Calculation of Conduction Spectra in Quantum Dot Composed of Penrose Lattice

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Abstract. Conductance through finite two-dimensional Penrose lattices (PLs) are calculated as a function of gate voltage. To investigate effects of lattice defects and lattice vibrations, three types of PLs are taken into account; (A) PL without lattice defects, (B) PL with lattice defects, and (C) PL with lattice vibrations, which is applied the electric field across the conductor. When energy levels of PL coincides with the chemical potential of the electrodes with increasing gate voltage, electron transfer through PL takes place. However, electron transfer is forbidden at certain states; These states have confined states, which have multiple-degeneracy in their electronic states. In addition, the states are localized due to interference of their wave-functions though the wave-function of each state is extended. We would like to point out that rigidity of confined states with respect to lattice defects and lattice vibrations.

1. Introduction
Artificial lattices have two fascinating characteristics; (1) Flexibility to design various lattice shapes. (2) Controllability of the number of electrons in a lattice by applying a gate voltage. For example, by the use of patterning techniques, Kagome-lattice was made of InAs wires on a GaAs substrate by Fukui et al. [1–3]. In particular, Kagome-lattice has a complete flat-band in its electronic structure. Eigenstates of the flat-band are completely localized within the unit cell. The characteristics of the flat-band states in two-dimensional Kagome-lattice are maintained in quasi-one-dimensional Kagome-lattice chain. In fact, the flat-band-like states appear in the Kagome-lattice chain. When the electric field is applied along the chain, the finite current is obtained. In contrast, no current is generated for the case where an electric field is applied perpendicular to the chain [4]. This is remarkable result from the viewpoint of the manipulation of switching process.

In our study, we calculate current for artificial lattice composed of finite two-dimensional Penrose lattice (PL) with fixed boundary condition. Here, the two-dimensional PL is described by the tight-binding model, where one electronic basis state is positioned on each vertex. The following properties of two-dimensional PL are confirmed [5, 6]; (1) This PL has degenerate state at an energy E=0, which appears at the center of the spectrum. (2) The states with E=0 are all strictly localized and have amplitudes only on three-edge vertices and some non-three-edge vertices. (3) The states named confined states have finite regions, which are nonzero amplitudes on these specific vertices. (4) The confined states survive independently in the magnetic field. Considering these remarkable properties, we investigate PL as the subject of
challenging research; the behavior of the current as a quantum dot whose edges are connected with electrodes is discussed in the present paper.

2. Model and Method

Our purpose is to make clear the behavior of conductance for the artificial lattice composed of PL. We give following definitions; (1) The lattice defects means that the electron cannot transfer from the $i$ sites of lattice defects to surrounding $j$ sites, i.e. $t_{i,j} = 0$. (2) 126 sites are used. (3) The energy for degenerate states having confined states ($E_C$) of PL is determined to be zero. We analyze the following situations for finite two-dimensional PL; (A) PL without lattice defects. (B) PL with lattice defects. We put the lattice defects on the sites of nonzero amplitudes of wave-function at $E_C$ of PL. Moreover, the lattice defects are given in order to break confined states for $E_C$ of PL. We consider the behavior of current influenced by the lattice defects. (C) PL with lattice vibrations in the electric field. In detail, the lattices vibrate between center sites of pentagon and surrounding sites. We give this condition. Because Abe et al. found that specific sites have the local thermal vibration anomalies [7]. We would like to know the behavior of current when the vibrations are given. In our model, the lattice vibrations between center sites of pentagons and surrounding sites are taken into account. Furthermore, we adopt the tight-binding approximation and Green’s function method for these systems. Hamiltonian for the situation (A) or (B) is

$$H = -t \sum_{<i,j>} (c_i^\dagger c_j + h.c.) + \sum_i eV_i c_i^\dagger c_i,$$

where $t$ is a transfer energy between nearest neighbor sites. Second term of the Eq. (1) describes potential energy, where $V_i$ is electric potential at the $i$ site. In the case of (A) and (B), the potential energy is not taken into account. This term is only valid in the case of (C).

In addition, the Green’s function for situations (A) and (B) is expressed as

$$G(\epsilon) = \sum_m \frac{\langle L |m\rangle \langle m |R\rangle}{\epsilon - \epsilon_m + eV_{\text{gate}} + i\Gamma/2}.$$  

Here, $\epsilon_m$ and $|m\rangle$ are eigenenergy and eigenstate of Eq. (1), respectively. Gate potential $V_{\text{gate}}$, which is shown in the denominator of Eq. (2), shifts the energy levels of the PL. Furthermore, $\Gamma$ is the width caused by the coupling between PL and two electrodes.

For situation (C), we introduce electric potential $V_i$ applied to the system and a perturbative Hamiltonian($H'$) as the deviation of transfer energies between specific sites and their surrounding sites by the effect of vibrations. As shown in Fig. 3, $V_i$ is given various values for position. The Hamiltonian of the case (C) is shown below:

$$\tilde{H} = H + H', \quad H' = -\delta \sum_{<i,j>} (c_i^\dagger c_j + h.c.).$$

For this situation (C), The Green’s function is expressed as

$$G(\epsilon) = \sum_m \frac{\langle L |m\rangle \langle m |R\rangle}{\epsilon - \epsilon_m + eV_{\text{gate}} + i\Gamma/2} \left[ 1 + \sum_{k \neq m} \frac{|\langle k |H'|m\rangle|^2}{(\epsilon_k - \epsilon_m)^2} \right],$$

where the first term already given in Eq. (2), the second term means that electrons transfer from energy level $|m\rangle$ to $|k\rangle$ by the lattice vibration.
In the case of Penrose lattice. The dashed and solid lines mean conductances without and with lattice defects, respectively. The manner of doping of the lattice defects is shown in the inset. Stars mean the lattice defects. The lattice defects are adopted at the sites where the amplitudes of wave-functions at $E$ of PL are not zero. The conductance peaks appear around $eV_{\text{gate}}/t = \pm 0.1$.

3. Results and Discussion
We calculate the current of PL for each situation (A), (B) and (C). In particular, we pay attention to the current of $E$ of PL. We make clear the unique current of this PL, comparing with square lattice consisted of periodic structure. We define that energy level of confined states $E$ of PL and the highest occupied levels for the case of half-filling in square lattice are zero. The numerical calculation is made by 126 sites in PL and $11 \times 11$ sites for square lattice.

The dashed line in Fig. 1 denotes the conductance of PL without lattice defects. The solid line means that PL with the lattice defects of which concentration is 5 %. It should be noted that the conductance gap of dashed line is larger than that of solid line. This feature is caused by the fact that some of degenerate states split and other electronic states appear with increasing lattice defects. However, the conductance at $E$ of PL is zero for situation (A) and (B). We would like to point out that the electrons at $E$ of PL do not contribute to the current, because of the confinement of their electronic states. The localization of wave-functions satisfies topological rules of PL. Arai et al. has suggested the rules for PL in details [5]. For PL, the eigenvalue equation $\sum_j t_{i,j}\phi_j = E\phi_i$ for the Hamiltonian of PL splits into two groups as for $E$ of PL. Nonzero amplitudes of wave-functions exist on one sublattice and those for all vertices on another sublattice are zero amplitude. Consequently, the current around $E$ of PL is not sensitive to the lattice defects.

As shown in Fig. 2, the lines show the current of square lattice. The dashed line denotes conductance of square lattice without lattice defects and the solid line means conductance with...
lattice defects. Here, the lattice defects are given in the inset. The shapes of conductance are seriously affected by lattice defects. The wave-function spreads to the whole lattice by the non-local property, because the wave-function of the periodic structure is Bloch state.

Comparing Fig. 1 with Fig. 2, conductance peaks at $E_C$ does not appear and conductance gap always appears around $eV_{\text{gate}}/t = 0$ for the PL with lattice defects. In contrast, position and values of conductance peaks for the square lattice change depend on the lattice defects. It means that periodic structures, which have Bloch wave, are sensitive to the lattice defects.

Calculated conductance of PL with lattice vibrations and the electric field are shown in Fig. 3, where the patterns of vibration are illustrated in the inset. In order to resolve the degeneracy at $E_C$, we apply an electric field across the system as shown in the inset of Fig. 3. The solid and dashed lines denote the conductance of PL without and with lattice vibrations, respectively. The localization of wave-functions at $E_C$ survives in spite of adopting lattice vibrations. The conductance around $0 \leq eV_{\text{gate}}/t \leq 0.2$ is small in comparison with the conductance appearing outside of the conductance gap. In other words, the conductance around $eV_{\text{gate}}/t = 0 \sim 0.2$ is reflected by the localization of wave-functions. Consequently, the localization of wave-functions at $E_C$ survives and shows small conductance.

4. Conclusions
We point out that the localization of wave-functions belong to the confined states of PL survives persistently with the lattice defects and the lattice vibrations. In fact, the conductance gap appears around $E_C$ of PL, because the wave-functions destructively interfere with each other.
Figure 3. The dashed line is the conductance through PL which apply an electric field. In addition, the solid line shows the conductance with lattice vibrations as well as the electric field. The conductance of solid lines around $0 \leq eV_{\text{gate}}/t \leq 0.2$ is small in comparison with that of other areas. As a result, the localization of wave-function of $E_C$ of PL remains strongly with the lattice vibrations.

We confirm that rigidity of confined states with respect to lattice defects and lattice vibrations. On the other hand, the current is obstinately obtained except for the region of the gap. As a result, we could control current by utilizing the energy level of the confined states $E_c$ and the other levels. Accordingly, it has possibility to apply this artificial lattice composed of PL to be a manipulation of switching process, though there remains much problem to be attacked.

5. References
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