Symmetry Breaking and Electron Transport in Kagomé-Chain Systems *

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Among various lattices, the Kagomé lattice is special because it has a completely flat electronic band whose eigenstates have both localized and itinerant characters. We investigate electron transport properties of finite-size Kagomé-lattice-chain systems, which have multi-degenerate flat-band-like states, using a simple tight-binding model and a nonequilibrium Green function method. It is found that the flat-band-like-state channel in a Kagomé-lattice-chain system generates a large electronic current along the chain when a small electric field is applied perpendicular to the chain, while no current is generated along the chain when an electric field is applied along the chain. We show that such unique transport characteristics originate from the symmetry breaking of flat-band-like states by the external electric fields. [DOI: 10.1380/ejssnt.2005.399]

Keywords: Green’s function method; Models of non-equilibrium phenomena; Electrical transport; Quantum conductance

I. INTRODUCTION

Recent advances in the field of nanotechnology have made it possible to arrange semiconductor quantum wires periodically on semiconductor substrates. These systems are sometimes called artificial lattices. The artificial lattices have two fascinating characteristics that are different from those of real crystals. One is the flexibility to design various lattice shapes [1–3]. The other is the controllability of the number of electrons in a lattice, which is realized by applying a gate voltage [4]. From these characteristics, the artificial lattices provide new stages to demonstrate exotic theoretical predictions for lattice systems [5, 6].

Among various lattices, the Kagomé lattice is located at a special position because it has a complete flat band in an electronic structure. Flat-band electronic states have the following unique features [7, 8]. (i) One can choose eigenstates of a flat band completely localized around one unit cell such that they have no wave-function amplitude outside the unit cell. On the other hand, these localized eigenstates are nonorthogonal and have finite overlaps with each other. On the basis of these facts, one can say that the flat-band electronic states have both localized and itinerant characteristics. (ii) Since each unit cell has a localized eigenstate, the sum of such eigenstates becomes a complete set of flat-band states having the same eigenenergy. This feature produces a macroscopic degree of energy degeneracy and becomes the origin of a flat band. The above-mentioned features of flat-band states promote the appearance of interesting magnetic and optical properties [4, 7–11].

The motivation of the present work arises from the simple question whether we can observe the unique features originating from the flat-band states in transport properties. In this study, we investigated the transport properties of the finite-size Kagomé-lattice system under small electric fields, by employing the simple tight-binding model and the nonequilibrium Green function method.

II. MODEL AND METHOD

We consider Kagomé-lattice systems made of semiconductor quantum wires. The electrons are mainly localized at the cross points of wires [4] and move along the wires. Thus, we reasonably assume that the use of the simple tight-binding model to describe the electronic states of these systems is effective [9]. To apply a small finite-magnitude electric field to the Kagomé lattice while keeping the flat-band features, we employ the finite-size Kagomé-lattice chain shown in Fig. 1(a). When the Kagomé-lattice chain has an infinite length, the electronic structure has the flatband at 2t as shown in Fig. 1(b), where t is the electron transfer energy. However, in the case of the Kagomé-lattice chain with a finite M plaquette length, M-fold degenerate states appear at the same energy.

Fig. 1: (a) Schematic pictures of M-plaquette Kagomé-lattice chain. (b) Electronic band structure of $M = \infty$ one-dimensional Kagomé-lattice chain. (c) Energy levels of four-plaquette ($M = 4$) Kagomé-lattice chain. The numbers in parentheses indicate the degree of energy degeneracies of individual energy levels.
The other flat-band eigenstates are localized in the other plaquettes, similarly. In this way, the unique features of flat band are well reproduced even in the electronic states in finite-size Kagomé-lattice chain.

To study the transport properties of electrons, the edges of the finite-size Kagomé-lattice chain are connected to the source and drain electrodes, as shown in Fig. 2(a). Figure 2(b) shows the schematic energy diagram of this joint system. To simplify, we treat electrons as spinless fermions having no Coulomb repulsive interactions. We assume that both electrodes are one-dimensional lattices having a half-infinity length. When we number the sites in the joint system, as shown in Fig. 2(a), the total Hamiltonian of the joint system is written as

$$\hat{H} = \hat{H}^C + \sum_{\xi=L,R} \hat{H}^\xi + \hat{W},$$  \hspace{1cm} (1)

$$\hat{H}^C = -\sum_{1\leq i,j\leq N} t_{ij} c_i^\dagger c_j + \sum_{1\leq i\leq N} V_i c_i^\dagger c_i,$$  \hspace{1cm} (2)

$$\hat{H}^\xi = -\sum_{i,j} \xi^{\xi} c_i^\dagger c_j + \mu^\xi \sum_i c_i^\dagger c_i,$$  \hspace{1cm} (3)

$$\hat{W} = -t'(c_i^\dagger c_1 + c_1^\dagger c_0 + c_{N+1}^\dagger c_N + c_{N+1}^\dagger c_N).$$  \hspace{1cm} (4)

where $c_i^\dagger$ and $c_i$ are the creation and annihilation operators of the electron at the $i$-th site, and $N$ the number of sites in the Kagomé-lattice chain. $V_i$ describes the on-site energy of the $i$-th site, which represents the effects of external fields. In this case, $V_i$ is written as $V_i = V^G + V^E_i$, where $V^G$ is the applied uniform gate voltage, and $V^E_i$ represents the potential due to the electric field. $\xi$ denotes either left (L) or right (R) electrode, and the summation runs over the sites with $i \leq 0$ ($i \geq N + 1$) for the $\xi = L$ (R) electrode. $t'$ is the transfer energy in the $\xi$ electrode, and $\mu^\xi$ is the chemical potential. The source-drain voltage $V^sd$ is given as $V^sd = \mu^L - \mu^R$. $t'$ indicates the coupling between the Kagomé-lattice chain and two electrodes.

The electronic current along the Kagomé-lattice chain is calculated by employing the nonequilibrium Green function method [12, 13]. In this method, the Green functions of the electrode and chain systems, $g(E)$, are separately calculated, assuming that these systems are isolated. Then, we connect the electrodes and chain to calculate the Green functions of the joint system, $G(E)$, by solving the Dyson equations with the connection $\hat{W}$ as a self-energy. The electronic current is calculated using a following formula,

$$\langle I \rangle = 4 e \frac{\mu^L}{h} t'^4 \int_{-\infty}^{+\infty} dE \left( f^L(E) - f^R(E) \right) \text{Im}[g^R_0(E)] G^l_{1N}(E) G^R_{1N}(E) \text{Im}[g^R_{N+1,N+1}(E)],$$  \hspace{1cm} (5)

where $h$ is a Planck constant [13]. In this formula, $f^L(E)$ and $f^R(E)$ are Fermi distribution functions of left and
right electrodes, respectively. \( \text{Im}[g_{60}^{\alpha}] \) and \( \text{Im}[g_{N+1, N+1}^{\gamma}] \) are the electron densities of states of the left and right electrodes. \( G_{tN}^{\alpha}G_{tN}^{\gamma} \) is the transport probability from the left edge to the right edge of the Kagomé-lattice chain.

Calculations are performed at \( t^L = t^R = 60t \), \( t' = 0.1t \), \( \mu^L = 0.05t \), \( \mu^R = 0 \), and inverse temperature \( \beta^{-1} = 0.01t \).

For later discussions, we estimate an analytic form of \( G_{tN}^{\alpha} \) which corresponds to the transport probability of an \( \alpha \)-th resonance level, using approximate Green functions. For the isolated Kagomé-lattice chain, when the \( \alpha \)-th eigenstate has the energy \( E_{t\alpha} \) with no degeneracy, the Green function around \( E = E_{t\alpha} \) is approximately given as

\[
g_{t\alpha}^{\alpha}(E \sim E_{t\alpha}) = \sum_\gamma \frac{\chi_{t\alpha}^{\gamma} \chi_{t\gamma}^{\alpha}}{E - E_{t\gamma} - i\delta} \approx \frac{\chi_{t\alpha}^{\alpha}}{E - E_{t\alpha} - i\delta}.
\]

(6)

\[
G_{tN}^{\alpha}(E) = \frac{1}{1 - t'^2(g_{60}^{\alpha}g_{11}^{\alpha} + g_{NN}^{\alpha}g_{N+1, N+1}^{\alpha}) + t't^2g_{60}^{\alpha}(g_{11}^{\alpha}g_{NN}^{\alpha} - g_{tN}^{\alpha}g_{N+1, N+1}^{\alpha})g_{N+1, N+1}^{\alpha}} \\
\approx \frac{\chi_{tN}^{\alpha} \chi_{tN}^{\gamma}}{E - E_{tN} - i\Delta_e}.
\]

(8)

where \( \Delta_e \) is given by

\[
\Delta_e = \delta + t'^2\frac{\chi_{tN}^{\alpha} \chi_{tN}^{\gamma}}{E - E_{tN} - i\Delta_e} + \frac{\mu^2}{tR} \chi_{tN}^{\alpha} \chi_{tN}^{\alpha}.
\]

(9)

\[\text{Eq. (9) represents the broadening of the energy-level width due to the contact to the electrodes.}\]

### III. RESULTS AND DISCUSSION

We first study the general features of the electronic current flowing through the Kagomé-lattice chain in the case when there is no external electric field. Figure 3 shows the calculated currents of the four-plaquette Kagomé-lattice chain as a function of the gate voltage. In the figure, the flat-band channel is located at \( V^G = -2t \), which is recognized by observing the energy spectra in Fig. 1(c). It is seen that the current through the flat-band-like channel is almost zero. This result occurs because of the infinite effective mass, i.e., localized nature, of the flat-band-like states. The other current peaks seen in the region from \( V^G = -1.3t \) to \( 0 \) originate from normal-band-like channels.

We then study how the current spectra change when a small external electric field is applied to the Kagomé-lattice chain. Two cases are considered: the uniform electric field along the chain and that perpendicular to the chain, i.e., the \( x \) and \( y \) directions in Fig. 2(a), respectively. In the former case, we assume that the on-site potential is given by

\[
V^E_x = V^x (2Ma - x_i)/(2Ma),
\]

where \( x_i \) is the \( x \)-coordinate of the \( i \)-th site in a chain and \( V^x \) represents the electric-field magnitude. The electric field magnitude is set to \( V^x = 0.05t \). In this case, we found that the overall spectra are similar to those in the case with no electric field shown in Fig. 3.

In the case of the electric field along the \( y \) direction, we assume the on-site potential as

\[
V^E_y = V^y y_i/(\sqrt{3}a),
\]

where \( y_i \) is the \( y \)-coordinate of the \( i \)-th site in a chain and \( V^y \) represents the electric-field magnitude. Figure 4 shows the calculated current vs gate-voltage spectrum for the four-plaquette Kagomé-lattice chain, where \( V^y = 0.05t \) is employed. Since the electric field is small, the currents through the normal-band-like channels have almost the same position and spectral magnitude as those in Fig. 3.

On the other hand, it is noteworthy that a large current peak appears at \( V^G = -2t \), i.e., at the position of the flat-band-like channel.

To understand the anisotropy of transport properties

![FIG. 4: Calculated current vs gate-voltage characteristic of four-plaquette Kagomé-lattice chain when electric field is applied perpendicular to chain, i.e., along \( y \) direction, with \( V^y = 0.05t \). The unit of current is \( 10^{-4}|t|^2e/h \).](http://www.sssj.org/ejssnt)
FIG. 5: Eigenfunctions of four-plaquette Kagomé-lattice chain corresponding to flat-band-like states, when an electric field is applied along the chain, i.e., along the $x$ direction. $+$ and $-$ in circles are the signs of wave functions, while the tone represents their amplitude.

FIG. 6: Eigenfunctions of four-plaquette Kagomé-lattice chain corresponding to flat-band-like states, when an electric field is applied perpendicular to the chain, i.e., along the $y$ direction.

with respect to electric fields, we investigate the wave functions. In the case of the four-plaquette Kagomé-lattice chain, for example, fourfold degenerate flat-band-like states change to have different energies under an electric field. The wave functions of these states are shown in Figures 5(a) to 5(d) when an electric field is applied along the chain. In these figures, $+$ and $-$ are the signs of the wave functions, while the tone represents their amplitude magnitudes. It is seen that all these states are localized around one of the plaquettes in the Kagomé-lattice chain. This is because each plaquette has a different on-site energy when the electric field is along the chain direction. Reflecting such a localized nature of the wave functions, the electron transport probability of these channels is considerably small. Therefore, one cannot see current through the flat-band-like channel.

When the electric field is applied perpendicular to the chain, fourfold-degenerate eigenstates change to have different energies and have wave functions shown in Figs. 6(a) to 6(d). It is seen that all these states are extended over the Kagomé-lattice chain. Thus, the current channels originating from these states are opened and induce the sudden appearance of large current peaks at $V^G = -2t$, as shown in Fig. 4.

Remembering that the flat-band-like states have both localized and itinerant characteristics, one can say that the electric field along the chain direction induces the localized characteristic and thus no current. On the other hand, the electric field perpendicular to the chain promotes the emergence of the itinerant characteristic and produces the large current.

Next, we study how the current through the flat-band-like channel vary as the magnitude of the electric field, $V^y$, gradually changes from zero to finite values. Figure 7 shows the current magnitude of the four-plaquette Kagomé-lattice chain for various values of $V^y$. The current variation can be categorized into two regimes, I and II, in Fig. 7 depending on the magnitude of the electric field. In regime I, the current quickly increases with increasing the electric field. On the other hand, in regime II, the current has almost the similar magnitude.

We first consider the regime II. Figure 8(b) shows the calculated imaginary parts of the $G^{a}_{1N}(E)$ at $V^y = 0.05t$, which denotes the transport amplitude. The four positive and negative peaks from $E = 0.025t$ to $0.03t$ correspond to flat-band-like channels. As seen in Eq. (8), the sign of peak reflects the product of wavefunction amplitudes at two edge sites, $\chi_1\chi_N$. As shown in Figs. 6(a) to 6(d), such product alternatively has positive and negative signs. Since the energy degeneracy of these channels is removed by the applied electric field, all peaks appear separately. Since square of the peak magnitude becomes the transport probability of the channel and the bias voltage is much larger than the energy separation of these peaks, all these four channels contribute to the current independent of the electric-filed magnitude. This is the reason why the

http://www.sssj.org/ejssnt (J-Stage: http://ejssnt.jstage.jst.go.jp)
current in the regime II is large and has a small variation.

However, when we decrease the electric field and enter the regime I, the energy separation among four flat-band-like states becomes small. Thus, the positive and negative peaks observed in Fig. 8(b) overlap with each other and decrease the magnitude as shown in Fig. 8(a). Such cancellation of peaks occurs apparently due to the quantum interference between the wave functions of flat-band-like states. In other words, the large variation of current in the regime I originates from the quantum interference. In this sense, one can say that the regime I is the quantum regime, while the regime II corresponds to the classical one.

Finally, we shortly comment on the experimental conditions to observe exotic transport properties studied in this work. To realize the flat-band-like states, the quantum coherence of electron wavefunction is essential. Therefore, various scattering effects for electrons encountered in Kagome-lattice chains should be enough small. From the energy-perturbation viewpoints, since the coherence of flat-band-like states is broken by the mixing of wavefunction components with normal-band-like states, the energy change by scattering, $\Delta E$, should be smaller than the representative energy difference between flat-band-like and normal-band-like states, $\delta E$. Here, we consider the Kagome-lattice chain having $72\text{nm}$ lattice constant and made of InAs quantum wires as an example. In this system, the energy transfer and energy difference, $t$ and $\delta E$, are estimated as $1.7\text{meV}$ and $0.3\text{meV}$, respectively [9]. With respect to the phonon scatterings, $\Delta_{\text{ph}}$ typically has the energy roughly corresponding to the sample temperature, $k_B T$. Thus, the experimental temperature should be lower than $1\text{K}$. On the other hand, the energy change due to the impurity or structure-randomness scattering is written by the relaxation time, $\tau$, as $\Delta_{\text{imp}} = \hbar/\tau$, while the system mobility, $\mu$, is also related to $\tau$ as $\mu = e\tau/m$. In order that $\Delta_{\text{imp}}$ becomes less than $0.3\text{meV}$, the system mobility should be larger than $1 \times 10^5 \text{cm}^2/\text{Vs}$ for InAs wires. Due to the similar reason, one might need high quality contacts to electrodes. However, it is noted here that these conditions are relaxed if one can prepare the Kagome-lattice chains with much shorter lattice constants; for example, the energy difference, $\delta E$, becomes about $30\text{meV}$ for the Kagome-lattice chain with $7\text{nm}$ lattice constant.

**IV. CONCLUSION**

Electron transport properties are investigated in the Kagomé-lattice-chain systems, using the simple tight-binding model and nonequilibrium Green function method. We found that the current through the flat-band-like channel is sensitive to the direction of the applied electric field; a large current is observed to flow along the chain when the electric field is applied perpendicular to the chain, while no current is observed to flow along the chain when the electric field is applied along the chain. By analyzing how the degeneracy of flat-band-like states is broken, this strange anisotropy is shown to originate from the unique feature of the flat-band states; that is, they have both itinerant and localized characteristics. Moreover, we found that the transport characteristic changes from the quantum interference to noninterference regimes with increasing electric field.

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