Numerical study of electronic structure under uniform magnetic field and quantized Hall conductance for multi-band tight-binding models

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Abstract. The electronic structure of periodic lattice under uniform magnetic field was studied numerically for multi-band tight-binding models with non-orthogonal basis sets. When magnetic translational symmetry is fully taken into account, computational time can be greatly reduced. Quantized Hall conductance was evaluated by robust multi-band formulation of Chern number. We found that calculated quantized Hall conductance coincides with the semi-classical results. Discontinuous jumps of Hall conductance occur at van-Hove singularities and correspond to mod $q$ ambiguity of the Diophantine equation of Chern number.

1. Introduction

The electronic structure of periodic lattice under uniform magnetic field has been attracted continued interest for several decades. Early numerical calculations have revealed exotic characters such as self-similar energy spectrum, which is called Hofstadter’s butterfly [1]. The quantized Hall conductance of periodic system has been explained from Chern number defined for occupied energy bands [2]. In addition, topological correspondence between bulk and edge states has been identified in this context. While these studies open new paradigm in electronic states under magnetic field, most of numerical calculations have been performed for simplified models under strong magnetic field which far exceeds experimental range. Therefore, these calculations have not been directly compared with experimental observation. This limitation partly arises from the symmetry restriction of magnetic translational group [3] as we must treat a large magnetic unit cell instead of the original cell. When magnetic flux penetrating into two dimensional unit cell is $\varphi = p/q$, where $p$ and $q$ are relatively prime integer, the magnetic unit cell becomes $q$ times larger than the original cell. Thus, computational efforts increase significantly for small magnetic field with a large denominator $q$.

In this paper, we present detailed formulation for the electronic structure under uniform magnetic field. General tight-binding approximations with overlap integrals are employed to model the realistic energy bands. Uniform magnetic field is included as phase factors of both hopping and overlap matrix elements. We show that computational time can be greatly reduced by magnetic translational symmetry. As an example of such calculation, we present the calculated results for graphene with magnetic field of $\varphi = 1/200$. 

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2. Calculation method

Let us consider two-dimensional periodic system with primitive translational vectors $a_1$ and $a_2$. We adopt general tight-binding models because fully self-consistent calculations under uniform magnetic field [5] are not feasible for realistic compounds with current computer facilities. The electronic structure is calculated non self-consistently under uniform magnetic field perpendicular to the two-dimensional plane. This treatment may be justified if the magnetic field does not alter charge density significantly.

We assume that energy bands in the absence of magnetic field can be constructed from localized orbitals $\phi_\nu R(r)$, which may not be orthogonal. Here, $R$ and $\nu$ denote atomic positions and other quantum numbers such as angular momentum, respectively. Multi-band models are needed in general since energy bands degenerate typically at several symmetric points in Brillouin zone. The tight-binding models are parameterized by following matrix elements:

$$H_0(\nu, R; \nu', R') = \langle \phi_{\nu R} | \hat{H} | \phi_{\nu' R'} \rangle$$
$$S_0(\nu R; \nu', R') = \langle \phi_{\nu R} | \phi_{\nu' R'} \rangle .$$

They may be obtained from first-principles calculations by fitting of energy bands or several other methods which directly generate tight-binding parameters.

Under uniform magnetic field represented by the vector potential $A(r) = \frac{1}{2} B \times r$, the localized basis sets are modified as [6, 7]

$$\tilde{\phi}_\nu R(r) = \exp\{i I_{r, R}\} \phi_\nu R,$$ 

where

$$I_{r', r} \equiv \frac{ie}{\hbar c} \int_r^{r'} A(s) ds.$$ 

Then, the matrix elements under uniform magnetic field may be evaluated as

$$H(\nu', R'; \nu, R) \approx \exp\{i I_{R', R}\} H_0(\nu', R'; \nu, R),$$
$$S(\nu', R'; \nu, R) \approx \exp\{i I_{R', R}\} S_0(\nu', R'; \nu, R).$$

Here, we should note that above approximation is considered valid only if basis sets $\phi_\nu R(r)$ are well localized around $R$. Therefore, non-orthogonal orbitals are suitable for present calculations because they can be more localized than orthogonalized orbitals.

Since $A(r)$ is not invariant with translation $\hat{T}(a_i)$, we must consider magnetic translation [3] defined as

$$\hat{T}_M(a_i) \equiv \exp\left\{ \frac{ie}{2c} B \cdot (a_i \times r) \right\} \hat{T}(a_i).$$

Because of additional phase factors, the magnetic translation operators do not commute each other and satisfy

$$\hat{T}_M(a_1) \hat{T}_M(a_2) = e^{i \varphi} \hat{T}_M(a_2) \hat{T}_M(a_2),$$

where $\varphi$ is flux quanta penetrating into the unit cell spanned by $a_1$ and $a_2$. When $\varphi = p/q$ is a rational number, we can define enlarged magnetic unit cell with $\tilde{a}_1 = q_1 a_1$ and $\tilde{a}_2 = q_2 a_2$, where $q_1$ and $q_2$ are integers which satisfy $q_1 q_2 = q$. Since the magnetic translation operators for the enlarged cell commute each other, eigen functions can be chosen to the form of magnetic Bloch function:

$$\hat{T}_M(T) \Psi_k = (-1)^{n_1 n_2} e^{-ik \cdot T} \Psi_k,$$
where $T = n_1\hat{a}_1 + n_2\hat{a}_2$ is a translational vector and $k$ is in magnetic Brillouin zone defined by reciprocal vectors $\hat{g}_1 = g_1/q_1$ and $\hat{g}_2 = g_2/q_2$. The additional prefactor $(-1)^m n_2$ arises from the relation $\hat{T}_M(T) = (-1)^m n_2 \hat{T}_M(n_1\hat{a}_1)\hat{T}_M(n_2\hat{a}_2)$. Furthermore, the eigen function $\Psi$ satisfies

$$\hat{T}_M(a_1)\Psi_k = \Psi_{k + \frac{a_1}{q_1} \hat{g}_2},$$

$$\hat{T}_M(a_2)\Psi_k = \Psi_{k + \frac{a_2}{q_2} \hat{g}_1}.\quad (10)$$

Namely, magnetic translations for $a_1$ and $a_2$ generate eigen functions at different k-points with the same energy eigenvalue. Using this relation, we need to calculate eigen functions only in $1/q$ area of magnetic Brillouin zone and can generate eigen functions in other area by above formula. This relation reduces the computational requirement to $1/q$ and enables us to treat larger magnetic unit cell, i.e., small flux quanta $\varphi$.

Under uniform magnetic field $\varphi = p/q$, each band splits into $q$ Landau subbands. When the chemical potential is located within an energy gap between Landau subbands, quantized Hall conductance $\sigma_{xy}$ is given as $[2, 4, 8, 9]$

$$\sigma_{xy} = -\frac{e^2}{h} c_F(\mu),\quad (12)$$

where $c_F$ is a topological integer called Chern number defined for the filled bands. The $c_F$ can be calculated numerically by discretizing the magnetic Brillouin zone into mesh $\{k_\ell\}$ as $[9]$

$$c_F(\mu) = \frac{1}{2\pi} \sum_{\ell} F(k_\ell),\quad (13)$$

$$F(k) = \text{Arg} \left[ u_1(k)u_2(k + \Delta k_1)u_2(k + \Delta k_2)^*u_2(k)^* \right],\quad (14)$$

$$u_{\mu}(k) = \det_{n,m \in \text{occupied}} \left[ \langle \Psi_{n,k} | \Psi_{m,k+\Delta k_\mu} \rangle \right],\quad (15)$$

where $n$ and $m$ are band indices and $\Delta k_\mu$ is a discretized momentum along $\hat{g}_\mu$ direction. As the $c_F$ is integer, this expression rapidly converges with the Brillouin zone mesh and is thus suitable for numerical calculations.

3. Results and discussion
We have calculated energy bands under uniform magnetic field for several models $[10, 11]$. For graphene, we have treated a realistic multi-band model which consists of 4 non-orthogonal orbitals per carbon atom $[10]$. In Fig. 1, we show calculated Chern numbers for $\varphi = 1/200$. The energy bands split into $8 \times 200 = 1600$ Landau subbands. Since the energy gaps are small, the Chern numbers look almost continuous and are indistinguishable from semi-classical estimation of Hall conductance $[10]$. The Chern number changes discontinuously at the van-Hove singularities of energy bands without magnetic field.

We found that the pronounced Landau quantization occurs in whole energy region. The band widths of individual Landau subbands are negligibly small compared with the energy gaps between them except near van-Hove singularities. In some cases, several consecutive Landau subbands appear at almost same energies. Such pseudo degeneracy corresponds to the existence of multiple equivalent segments in Fermi surface without magnetic field. For example, two Landau subbands degenerate at Dirac particle region near $\varepsilon = 0$. The degeneracy of Landau subbands also occurs in other energy regions where electron or hole pockets of Fermi surface appear around $K$ or $M$ points.

Each Landau subband contributes to Chern number with $c_F = 1$ except at the van-Hove singularities. This is consistent with the requirement of Diophantine equation that each Landau
Figure 1. Calculated Chern numbers for graphene with $\varphi = 1/200$ are plotted as a function of chemical potential in upper panel. The Chern numbers for adjacent energy gaps are connected with straight lines. For comparison, lower panel shows energy bands without magnetic field with vertical dashed lines at van-Hove singularities.

subband gives $c_F = 1 + Nq$ for $\varphi = 1/q$ where $N$ is an integer [12]. We found that the large jumps of Chern number at the van-Hove singularities can be explained by the additional factor $-q$ which corresponds to $N = -1$ solution of the Diophantine equation.

4. Summary
In this paper, computational methods for energy bands under uniform magnetic field were explained. Realistic energy bands can be treated easily with multi-band tight-binding model formulated by non-orthogonal basis sets. The calculated results for graphene with $\varphi = 1/200$ was shown as an example.

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