Upper and Lower Bounds on the Partition Function of the Hofstadter Model

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UPPER AND LOWER BOUNDS ON THE PARTITION FUNCTION OF THE HOFSTADTER MODEL

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ABSTRACT

Using unitary equivalence of magnetic translation operators, upper and lower bounds on
the partition function of the Hofstadter model are derived for any rational “flux” and
any value of Bloch momenta. These bounds generalize straightforwardly to the case of a
general asymmetric hopping and to the case of hopping of the form \( t_{jn}(S_j^n + S_j^{-n}) \) with \( n \)
arbitrary integer larger than or equal 2.

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1. Introduction.- In what follows, we shall consider the Hofstadter model [1] described by the Hamiltonian

\[ H = t_1(S_1 + S_1^*) + t_2(S_2 + S_2^*), \]  

(1)

where unitary operators \( S_1 \) and \( S_2 \), sometimes called magnetic translation operators, satisfy the commutation relation

\[ S_1 S_2 = \omega S_2 S_1, \]  

(2)

with

\[ \omega = \exp(-2\pi i \alpha), \]  

(3)

\( \alpha \) being a real number. In general we shall allow for additional hopping terms of the form \( t_{jn}(S_j^n + S_j^{-n}) \) with \( n \) arbitrary integer larger than or equal to 2. However, as will become clear later, our results generalize straightforwardly the symmetric case \( t_1 = t_2 \) with nearest-neighbour hopping. Therefore, for the sake of clarity, we shall firstly derive our bounds for \( t_1 = t_2 \) and then the relevant generalization for the case \( t_1 \neq t_2 \) and additional hopping terms is discussed afterwards.

The model (1) appears in many physical problems. Originally, it appeared in the study of the behaviour of electrons moving simultaneously in a periodic potential and an uniform magnetic field \( B \) [2]. Subsequently, it has been also used in early discussions of the integer quantum Hall effect [3], to describe superlattices and quasicrystals [4], and flux phases in the high-\( T_c \) superconductors [5]. In the case of lattice electrons moving in an uniform magnetic field \( B \), the parameter \( \alpha(= \Phi/\Phi_0) \) is the flux per unit cell measured in units of flux quantum \( \Phi_0(= \hbar c/|e|) \), and, in the Landau gauge \( \mathbf{A} = (-B y, 0, 0) \),

\[ S_1 = e^{\frac{i}{\hbar}(\hat{p}_1 + eB y)} = e^{\hat{\beta}_1 + 2\pi i \alpha y}, \]  

(4)

and

\[ S_2 = e^{\frac{i}{\hbar} \hat{p}_2} = e^{\hat{\beta}_2}. \]  

(5)

Despite its simple form and the extensive numerical knowledge available, the Hofstadter model defies exact solution (see Ref. [6] for a recent progress). Here, we shall concentrate on the partition function,

\[ Z(\beta) = \text{Tr} e^{-\beta H}, \]  

(6)
where $\beta = 1/T$ and $T$ is temperature. The calculation of the partition function $Z(\beta)$ can be viewed as a technical tool to calculate the density of states $\rho(E)$ [7], because $Z(\beta)$ is nothing but the Laplace transform of $\rho(E)$,

$$Z(\beta) = \int_0^\infty e^{-\beta E} \rho(E) \, dE. \quad (7)$$

2. Results.- We are not yet able to calculate the partition function $Z(\beta)$ exactly, however, we shall formulate upper and lower bounds on $Z(\beta)$ which hold for any rational $\alpha = p/q$, with $p$ and $q$ relative prime integers. In the case where $\alpha$ is rational, the model is known to enjoy $SL(2, \mathbb{Z})$ symmetry [8], and, because of the periodicity over an enlarged unit cell [9], one can define Bloch momenta, $k = (k_1, k_2)$, and a corresponding magnetic Brillouin zone [1]. In momentum space, the Hamiltonian $H$ and operators $S_1$ and $S_2$ can be written as $q \times q$ traceless matrices,

$$H(k_1, k_2) = \begin{pmatrix}
2 \cos k_1 & e^{ik_2} & \cdots & e^{-ik_2} \\
e^{-ik_2} & 2 \cos(k_1 + 2\pi \alpha) & \cdots & 0 \\
0 & e^{-ik_2} & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
e^{ik_2} & \cdots & e^{-ik_2} & 2 \cos[k_1 + 2(q - 1)\pi \alpha]
\end{pmatrix}, \quad (8)$$

$$S_1 = e^{ik_1} S_1 = e^{ik_1} \begin{pmatrix}
\omega^q & 0 & \cdots & 0 & 0 \\
0 & \omega & \cdots & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0 & \cdots & 0 & \omega^{(q-2)} & 0 \\
0 & \cdots & 0 & 0 & \omega^{(q-1)}
\end{pmatrix}, \quad (9)$$

$$S_2 = e^{ik_2} S_2 = e^{ik_2} \begin{pmatrix}
0 & 1 & 0 & \cdots & 0 & 0 \\
0 & 0 & 1 & \cdots & 0 & 0 \\
0 & 0 & 0 & 1 & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & \cdots & 0 & 0 & 0 & 1 \\
1 & 0 & \cdots & 0 & 0 & 0
\end{pmatrix}. \quad (10)$$

Let us introduce $A \equiv S_1 + S_1^*$ and $B \equiv S_2 + S_2^*$. Our main result is that for all $\beta$, $k_1$, and $k_2$,

$$q \leq \max \left(\text{Tr} \, e^{-\beta A}, \text{Tr} \, e^{-\beta B}\right) \leq Z(\beta) \leq \frac{1}{q} \left(\text{Tr} \, e^{-\beta A}\right) \left(\text{Tr} \, e^{-\beta B}\right), \quad (11)$$

where

$$\text{Tr} \, e^{-\beta A} = \sum_{l=1}^q Q(k_1, l), \quad \text{Tr} \, e^{-\beta B} = \sum_{l=1}^q Q(k_2, l), \quad (12)$$

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and $Q(k, l) = \exp\{-2\beta \cos[k + 2\pi \alpha(l - 1)]\}$. Bounds (11) are valid for $\beta$ of both sign, positive and negative, and they are saturated for $\beta = 0$, i.e., at infinite temperature. Given convexity of $e^{-x}$, the first inequality (from the left) follows from the Jensen inequality [10] and the fact that $\sum_{k=1}^{n} \cos[k + 2\pi \alpha(l - 1)] = 0$ for all $k$. The lower bound on $Z(\beta)$ in (11) is a consequence of the Peierls variational principle [11] which states that

$$Z(\beta) = \text{Tr} \exp(-\beta H) \geq \sum_{n} e^{-\beta (\Phi_{n}, H \Phi_{n})},$$  \hspace{1cm} (13)$$

where $\{\Phi_{n}\}$ is an arbitrary set of linearly independent normalized vectors in a Hilbert space. Eventually, the upper bound on $Z(\beta)$ follows from the Golden-Thompson inequality [12],

$$\text{Tr} e^{A+B} \leq \text{Tr} \left(e^{A} e^{B} \right).$$  \hspace{1cm} (14)

3. **Derivation of bounds.** The main step in deriving bounds (11) is to use the unitary equivalence of operators $\bar{S}_{1}$ and $\bar{S}_{2}$ defined by relations (9) and (10). Indeed, one has

$$\bar{S}_{2} = U \bar{S}_{1} U^{-1},$$  \hspace{1cm} (15)$$

where $U$ is the unitary matrix with elements given by

$$U_{lm} = \frac{1}{\sqrt{q}} \omega^{-(l-1)(m-1)} \omega \ldots \omega^{(m-1)} = \frac{1}{\sqrt{q}} \omega^{-(l-1)(m-1)+m(m-1)/2}.$$  \hspace{1cm} (16)$$

By direct calculation,

$$[U \bar{S}_{1} U^{-1}]_{ik} = \sum_{l=1}^{q} U_{il} U_{kj}^{*} \omega^{-(i-1)} = \frac{1}{q} \sum_{l=1}^{q} \omega^{(l-1)(k-i)} \omega^{-(i-1)} = \delta_{i,k-1}.$$  \hspace{1cm} (17)$$

One can verify that $U_{i+,m} = U_{i,m}$ and

$$U_{i,m+q} = \begin{cases} U_{i,m}, & q \text{ odd} \\ -U_{i,m}, & q \text{ even.} \end{cases}$$  \hspace{1cm} (18)$$

For all $j$ and $l$,

$$U_{ji}^{*} U_{jl} = \frac{1}{q}.$$  \hspace{1cm} (19)$$

In general,

$$U_{ji}^{*} U_{jk} = \frac{1}{q} \omega^{-(j-1)(k-j)} \left[\omega \ldots \omega^{(k-j)}\right]^{1 \times \text{sgn}(k-j)} = \frac{1}{q} \omega^{-(j-1)(k-j) + \text{sgn}(k-j) \times (k-j)(k-j+1)/2}. \hspace{1cm} (20)$$
The action of $U$ on the Hamiltonian $H$, $U H U^{-1}$, interchanges momenta $k_1$ and $k_2$ and implies that the spectrum of $H$ is symmetric under this interchange. It also allows to show that the spectrum of $H$ is equivalent to the spectrum of the Hamiltonian $\tilde{H}$ of the form

$$\tilde{H} = U^{-1/2} D_1 U^{1/2} + U^{1/2} D_2 U^{-1/2},$$

(21)

where $D_1$ and $D_2$ are real diagonal matrices, $(D)_{lm} = 2 \cos (k + 2\pi \alpha l) \delta_{lm}$, with subscript labelling the dependence on either $k_1$ or $k_2$.

Due to (15), both $S_1$ and $\tilde{S}_2$ have the same spectrum $\Sigma$ [13] which can be read off from (9), i.e.,

$$\Sigma = \{\omega^{-j} \mid j = 0, 1, \ldots, q - 1\}.$$  

(22)

Normalized eigenvectors of $S_1$ are $(\Phi_j)_i = \delta_{ji}$, and corresponding normalized eigenvectors of $\tilde{S}_2$ are

$$\Psi_j = \frac{1}{\sqrt{q}} \left(1, \omega^{-j}, \omega^{-2j}, \ldots, \omega^{-(q-1)j}\right).$$

(23)

One can verify that, in the standard scalar product in $C^q$, $(\Phi_j, \Phi_i) = (\Psi_j, \Psi_i) = \delta_{ji}$. The lower bound on $Z(\beta)$ in (11) then follows from the Peierls variational principle (13) by taking the complete set of vectors to be the set of eigenvectors of either $S_1$ or $\tilde{S}_2$. Indeed, one has

$$(\Phi_j, H \Phi_j) = 2 \cos (k_1 + 2\pi \alpha j), \quad (\Psi_j, H \Psi_j) = 2 \cos (k_2 + 2\pi \alpha j).$$

(24)

The same lower bound can be also obtained from the Bogoliubov variational principle [14],

$$-\beta F \geq \ln \text{Tr} \exp(-\beta \tilde{H}) - \beta \left\{ \frac{\text{Tr} \left[ \exp(-\beta \tilde{H}) (H - \tilde{H}) \right]}{\text{Tr} \exp(-\beta \tilde{H})} \right\},$$

(25)

where $\tilde{H}$ is a trial Hamiltonian which is not necessarily a dynamical operator. One uses the Bogoliubov variational principle (25) with $\tilde{H}$ to be chosen either of the operators $A$ and $B$. In the case of general Bloch momenta $k_1$ and $k_2$, one has

$$e^A = e^{S_1 + S_1^*} = \text{diag} \left\{ e^{2\cos[k_1 + 2\pi (l-1)\alpha]} \right\}, \quad e^B = e^{S_2 + S_2^*} = U \text{diag} \left\{ e^{2\cos[k_2 + 2\pi (l-1)\alpha]} \right\} U^{-1}.$$

(26)

The second term on the right side of Eq. (25) then vanishes [15] and the remaining term gives the lower bound in (11) on the partition function $Z(\beta)$, valid for any rational $\alpha$ and for all $\beta$, $k_1$, and $k_2$. 

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As for the upper bound \((11)\) on \(Z(\beta)\), using Eqs. \((26)\) and \((19)\) one has

\[
\text{Tr } (e^{-\beta A} e^{-\beta B}) = \sum_{j<l} Q(k_1,l)Q(k_2,j)U_{lj}^* U_{lj} = \frac{1}{q} \sum_{j<l=1}^q Q(k_1,l)Q(k_2,j)
\]

\[
= \frac{1}{q} \left( \text{Tr } e^{-\beta A} \right) \left( \text{Tr } e^{-\beta B} \right).
\]

(27)

Combining Eq. \((27)\) with the Golden-Thompson inequality \((14)\) then gives the upper bound \((11)\) on \(Z(\beta)\),

\[
Z(\beta, \alpha) \leq \frac{1}{q} \left( \text{Tr } e^{-\beta A} \right) \left( \text{Tr } e^{-\beta B} \right),
\]

(28)

valid for any rational \(\alpha = p/q\) and for all \(\beta, k_1,\) and \(k_2\).

3. Further generalizations.- For a given \(\beta\), one can check numerically that [after dividing \((11)\) by \(q\)] the upper and lower bounds on \(Z(\beta)\) depend only very weakly upon \(q\) and Bloch momenta. The dependence of the bounds on \(\beta\) is much stronger. As \(\beta\) increases,

\[
\max \left( \text{Tr } e^{-\beta A}, \text{Tr } e^{-\beta B} \right) / Z(\beta) \approx e^{-2\beta} \to 0.
\]

(29)

Therefore, the lower bound is far from being optimal and, in principle, it can be further improved using the Peierls variational principle \((13)\) with a better choice of the complete set of vectors than used here. With respect to large \(\beta\) behaviour, the upper bound \((11)\) on \(Z(\beta)\) is much better because it mimics the large \(\beta\) behaviour of \(Z(\beta)\). The upper bound can also be further improved: by repeatedly using inequality \([12]\)

\[
\text{Tr } (XY)^{2m+1} \leq \text{Tr } (X^2Y^2)^{2m}
\]

(30)

for nonnegative matrices \(X\) and \(Y\), with \(m\) integral and \(\geq 0\), together with the Trotter formula,

\[
e^{A+B} = \lim_{n \to \infty} \left( e^{A/n} e^{B/n} \right)^n.
\]

(31)

One finds for \(2 \leq l \leq m\) that

\[
\text{Tr } (e^{-\beta A} e^{-\beta B}) \geq \text{Tr } (e^{-\beta A/2} e^{-\beta B/2})^\ell \geq \text{Tr } (e^{-\beta A/l} e^{-\beta B/l})^\ell
\]

\[
\geq \left( e^{-\beta A/m} e^{-\beta B/m} \right)^m \geq \text{Tr } e^{-\beta H} = Z(\beta).
\]

(32)

Note that relation \((20)\) enables us to calculate explicitly

\[
\left[ e^{-\beta (S_1 + S_1^{-1})} e^{-\beta (S_2 + S_2^{-1})} \right]_{lm} = \omega^{\text{sgn}(m-l)} |m-l|^{m-l|m-l|+1/2} Q(k_1,l) \hat{Q}(k_2, m-l),
\]

(33)
where \( \tilde{Q}(k_2, m - l) \) is a discrete Fourier transform,

\[
\tilde{Q}(k_2, m - l) \equiv \frac{1}{q} \sum_j \omega^{-(j-1)(m-l)} Q(k_2, j).
\]  

(34)

Obviously, in the asymmetric case, \( t_1 \neq t_2 \), and even in the case where hopping has the form \( t_{jn}(S_j^n + S_j^{-n}) \) with \( n \geq 2 \) arbitrary integer, one can still use the unitary equivalence (15) with the matrix \( U \) given by Eq. (16). One writes \( H = A + B \), where matrix \( A \) (\( B \)) now includes all hopping terms in the \( x \)-direction (\( y \)-direction) and proceeds with matrices \( A \) and \( B \) as before, i.e., uses them as the trial Hamiltonian \( \tilde{H} \) in the Bogoliubov variational principle (25) and in the Golden-Thompson inequality (14). Inclusion of hopping terms \( t_{jn}(S_j^n + S_j^{-n}) \) in the Hamiltonian \( H \) does not change the form of bounds (11) and involves only modification of \( Q(k, l) \). For example, in the asymmetric case, \( t_1 \neq t_2 \), with the nearest-neighbour hopping, the only change in bounds (11) consists in replacing \( A \) by \( t_1 A \) and \( B \) by \( t_2 B \).

4. Conclusions.- To conclude, we have formulated upper and lower bounds on the partition function of the Hofstadter model, valid for any rational “flux” \( \alpha \), inverse temperature \( \beta \), and Bloch momenta \( k \). These bounds imply constraints on the density of states of the Hofstadter model and supply constraints imposed by the coefficients of the secular equation for the Hofstadter model,

\[
\lambda^l + a_{-2} \lambda^{l-2} + a_{-4} \lambda^{l-4} + \ldots + \det H = 0.
\]  

(35)

Here, depending on whether \( q \) is odd or even, either \( \det H = 2[\cos(qk_1) + \cos(qk_2)] \) or \( \det H = 4 - 2[\cos(qk_1) + \cos(qk_2)] \). One can show that \( a_{-(2i+1)} \equiv 0, a_{-2} = -2q \),

\[
a_{-4} = q(2q - 7) - 2q \cos(2\pi \alpha),
\]

\[
a_{-6} = -\frac{2}{3} q(2q^2 - 21q + 58) + 4q(q - 6) \cos(2\pi \alpha) - 4q \cos(4\pi \alpha),
\]  

(36)

and that except for the constant term, \( \det H \), none of the coefficients \( a_j \) depends on the Bloch momenta [16].

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[7] Using transfer matrix [1], it can be shown that the spectrum of the Hamiltonian $H$
lies within the interval $[-4, 4]$. Therefore, in order to use the formula (7), one must,
instead of $H$, consider the Hamiltonian $H = H + 4 \geq 0$.


[9] One possible choice is, for example, a unit cell with $q$ lattice spacings in the $y$ direction
and one lattice spacing in the $x$ direction.

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[13] Provided $q$ is a prime number then all nontrivial powers $S_j^l$, $j = 1, 2$, $l \neq 0 \mod q$, of these operators have the same spectrum $\Sigma$.

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[15] One can check by direct calculation that $\text{Tr} \, D B = 0$ for any diagonal matrix $D$.