Fractality of Hofstadter Butterfly in Specific Heat Oscillation

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We calculate thermodynamical properties of the Hofstadter model using a recently developed quantum transfer matrix method. We find intrinsic oscillation features in specific heat that manifest the fractal structure of the Hofstadter butterfly. We also propose experimental approaches which use specific heat as an access to detect the Hofstadter butterfly.

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The interplay between crystalline potential and magnetic field on a two-dimensional electronic gas remains a nontrivial problem for decades. This issue provides a stage on which purely mathematical concepts, i.e., the irrationality of a real number, interrupts our intuition of physical reality. Hofstadter studied the energy spectrum of the tight-binding limit of this problem, namely, the Hofstadter model. He proposed a fractal topology for the spectrum (Hofstadter butterfly), which reconciled the paradox raised by the irrationality. The experimental verification of the Hofstadter butterfly is challenging but some hints of the fractal structure have been observed in microwave measurements, Hall conductivity and magnetic transport measurements in analogous systems.

In this paper, we adopt a recently developed quantum transfer matrix method to study thermodynamic properties of the Hofstadter model. We focus on the behavior of internal energy and specific heat as functions of magnetic field. As far as we know, this is the first report that by theoretical method, the fractal structure in the Hofstadter butterfly can be studied by computing the specific heat in a magnetic field of a generic value. We also briefly discuss the feasibility of experimental observations of these features.

In a previous publication, we had used the quantum transfer matrix method to study the magnetic properties of Hofstadter model. The advantage of this method lies in that it directly computes the partition function of the model for arbitrary magnetic flux quanta through a unit cell, then the thermodynamic properties can be studied steadily. Conventional theoretical methods, such as Bethe ansatz and exact diagonalization, are mostly applied to the cases, where and are mutually prime numbers, and is relatively small. Although detailed information of energy spectrum and wavefunction can be obtained with these methods, only limited cases of can be studied and most discussion was focused on ground state properties. Besides, at ground states, due to the fractality of the Hofstadter butterfly, the smoothness of physical quantities as functions of magnetic field, such as total energy, static magnetic susceptibility are significantly diminished. However, within the quantum transfer matrix formulation, the effect of finite temperature is embodied in the partition function at the beginning, and the singularities due to the fine fractality will be smeared out and the smoothness of physical quantities can be recovered, which makes the comparison to experimental results more straightforward.

Hofstadter model describes the dynamics of two-dimensional tight binding electrons in a uniform magnetic field. By applying Landau gauge, i.e., , the Hamiltonian is explicitly translationally invariant along the direction. Fourier transformation along the -axis will then decouple the two-dimensional model into a series summation of one-dimensional Hamiltonian :
temperature), which is the key point leading us to the transfer matrix representation and to significantly simplify the calculation in Ref.\[7,\ 8\]. Given \( k \), the partition function of \( H_k \) is defined by

\[
Z_k = \text{Tr} \exp(-\beta H_k),
\]

(3)

where \( \beta = 1/k_B T \). The partition function of the whole system is simply a product of all \( Z_k \)s. By making use of the translational invariance along the imaginary time, \( Z_k \) can be expressed as a product of \( N_\pi \) \( 2 \times 2 \) matrices. After multiplying different \( k \) components, we can obtain the partition function of the system, from which one can calculate the free energy by \( F = -(1/\beta) \ln Z \), and other thermodynamic quantities such as magnetic susceptibility and specific heat.

In Ref.\[8\], the authors have discussed the effect of lattice size on the numerical results. Accordingly, we choose here \( N_\pi = 50000 \) and \( N_y = 100 \) to ensure the numerical accuracy as well as computational efficiency for the temperature range in this paper. For simplicity, we only consider the half-filling case, which corresponds to a particle-hole symmetry and automatically sets chemical potential \( \mu \) to 0.

First, we calculate the average internal energy as a function of \( \phi \) at \( T = 0.01 \). As shown in Fig. 1 at the local minima of the internal energy, the electron count \( \nu = 0.5 \) for half-filling) and \( \phi \) satisfy the relation in (4), which was given Ref.\[11\]. These minima are cusp-like.

\[
\nu = M + N\phi, \quad M, N \in \mathbb{Z}.
\]

(4)

The global minimum in Fig. 1 is consistent with the conclusion that there is an global minimum of the average energy\[12,\ \text{13}\] when \( \phi = \nu = 1/2 \), that is, each electron carries one flux quanta. We have marked the values of \( \phi \)(the red number on the top axis) located at distinguishable minima and the corresponding integers \( M \) and \( N \) in Fig. 1. At zero temperature, the average energy will not be smooth almost everywhere because there are infinite number of rational \( \phi \)'s that satisfy (4). But here the temperature will erase minor singularities and only keep the significant ones.

Then we compute the specific heat from the first order derivative of the internal energy with respect to the temperature. Fig. 2 shows the specific heat \( C \) as a function of temperature \( T \) for some special \( \phi \)'s. The chosen three \( \phi \)'s belong to the pure cases in Hofstadter’s proposal\[2\], i.e., \( \phi = 1/N \), or \( 1 - 1/N \) when \( N \geq 2 \). Under magnetic field of these values, the single Bloch band in zero magnetic field is split into \( N \) subbands. If \( N \) is odd, the central subband has a van-Hove singularity at the center point of the energy spectrum\((E = 0)\). If \( N \) is even, the density of states\(\text{(DOS)} \) goes to zero at \( E = 0 \). When the temperature is so high that the thermal fluctuations are comparable to the energy difference between the lowest and the highest subband, the subbands will not be able to manifest their internal fine structures from specific heat. This can be observed from the high temperature tail in Fig. 2.

The difference in the specific heat for various values of \( \phi \) will emerge with the decreasing temperature. First, at low temperature, the behavior of specific heat can tell the singularity of DOS at the energy spectrum center point\(\text{(the Fermi surface\(\text{(FS)} \) in our half-filling case). In the regime near zero temperature, the } \phi = 1/2 \) and \( \phi =
1/4 curves are decreasing faster than that of \( \phi = 1/3 \). A closer observation indicates that \( \phi = 1/2 \) and \( \phi = 1/4 \) decrease exponentially-like, while \( \phi = 1/3 \) is linear-like. This is because of the different behavior of DOS at the spectrum center point \( \frac{1}{2} \). For \( \phi = 1/2 \) and \( \phi = 1/4 \), the original single band in zero field splits up into 2 and 4 bands. But the centermost two bands are not completely separated by a gap, rather they “kiss” at the center point, where DOS of both bands goes to zero. Therefore, we will expect a gap-like behavior at low temperature, which shows up as an exponential-like decrease in specific heat. For \( \phi = 1/3 \), the Bloch band splits into 3 bands, and DOS of the center band is singular at the center point. Thus we expect a much slower decrease near zero temperature, which is also observed in Fig. 2.

In the intermediate temperature regime, the specific heat tells the information about gaps and redistribution of DOS along the energy spectrum. In Fig. 2(a), the curves of \( \phi = 1/3, 1/4 \) show some similar minor hump structures, which is different from the case of \( \phi = 1/2 \). For \( \phi = 1/2 \), two subbands touch at FS, where DOS is zero, and there is no finite gap in the energy spectrum. Thus there is only one major hump in specific heat curve. For both \( \phi = 1/3 \) and \( \phi = 1/4 \), there is a finite gap lying above FS \( \frac{1}{11} \), which separates the subband on(\( \phi = 1/3 \)) or near(\( \phi = 1/4 \)) FS from the higher band, and gives the extra minor hump in the specific heat curve.

Fig. 3(a) shows the specific heat coefficient \( C/T \) as a function of \( 1/\phi \), so that the conventional de Haas-van Alphen (dHvA) -like oscillations are shown distinctly in the figure. The period \( \Delta (1/\phi) \) of this oscillation is about 2 in both cases, which is consistent with that obtained from textbook formula [14]. \( \Delta (1/\phi) = 4\pi^2/S_F \), where \( S_F \) is the Fermi volume. At half filling, \( S_F = 2\pi^2 \), thus \( \Delta (1/\phi) = 2 \) in Fig. 3(a).

However, a more important observation is that subtle oscillations emerge within the dHvA-type period with decreasing temperature and strong field. The specific heat at \( T = 0.1 \) displays a clean periodic oscillation on the weaker field side(large \( 1/\phi \)), while this periodicity is disturbed in the stronger field regime(small \( 1/\phi \)). This becomes more explicit with lower temperature \( T = 0.01 \). In the first three periods, very sharp peaks and dips show up, and they make a peculiar type of oscillations within the period. Even for weaker field regime, some sharp structures are still observable.

For the purpose of comparison, Fig. 3(b) shows the magnetization oscillation with respect to the magnetic field. Similar to the specific heat, the main envelope of oscillation is the conventional dHvA oscillation. Besides, subtle structures emerge within the dHvA period. By comparing the results for magnetization and specific heat, we find that the specific heat oscillations are more distinct and drastic.

![Figure 3](image3.png)

**FIG. 3:** (Color online) (a) The specific heat coefficient \( C/T \) as a function of \( 1/\phi \). Two different temperatures \( T = 0.01, 0.1 \) are compared; (b) Magnetization at \( T = 0.01 \) as a function of \( 1/\phi \).

![Figure 4](image4.png)

**FIG. 4:** (Color online) Specific heat coefficient(black line) and magnetic susceptibility(red line) for the Hofstadter model at half-filling. The numerical values of specific heat are 6000 times larger than the original ones for comparison. The values of \( \phi \) marked corresponds to some local maxima and minima in both specific heat and magnetic susceptibility.
To explore the information about the fractal structure of Hofstadter butterfly from specific heat, we zoom in the first period in Fig.3 and then have Fig.4 for low temperature specific heat $C$ and magnetic susceptibility $\chi$. The numerical values of the specific heat are enlarged to 6000 times of the original values for a clear comparison. Here $\phi$ is chosen to be the horizontal axis. The consistency between $C$ and $\chi$ is obvious if we compare the positions of local maxima and minima of both quantities. In Fig.3 some fractional values of $\phi s$ are marked where they are close to the local maxima and minima. Applying Hofstadter’s proposal of constructing the butterfly, we can extract the structure of energy spectrum at these $\phi s$ and understand why the extrema of $C$ and $\chi$ are close to them. With Hofstadter’s proposal, each fractional $\phi$ can be decomposed to a set of more “fundamental” fractions, or, “local variable” as in Ref.[2], which then directly displays the splitting of subbands in the energy spectrum. For example, for $\phi = 4/13$, the center local variable is $4/5$, which means there is a cluster of 5 subbands centered at FS. Consequently, a van-Hove singularity of DOS shows up at FS and causes the local maximum in $C$ and the strong paramagnetism (local maximum in $\chi$)[8], while for $\phi = 3/8$, the center local variable is $1/2$, thus there are two subbands lying above and below FS with a zero DOS at FS and consequently in Fig.4 $C$ shows a small value (close to 0) around $\phi = 3/8$ and $\chi$ is strongly diamagnetic around $\phi = 3/8$.

Therefore, by decreasing the temperature, fractal structures of the Hofstadter butterfly manifest themselves by producing peculiar oscillatory features within conventional dHvA period. This emergence along with decreasing temperature is due to the fact that temperature provides the only energy scale that sets up the resolution of the spectrum. Temperature erases minor bands and gaps that are smaller than the scale of temperature and restores the smoothness of physical quantities. But fractal structures with an energy scale larger than the temperature survive, and are able to manifest themselves by displaying smoothened singularities in thermodynamic quantities. Thus the subtler fractal structures of Hofstadter butterfly can be probed by the measurement of the specific heat at lower temperatures.

We propose to adopt the superconducting thin films (for example the element Nb) with periodic arrays of pinning sites[15] to realize this temperature-dependent emergence of fractal structures in specific heat. The artificial pinning centers hold great potential. Just below the onset temperature of superconducting transition, the electrons possess long mean free path. When the interval between adjacent sites comes to the order of 100nm, the experimentally accessible steady fields can enter the interesting regime of $\phi$. The resulting effective lattice subjected to perpendicular magnetic field is probably able to show the fractal properties of the Hofstadter model. In addition, the purity requirement of the sample is relaxed when considering the specific heat measurement.

In summary, adopting the quantum transfer matrix method, we compute the internal energy and specific heat of the Hofstadter model, and for the first time we study the oscillation of the specific heat with varying magnetic field as a signature of fractal structure of the Hofstadter butterfly. In low field regime, the oscillation period of specific heat is consistent with the conventional dHvA oscillation. When the temperature is decreased, sharp peaks and dips emerge in addition to the dHvA-type background. These peculiar oscillatory behaviors are direct indications of DOS in the fractal energy spectrum. We also suggest the possibility of making use of superconducting films to detect this fractal structure by measuring the specific heat.

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