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A sum rule on Hofstadter spectrum and its application

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Abstract. Some time ago, in a remarkable paper, Hofstadter showed that the energy spectrum of a spinless tight-binding electron, moving in a constant magnetic field B, has a very complicated recursive structure. In this article, we shall show that, these energy levels satisfy a simple sum rule. Then, as an application of this sum rule, we show why a proposition on the absolute minimum of the energy of this system, which was made by Hasegawa *et al*, holds in general cases.

Hofstadter showed [1] some very interesting results on the dependence on the magnetic field of the energy spectrum of a two-dimensional tight-binding electron system. In particular, he found that, when the number of flux quanta per unit cell, ϕ/ϕ_0 ($\phi_0 = hc/e$ is the quantum of the magnetic flux), is a rational number p/q, the tight-binding band is split up into q non-overlapping subbands. He also showed that the energy spectrum as a function of the magnetic field exhibits a recursive structure. Since then, this recursive structure has been vigorously studied [2–5].

In a recent article [6], Hasegawa *et al* made an interesting observation about the energy of the ground state of this system. By numerical calculations for several specific rational values of flux quanta per unit cell, they found that, for a fixed electron filling $\alpha = p/q$ of the lattice, the total energy E of the electrons has an absolute minimum at $\phi/\phi_0 = \alpha$. Based on this observation, Lederer, Poilolanc and Rice proposed a new mechanism for superconductivity [7]. The result of Hasegawa *et al* has been conformed by other authors [8–10].

In this article, we would like to reveal another interesting property of the energy spectrum of this system. We shall first show that, although the energy spectrum has a very complicated recursive structure, the energy levels satisfy a simple sum rule. Then, as an application of this sum rule, we show that the total energy E of the electrons has indeed an absolute minimum at ratio $\phi/\phi_0 = \alpha$, which is the electron filling of the lattice.

We take a finite square lattice Λ with $N_\Lambda = L \times L$ sites and impose the periodic boundary condition on it. Assume that the constant magnetic field B is perpendicular to the lattice plane. Then, the motion of a spinless free electron in the lattice is described by the following Hamiltonian

$$H = \sum_{\langle ij \rangle} t_{ij} c_i^+ c_j \tag{1}$$

where $c_i^+ (c_i)$ is the electron creation (annihilation) operator at site i and $\langle ij \rangle$ denotes a pair of nearest-neighbour sites of the lattice. The hopping constants $\{t_{ij}\}$ are

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determined by the so-called 'Peierls substitution'. In the simplest case, they are defined by

$$t_{ij} = \begin{cases} t \exp\left\{-2\pi \mathrm{i} \int_i^j \boldsymbol{A} \cdot \mathrm{d}\boldsymbol{l}/\phi_0\right\} & \text{if } i \text{ and } j \text{ are the nearest neighbours} \\ 0 & \text{otherwise} \end{cases} \tag{2}$$

where $\boldsymbol{A}$ is the vector potential of the magnetic field $\boldsymbol{B}$. In the following, we shall use the Landau gauge $\boldsymbol{A} = B(0, x, 0)$. Notice that, due to the periodic boundary condition, there will be an additional phase factor to the hopping constants $\{t_{ij}\}$ associated with the boundary bonds. But, as we shall show in the following, all the phase factors will be cancelled out in the final result. Therefore, we can ignore these additional phase factors from the beginning. We further notice that the lattice Λ is bipartite with respect to the Hamiltonian (1), i.e. its sites can be divided into two groups, A and B. For two lattice sites i and j in the same group, the hopping constant t_{ij} is identically zero. This observation is indispensible for the proof of our sum rule. It is not difficult to see that we have a natural partition of the square lattice Λ in terms of the definition of $\{t_{ij}\}$.

Now, we can summarize our main result in the following theorem;

Theorem. For an arbitrary constant magnetic field $\boldsymbol{B}$, the eigenvalues of Hamiltonian (1) are paired, i.e. for any positive eigenvalue ϵ of the Hamiltonian, there is also a negative eigenvalue $-\epsilon$. The total number of the eigenvalues is N_Λ. Furthermore, these eigenvalues satisfy the following sum rule

$$\sum_{i=1}^{N_\Lambda} \epsilon_i^2 = z t^2 N_\Lambda \tag{3}$$

where z is the coordination number of the lattice.

Proof. By choosing a basis of the state vectors, we can write the Hamilonian in a matrix. Let $\epsilon_1 \leqslant \epsilon_2 \leqslant \cdots \leqslant \epsilon_{N_\Lambda}$ be the eigenvalues of H. Then, they are given by the solutions of the following algebric equation

$$\det(\lambda I - H) = 0. \tag{4}$$

It is not difficult to see that the set of the state vectors defined by

$$\Psi_i = C_i^\dagger |0\rangle \qquad i \in \Lambda \tag{5}$$

where $|0\rangle$ is the vacuum state, is a basis of the Hilbert space of this system. The total number of these vectors is N_Λ. We now divide $\{\Psi_i\}$ into two groups $\tilde{A}$ and $\tilde{B}$ in the following way. If i belongs to set $A(B)$ of the partition of lattice Λ, then Ψ_i is defined to be in $\tilde{A}(\tilde{B})$. By the definition of $\{t_{ij}\}$, we can easily see that $\langle \Psi_i | H | \Psi_j \rangle = 0$ if Ψ_i and Ψ_j are in the same group. Therefore, the matrix of Hamiltonian (1) has a block form

$$H = \begin{bmatrix} H_{\tilde{A}\tilde{A}} & H_{\tilde{A}\tilde{B}} \\ H_{\tilde{B}\tilde{A}} & H_{\tilde{B}\tilde{B}} \end{bmatrix} = \begin{bmatrix} 0 & T \\ T^\dagger & 0 \end{bmatrix} \tag{6}$$

where each block is an $N_\Lambda/2 \times N_\Lambda/2$ submatrix and 0 denotes the zero submatrix. Furthermore, a direct calculation shows that there are exactly z non-zero elements in each row of submatrix T. To determine the eigenvalues of H, the following lemma is very useful.

Lemma. Let M be an $2N \times 2N$ matrix with a block form

$$M = \begin{bmatrix} A & B \\ C & D \end{bmatrix} \tag{7}$$

where A, B, C and D are $N \times N$ square submatrices. Then, the determinant of M is given by

$$\det M = \det A \det(D - CA^{-1}B). \tag{8}$$

In particular, if A commutes with C, then $\det M = \det(AD - CB)$ and it holds even if A has no inverse.

A proof of this lemma can be found in [12] page 17.

Applying this lemma to matrix $M = \lambda I - H$, we immediately obtain

$$\det(\lambda I - H) = \det(\lambda^2 I - T^\dagger T) \tag{9}$$

since λI commutes with any matrix. Therefore, if $\tilde{\lambda}$ is a root of the characteristic equation of H, $-\tilde{\lambda}$ is also a root, i.e. the eigenvalues of H are paired. Furthermore, by using the well known relation between the trace and the eigenvalues of a matrix, we obtain the following identity from equation (9)

$$\sum_{i=1}^{N_\Lambda} \epsilon_i^2 = 2 \operatorname{tr} (T^\dagger T). \tag{10}$$

The factor 2 is due to the fact that each eigenvalue of $T^\dagger T$ is counted twice in the sum of (10). The right-hand side of the above equation can be easily evaluated. Since H contains only hopping terms, each diagonal element $\langle \Psi_i | T^\dagger T | \Psi_i \rangle$ is a sum of the contributions from those two-steps-returning walks. A little algebra yields its value, zt^2, which is a positive quantity independent of the magnetic field. Therefore

$$\operatorname{tr} (T^\dagger T) = \tfrac{1}{2} z t^2 N_\Lambda \tag{11}$$

Substituting (11) into equation (10), we obtain sum rule (3).

Our proof is thus accomplished. □

Some remarks are in order.

Remark 1. Following the above proof, one can easily generalize sum rule (3) to other type of lattices as long as they are bipartite with respect to the Hamiltonian. In other words, the hopping coefficients $\{t_{ij}\}$ can be more complicated than those given by definition (2). Consequently, the constant $zt^2 N_\Lambda$ on the right-hand side of equation (3) must also be changed.

Remark 2. In our proof, we have assumed that the spin-freedom of electrons is polarized by the external magnetic field $\boldsymbol{B}$. Therefore, we can treat them as spinless fermions. If $\boldsymbol{B}$ is weak and the spin of electrons is unpolarized, the constant $zt^2 N_\Lambda$ of equation (3) should be multiplied by a factor 2.

Remark 3. For technical convenience, we let N_Λ, the number of lattice sites, be an even number in the proof. In the thermodynamic limit, this should not put real restriction on our theorem.

Next, as an application of sum rule (3), we would like to argue why the absolute minimum of the energy E of electrons in this system is attained when the number of the magnetic flux quanta per cell ϕ_0/ϕ equals p/q, the electron filling of the lattice. In the following, we shall only consider a finite lattice while Hasegawa *et al* did their calculations directly for an infinite lattice. In this way, we make our argument more intuitive. One can easily see that the final conclusion should still hold in the thermodynamic limit. Another point is worthwhile mentioning. Notice that E is symmetric about the half-filling point $\alpha = 1/2$. Therefore, we need only consider these fillings which is less than one half in the following.

First, we introduce a $N_\Lambda/2$–dimensional space and give sum rule (3) a geometric explanation. By setting up a coordinate system, we see that, as the magnetic field $\boldsymbol{B}$ changes, the corresponding sets of the ordered non-positive eigenvalues $\epsilon_1 \leqslant \epsilon_2 \leqslant \cdots \leqslant \epsilon_{N_\Lambda/2} \leqslant 0$ (other eigenvalues are non-negative since the eigenvalues are paired) of the Hamiltonian can be represented by points in this space. Geometrically, sum rule (3) tells us that the totality of these points is, in fact, a subset of the $N_\Lambda/2$–dimensional sphere defined by

$$\sum_{i=1}^{N_\Lambda/2} \epsilon_i^2 = \frac{zt^2 N_\Lambda}{2} \equiv R^2. \tag{12}$$

When the electron filling equals $\alpha \equiv N/N_\Lambda \leqslant 1/2$, the energy of the ground state is given by

$$E = \epsilon_1 + \epsilon_2 + \cdots + \epsilon_N = -(|\epsilon_1| + |\epsilon_2| + \cdots + |\epsilon_N|) \tag{13}$$

and it is a continuous function of the magnetic field $\boldsymbol{B}$. Assume that E reaches its absolute minimum at $\phi/\phi_0 = \beta$. Then, the projection of the radical vector

$$\boldsymbol{R} \equiv (-\epsilon_1(\phi/\phi_0), -\epsilon_2(\phi/\phi_0), \cdots, -\epsilon_{N_\Lambda/2}(\phi/\phi_0)) \tag{14}$$

into the subspace V spanned by $(e_1, e_2, \cdots, e_N)$, where e_i is the unit vector in the ith direction, should be maximal at $\phi/\phi_0 = \beta$. Consequently, by sum rule (3), the projection of $\boldsymbol{R}$ into the complementary subspace $V^\perp$ spanned by $(e_{N+1}, \cdots, e_{N_\Lambda/2})$ should be minimal. In other words, a gap developes between the energy levels ϵ_N and ϵ_{N+1} and this gap should reach its maximum when $\phi/\phi_0 = \beta$. On the other-hand, by Wannier's work [2], we know that the largest gap in the recursive structure of the energy spectrum appears at $\beta = \alpha$. Therefore, for a fixed electron filling α, the maximal projection of $\boldsymbol{R}$ into the subspace V is achieved at $\phi/\phi_0 = \beta = \alpha = p/q$. That explains the observation made by Hasegawa *et al* [6].

Although we do not claim that the above argument is rigorous, we do hope that it sheds some light on the relation between the recursive structure of the energy spectrum and the exact energy of the gound state of this system.

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Note added in proof. After submission of this work, I received a preprint by E Lieb and M Loss. They studied the half-filled case. They have partially solved the problem of the lowest total energy and completely solved the problem for determinants (i.e. for products of eigenvalues instead of sums of eigenvalues) on bipartite planar graghs. I would like to thank them for their encouragement.

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