Edge-dependent optical absorption of silicene nanoribbons in an in-plane magnetic field

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Abstract. We theoretically study the low energy electronic structures and optical conductivities of silicene nanoribbons (SiNRs) with zigzag and armchair edges in the presence of an in-plane magnetic field. It is found that the absorption spectrum exhibits a rich structure and remarkably depends on the edge types and the width of the SiNRs. In particular, the helical edge states for the zigzag SiNRs is gapped by the magnetic field, whereas those for the wide armchair SiNRs remain gapless, which could be demonstrated by the optical absorption measurement in experiments.

1. Introduction
Silicene, a single layer of silicon atoms closely packed in a two-dimensional (2D) honeycomb lattice, has recently attracted much interest since its successful fabrication in experiments [1-3]. In contrast to its counterpart of carbon, namely graphene, silicene has a buckled structure and a relatively large spin-orbit interaction (SOI) [4]. Consequently, silicene shows unusual electronic structures, which are characterized by the spin-orbital gap at the K points in the Brillouin zone. It has been predicted that the SOI could bring about exotic phenomena, such as the quantum spin Hall effect [4,5] and spin-valley coupled optical response [6-9]. What is more, the combination of the SOI and a perpendicular electric field or exchange field in silicene sheet could give rise to a rich variety of phases: a quantum spin Hall insulator, a quantum anomalous Hall insulator, a valley-polarized metal and a band insulator [10].

Silicene nanoribbons (SiNRs) are quasi-one dimensional (1D) strips of monolayer silicene with nanometer width, which have also been synthesized in experiments [11,12]. Distinct from 2D silicene sheets, 1D SiNRs have richer physics because of the quantum confinement and edge effects. It has been found that the quantum spin Hall edge states at zigzag and armchair terminations of honeycomb lattice are fundamentally different [13,14]. Akin to graphene nanoribbons [15,16], the energy gap of silicene and its nanoribbons can be modulated by applying electric field [17], adsorption [18], and doping [19], that makes them promising for the electronic and optical applications. It is well known that the optical absorption measurement has become an important tool to reveal the electronic structures and the topological states of the materials. There have been numerous works on the optical properties of graphene nanoribbons [20-26], but a few researches on that of SiNRs. Bao and his collaborators have predicted selection rule for the optical spectrum of armchair SiNRs (ASiNRs) [27]. Shyu has studied the electric field-modulated optical properties of armchair SiNRs (ASiNRs) [28] and the magneto-optical properties of zigzag SiNRs (ZSiNRs) [29].

In this work, we study the low energy electronic and optical properties of the SiNRs with zigzag and armchair edges in the presence of an in-plane magnetic field. It is found that the effects of the in-plane...
magnetic field on the properties of the zigzag and armchair SiNRs, especially on the edge states, completely differ. The rest of the paper is organized as follows. In section 2, we introduce the tight-binding model for the SiNRs and the formulism for the optical absorption. In section 3, we show the numerical results of the electronic structure and the optical conductivity, as well as some theoretical analysis. Finally, a brief summary is provided in section 4.

2. Model and formulism

Now we consider the single layer SiNRs with two edges run along the x direction, as shown in figure 1. The width of a SiNR in the y direction is defined as the number of the longitudinal diatomic chains. In the tight binding approximation, the π electrons in a pristine SiNR can be described by the following Hamiltonian [30,31]

\[ H_0 = -t_0 \sum_{\alpha, j, \alpha'} c_{i, \alpha}^\dagger c_{j, \alpha} + \frac{i\lambda_{SO}}{3}\sum_{\alpha, \alpha' j, \alpha' > \alpha} V_j c_{i, \alpha}^\dagger s_{\alpha' j, \alpha} c_{i, \alpha}, \quad (1) \]

where \( c_{i, \alpha}^\dagger (c_{i, \alpha}) \) is the creation (annihilation) operator of an electron with spin index \( \alpha \) at site \( i \) in the honeycomb lattice, and \((i, j) \) runs over the pairs of nearest (next-nearest) neighbor sties. \((s_x, s_y, s_z)\) is a vector of Pauli matrix for electron spin. The first term in equation (1) represents the standard nearest-neighbor hopping with the transfer energy \( t = 1.6 \text{ eV} \), while the second term accounts for the intrinsic SOI with its strength \( \lambda_{SO} = 3.9 \text{ meV} \) and the factor \( v_{ij} = 1 \) \((-1)\) if the next-nearest neighbor hopping is anticlockwise (clockwise) with respect to the positive \( z \) axis. Here we ignore the intrinsic Rashba SOI since it is very tiny in silicene (about 0.7 meV) [10]. For simplicity the change of the transfer energy at edges is also not considered.

![Figure 1](image_url) (Color online)

Schematics of (a) zigzag and (b) armchair SiNRs. Here we set the width \( W = 6 \) for the zigzag and \( W = 10 \) for the armchair nanoribbons, respectively. A unit cell consisting of \( 2W \) atoms is denoted by a rectangle. The lattice constant \( a = 3.86 \text{Å} \) for the zigzag and \( b = \sqrt{3}a \) for the armchair SiNRs. An in-plane magnetic field is applied along the x direction.

As the SiNR is subjected to an externally static in-plane magnetic field along the x direction, an additional term due to Zeeman effect should be added to the Hamiltonian above, which has the form

\[ H_1 = \lambda_m \sum_{i, \alpha \beta} c_{i, \alpha}^\dagger s_{\alpha \beta} c_{i, \beta}. \quad (2) \]

Here the parameter \( \lambda_m \) represents the Zeeman splitting induced by the in-plane magnetic field. Therefore the total Hamiltonian for the system is written as \( H = H_0 + H_1 \). It should be noted that the in-plane magnetic field could not cause orbital effect in the SiNR but plays a role like an exchange field in a ferromagnet. Besides, the direction of the in-plane magnetic field is irrelevant to the results.
of this paper. The Zeeman (exchange) field in the SiNR maybe also arise via proximity coupling to a ferromagnetic insulating substrate [10].

Since the nanoribbon is translationally invariant along the $x$ direction, we can perform the partial Fourier transformation on the tight binding Hamiltonian $H$ to rewrite it as $H(k_x)$, in which $k_x$ is the Bloch wavevector in the longitudinal direction. And then numerically diagonalizing the Hamiltonian, one can obtain the energy bands $E_n(k_x)$ and the corresponding eigenstates $|n, k_x\rangle$. Here the letter $n$ denotes the band index according to the minimum energy spacing between the subband and Fermi level. We will show the bandstructures of SiNRs with different width and edge types in the next section.

Now we irradiate the SiNRs by using a beam of monochromatic light with a linear polarization along the longitudinal direction of the nanoribbon. In order to investigate the optical response of SiNRs, one should calculate the real part of the dynamical conductivity $\sigma(\omega)$, which describes the optical absorption. Within the linear response theory, it can be expressed as

$$\sigma(\omega) = \frac{2e^2}{A \omega} \sum_{n, n', x} \left[ \langle n', k_x | \hat{v}_x | n, k_x \rangle \right]^2 \left[ f(E_{n, k_x}) - f(E_{n', k_x}) \right] \delta(E_{n, k_x} - E_{n', k_x} - \hbar \omega)$$

where $e$ is the electron charge, $A$ is the area of the sample, and $\omega$ is the irradiation frequency. $\langle n', k_x | \hat{v}_x | n, k_x \rangle$ is the matrix element for the $x$ component of the velocity operator $\hat{v}_x = \frac{\partial H}{\partial k_x}. f(E_{n, k_x})$ is the Fermi-Dirac distribution function. At low temperature, one can assume $f(E_{n, k_x}) = 1$ for $E_{n, k_x} < E_F$ and $f(E_{n, k_x}) = 0$ for $E_{n, k_x} > E_F$, where $E_F$ is the Fermi level. Here we study an undoped SiNR at low temperature such that $E_F = 0$.

3. Results and discussion

In the following, we will show some numerical results of the bandstructure and optical conductivity for the zigzag and armchair SiNRs. For clear illustration of the effects of the SOI and the in-plane magnetic field, we use the reduced parameters and enlarge the strength of the SOI. Besides, the Dirac delta function in equation (3) is approximated by a Lorentz function with its broadening parameter $\eta = 0.003t_0$. Hereafter we refer to a zigzag SiNR with $W$ zigzag chains as a $W$-ZSiNR and an armchair SiNR with $W$ dimer lines as a $W$-ASiNR.

3.1. Zigzag nanoribbons.

In figure 2(a) and (b), we present the low energy bandstructures of an 11-ZSiNR in the absence and presence of the in-plane magnetic field, respectively. The physical width for the 11-ZSiNR ($W = \sqrt{3}W a/2$) is about 3.68 nm. In figure 2(a), it is seen that the band structure with spin degeneracy is symmetric about the wavevector $k_x = \pi/a$. Moreover, the highest occupied subband ($n_o = 1$) and the lowest unoccupied subband ($n_c = 1$) touch at $k_x = \pi/a$ and their corresponding dispersions near the zero energy are linear. It can be demonstrated that the gapless states are quantum spin Hall edge states [4]. As the in-plane magnetic field is applied in the nanoribbon, each subband with spin degenerate in figure 2 (a) splits into two subbands in figure 2(b). More importantly, the Zeeman field leads to a gap of the edge states, which is about 0.1$t_0$ as illustrated in figure 2(b). That could be reflected in the low frequency optical absorption. By the way, one should note that the out-of-plane Zeeman field only results in a shift of the subbands with spin up (down) by an half positive (negative) Zeeman energy, so that it could not open a gap in our system.
Figure 2. (Color online) Band structures of 11-ZSiNR (a) with and (b) without the in-plane magnetic field. The up arrows denote the optical transitions between the edge states. (c) Spectra of optical conductivity in different cases.

Figure 2(c) displays the corresponding optical conductivities in different cases which are denoted by the different lines. The solid line stands for the spectrum of a pristine 11-ZSiRN without SOI, which is similar to that of a zigzag graphene nanoribbon [23]. The three absorption peaks come from the optical transitions satisfying the selection rule: Δn = n_e − n_o = odd. As the SOI is considered, all the original peaks exhibit the blue shift, meanwhile three additional peaks generating from a new selection rule Δn = even emerge [29]. It should be noted that the first new peak A_1 at ω = 0.2t_0 is predominated by the optical transitions between the edge states at the vicinities of the K points (k_x = 2π/3a, 4π/3a). When the in-plane magnetic field is applied in the sample, the Zeeman field leads to a richer optical spectrum due to the band splitting. It is clearly seen that each of the first three peaks, which is in the dashed line for the free 11-ZSiRN without the Zeeman field, splits into two peaks in the dash-dotted line. In particular, the two subpeaks B_1 and B_2 emerge at hω = 0.10t_0, 0.17t_0, which are contributed by the transitions at the vicinities of the center of Brillouin zone (k_x = π/a) and K points, respectively. The threshold peak B_1 at hω = 0.10t_0 is the signature for the energy gap of the edge states induced by the in-plane Zeeman field.
Figure 3. (Color online) Band structures of 50-ZSiNR (a) with and (b) without the in-plane magnetic field. (c) Spectra of optical conductivity in different cases. The arrows in (a) and (b) denote the first absorption shoulder and peak in (c), respectively.

We also calculate the band structures and optical conductivities for a 50-ZSiRN ($W' = 16.7$ nm), as illustrated in figure 3. In the wide ZSiRN without a magnetic field, the matching frequency for the optical transition between the edge states at the $K$ points is near that for the transitions involving the bulk states, as seen in figure 3(a), such that the corresponding absorption peaks almost overlap as shown on the dashed line in figure 3(c). In fact one can see a shoulder $A_1$ at $\hbar\omega = 0.20t_0$, which is attributed to the transition between the edge states near the $K$ points. As the in-plane magnetic field is considered, there exists a tiny peak $B_1$ at $\hbar\omega = 0.10t_0$, same as that for 11-ZSiRN, which indicates the width-independent energy gap of the edge states opened by the Zeeman field (shown in figure 3(b)), while the second peak $B_2$ remains at the frequency $\hbar\omega = 0.20t_0$. Actually, if consider a semi-infinite silicene sheet with a zigzag edge along the $x$ direction, we can obtain an effective Hamiltonian for the helical edge states: $H_e = \hbar v_F k_x s_z + \lambda_m s_x$, where $v_F$ is the Fermi velocity of the edge states dependent on the SOI [14]. Consequently, one gets the dispersion for the edge states: $\epsilon = \pm \sqrt{(\hbar v_F k_x)^2 + \lambda_m^2}$ and the gap: $\Delta E_e = 2\lambda_m$, which could be identified by the threshold peak of the optical absorption.

3.2. Armchair nanoribbons.

Now we turn to the armchair nanoribbons. It has been confirmed that the armchair graphene nanoribbons can be divided into two families: one family with $W = 3p, 3p + 1$ (p is an integer) are semiconductors, while the other with $W = 3p + 2$ are semimetals. This classification is also suitable for the ASiNRs with a weak SOI. Figure 4(a) and (b) exhibit the low energy bandstructures for a semiconducting 15-ASiRN with and without the in-plane magnetic field, respectively. Its physical width ($W' = Wa/2$) is about 2.90 nm. One can find that the free 15-ASiRN is a semiconductor with
the gap about $0.18t_0$, while the 15-ASiRN under the in-plane Zeeman field gets a narrower gap about $0.11t_0$ due to the breaking of the spin degeneracy.

\[ \Delta n = n_v - n_c \]

In figure 4(c), we plot the corresponding optical conductivities for the 15-ASiRN. In this figure, the solid line represents the spectrum for a pristine armchair nanoribbon without the SOI, which is consistent with the result for the armchair graphene nanoribbon [23]. On this line, one can see three absorption peaks resulting from the direct interband transitions: $\Delta n = 0$. As the SOI is introduced in the armchair nanoribbon, the first original peak shifts to the lower frequency, while the others shift to the higher. However, there is no additional peak, which indicates that the selection rule $\Delta n = 0$ still holds in the presence of the SOI [28]. This is quite distinct from the results for the ZSiNRs. After the application of the in-plane magnetic field in the sample, more absorption peaks appear since the selection rule is altered. It is obvious that there exist two subpeaks, which are labelled as $B_2$ at $\hbar \omega = 0.30t_0$ and $B_3$ at $\hbar \omega = 0.42t_0$ between the first two adjacent principal peaks $B_1$ and $B_4$. This two subpeaks are from the optical transitions $\Delta n = \pm 2 (n_v \rightarrow n_c; 1(3) \rightarrow 3(1))$ and $\Delta n = \pm 2, \pm 4 (n_v \rightarrow n_c; 2(4) \rightarrow 4(2), 1(5) \rightarrow 5(1))$ respectively. Furthermore, it is noted that the frequency $\hbar \omega = 0.17t_0$ for the first main peak $B_1$, which responses to the transition $\Delta n = \pm 1 (n_v \rightarrow n_c; 1(2) \rightarrow 2(1))$, is larger than the energy gap $\Delta E_g = 0.11t_0$. The transition between the highest occupied subband ($n_v = 1$) and the lowest unoccupied subband ($n_c = 1$) is forbidden.
Figure 5. (Color online) Band structures of 54-ASiNR (a) with and (b) without the in-plane magnetic field. The insets zoom in on the region near the Dirac points. (c) Optical conductivity versus light frequency in different cases. The arrows in (a) and (b) denote the first absorption peak and shoulder in (c), respectively.

Figure 5 exhibits the bandstructures and the optical conductivities for a semiconducting 54-ASiRN with physical width $W = 10.4$ nm. In figure 5(a), it is seen that a tiny gap about $0.015t_0$ for the free 54-ASiRN is opened by the weak coupling between edge states localized at opposite edges. One can infer that the gap of the edge states approaches to zero as the ASiRN gets wider. The absorption peak $A_1$ near the long wave limit, as illustrated in figure 5(c), is the signature of the existence of the edge states with the tiny gap. As the in-plane magnetic field is applied in the 54-ASiNRs, the gap of the edge states is close to zero. Actually it is about $0.002t_0$, as shown in the inset of figure 5(b). Consequently, one can see a wide shoulder $B_2$ extended from $0.15t_0$ to $0.25t_0$ in figure 5(c), which is attributed to the transitions between the edge and bulk states.

We also calculate the bandstructures and optical conductivities for the metallic 14-ASiRN and 53-ASiRN (not shown here). It is found that the absorption spectrum for the 14-ASiRN is almost unaffected by the in-plane magnetic field, although the energy bands are split. However, the absorption spectrum for the 53-ASiRN in the Zeeman field is similar to that for the 54-ASiRN, since the effect of the hybridization between the edge states at opposite boundaries in the wide ASiRRs is faint. We could infer that the edge states for the wide enough ASiRRs remain gapless if even the in-plane magnetic field is applied. This is quite distinct from the result for the ZSiRNs. Indeed, we can analytically obtain the dispersion of the gapless edge states for a semi-infinite silicene sheet with an armchair edge along the $x$ direction. Considering the effective Hamiltonian near the K points for a silicene sheet under an in-plane magnetic field, and using the approach proposed in the previous works [14,32], one can derive an approximate dispersion for the gapless edge states: $\epsilon = \pm \hbar v_F t_0 \lambda_{sp} k_x \sqrt{\lambda_m^2 + \lambda_{so}^2}$, where $v_F = \sqrt{3} t_0 a / 2$ is the bare Fermi velocity in the freestanding silicene sheet. It is concluded that the effect of the in-plane Zeeman field on the edge states at the
armchair edges is to decrease their velocities but not open a gap.

4. Conclusion
We have investigated the bandstructures and optical conductivities for SiNRs including both zigzag and armchair types in the presence of an in-plane magnetic field. It is found that the Zeeman field induces a gap of the edge states for the ZSiNRs, but decreases the gap for the ASiNRs. We infer that the gapless edge states in the wide ASiNRs are robust to the in-plane magnetic field, but the ones in the ZSiNRs are not. Furthermore, the absorption spectrum becomes richer and remarkably depends on the edge types and the width of the SiNRs. Some particular absorption peaks are attributed to the transitions involving the edge states. The fundamental difference of the effects of the in-plane magnetic field on the topological edge states in the zigzag and armchair SiNRs could be identified by the optical absorption measurement in experiments. We expect that our research is useful for designing the Si-based optoelectronic nanodevices in the future.

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