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Topological map of the Hofstadter butterfly: Fine structure of Chern numbers and Van Hove singularities

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A B S T R A C T

The Hofstadter butterfly is a quantum fractal with a highly complex nested set of gaps, where each gap represents a quantum Hall state whose quantized conductivity is characterized by topological invariants known as the Chern numbers. Here we obtain simple rules to determine the Chern numbers at all scales in the butterfly fractal and lay out a very detailed topological map of the butterfly by using a method used to describe quasicrystals: the cut and projection method. Our study reveals the existence of a set of critical points that separates orderly patterns of both positive and negative Cherns that appear as a fine structure in the butterfly. This fine structure can be understood as a small tilting of the projection subspace in the cut and projection method and by using a Chern meeting formula. Finally, we prove that the critical points are identified with the Van Hove singularities that exist at every band center in the butterfly landscape.

1. Introduction

Discovered by Belgian physicist Leon Van Hove in 1953, Van Hove singularities are singularities in the density of states (*DOS*) crystalline solid [1]. These singularities are known to be responsible for various anomalies provided the Fermi level lies close to such a singularity. Electronic instabilities at the crossing of the Fermi energy with a Van Hove singularity in the DOS often lead to new phases of matter such as superconductivity, magnetism, or density waves [2].

A two-dimensional electron gas (2DEG) in a square lattice provides a simple example of Van Hove singularities in the energy dispersion of a crystal. For a tight binding model of a square lattice the energy dispersion is given by,

$$E = -2J[\cos k_x a + \cos k_y a] \quad (1)$$

Here $\vec{k} = (k_x, k_y)$ is the wave vector in the first Brillouin zone, a is the lattice spacing of the square lattice and J is the nearest-neighbor hopping parameter which defines the effective mass m_e of the electron on the lattice by the relation $J = \frac{\hbar^2}{2m_e a^2}$. This single band Hamiltonian has band edges at $E = \pm 4J$. It can be shown that the DOS at the band edges approaches a constant equal to $\frac{1}{4\pi a^2 \hbar^2}$. However, it diverges at the band center as DOS $\approx \frac{\ln J}{E}$. Such a divergence is an example of a Van Hove singularity. Fig. 1(a) shows the energy contours in (k_x, k_y) plane, where the almost free-electron concentric circles are transformed into a diamond shape structure that corresponds to saddle points in the energy surface. We note that the lattice structure is essential for the existence of Van Hove singularities. Van Hove singularities have been given a topological interpretation in terms of a switching of electron orbits from electron like to hole like [3]. It is worthwhile mentioning that the topological properties of Van Hove singularities in lattices without magnetic fields have been known since long time ago using a theory developed by Morse [4] and applied to solid state physics by J.C. Phillips [5].

In this paper we investigate the Van Hove anomalies of a 2DEG in transverse magnetic fields. Such a system describes all phases of non-interacting electrons as one varies the chemical potential and magnetic field. The phase diagram, known as the Hofstadter butterfly [19] represents various quantum Hall states, each characterized by a quantum number, the Chern number, that has its roots in the nontrivial topology of the underlying Hilbert space [9]. Several aspects of this quantum Hall effect are well understood

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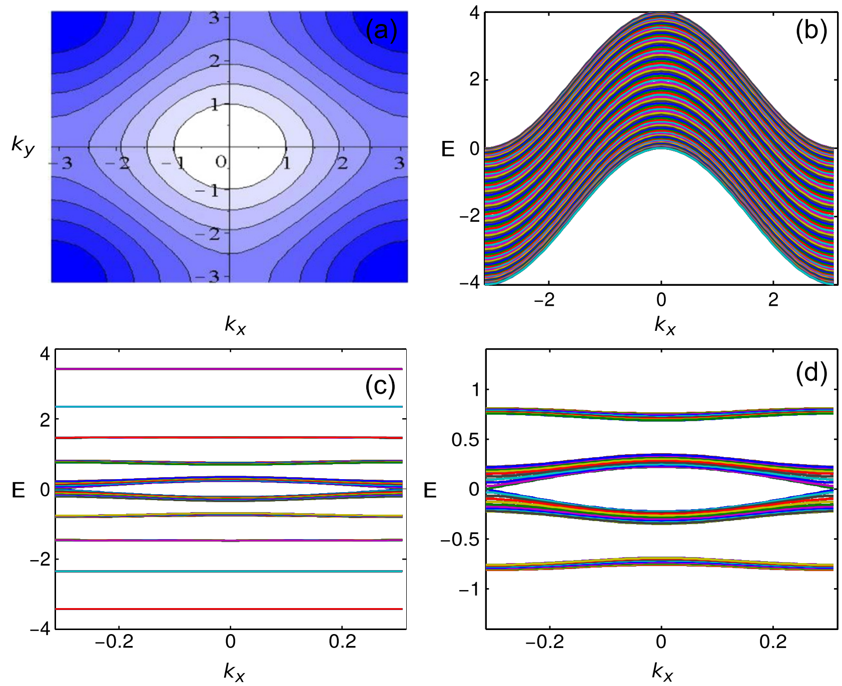

Fig. 1. (a) Contour plot of the energy E in the (k_x, k_y) plane, illustrating the saddle character of the band center for a 2DEG on a square lattice. (b) Shows the corresponding band as a function of k_x. (c) Shows the spectrum for small magnetic flux $\phi = 0.1$. Landau levels correspond to the horizontal flat bands. In (d) we show a blow up of (c) near the band center, illustrating the deviation from the Landau level picture near the band center that hosts a Van Hove singularity. In (b), (c) and (d), the colors represent different values of k_y.

[2] and recently there has been a reemergence of the field due to the first experimental observation of the Hofstadter butterfly [10], leading to perform band-structure engineering [11]. Many of these properties have been measured in graphene over a substrate, since strain in graphene acts as a pseudo magnetic field [12–14]. Also, there is an interest in artificial systems which share the same phenomenology, like ultra cold bosonic atoms [15].

The key result of this paper is the characterization of Van Hove singularities that are nested in the topological hierarchical pattern of the butterfly spectrum. We show that in the two-dimensional energy-flux space, every vicinity of a Van Hove consists of interlacing sequences of Chern numbers. In other words, the Van Hove singularities separate different topological sequences. To achieve this goal, we calculate Chern numbers in the neighborhood of Van Hove singularities, facilitated by simple rules that are derived for determining the entire topological map of the butterfly fractal at all scales.

Notice that there are other previous classic works that studied in detail the layout of the Hofstadter butterfly [16,17] and its relationship with the density of states, however, the fine structure around Van Hove singularities has not been tackled previously. Furthermore, our analysis begins with a simple geometrical approach, based on a method to treat the structure of quasicrystals, that sets the stage for determining the Chern numbers of all the gaps and its associated fine structure. Although this functional relationship is known [18], our geometrical approach allows to find it in a simple way. It also provides a powerful, intuitive and simple geometrical interpretation for the more complicated number theory approach [17]. In fact, we will show that the fine structure of the Hofstadter butterfly can be explained in terms of a simple tilting of the projection subspace used in the cut and projection method.

It is the orderly patterns of topological integers that characterize the fine structure that gets linked to the Van Hove anomalies of a two dimensional crystalline lattice in a magnetic field. Moreover, a very recent study of the 2DEG when subjected to a weak magnetic field, revealed the importance of Van Hove singularities in inducing changes in localization characteristics of the system [6].

In a continuum system, that is, in the absence of any lattice structure, the magnetic field B introduces a magnetic length $l_B = \sqrt{\frac{\Phi_0}{2\pi B}}$ (where Φ_0 is the magnetic flux), reincarnation of the cyclotron radius of the corresponding classical problem. In this limit, the energy spectrum consists of equally spaced harmonic oscillator levels known as the Landau-levels. Interestingly, in a lattice with weak magnetic flux, the Landau level picture breaks down near the band center as illustrated in the Fig. 1. As we will discuss, this is due to the saddle points of the energy dispersion surface. This is in sharp contrast to the parabolic dependence of the energy near the band edges that leads to the Landau levels.

The model system that we study here consists of (spinless) fermions in a square lattice. Each site is labeled by a vector $\mathbf{r} = l\hat{x} + m\hat{y}$, where l, m are integers, and $\hat{x}$ ($\hat{y}$) is the unit vector in the x (y) direction. The tight binding Hamiltonian has the form

$$H = -J_x \sum_{\mathbf{r}} |\mathbf{r}+\hat{x}\rangle\langle\mathbf{r}| - J_y \sum_{\mathbf{r}} |\mathbf{r}+\hat{y}\rangle e^{i2\pi l\phi}\langle\mathbf{r}| + h.c. \qquad (2)$$

Here, $|\mathbf{r}\rangle$ is the Wannier state localized at site $\mathbf{r}$. J_x (J_y) is the nearest neighbor hopping along the x (y) direction. With a uniform magnetic field B along the z direction, the flux per plaquette, in units of the flux quantum Φ_0, is $\phi = -Ba^2/\Phi_0$. The field B gives rise to the Peierls phase factor $e^{i2\pi l\phi}$ in the hopping.

Within the Landau gauge, the above Hamiltonian has been engineered in cold atom experiments [7]. Using this gauge, the vector potential is given by $A_x = 0$ and $A_y = -\phi x$ resulting in a Hamiltonian that is cyclic in y. Therefore, the eigenstates of the system can be written as $\Psi_{l,m} = e^{ik_y m}\psi_n$ where ψ_l satisfies the Harper equation [19]

$$\psi_{l+1} + \psi_{l-1} + 2\lambda\cos(2\pi l\phi + k_y)\psi_l = E\psi_l. \qquad (3)$$

Here l (m) is the site index along the x (y) direction and $\lambda = J_y/J_x$. For a rational $\phi = p/q$, where p and q are relatively prime integers, the solutions are periodic resulting in the condition $\psi_{l+q} = \exp(k_x qa)\psi_l$.

At the rational flux $\phi = p/q$, the energy spectrum has $q-1$ gaps, although for even q the central gap is closed. These spectral