Characterizing the Hofstadter butterfly’s outline with Chern numbers

N Goldman

Center for Nonlinear Phenomena and Complex Systems, Université Libre de Bruxelles (ULB), Code Postal 231, Campus Plaine, B-1050 Brussels, Belgium

Received 11 December 2008, in final form 12 January 2009
Published 16 February 2009
Online at stacks.iop.org/JPhysB/42/055302

Abstract

In this work, we report original properties inherent to independent particles subjected to a magnetic field by emphasizing the existence of regular structures in the energy spectrum’s outline. We show that this fractal curve, the well-known Hofstadter butterfly’s outline, is associated with a specific sequence of Chern numbers that correspond to the quantized transverse conductivity. Indeed the topological invariant that characterizes the fundamental energy band depicts successive stairways as the magnetic flux varies. Moreover each stairway is shown to be labelled by another Chern number which measures the charge transported under displacement of the periodic potential. We put forward the universal character of these properties by comparing the results obtained for the square and the honeycomb geometries.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The energy spectrum associated with charged particles moving in a two-dimensional lattice and subjected to a high-magnetic field has inspired numerous works, since the seminal papers of Hofstadter [1] and Wannier [2]. When the magnetic flux penetrating the lattice is a rational number, namely \( \Phi = \frac{p}{q} \) where \( p,q \) are integers, the spectrum splits into \( q \) subbands. The representation of the spectrum as a function of the flux shows a recursive structure with clear self-similarities [3], and adopts the shape of an intriguing insect: the so-called Hofstadter butterfly [1]. The infinitely many gaps which compose this surprising figure are known to follow a simple rule: each gap is labelled by two integers \((tr, sr)\) which satisfy a Diophantine equation [2, 5]. In a fundamental work, Thouless et al have emphasized that the Hofstadter butterfly plays a key role in the quantum Hall effect theory: when the Fermi energy of the system lies in a gap, the transverse conductivity of the system is quantized and is given by \( \sigma_{xy} = \left( \frac{e^2}{h} \right) tr \), where \( e \) is the particle’s charge, \( h \) is Planck’s constant and \( tr \) satisfies the aforementioned Diophantine equation [6].

In this context, the Green–Kubo expression for the transverse conductivity has an elegant topological interpretation: when the Fermi energy of the system lies in a gap, the transverse conductivity is given by a sum of Chern numbers. The latter are associated with the filled bands that are situated below the gap [4]. From a mathematical point of view, the Chern number is an integral invariant characterizing the topology of a fibre bundle which is defined on each energy band [4, 7]. Moreover, these topological invariants are known to be the only quantized quantities which can be associated with the energy bands [8]. The Diophantine equation, which describes any 2D electronic systems subjected to a magnetic field [5], is highly connected to topology since both integers \((tr, sr)\) can be interpreted as Chern numbers [9, 10]. As pointed out by MacDonald and Kunz, the Chern number \( sr \) measures the charge transported when the periodic potential is adiabatically displaced [3, 9].

Recent advances in cold atom physics [11, 12] allow us to carry out experimental exploration of the Hofstadter butterfly using atoms trapped in optical lattices [13]. Different arrangements, which indeed mimic the presence of an artificial ‘magnetic’ field in the dynamics of neutral particles [13, 14–17], are nowadays studied in laboratories. With such setups one expects to explore new features in the fields of vortex physics [12, 19–21] and quantum Hall systems [17, 22–26]. In particular, we have suggested that an integer quantum Hall-like effect for neutral fermionic particles should be observed in optical lattices [22].

Recently, we have also shown that fermionic atoms trapped in 2D optical lattices and subjected to an artificial...
‘magnetic’ field should undergo a Mott metal-insulator transition and that the phase boundary depicts the Hofstadter butterfly’s outline [27]. Although the Mott-insulator phase transition occurs in the system when the interaction between the particles is taken into account, the phase boundary only depends on the underlying single-particle physics. A similar result has been obtained by Oktel et al [28, 29] and by Goldbaum et al [30] in the context of the bosonic superfluid-insulator transition.

Motivated by the important role played by the Hofstadter butterfly’s outline in this theoretical framework, and by the recent experimental advances in the field of ultracold atoms, we investigate intrinsic properties associated with this fractal outline, which corresponds to the fundamental energy band for a 2D square lattice subjected to a magnetic field. The butterfly’s outline, which corresponds to the fundamental energy band \( E_k(k_x, k_y) \), is coloured in red. The energy is expressed in units of the hopping parameter \( t \).

\[ e^{i2\pi \frac{m}{p}} \psi_{m+1} + e^{-i2\pi \frac{m}{p}} \psi_{m-1} + 2 \cos(2\pi \frac{m}{p} - k_x) \psi_m = E \psi_m, \]

where \( \psi_m \) is a \( q \)-periodic wavefunction, \( k \) is the wave vector and \( E \) is the single particle energy. The wave vector belongs to the magnetic Brillouin zone, a two-torus defined as \( k_x \in [0, \frac{2\pi}{a}] \) and \( k_y \in [0, 2\pi/a] \). The energy spectrum associated with equation (2) has a band structure, composed of \( q \) subbands, which has been extensively studied in the literature [1–3, 34–36]: the representation of the energy as a function of the flux leads to the Hofstadter butterfly (figure 1). This striking fractal figure, which illustrates the infinitely many gaps of the spectrum, exhibits a recursive structure and is described through a simple rule [3]: for \( \Phi = \frac{p}{q} \), the \( r \)th gap of the spectrum is labelled by two integers \((t_r, s_r)\), which satisfy a Diophantine equation [2, 5]

\[ r = pt_r + qs_r. \]

In the square lattice case, the condition \(|t_r| \leq q/2\) determines the solution unambiguously [5].

In this work, we focus our attention on the outline of the butterfly (red curve in figure 1), which is known to play a key role in the field of quantum phase transitions [27–33]. Our aim is to investigate the structures characterizing this non-trivial curve, which is formed by the fundamental band \( E_k(k_x, k_y) \), where \( H|\psi_1\rangle = E_1|\psi_1\rangle \), in the range \( \Phi = \frac{p}{q} \in [0, 1] \). As \( q \) increases, the butterfly’s outline does not seem to smoothen because of its fractal nature [1]. In order to maintain the system along this irregular curve, we suppose that the Fermi energy lies inside the first gap of the single particle spectrum for all \( \Phi \in [0, 1] \). Under this assumption, we are able to compute the analogue of the transverse conductivity for neutral currents [22], which is associated with the energy band \( E_k(k_x, k_y) \) for a given value of the flux \( \Phi \). In this context, the transverse
conductivity can be computed with Kubo’s formula and is expressed as [6, 36]
\[
\sigma_{xy} = \frac{1}{2\pi i} \int C S \left( \frac{\partial \psi}{\partial k_x} \right) \left( \frac{\partial \psi}{\partial k_y} \right) - \left( \frac{\partial \psi}{\partial k_y} \right) \left( \frac{\partial \psi}{\partial k_x} \right),
\]
where the fundamental state \(|\psi_1\rangle\) alone contributes.

The quantization of this quantity follows from the topological interpretation of equation (4): the transverse conductivity is related to the topologically invariant Chern number \(C_S\),
\[
C_S = \frac{1}{2\pi} \int \mathcal{F} = \frac{1}{2\pi} \int \left( \frac{\partial \psi_1}{\partial k_x} \right) \left( \frac{\partial \psi_1}{\partial k_y} \right) \left( \frac{\partial \psi_1}{\partial k_y} \right) \left( \frac{\partial \psi_1}{\partial k_x} \right),
\]
where \(\mathcal{F}\) is the so-called Berry’s curvature associated with the band \(E_1(k_x, k_y)\). According to [6, 36], one finds that \(C_S = -t_1\), and therefore this invariant integer satisfies the Diophantine equation (3) with \(r = 1\),
\[
C_S = \Phi^{-1} s_1 = \frac{1}{p},
\]
with the condition \(|C_S| \leq q/2\).

One can solve equation (6) for all \(\Phi = p/q \in [0, 1]\), in order to obtain the many Chern numbers associated with the Hofstadter butterfly’s outline. Technically one fixes a high value for the denominator \(q\) and computes the Chern number \(C_S\) for \(p = 1, 2, \ldots, q\), such that \(p\) and \(q\) are mutually primes.

The illustration of these integers as a function of the effective magnetic flux is quite surprising. All along the irregular outline \(E_1 = E_1(\Phi)\), the Chern numbers computed for the various \(\Phi\) follow a very regular law: the representation of the Chern numbers as a function of the flux \(C_S = C_S(\Phi)\) depicts plateau sequences, adopting the shape of successive stairways. In figure 2, we show this structure in a compact way, by plotting \(|C_S|\) as a function of the flux \(\Phi\). We note that this figure is symmetric with respect to \(\Phi = 0.5\).

The numerical result illustrated in figure 2 is already interesting since it underlines the complexity of the Hofstadter 2 We use the notation \(C_S\) (resp. \(C_M\)) in order to denote the Chern numbers computed in the square (resp. honeycomb) lattice case.

Figure 2. Chern numbers as a function of the magnetic flux, \(|C_S| = |C_S|_{\Phi}\), for \(\Phi = \frac{p}{q}\) with \(q < 77\).
which is associated with the first energy band, and which takes infinitely many different values as a function of the flux. Surprisingly, these many values give rise to a structure consisting of successive stairways which are characterized by the number \( s_1 \).

3. The honeycomb lattice

In this section, we consider the case of a 2D honeycomb lattice subjected to a magnetic field. The honeycomb has a bipartite structure and it is common to define two fermion operators \( a^\dagger_A(r) \) and \( a^\dagger_B(r) \), where \( r = me_1 + ne_2 \) (see for example [37]). The unit vectors are chosen as \( e_1 = (3/2, \sqrt{3}/2) \) and \( e_2 = (0, \sqrt{3}) \). In the tight-binding approximation, the many-body Hamiltonian reads

\[
\mathcal{H}(r) = a^\dagger_A(r)a_B(r) + e^{i\pi\Phi}a^\dagger_A(r)a_B(r - e_2) + a^\dagger_A(r + e_1)a_B(r) + \text{h.c.,}
\]

and \( \Phi = p/q \) is the effective magnetic flux quanta per unit cell. The single-particle Schrödinger equation associated with equation (8) yields

\[
(1 + e^{i2\pi\Phi m - ik})\psi_A(m) + e^{ik}\psi_A(m + 1) = \frac{E}{t}\psi_B(m),
\]

\[
(1 + e^{-i2\pi\Phi n + ik})\psi_B(m) + e^{-ik}\psi_B(m - 1) = \frac{E}{t}\psi_A(m),
\]

where \( \psi_A(m) \) and \( \psi_B(m) \) are \( q \)-periodic wavefunctions, \( k \) is the wave vector and \( E \) is the single-particle energy. The wave vector belongs to the magnetic Brillouin zone defined as \( k_x \in [0, \frac{2\pi}{\sqrt{3}}] \) and \( k_y \in [0, 2\pi] \). The spectrum is depicted in figure 5 as a function of the effective magnetic flux \( \Phi \), and illustrates a modified version of the Hofstadter butterfly. The band structure associated with equation (9) has been extensively studied in order to investigate the very rich physics of graphene [37–39]. The Chern numbers associated with the energy bands have been computed numerically by Hatsugai et al and give rise to the anomalous quantum Hall effect: around \( E = 0 \), the transverse conductivity evolves by steps according to \( \sigma_{xy} = \pm (2N + 1)e^2/h \) where \( N \) is an integer [37].

Figure 4. Chern numbers (black dots) as a function of the magnetic flux, \( |C_3| = |C_3| (\Phi) \), for \( \Phi = \frac{p}{q} \) with \( q < 157 \). The dots are connected by colored lines according to the topological invariant \( s_1 \) to which they are associated through the Diophantine equation (6). Note that the Chern numbers are single-valued.

Figure 5. Butterfly spectrum \( \Phi = \Phi(E) \) for the 2D honeycomb lattice subjected to a magnetic field. The butterfly’s outline is coloured in red. The energy is expressed in units of the hopping parameter \( t \).

The outline of the honeycomb butterfly (red curve in figure 5) is highly irregular and differs from the square lattice case in regards to its general shape. In order to characterize this other irregular curve, and compare it to the Hofstadter butterfly’s outline, one has to evaluate the Chern numbers \( C_H \) associated with the fundamental band \( E_1(k_x, k_y) \) for the honeycomb lattice case. Unfortunately, in contrast to the square lattice case, no Diophantine equation is known to describe the entire honeycomb butterfly [37]: the gaps are labelled by two integers \((t_r, s_r)\) which satisfy equation (3), but the condition \(|t_r| \leq q/2\) is not always satisfied. Thus the Chern numbers cannot be unambiguously determined on the basis of the Diophantine equation. In the lack of such an equation, one has to compute the Chern numbers numerically. This can easily be achieved thanks to an efficient method developed by Fukui et al [40].

The numerical results are shown in figure 6. A new sequence of plateaux is observed in the honeycomb case, for which the transverse conductivity evolves by steps according to \( \sigma_{xy} = \pm (2N + 1)e^2/h \), where \( N \) is an integer. This is already surprising, because the fundamental band \( E_1(k_x, k_y) \) corresponds to energies which are far from \( E = 0 \), where the anomalous behavior of double steps is expected [37]. From this observation, it seems that the main signature of the anomalous quantum Hall effect is already contained in the edge of the butterfly: if the Fermi energy of the system lies in the first gap while varying \( \Phi \), one should observe this fascinating property proper to graphene. From a topological point of view, this particular sequence of Chern numbers suggests that the honeycomb butterfly’s outline radically differs from the Hofstadter butterfly’s outline.

However, it is worth noticing that the general structure depicted in figure 6 is remarkably similar to the results shown in figures 2 and 4 in the context of the square lattice case. The universality arising from these figures indicates that the Diophantine equation also plays a key role in the honeycomb system.
Although the condition $|C_H| \leq q/2$ is not fulfilled, we have verified that all the solutions $C_H(\Phi)$ satisfy the Diophantine equation (3), and that each stairway is again characterized by the other number $|s_1|$.

In order to emphasize the universality suggested by figures 2 and 6, we have connected with a coloured line the solutions $C_H(\Phi)$ according to their associated number $|s_1|$ (see figure 6). As in the square lattice case, the successive stairways are indeed characterized by increasing values of the Chern number $|s_1|$.

4. Conclusion

In this work, we have put forward the existence of strong and regular structures associated with the highly irregular Hofstadter butterfly’s outline. These structures, which arise in square and honeycomb lattices, have a universal character and are related to the underlying topology of the system’s fundamental energy band. The topology of the system is designated through the Chern number which gives its value to the quantized transverse conductivity. The correspondence between the results obtained for the square and the honeycomb lattices has been confirmed through numerical computations of the Chern numbers in the honeycomb case. We have verified that these solutions indeed satisfy the general Diophantine equation. It has been shown, for both geometries, that when the Fermi energy remains in the first gap, the transverse conductivity is highly irregular but evolves on stairways labelled by the other number that satisfies the Diophantine equation. We believe that these structures might play a role in the Mott-insulator transitions observed in rotating atomic systems, where single-particle properties are known to be dominant. We eventually point out that the properties emphasized in this work are not restricted to the field of cold atoms physics and could also be found in superconducting networks or 2D electronic systems.

Acknowledgments

NG thanks P Gaspard, A Astudillo Fernandez, P de Buyl, S Goldman, R Matos Alves, J-S Mc Ewen, N Tabti and V Wens for their support. The author also thanks A Kubasiak and M Lewenstein for their valuable comments and encouragements. NG is financially supported by the FRS-FNRS Belgium.

References

[1] Hofstadter D 1976 Phys. Rev. B 14 2239
[2] Wannier G H 1978 Phys. Status Solidi B 88 757
[3] MacDonald A H 1983 Phys. Rev. B 28 6713
[4] Kohmoto M 1989 Ann. Phys. 160 343
[5] Kohmoto M 1992 J. Phys. Soc. Jpn 61 2645
[6] Thouless D J, Kohmoto M, Nightingale M P and denNijs M 1982 Phys. Rev. Lett. 49 405
[7] Simon B 1983 Phys. Rev. Lett. 51 2167
[8] Avron J E, Seiler R and Simon B 1983 Phys. Rev. Lett. 51 51
[9] Kunz H 1986 Phys. Rev. Lett. 57 1095
[10] Tesanovic Z, Axel F and Halperin B I 1989 Phys. Rev. B 39 8525
[11] Bloch I, Dalibard J and Zwerger W 2008 Rev. Mod. Phys. 80 885
[12] Lewenstein M et al 2007 Adv. Phys. 56 243–379
[13] Jaksch D and Zoller P 2003 New J. Phys. 5 56
[14] Ho T-L 2001 Phys. Rev. Lett. 87 060403
[15] Polini M, Fazio R, MacDonald A H and Tosi M P 2005 Phys. Rev. Lett. 95 010401
[16] Klein A and Jaksch D 2009 Europhys. Lett. 85 13001
[17] Sørensen A S, Demler E and Lukin M D 2005 Phys. Rev. Lett. 94 086803
[18] Lin Y-J, Compton R L, Perry A R, Phillips W D, Porto J V and Spielman I 2008 arXiv:0809.2976
[19] Bhat R, Carr L D and Holland M J 2006 Phys. Rev. Lett. 96 060405
[20] Goldman N 2007 Europhys. Lett. 80 2001
[21] Goldman N and Gaspard P 2008 Phys. Rev. A 77 053629
[22] Goldman N, Kubasiak A, Gaspard P and Lewenstein M 2007 arXiv:0712.2571v4 at press
[23] Goldman N 2008 Phys. Rev. A 77 053406
[24] Oktel M Ö, Nita M and Tanatar B 2007 Phys. Rev. B 75 045133
[25] Umucalilar R O and Oktel M Ö 2007 Phys. Rev. A 76 055601
[26] Goldbaum D S and Mueller P 2008 Phys. Rev. A 77 033629
[27] Fink H J, López A and Maynard R 1982 Phys. Rev. B 26 5237
[28] Ramrak R, Lubensky T C and Toulouse G 1983 Phys. Rev. B 27 2820
[29] Alexander S 1983 Phys. Rev. B 27 1541
[30] Petschel G and Geisel T 1993 Phys. Rev. Lett. 71 239
[31] Springsguth D, Ketzmerick R and Geisel T 1997 Phys. Rev. B 56 2036
[32] Kohmoto M 1989 Phys. Rev. B 39 11943
[33] Hatsuui Y, Fukui T and Aoki H 2006 Phys. Rev. B 74 205414
[34] Gusynin V P and Sharapov S G 2005 Phys. Rev. Lett. 95 146801
[35] Park C-H, Yang L, Son Y-W, Cohen M L and Louie S G 2008 Phys. Rev. Lett. 101 126804
[36] Fukui T, Hatsuui Y and Suzuki H 2005 J. Phys. Soc. Jap. 74 1674

J. Phys. B: At. Mol. Opt. Phys. 42 (2009) 055302

N Goldman