Valley-dependent electronic transport in quantum Hall systems of $\alpha$-T$_3$ model

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Abstract. We study the quantum transport in $\alpha$-T$_3$ model lattice in the presence of a perpendicular magnetic field. It is found that valley pseudospin is also a very important degree of freedom for electrons in $\alpha$-T$_3$ model lattice, which can be modulated by the magnetic field. When a perpendicular magnetic field is applied to $\alpha$-T$_3$ model lattice, the electrons in the two valleys have different responses to the magnetic field. We found that the continuous subbands of $\alpha$-T$_3$ model lattice are splitted into discrete Landau levels by the perpendicular magnetic fields, and the Landau levels for the two valleys are different, which leads to high valley polarization. Our results may stimulate further experimental studies of the realization of valleytronic devices.

1. Introduction

As we know, electrons have two degrees of freedom, namely charge and spin [1], but another degree of freedom valley also plays important role in graphene-like materials with hexagonal lattice. Valley degrees of freedom can be used as information carriers just like charge and spin, which is referred as valleytronics. In valleytronics, the valley degree of freedom is controlled to design and realize related functional devices, and this offers us new opportunities to develop valley-based electronic devices. Many different methods have been used to control the valley-dependent quantum transport in graphene [2, 3], such as line defect [4, 5], trigonal warping [6], and lattice strain [7]. Besides, valley-dependent quantum transport has also been investigated in other materials such as silicene [8], bilayer graphene and black phosphorus [9]. Zhang et al. proposed a valley filter in silicene by adding a magnetic barrier and a perpendicular electric field [8]. Park et al applied a potential barrier and a magnetic field to a bilayer graphene and a valley filter is obtained [10].

In 2004, graphene was successfully obtained in the experiments by mechanical stripping method [11], and it has attracted great attentions in the scientific field [12-16]. Graphene is a two-dimensional carbon nanomaterial with beehive-shaped lattice, and it has been regarded as a promising candidate for optoelectronic applications [17], valleytronics [18] and spintronics [19]. Because of the unique properties of graphene, other two-dimensional materials such as silicene, phosphorene and TMDs are also investigated intensively. In recent years, another two-dimensional material $\alpha$-T$_3$ was proposed by coupling the honeycomb lattice to an additional atom, and the atom is located at the centre of the hexagons [20]. In the $\alpha$-T$_3$ lattice, the parameter $\alpha$ is used to describe the coupling strength between the atoms on the honeycomb lattice and atoms in the centre of the hexagons, which evolves
continuously from 0 (graphene) to 1 (dice lattice). The $\alpha$-T$_3$ lattice is an interpolation between graphene and dice lattice, so it has attracted considerable attention in the field of physics [21-24]. The $\alpha$-T$_3$ lattice can be realized by growing a three-layer structure of SrTiO3/SrO3/SrTiO3 in the (111) direction. [25] Recently, a $\alpha$-T$_3$ lattice was obtained in Hg$_{1-x}$Cd$_x$Te with a critical value $x=0.17$, and the intermediate parameters $\alpha=1/\sqrt{3}$. [24] In $\alpha$-T$_3$ model, the energy band spectrum also has K and K’ valleys, which is similar with graphene. The valley-dependent transport [26, 27] in $\alpha$-T$_3$ model has become one of the important research direction. Xu et al. study the valley Hall effect in $\alpha$-T$_3$ model, and valley filtering effects was obtained [28]. Bouhadida et al. study the valley-dependent quantum transport in $\alpha$-T$_3$ model with electric and magnetic barrier [29].

In this study, we investigate the valley-dependent quantum transport in $\alpha$-T$_3$ model under a magnetic field. Since the energy band spectrum of $\alpha$-T$_3$ model also has K and K’ valleys, it is of great interest to find the methods to generate valley polarization or valley filtering in $\alpha$-T$_3$ model. We found that the magnetic field will generate uneven distribution of electrons in K and K’ valleys, and the conductance for K and K’ valley electrons are different. The energy band spectrum of $\alpha$-T$_3$ model under magnetic field shows us the different subbands in K and K’ valleys, so valley polarization and valley filtering effects are obtained. Our proposed device can work as a valley filter and our study may be useful for the development of valleytronic devices in $\alpha$-T$_3$ model.

2. Model and methods
In Figure 1(a) we show a schematic of $\alpha$-T$_3$ model, and we can see that an atom is added to the geometry of the honeycomb lattice. This atom is located at the centre of each hexagon and is coupled to one of the two atoms in one unit cell. In each unit cell of the $\alpha$-T$_3$ lattice, it contains three lattice points. Atoms A and B form a hexagon lattice, which is same as graphene, and the nearest hopping amplitude between A and B is t. The additional atom C only couples to B atom, and this additional atom offers $\alpha$-T$_3$ model a lot of new properties that graphene does not have. The hopping amplitude between C and B is $t\alpha$, where the value of $\alpha$ changes in the region $0\leq\alpha\leq1$. When $\alpha=0$ we have graphene, and we will have dice lattice when $\alpha=1$. It is noted in Figure 1(a) that we have a zigzag edge along x-direction. The atoms on the top and bottom edges are C and A atoms respectively, and we call it C-A edged zigzag ribbon. In this study, we investigate the quantum transport properties of a $\alpha$-T$_3$ model nanoribbon with C-A edges. A magnetic field is applied perpendicular to the C-A edged zigzag nanoribbons. Due to unique lattice structure of $\alpha$-T$_3$ model, the transport properties are different from graphene and other graphene-like two dimensional materials. The tight-binding Hamiltonian for $\alpha$-T$_3$ model under a perpendicular magnetic field can be written as

$$H = -\sum_{\langle ij \rangle} t e^{i\phi} a^+_i a_j + \sum_{\langle jk \rangle} \alpha t e^{i\phi} b^+_j b_k + H.c.$$  

where $a_i$ ($a^+_i$), $b_j$ ($b^+_j$) and $c_k$ ($c^+_k$) are annihilation (creation) operators at site i, j and k respectively. The effects of the magnetic field is included Peierls’ substitution $\phi_{ij(k)} = (2\pi / \phi_0)\int_{j(k)}^{(i)} A \cdot d\vec{r}$ with the quantum of magnetic flux $\phi_0 = h / e$. In the Landau gauge, the perpendicular magnetic field can be described by a vector potential $\vec{A} = (-B, 0, 0)$. The tight-binding model in this study is constructed using the Kwant tight-binding code [30]. The conductance for K and K’ valleys is calculated by the nonequilibrium Green’s function (NEGF) formalism

$$G(E) = \frac{e^2}{h}\text{Tr}[\Gamma^r(E)G^r(E)\Gamma^l(E)G^a(E)]$$

where $\Gamma^r_{L(R)} = \{\Sigma^r_{L(R)} - \Sigma^a_L\}$ which is written in terms of self-energies of the left lead ($\Sigma^r_L$) or right lead ($\Sigma^r_R$). $G^\alpha(E)$ is the retarded (advanced) Green’s functions. The band structures and the current of the device is calculated using Kwant. In our numerical calculations, the distance between A
site and B site is chosen to be 0.142nm, which is the carbon-carbon bond distance. It will be convenient for us to compare the results with graphene. In this study, we consider a small size device, and we only investigate the ballistic transport properties of electrons in our proposed device. The nonlocal transport properties are not considered.

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Figure 1. (a) Schematic of $\alpha$-T$_3$ model. Colours denote the three atoms in each unit cell, ie. A (blue), B atom (red) and C (green) (b) Schematic of the low-energy dispersion for $\alpha$-T$_3$ model at a single K point.

3. Result and discussion
In this section, we take into account the valley degree of freedom and investigate the transport properties for a structure of $\alpha$-T$_3$ nanoribbon shown in the inset in Figure 2(a). In the scattering region a perpendicular magnetic field is considered, and no magnetic field is included in the leads. The sample size is chosen to be $L=120$nm and $W=30$nm. The parameter $\alpha$ is chosen to be 0.5. In Figure 2(a), we show the valley resolved conductance for a C-A edged ribbon in the absence of a magnetic field. We can see that the conductance in the low energy region is zero, which means that there is a band gap for C-A edged ribbon with $\alpha=0.5$. The conductance increases with the increasing of the Fermi energy, because more electron conduction channels contribute to the transport when Fermi energy increases. Since we do not consider the effects of magnetic field, there is no scatterings in the device region. So, we have perfect conductance plateaus. More importantly, we find that the conductance for K and K' valleys are the same. We do not have valley filtering or valley polarization when no magnetic field is applied, and the valley degree of freedom can not act as information carriers.

In Figure 2(b), we plot the valley resolved conductance as a function of Fermi energy when a perpendicular magnetic field $B=120$T is applied. It is found that the conductance for K and K' valleys are not the same anymore. For the system without valley polarization, the conductance is contributed from both K and K' valleys. For our present work, the valley polarization will affect the electronic transport measurements. It is noted that the conductance $G=1e^2/h$ is obtained in the region $0.06t<E<0.125t$, which is the effect of valley polarization. In this region, the K' valley electrons are all filtered, and we have 100% valley polarization. In the energy region $0.0t<E<0.125t$, the conductance for K' valley is zero, which means a band gap is induced by magnetic field in K' valley. A band gap also induced in K valley, but the band gap is smaller. At last, we want to point out that the transport is robust, and the conductance for K and K' valleys only have very small oscillations. As we know we only considered a magnetic field in the device region, but we do not have magnetic field in the leads. The scatterings between the device region and the leads are very small.
Figure 2. (a) The valley resolved conductance is plotted as a function of the Fermi energy without magnetic field. The inset illustrates schematically the system under consideration. (b) The valley resolved conductance is plotted as a function of Fermi energy with magnetic field $B=120T$.

Figure 3. Band structures of C-A edged zigzag ribbons with various parameters $\alpha=0$, 0.5, 1, and magnetic field $B=0T$, 120T.

To understand the transport properties discussed above, we plot the band structures with various parameters $\alpha=0$, 0.5, 1, for a strong magnetic field $B=0T$ and 120T. Figure 3 shows the evolution of the band structure of the metal zigzag ribbon with different parameters $\alpha$ at different magnetic fields. In Figure 3(b), the band structure of C-A edged zigzag ribbons with $\alpha=0.5$ is presented. We can see that the subbands in K and K' valleys are the same, and no valley filtering can be obtained, which agrees well with the results shown in Figure 2(a). In Figure 3(e), the parameters $\alpha$ is still 0.5 but a perpendicular magnetic field $B=120T$ is applied to $\alpha$-T$_3$ model. The presence of flat energy bands in Figure 3(e) signaled the formation of Landau levels. For a smaller magnetic strength, we can also obtain valley polarization in $\alpha$-T$_3$ model. Flat energy bands can also be found in low energy region for
smaller magnetic field strength. The Hall conductivity can be obtained by counting the number of the energy levels. Furthermore, we find that the energy levels in K and K' valleys are different. In the energy region $0.06t < E < 0.125t$, we have energy levels in K valley, but no energy levels are found in K' valley. The band structure can explain the results in Figure 2(b).

For $\alpha=0$, the band structures for B=0T and B=120T are presented in Figure 3(a) and (d) respectively. In this case, we actually have a zigzag graphene nanoribbon. The band structures are the same as some previous studies [31]. For $\alpha=1$, we have a dice lattice. We can see from Figure 3(c) that there is a band gap between the conduction and valence bands. When magnetic field is applied, the band gap is enlarged, but the energy levels for K and K' valleys are the same. Comparing the band structures in Figure 3(e) with band structures of graphene nanoribbon shown in Ref. [31], we can see that magnetic field can not induce the differences in K and K' valleys in graphene. These special properties of $\alpha$-$T_3$ model are caused by its unique lattice structure. In Ref. [3], valley polarization is obtained in a T junction of graphene nanoribbons without magnetic field, but this can not be realized in $\alpha$-$T_3$ model because the subbands in K and K' valleys are the same when no magnetic field is applied (see Figure 3(b)). In Refs [2, 8], the valley-dependent transports in bulk systems are studied, and ferromagnetic stripes are considered to separate the electrons in K and K' valleys. In our present work, valley filtering effects is realized in a quantum Hall system of $\alpha$-$T_3$ model, which has not been reported in these studies.

![Figure 4](image_url)  
**Figure 4.** Current flow in the C-A edged zigzag ribbons with magnetic field B=120T. The energy is chosen to be E=0.2t and 0.1t.

It is important to know how current flows in a quantum Hall system, so we show the current of C-A edged zigzag ribbons when the magnetic field is 120T. In the absence of a magnetic field, the current is evenly distributed in the nanoribbon, however, current flows on the edge of the nanoribbon when a magnetic field is applied. In Figure 4(a) and (b), we can see that current flows on the top edge when it comes from the left lead, but the current flows on the bottom edge when it comes from the right lead. No current exists inside the ribbon. The electrons only transport on the edges, which is one of the very important properties for quantum Hall systems. In Figure 4(c) and (d), we show the current for E=0.1t, and it is noted in Figure 3(e) that the current for E=0.1t is only contributed from the K valley electrons, and we only have one conduction channels for the transport of electrons. This is different from the current at E=0.2t. For E=0.2t, the current is contributed from both K and K' valleys, and we can see in Figure 3(e) that we have two conduction channels in K and K' valleys respectively.

4. Conclusion

In conclusion, we study the valley-dependent quantum transport in nanoribbons of $\alpha$-$T_3$ model. When an external magnetic field is applied to a $\alpha$-$T_3$ nanoribbon, discrete Landau levels are obtained, and the energy levels in K and K' valleys are different. For a ribbon with magnetic field, we calculate the conductance for K and K' valleys and find that valley filtering effects can be obtained. A
perpendicular magnetic field can induce valley filtering $\alpha$-$T_3$ model. The band structures of $\alpha$-$T_3$ nanoribbons under magnetic field are plotted to explain the transport properties. We also note that current flows only on the edge of the ribbon, and no current flows inside the ribbon. These findings paved the way for the design of valleytronics devices based on $\alpha$-$T_3$ model materials.

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