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Spin helical states and spin transport of the line defect in silicene lattice

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ABSTRACT

We investigated the electronic structure of a silicene-like lattice with a line defect under the consideration of spin–orbit coupling. In the bulk energy gap, there are defect related bands corresponding to spin helical states localized beside the defect line: spin-up electrons flow forward on one side near the line defect and move backward on the other side, and vice versa for spin-down electrons. When the system is subjected to random distribution of spin-flipping scatterers, electrons suffer much less spin-flipped scattering when they transport along the line defect than in the bulk. An electric gate above the line defect can tune the spin-flipped transmission, which makes the line defect as a spin-controllable waveguide.

1. Introduction

A variety of two-dimensional materials of the lattice structure similar to graphene have drawn intensive attention in recent years. Silicene, germanene, and stanene have the buckled honeycomb lattice, and Dirac points were found in their electronic structures [1]. Comparing to graphene, there are advantages of these materials stemming from the lattice buckling. A normally applied electrical field induces a stagger potential and causes a band gap [2], which is essential for the application. The buckling dramatically increases the spin–orbit coupling (SOC) [3], while it is too weak to induce observable effect in graphene [4]. The SOC in a honeycomb lattice material makes it a topological insulator and spin helical edge states exist in the edges [5]. The combination of the stagger potential and the SOC results in valley polarization [6,7], and various spin and valley related physics can be found in junction systems [8–10]. Recently, researchers successfully fabricated line defects in honeycomb lattices [11,12], which has spurred lots of discussions on their electronic properties. A tight-binding investigation reveals that the system is gapless [13], and can be regarded as a quantum waveguide [14]. When a magnetic field is applied, localized states arise beside the defect line, like the edge states on the edges. The quantum states around the line defect can be described by the low energy continuum model with a proper wave connection condition [15,16]. An efficient valley filter effect can be caused by multiple defect lines due to the valley-dependent resonance [17,18]. The studies on the defect line are all based on graphene lattice, in which no SOC need to be considered. Due to the new features caused by lattice buckling, we expect more physics can be found in the silicene-like lattice with the defect line.

In this paper, we investigate the band structure of a silicene-like lattice with a line defect under the consideration of spin–orbit coupling. Fig. 1(a) shows the x–y projection of the investigated lattice, the defect atoms lie on the line $y = 0$ and the buckling amplitude for the defect atoms is assumed to be the same as that of the bulk lattice. We find there are two bands related with the line defect for each spin electrons between the bulk dispersions. The states of one band are most localized on the defect atoms themselves and the other most localized on the atoms nearest to the defect line (we refer these atoms closest to the line defect as the defect edge atoms). The spin-up defect edge states propagate along one defect edge and run back along the other defect edge, and the spin-down ones behave reversely, i.e., they are spin helical states. The stagger potential makes the bands asymmetric and alters the localization properties of the defect edge states. We study the spin-flipped transport when the lattice is subjected by random distribution of spin-flipped impurities. There always exists an energy interval within the bulk gap, in which the spin-flipped transmission is much smaller than that of the bulk electrons. This property stems from the separation in real space between the states of different spins.

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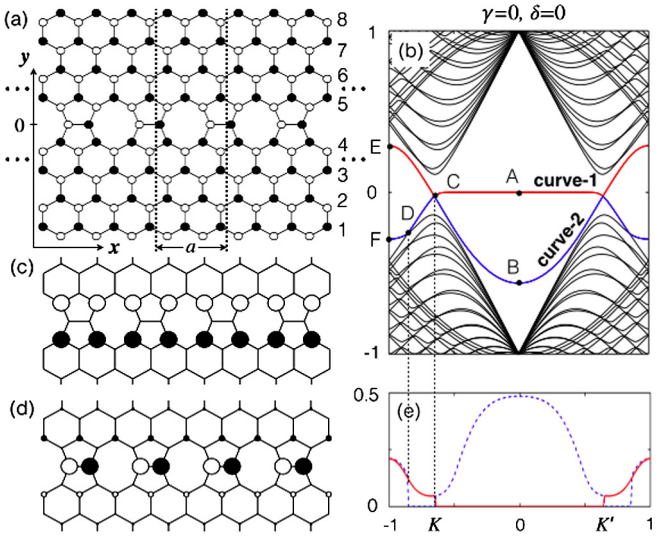

Fig. 1. (Color online.) (a) x–y projection of a silicene-like lattice with a line defect. The filled and empty circles represent atoms buckled-up and buckled-down respectively. (b) Dispersion $E(k)$ (in units of t) versus wavevector k (in units of π/a). The lateral atom number is 40. (c) The probability distribution of the eigen-state marked by point A in the dispersion. Larger atom circle radius means larger probability on the atom. (d) The probability distribution of the eigen-states marked by point B. (e) ρ_0 of the curve-1 (solid line) and curve-2 (dashed line) as functions of k.

2. Calculations and discussions

2.1. The Hamiltonian

The tight-binding Hamiltonian including the SOC reads

$$H = \delta \sum_{i\alpha} \nu_i c^+_{i\alpha} c_{i\alpha} - t \sum_{\langle ij\rangle\alpha} c^+_{i\alpha} c_{j\alpha} + i\gamma \sum_{\langle\langle ij\rangle\rangle\alpha\beta} \nu_{ij} c^+_{i\alpha} \sigma^z_{\alpha\beta} c_{j\beta} \quad (1)$$

where $c^+_{i\alpha}$ ($c_{i\alpha}$) is the creation (annihilation) operator for an electron with spin α on site i, σ^z is the z-component of Pauli matrix, and the summations with the brackets $\langle..\rangle$ and $\langle\langle..\rangle\rangle$ run over all the nearest and next-nearest neighbor sites, respectively. The first term is the Hamiltonian related with the stagger on-site potential, in which $\nu_i = 1$ when i represents a buckled up atom and $\nu_i = -1$ for buckled down atom, and δ is the stagger potential amplitude. The second term is the Hamiltonian of the nearest neighbor hopping with hopping energy t. The third term is the SOC Hamiltonian which involves the next-nearest neighbor hopping with amplitude γ and a path dependent amplitude ν_{ij}. For the electron couples form atom i, mediated by a nearest neighbor site and to a next-nearest neighbor atom j, we have $\nu_{ij} = 1$ if it makes a left turn and $\nu_{ij} = -1$ if goes a right turn. Since the line defect lies along x-direction, the wavevector in x-direction is a good quantum number. The calculation is conducted in a translational cell. In y-direction, the periodical edge condition is adopted to avoid the distraction of the edge states, which are not our targets.

2.2. The basic case: $\delta = 0$ and $\gamma = 0$

Firstly, we investigate the electronic structure of the system when both the stagger potential and the SOC are turned off (i.e., $\delta = 0$ and $\gamma = 0$). The dispersion is shown in Fig. 1(b). It can be seen that the dispersion is quite similar to that of a graphene ribbon, except that there are two additional curves lacking of electron–hole symmetry. The two bands are labeled by curve-1 and curve-2 in the figure and we will conduct detailed investigation on their properties for a variety of parameters. There is a flat part on curve-1, which implies that these states bear analogous properties of edge states. Fig. 1(c) shows the electron probability distribution of the eigen-state represented by point A on curve-1, and one can see that the density is most localized on the defect edge atoms. If we choose another point on the flat band apart from point A (a point between A and C) to study, we find the density decays away from the defect edge atoms to the bulk of either side, and the decay rate depends on the deviation of the point studied from point A (not shown in the figure). These features are just those of edge states for a zigzag graphene ribbon, which is not strange because the defect edge atoms are just the real edge ones if the defect atoms are removed. For this reason, we call these defect-nearest atoms as defect edge ones. The electron density of point B on curve-2 is shown in Fig. 1(d). The density is most localized on the defect atoms and slightly scattered on nearby atoms. For other points on the same curve near point B, the densities are more scattered on more atoms around the defect atoms, and decay away into the bulk (not shown in the figure). We also examine the properties of other parts of curve-1 and curve-2. The states of EC and FD are distributed on both the defect atoms and the defect edge atoms, as the states of part CB of curve-2, while, DC represents bulk states, which is result of the band crossing that occurs at point D. The density distributions of the two bands are symmetric with respect to the defect line.

To describe the localization on the defect atoms, we define quantity

$$\rho_0 = \rho(y = 0), \quad (2)$$

where ρ is the probability distribution. Fig. 1(e) shows ρ_0 of curve-1 and curve-2 as functions of k. From E to C, ρ_0 decreases continuously, abrupt change happens at point C because of the band crossing, and it vanishes for part CA (the flat part) since it represents defect edge states. ρ_0 of curve-2 experiences one more abrupt change because there is an additional crossing at point D besides of the crossing at point C; part FD of it is almost overlap with ρ_0 curve for curve-1 since they have similar localization properties; for part DC, ρ_0 is zero, which reflects the properties of the bulk states and the electron probability on the defect atoms is infinitesimal; and from C to B, the density on defect atoms is continuously increased.

2.3. The general cases

Now we turn the SOC term on to a small value. For this case the system is spin-dependent, we only study the properties for the spin-up electrons for now, and discuss spin-down electrons later. The SOC induces a gap $2\Delta_{SO}$ at each valley for a perfect bulk silicene-like lattice, which depends on the SOC by

$$\Delta_{SO} = 3\sqrt{3}\gamma. \quad (3)$$

The small gap can be found between curve-1 and curve-2 near valley K in Fig. 2(a), and it causes slightly smearing of the abrupt changes of ρ_0 versus k for both curve-1 and curve-2, as illustrated in Fig. 2(f). When we increase the SOC amplitude, the gap at valley K increases correspondingly, the smearing of ρ_0 is more apparently, the defect states around point C on curve-1 and the bulk states around the point on curve-2 are mixed with each other, and the $\rho_0 = 0$ part disappears. The bulk gap at valley K or K' is not the real gap between curve-1 and curve-2, because the bottom of curve-1 remains almost unchanged at $E = 0$ when γ changes.

In the energy gap, the SOC drives spin-up electrons piled up at one edge if edges exist, and spin-down electrons at the other edge.