Hofstadter butterfly as quantum phase diagram

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The Hofstadter butterfly is viewed as a quantum phase diagram with infinitely many phases, labeled by their (integer) Hall conductance, and a fractal structure. We describe various properties of this phase diagram: We establish Gibbs phase rules; count the number of components of each phase, and characterize the set of multiple phase coexistence. © *2001 American Institute of Physics.*
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I. INTRODUCTION

Azbel[1] recognized that the spectral properties of two-dimensional, periodic, quantum systems have sensitive dependence on the magnetic flux through a unit cell. A simple model conceived by Peierls and put to the eponymous Harper as a thesis problem, gained popularity with D. Hofstadter's Ph.D. thesis,[2] where a wonderful diagram, reminiscent of a fractal butterfly, provided a source of inspiration and a tool for spectral analysis.[3–9]

The Hofstadter butterfly can also be viewed as the quantum (zero temperature) phase diagram for the integer quantum Hall effect. It is a fractal phase diagram with infinitely many phases.[10,11] The diagram leads to certain natural questions: Count the number of components of a given phase; classify which phases coexist and where. It also leads to the general question: What form does the Gibbs phase rule[12,13] take for quantum phase transitions.

Fractal phase diagrams and/or infinitely many phases appear in dynamical systems.[14,15] In classical lattice systems fractal phase diagrams[12,16,17,13] are commonly viewed as a pathology due to either long range interactions, or, as is the case for spin glasses, loss of translation invariance. The Hofstadter model, when viewed as a statistical mechanical model, is both short range and translation invariant in a natural way. But, it is quantum and the translation group is noncommutative. It suggests that the fractal phase diagram may be more common in quantum phase transitions than in classical phase transitions.

II. THE HOFSTADTER MODEL

The model conceived by Peierls has two versions. For the sake of concreteness we shall focus here on the tight binding version. On the lattice $\mathbb{Z}^2$, define magnetic shifts

$$(U\psi)(n,m)=\psi(n-1,m),\quad (V(\Phi)\psi)(n,m)=e^{2\pi i n\Phi}\psi(n,m-1)\quad n,m\in\mathbb{Z}. \tag{1}$$

$2\pi\Phi$ is the magnetic flux through a unit cell. The Hofstadter model is

$$H(\Phi,a,b)=a(U+U^*)+b(V(\Phi)+V^*(\Phi)), \tag{2}$$

where $a,b>0$ are "hopping" amplitudes. $a=b$ is called the self-dual case[18] and we shall focus on that case in the following. We set $H(\Phi)=H(\Phi,1,1)$.

U and V, and therefore also $H(\Phi)$, commute with the (dual) magnetic translations $\mathcal{U}$ and $\mathcal{V}$,

$$(\mathcal{U}\psi)(n,m)=\psi(n,m-1)\quad (\mathcal{V}\psi)(n,m)=e^{2\pi i\Phi m}\psi(n-1,m). \tag{3}$$

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This makes $H(\Phi)$ translation invariant in a natural way. The group of magnetic translations[19] is noncommutative:

$$U^*V^*UV=\mathcal{U}\mathcal{V}\mathcal{U}^*\mathcal{V}^*=e^{-2\pi i\Phi}. \tag{4}$$

The one-particle representation of the Hofstadter model, Eq. (2), is natural for spectral studies. In the context of statistical mechanics the second quantized representation of the model is also instructive because it makes it clear that the model has short range, in fact, only on site and nearest neighbors, interactions. The fractal features of the phase diagram are, therefore, not a consequence of long range forces, as in some classical statistical mechanics models. The second quantized form is

$$\mathcal{H}(\Phi,\mu)=\sum e^{i\gamma(nm;n'm')}a^{\dagger}_{nm}a_{n'm'}+\mu\sum a^{\dagger}_{nm}a_{nm}, \tag{5}$$

where

$$e^{i\gamma(mn;m'n')}=\begin{cases}1, & n-n'=\pm 1,\ m=m'\\ e^{\pm 2\pi in\Phi}, & m-m'=\pm 1,\ n=n'\\ 0 & \text{otherwise.}\end{cases} \tag{6}$$

μ is the chemical potential and $a^{\dagger},a$ are the usual Fermionic operators.

Let us recall a few elementary features of the spectrum:

$$S(H(\Phi))=-S(H(\Phi))=-S(H(1-\Phi)). \tag{7}$$

The first is a consequence of $\mathbb{Z}^2$ being bipartite, and the second is a consequence of time reversal. Together, they imply a fourfold symmetry, manifest in the Hofstadter butterfly.

The electronic density, $\rho(\Phi,\mu)$ (=integrated density of state), is

$$\rho(\Phi,\mu)=\langle 0|\theta(\mu-H(\Phi))|0\rangle, \tag{8}$$

where $|0\rangle$ is Kroneker delta at the origin. $0\leqslant\rho(\Phi,\mu)\leqslant 1$ is an increasing function of μ. θ is the usual step function.

The gaps in the spectrum are labeled by an integer, k, which is a solution of[20,3]

$$\Phi\, k=\rho \bmod 1. \tag{9}$$

k is the Hall conductance. We picked the letter k because it is naturally associated with an integer, and it is also the first letter in von Klitzing's name. By Eqs. (9) and (7),

$$k(\mu,\Phi)=-k(\mu,1-\Phi)=-k(-\mu,\Phi), \tag{10}$$

which implies a fourfold (anti) symmetry of the butterfly.

We shall assume that the Ten Martini conjecture[21] holds. Namely, that for all irrational Φ's, all the gaps are open, so Eq. (9) has ρ in an open gap for all $k\in\mathbb{Z}$.

Figure 1 shows the Hofstadter butterfly, color coded according to the Hall conductance. Zero Hall conductance is left blank. The gross features of the diagram are associated with small integers where the color coding is faithful.

The colored picture emphasizes the gaps while the standard Hofstadter butterfly emphasizes the spectrum. The colored figure is prettier and displays the regular aspects of the diagram: Gaps are better behaved than spectra. The colored diagram is also more faithful to certain spectral characteristics. For example, the spectrum is a small set (in fact, one of zero Lebesgue measure), something that is manifest in the colored diagram, but is less obvious from the usual Hofstadter butterfly which plots the spectrum.

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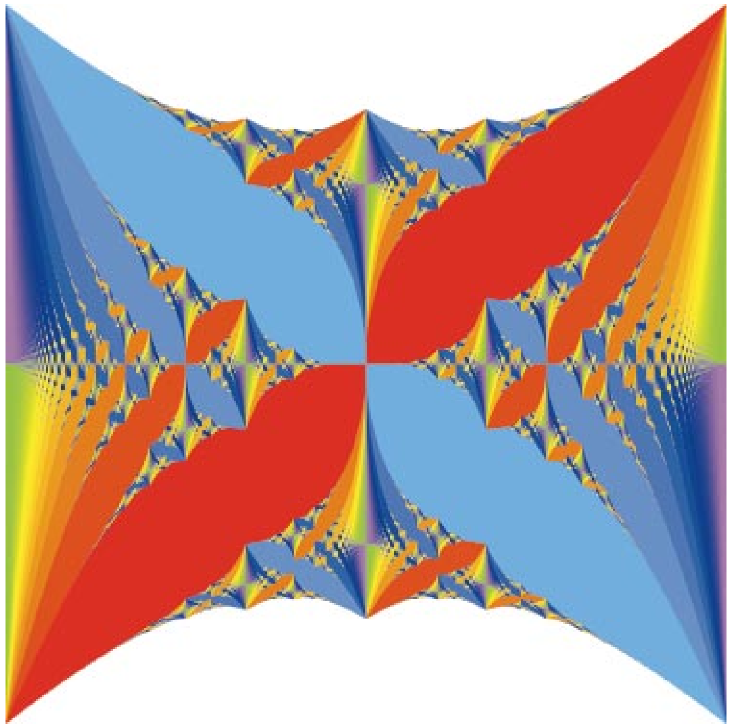

FIG. 1. (Color.) Hofstadter colored butterfly.

We also broke with tradition in that the colored Hofstadter butterfly is rotated by 90°: In Fig. 1 the horizontal axis is Φ and the vertical axis is the energy, or $S(H(\Phi))$. The reason we chose to do so is that this way emphasizes the fact that phase boundaries are functions (of Φ).

We denote by $P(k)$ the kth phase. Formally,

$$P(k)=\{\Phi,\mu|\Phi k=\rho(\Phi,\mu)\bmod 1,\mu\notin S(H(\Phi))\}. \tag{11}$$

$P(k)$ is an open set in the (Φ,μ) plane, with a finite number of components. For example, $P(1)$ is two of the four big wings of the butterfly. We call $P(k)$ a *pure phase* and denote its number of components $|P(k)|$. The closure of the pure phase is denoted $\overline{P}(k)$ and the phase boundary is $\partial P(k)$. We call $\cup_k \partial P(k)$ the total boundary.

III. COUNTING COMPONENTS

The kth pure phase is made of several components. The $k=0$ phase (blank) has two components. For $k\neq 0$ the number of components is

$$|P(k)|=\sum_{j=1}^{2|k|}\phi(j)=12\frac{k^2}{\pi^2}+O(k\log k), \tag{12}$$

where $\phi(j)$ is Euler (totient) function. Recall that $\phi(j)$ counts the number of integers, up to j (and including 1), that are prime to j: $\phi(1)=1$, $\phi(2)=1$, $\phi(3)=2$ etc.

To prove Eq. (12) note first that from Eq. (9)

$$k(\rho,\Phi)=k(\rho',\Phi)\Rightarrow\rho=\rho'. \tag{13}$$

Hence, a given color would appear *at most* once on any vertical line of fixed Φ.

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When $\Phi = p/q$ with $\gcd(p,q)=1$ [$\gcd(p,q)$ is the greatest common divisor of p and q], the spectrum of the Hofstadter model has q finite bands and $q-1$ gaps which are all open intervals (except when q is even the central gap is closed). We then number the gaps by their natural order $1,\ldots,q-1$. The semi-infinite interval below the spectrum is, formally, the 0th gap, and the semi-infinite interval above the spectrum as the qth gap. Equation (9), for the jth gap, can be written as

$$p\,k = j \bmod q. \tag{14}$$

Given $p,q,$ and j the equation has a unique solution for each open gap such that $|k|<q/2$. In particular, once q has been fixed, the Hall conductance takes all (nonzero) integer values, from $-\lfloor q/2 \rfloor$ to $\lfloor q/2 \rfloor$, and each value appears once. For even q, the central gap is closed and formally can be assigned a value of $\pm q/2$.

The number of components of the kth phase is the same as the number of flux values, Φ_{ℓ}, which accommodate the wing tips, minus one. The kth wing tips are located at those values of Φ where the kth color is absent (the kth color *is* present in any small neighborhood of those values of Φ, because this neighborhood contains fractions with arbitrary large q's). Given $k \neq 0$, it must appear once on a horizontal interval with $\Phi = p/q$ provided $q/2>|k|$. The tips of a wing with a given color must, therefore, be located at those values of Φ which do not admit k as solution of Eq. (14) for any ρ. In other words, the wing tips lie at those values of Φ where q is too small to accommodate $|k|$. This is the finite set, a Farey sequence,

$$F_{2|k|} = \left\{ \frac{p}{q} \,\middle|\, 0 \leq p \leq q, \gcd(p,q)=1, q \leq 2|k| \right\} = \bigcup_{q=1}^{2|k|} \left\{ \frac{p}{q} \,\middle|\, 0 < p \leq q, \gcd(p,q)=1 \right\} \bigcup \{0\}. \tag{15}$$

Let $|F|$ be the number of elements in F. Then from (15),

$$|P(k)| = |F_{2|k|}| - 1 = \sum_{q=1}^{2|k|} \phi(q) \tag{16}$$

essentially from the definition of the Euler function.

The asymptotic expansion for the sum in Eq. (12) is taken from Ref. 22.

IV. PURE PHASES AND PHASE BOUNDARIES

In thermodynamics and statistical mechanics, Gibbs phase rule is a statement about the structure of pure phases and their boundaries. A weak form of the Gibbs phase rule says that pure phases are a set of full measure; two phases coexist, generically, on a set of Hausdorff codimension one, etc.[12] This is the form that one gets if one considers general convex functions for thermodynamic potentials. The number of coexisting phases is related to the dimension of tangent planes, and the Gibbs phase rule is a consequence of theorems about convex functions. There is a stronger form of the rule[13] which posits, in addition, that the sets are (locally) manifolds. This form is a consequence of additional regularity of the thermodynamic potentials.

Gibbs phase rule is a consequence of the convexity of thermodynamic potentials and so is ultimately based on the second law of thermodynamics. It has nothing to say about the zero temperature phase diagram of quantum phase transitions in general,[23] and the Hofstadter model in particular (because the entropy vanishes identically). A question that arises is then what form might Gibbs phase rule take for quantum phase transition. The Hofstadter model restricts what could and what could not be true in general. As we shall see, the phase diagram of the Hofstadter model turns out to satisfy only a weak form of the Gibbs phase rules.

Figure 1 suggests that the set of unique phase is a set of full measure and that the phase boundaries, though fractal, are not too wild. More precisely, we have the following.

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Gibbs-like phase rule: The phase diagram of the self-dual Hofstadter model is such that pure phases, labeled by their Hall conductances, are full measure; phase boundaries are not manifolds—they are nowhere differentiable—but they are almost so in the sense that their Hausdorff co-dimension is integral, in fact:

$$\dim_H(\partial P(k)) = 1. \tag{17}$$

Since the number of phases is countable the total phase boundary $\cup_m(\partial P(m))$ *is a set of Hausdorff dimension one as well. Finally, infinitely many phases coexist on a countable set, and therefore a set of Hausdorff dimension zero.*

The first part of the Gibbs-like phase rule is an easy consequence of a result of Last,[6] which states that $|S(H(\Phi))| = 0$ for a set of Φ of full measure. That phase boundaries are nowhere differentiable follows from results of Wilkinson,[9] Rammal, and Helffer and Sjöstrand,[5] who showed that the phase boundaries $\partial P(k)$ possess distinct left and right tangent at every rational Φ. That the Hausdorff dimension of the boundary is one follows from results of Bellissard,[24] who showed that away from the wings tips, $\partial P(k)$ can be represented by functions of Φ that are *uniformly* Lipshitz. By standard results,[25] it then follows that the Hausdorff dimension is one. The set of infinite phase coexistence is analyzed in the following.

V. COEXISTENCE

In Ref. 15 the term lakes of Wada was used to describe dynamical systems with the property that any point on the boundary of the one basin of attraction is also on the boundary of all other basins. We shall say that a system is almost Wada of order m if every circle that contains two pure phases contains m pure phases.

The Hofstadter butterfly is almost Wada of infinite order. This is seen from the figure, and can also be shown to follow from Eq. (9).

We say that the two pure phases, $P(m)$, $P(n)$, coexist on

$$C(m,n) = \partial P(m) \cap \partial P(n). \tag{18}$$

No two phase coexists for any irrational flux. This is easily seen from Eq. (9): For irrational Φ the electron density ρ takes a dense set of values in the gaps. Therefore, any two phases, $P(m)$ and $P(n)$, are separated by infinitely many other phases. It follows that the set of phase coexistence is a countable set, and so of zero Hausdorff dimension.

The following result gives a complete characterization of phase coexistence:

Proposition: Consider a point $x \in \partial P(k)$ *with* $\Phi(x) = p/q$ *with* $\gcd(p,q) = 1$. *Then* $x \in \partial P(k + \ell q)$ *for all* $\ell \in \mathbb{Z}$. *Moreover* $x \notin \partial P(k')$ *if* $k' \neq k + \ell q$ *for each* $\ell \in \mathbb{Z}$

Proof: Since $\gcd(p,q) = 1$ the equation

$$pa - qb = 1 \tag{19}$$

has a solution with integer a and b (where a is nonunique mod q). Let $p_n/q_n = (np - b)/(nq - a)$ with $n \in \mathbb{Z}$. Then

$$p_n q - q_n p = 1. \tag{20}$$

From Eq. (14) it follows that each band at p_n/q_n carries Hall conductance $q \pmod{q_n}$.

Now consider a point x on the right boundary of $P(k)$. We shall first show that x is also on the left boundary of $P(k+q)$. Since $P(k+q)$ has a finite set of wing tips, Eq. (15), when n is large enough, the gap with label (=Hall conductance) $k+q$ at flux p_n/q_n must be open, and must remain open for all large n. By a bound of Last and Wilkinson[26] for the total width of the spectrum at p_n/q_n, each band is small and hence

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$$\mathrm{dist}(P(k),P(k+q))<\frac{24}{q_n}. \tag{21}$$

Taking $n\to\infty$ we see that $x\in\partial P(k+q)$ as claimed.

By considering the next band we shall now show that x also lies on the boundary of $P(k+2q)$. Now, $P(k+2q)$ at p_n/q_n is separated from $P(k)$ by two bands and a gap. The bands are small by the Last–Wilkinson bound. The gap is also small by the Hölder continuity of the spectrum:

$$|\mathrm{gap}|<18\sqrt{\frac{p_n}{q_n}-\frac{p}{q}}=\frac{18}{\sqrt{qq_n}} \tag{22}$$

and from this

$$\mathrm{dist}(P(k),P(k+2q))<\frac{24}{q_n}+\frac{18}{\sqrt{qq_n}}. \tag{23}$$

Taking the limit $n\to\infty$ yields the result. The argument can be repeated for any $P(k+\ell q)$ with ℓ finite and positive. Negative values $P(k-\ell q)$ are obtained by letting $n\to-\infty$ in the abovementioned argument.

For the left boundary point of $P(k)$, $n\to\infty$ will give $P(k-\ell q)$ and $n\to-\infty$ will give $P(k+\ell q)$. This formula applies also to the phase $k=0$, with its right boundary being the leftmost point of the spectrum and vice-versa. The Hall conductance for the middle gap with even q (which is closed) is formally $\pm q/2$, so it is common to phases $P(\pm q/2+\ell' q)$ which is the same as $P(q/2+\ell q)$ for $\ell,\ell'\in\mathbb{Z}$.

The second part of the proposition follows from the equality

$$\bigcup_{k\leqslant|\frac{q}{2}|}\ \bigcup_{\ell\in\mathbb{Z}} P(k+\ell q)=\bigcup_{k\in\mathbb{Z}} P(k)$$

and the fact that for fixed Φ, each Hall conductance k can appear only once.

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