-Bohm Cages in Two-Dimensional Structures. *Phys. Rev. Lett.*, 81:5888, 1998.
- ¹⁸ A. Rauh. On the broadening of Landau levels in crystals. *Phys. Stat. Sol.*, 69:K9, 1975.
- ¹⁹ G. H. Wannier F. H. Claro. Magnetic subband structure of electrons in hexagonal lattices. *Phys. Rev. B*, 19, 1979.
- ²⁰ N. D. Mermin N. W. Ashcroft. *Solid State Physics*. Harcourt College Publishers, 1976.
- ²¹ J. T. Edwards and D. J. Thouless. Numerical studies of localization in disordered systems. *J. Phys. C*, 5:807, 1972.