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THE RESEMBLANCES BETWEEN FINITE AND INFINITE FORMULATION OF HOFSTADTER BUTTERFLY SPECTRUM

Ovidiu Borchin

Department of Theoretical Physics, Faculty of Physics, West University of Timişoara, Bul. Vasile Parvan nr. 4, 300223-Timişoara, Timiş, Romania

Abstract
Hofstadter butterfly's energy spectrum is discussed both for infinite and finite lattices types. For this purpose, a square, a triangular and a honeycomb lattice are accounted for. The set of the nested band structures is treated in same more detail.
Keywords: Hofstadter butterfly, nested bands, Landau levels.

1. Introduction

The studies, concerning the movement of the electrons under the simultaneous influence of a periodic potential and a magnetic field has received much interest [1-11]. Based on Peierls, Harper and Wannier work, D. Langbein, analyzing the Landau levels, discovered "the tips of the butterfly", in fact a new and profound connection between the admissible energy states and the form and size of the lattice pierced by the magnetic field. Since Landau discovered the electron classical energy levels, this investigation instrument evolved, into a complex mathematical description. D. Hofstadter analyzed numerically this kind of band spectrum predicted by M. Y. Azbel. His work led him to "the most fascinating spectrum in physics" as P. Miller [12] said. If Azbel treated as perturbation the periodic potential in a strong magnetic field, Hofstadter assumed as perturbation a weak magnetic field in a strong periodic potential. The numerical result obtained by D. Hofstadter, presented in *Fig.2*-left, shows that the spectrum is different from Landau energy bands and that the configuration of the energy bands looks like a butterfly. Later, it was found that the spectra obtained for another types of lattices, such as triangular and honeycomb ones, presented in *Fig.4*-left and *Fig.5*-left, have similar pattern. They all have a recursive subband structure with nesting effects within the energy bands. Using scattering theory and molecular orbitals, finite lattices have also been considered [13-19]. It has been found that the electron energy spectrum for a finite size lattice, the so-called finite butterfly, presented in *Fig.2*-right (square), *Fig.4*-right (triangular), *Fig.5*-right (honeycomb), looks like the Hofstadter butterfly. The aim of this article is to highlight the pattern resemblances between the infinite and finite energy spectra.

2. Electrons in magnetic fields

Motion of a charged particle in a 2D plane, under a $\perp$ magnetic field $\vec{B}$, represents the Landau two-dimensional problem. Viewed classically, the electrons move in a magnetic field in circles in a plane perpendicular $\vec{B} \parallel \vec{z}$ to the field direction. As their velocity increases, the movement takes place on larger circles, its rotational period [20] remaining the same. The electron Hamiltonian is $H = \frac{1}{2m}\left(\vec{p} + \frac{e}{c}\vec{A}(r)\right)^2$. In case of a Landau gauge $\vec{A} = \frac{1}{2}(\vec{B} \times \vec{r})$, the energy levels split up into an equidistant series of levels similar to the harmonic oscillator. As a result, the electron energy E_n becomes quantized into discrete levels $E_n = \left(n + \frac{1}{2}\right)\hbar \cdot \frac{e\vec{B}}{m}$.

In the case of a tight-binding approximation [21], and for a quadratic dispersion law $E\left(\vec{k}\right) = \frac{\hbar^2 k^2}{2m}$ the base of energy levels will be described by the equation given above.

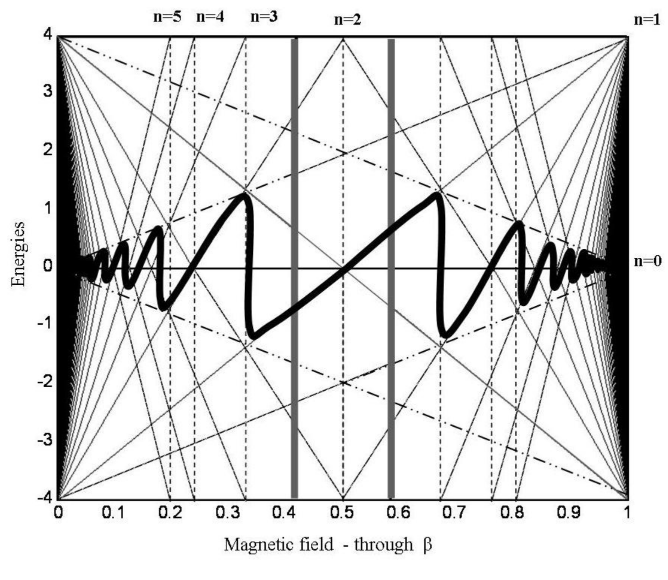

Fig.1 Landau fan energy levels. In the corners are the LLL, the thick line represent the oscillations of the chemical potential

If we take mass as the effective mass $m \text{ ® } m^*$ since $m^* = 0,95 \times m$ the cyclotron frequencies $f_c = \frac{e\vec{B}}{m}$, transforms into $f_c^* = \frac{e\vec{B}}{|m^*|} = \frac{4|t|\beta}{\hbar}$, [22] ($t$ hopping parameter and β the commensurability parameter) results the equation:

$$E(\vec{k}) \cong -4|t| + \frac{\hbar^2}{2|m^*|}\left(k_x^{\ 2} + k_y^{\ 2}\right) \quad \Rightarrow \quad \frac{E}{|t|} = -4 + 4\pi\beta \cdot \left(n + \frac{1}{2}\right) \tag{1}$$

These discrete levels with the shape of a fan make up the Landau Fan [23], being presented in $Fig.1$ as broadened Landau levels. In corners, we may see the lowest Landau levels (LLL), while the energy of the lowest states is raised with $\hbar f_c^*$ being no longer zero. These energy levels are highly degenerated levels, being proportional with the strength of the magnetic field. At $T = 0K^0$ in the absence of any external field, the Fermi energy E_F is equal with the chemical potential $\mu(B,T)$ thus it is convenient to keep the Fermi energy as a point of reference and to establish the chemical potential, as a magnetic field dependence. The large energy gaps between high degeneracy of the energy levels determine specific sharp oscillations of the chemical potential - thick line *Fig.1* crossing the Fermi energy set to zero. The amplitude of the oscillation is equal with the distance between two adjacent Landau levels. The location of the chemical potential is given by the fraction between (the number of electrons situated in the upper Landau levels) and (the number of holes situated in the lower Landau levels). The oscillations tend to become null in the point corresponding to the Fermi level set at zero.

3. Electrons in infinite and finite periodic potentials

In the case of a two-dimensional electronic system characterized by a particular type of infinite lattice, in the presence of a homogeneous perpendicular external magnetic field, the general hopping Hamiltonian [24] is described by:

$$H = -\sum_{\langle i,j \rangle} t_{ij} a_j^+ a_i e^{-i\theta_{ij}} + H.c. \tag{2}$$

The properties of such systems under a Landau gauge $\vec{A} = (0, B_x, 0)$ reveal that they are in direct dependence with the quotient $\beta = \frac{\Phi}{\Phi_0} = \frac{P}{Q}$,[25] as mutual prime integers P and Q. Numerical results show the energy spectrum for an infinite square, triangular and honeycomb types of lattices in *Fig.2,3,4,5*-left and that the energy bands are short range lines and points. In case of finite size system, the molecular wave function $|\psi\rangle$ is a linear combination of atomic orbitals $|\psi\rangle = c_A|\psi_{1s,A}\rangle + c_B|\psi_{1s,B}\rangle$. The Hamiltonian H of the nearly free electron, orbiting between two arbitrary atoms, corresponds to the molecular orbitals $H = -\frac{\hbar^2}{2m}\nabla^2 + U_A + U_B$,where U_A and U_B are the attraction energies. Treating the structure of the molecular orbitals with the help of Debye-Hückel approximation and taking the superposition integral as $S_{ij} = \langle\psi_i|\psi_j\rangle \cong 0$, the secular equation results, [26] under the determinant form with the solutions $E = E_0 \pm t$ and hopping integral $t = \langle\psi_A|H|\psi_B\rangle$. For an arbitrary site (ma, na), the only nontrivial matrix elements of the Hamiltonian wave function are:

$$\langle\psi_{m,n}|H|\psi_{m,n\pm1}\rangle = t \quad \text{and} \quad \langle\psi_{m,n}|H|\psi_{m\pm1,n}\rangle = t \tag{3}$$

$$\langle\psi_{m,n}|H|\psi_{p,r}\rangle = E_0\delta_{m,p}\delta_{n,r} \tag{4}$$

Including the magnetic field $\vec{A}$ and knowing that each plaquette contribute to the phase factor $e^{2\pi i\beta}$, due to the Aharonov-Bohm effect, [27], the above equation becomes:

$$\langle\psi_{m,n}|H|\psi_{m,n\pm1}\rangle = te^{\pm2\pi im\beta} \tag{5}$$

$$\langle\psi_{m,n}|H|\psi_{m\pm1,n}\rangle = t \tag{6}$$

The numerical representations of the energy eigenvalues as function of the magnetic field are presented in *Fig.5*-right*, Fig.6*-right*, Fig.7*-right corresponding to the finite square, triangular and honeycomb structure of the finite lattice spectra.

4. Pattern resemblances between the energy spectrum of an infinite and a finite lattice in accordance with the Landau fan levels

What's the difference between a finite and an infinite lattice when we view at a singular unit cell from the inner crystal? From a bird's eye view; it seems that there are no major differences, except their spatial extension given by the global characteristics. For us, they are identical. What seems evident for us is not valuable for the electrons. Under the simultaneous influences of neighbors (from the lattice part) and of the external magnetic field, the electrons behave differently. They get energy states which are in strong dependence with their characteristics given by the "neighbor's quality". The electrons "feel" if they are placed into an infinite size lattice or into a finite size one. The shape and the disposition of the energy bands in the spectrum reflect these differences.

The finite size lattice energy spectrum is completely different from the infinite size energy butterfly, due to the fact that the energy bands are sinuous lines for the finite size energy spectra, while for the infinite size energy spectra they are points or short-range lines. Band structures are highly sensitive to the relation between the geometric parameters of the periodic lattice and the magnetic length β, in both cases (of infinite and finite butterflies). These dependences explain the appearance of four distinct regions in the spectra:

Region A : is symmetrical situated by the low and high level of the commensurability parameter. It is a zone of highly disordered energy lines in case of finite spectrum and highly dotted in case of infinite spectrum. They are the *weak filed area*. The cyclotron radius is larger than that of the finite size lattice.

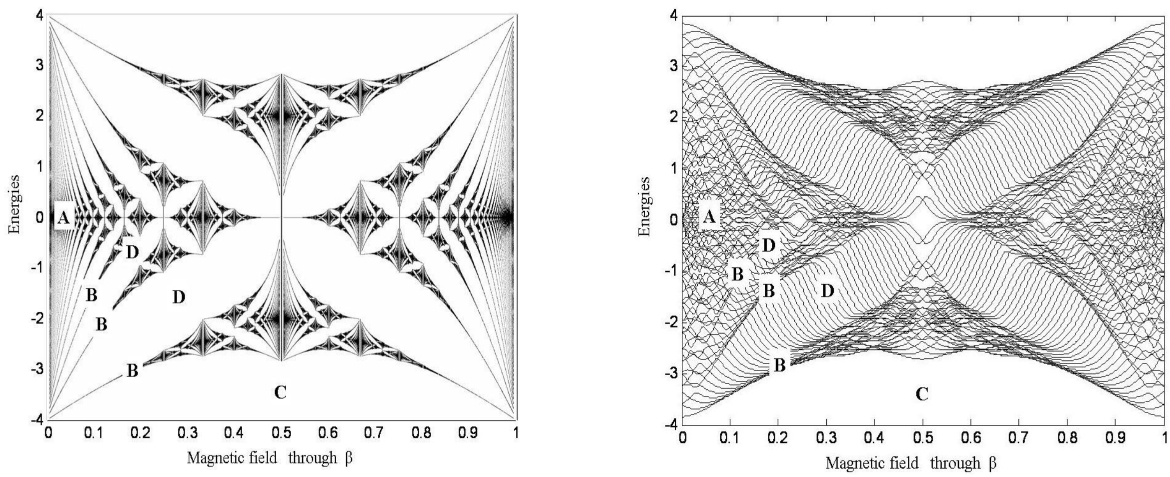

Fig.2 *The Hofstadter butterfly of a square infinite and finite 400 sites lattice*

Region B : in these areas, in the case of weak magnetic fields, the energies are given by the effective mass approximation. In case of strong magnetic fields, the energies change very rapidly revealing the Landau energies (for the finite butterflies the energy lines change rapidly, while for the infinite butterflies these is a region where the dots and the short range lines are gathered). All trajectories are limited to the bulk, to the interior, while in the exterior; there is not an intersection between them. These regions are the *bulk Landau levels*.

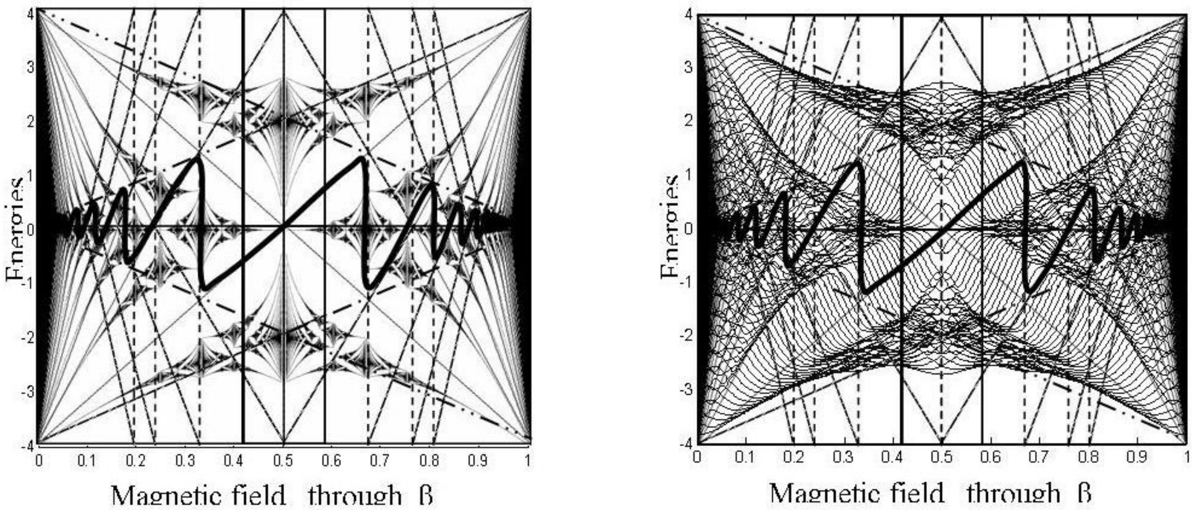

Fig.3 The Hofstadter butterfly of a square infinite and finite lattice

Region C : in these regions there are no energy lines or energy points or short range energy lines. The density of states vanishes here for lower energies. Around $\beta = 1/2$, the regions are symmetrical too. These regions are the *magnetic barrier*.

Region D : these regions, are also very intriguing, due to their role in revealing the major differences between the infinite and finite energy spectra. These energies correspond to the gap between Landau levels. These regions are the *edge state*.

The presented figures we obtained by overlapping the energy diagram revealing the Landau fan levels, with the spectrum of finite and infinite lattices as:

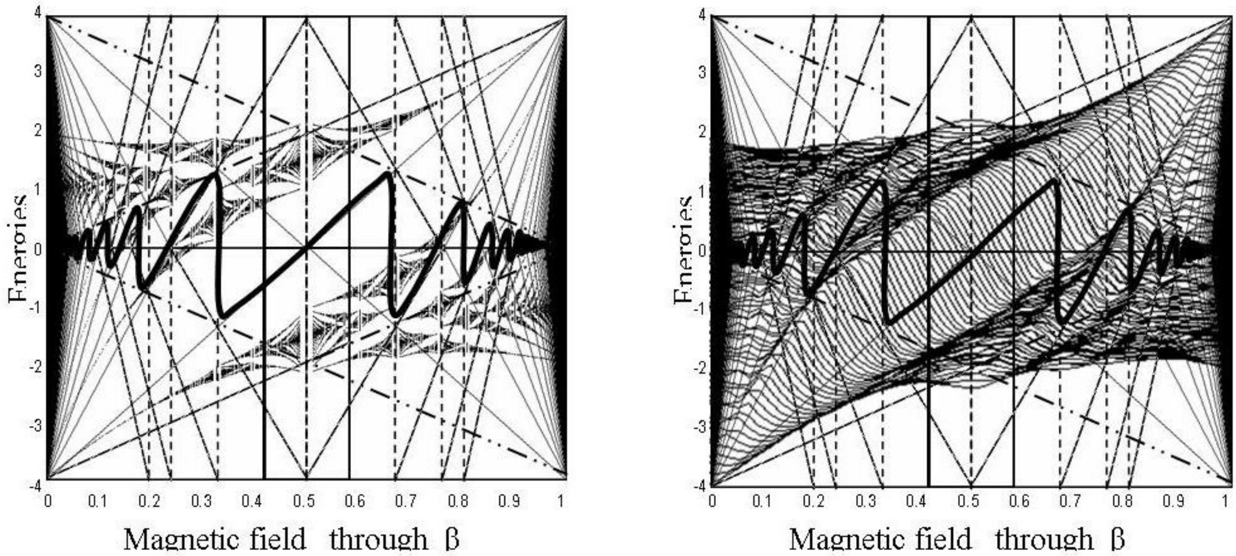

Fig.4 The Hofstadter butterfly of a triangular infinite and finite lattice

The numerical results show that the energy lines or energy bands are underlined at the Landau fan levels. Both types of lattices, determine the apparition of a highly similar pattern between allowed energies. The energy levels of the electrons are dense and highly degenerated or sparse and non-degenerated, depending on their bounding characteristics.

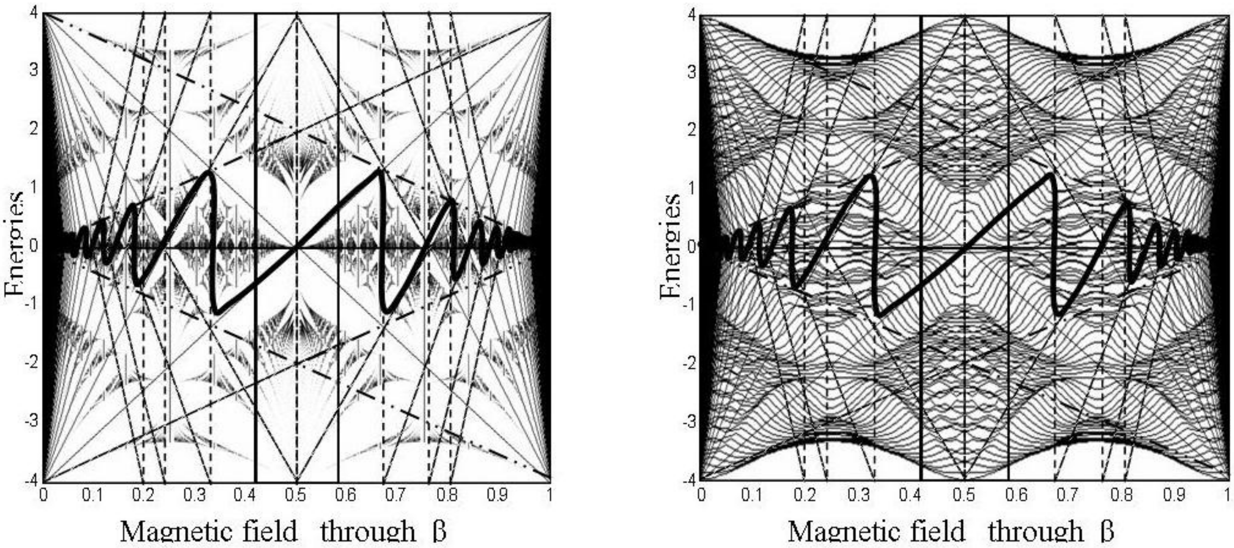

Fig.5 The Hofstadter butterfly of a honeycomb infinite and finite lattice

The finite size energy spectrum presents lines in the gap zones of the infinite size energy spectrum, characteristic to the region D. All these show that energies which are available for the infinite spectrum are not accessible for the finite size, and vice-versa, states which are not allowed in the infinite spectrum are permitted in the finite lattice. Accessible energies for the infinite lattice are highly dense and degenerated. Wide structures of the Landau levels for the infinite size lattice are marked by the energy spectrum of the butterfly for the finite size lattice too. We may see that the bands gaps from the “infinite butterfly” are completed with energy bands, [18], [19], corresponding to the "finite butterfly".

4. Conclusions

The electrons energy spectrum in the presence of both periodic potential determined by the characteristics of the lattice and the external homogenous magnetic field reveals sensitive cases of the “butterflies” spectrum appearances. Despite the differences, both butterflies present a similar pattern. From their individual patterns the infinite Hofstadter butterfly and the finite butterfly emerges the Landau fan energy levels.

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