Valley polarization in silicene induced by circularly-polarized resonance light

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In the presence of circularly-polarized resonance light, silicene develops dynamical band gaps in its quasi-energy band structure. Using numerical calculations, our results show that the gap appearing at \( h\omega/2 \), where \( h\omega \) is the photon energy. More importantly, we find that these gaps are non-symmetric for two inequivalent valleys. Therefore we can introduce light-controlled valley polarization in these dynamical band gaps. Different valleytronic devices can be realized using this technique.

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I. INTRODUCTION

Silicene is a promising material which consists of a honeycomb lattice of silicon atoms with buckled sublattices made of A and B sites as shown in Fig. 1(a). It has been synthesized recently and has attracted much attention. The states near the Fermi energy are \( \pi \) orbitals residing near the K and K’ valleys at opposite corners of the hexagonal Brillouin zone which is shown in Fig. 1(b). Because of the large separation in the momentum space of two valleys, inter-valley scattering is strongly suppressed when the sharp potential changes in distances of atomic order are absent.[1,2] This suggests a potential usage of the degree of freedom of valley index as a quantum identification of electron states, similar to the role of the spin degree of freedom in spintronics. For intrinsic silicene, these two valleys are degenerate, and the electronic quantities of silicene, such as the conductance, are usually twice the contributions from one valley due to the valley degeneracy. Valley polarization can only be entailed by applying external manipulations.[3-10]

A powerful method to modulate a band structure is to apply a coherent laser beam into the system. It has been proven to be very critical for topological phase transitions in the context of 2D[11,12] and 3D[13] systems. However, most of these proposals are focused on the change of the band gaps at the K and K’ points. It requires a very strong off-resonant light which might actually damage the material. In this paper, we have focused on the on-resonant region where the direct absorption of photons are allowed as shown in Fig. 1(c) and (d). In this region, when we increase the strength of the light, the biggest modulation of the band structure first appears at the resonance circle instead of the K/K’ points and the strength needed in on-resonance case is much less than in the off-resonance case.

In this paper, we use the Floquet theorem to calculate the band structure of the silicene manipulated by the on-resonance light. We find that on the resonance circle, dynamical gaps are opened for both K and K’ valleys. However, due to the intrinsic spin-orbital coupling, the dynamical gaps are non-symmetric for two inequivalent valleys. Within the dynamical gaps, we can define valley polarization if the fermi level only cross one valley whether in the valence band or the conduction band.

II. EFFECTIVE MODEL UNDER THE APPLICATION OF RESONANT PERTURBATION

The irradiating field is represented as a time-dependent vector potential which will modify the momentum via Peierl’s substitution \( \mathbf{\hat{P}} \rightarrow \mathbf{\hat{P}} + e \mathbf{A} \), where \( e > 0 \) is the magnitude of the electron charge and the vector potential can be written as \( \mathbf{A}(t) = [A_x(t), A_y(t)] \). The Hamiltonian of irradiated silicene is then given by

\[
H(t) = V_F \left( \tau (p_x - eA_x)\sigma_x + (p_y - eA_y)\sigma_y + \lambda \tau \sigma_z \right) + H_f
\]

(1)

instead of the static Hamiltonian given in reference [3,4,16], where \( \lambda = 3.9meV \) is the spin-orbit splitting term, \( V_f \approx 5 \times 10^5 m/s \) is the Fermi velocity and \( p_x, p_y \) are the components of the momentum relative to the K/K’ point. \( \sigma_i, (i = x, y, z) \) are Pauli matrixes for the two sublattices. And \( \tau = \text{sign}(t) \) is the valley index represents valley K (K’). The Rashba SOC is omitted since it is a factor of 10 smaller than the intrinsic SOC[3].

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FIG. 1: (a) and (b) show the basic structure of silicene in the real space and the momentum space. (c) shows the band structure of intrinsic silicene. If we apply a on-resonance light, direct photon absorption is allowed. (d) shows that the modulation of the band structure takes place on the resonance circle. We can see that dynamical gaps are opened on the resonance circle.

The information about the effect of the radiation is encoded in the time-dependent vector potential, such as the polarization of the light, the field strength and the radiation frequency. In the case of linearly polarized light, the vector potential can be written as $\mathbf{A} = A[\cos(\omega t), \sin(\omega t)]$, where $\theta$ is the angle of polarization in the plane of silicene and $\omega$ is the frequency. The strength of the vector is given by the parameter $A$. Furthermore, for the circularly polarized light, a phase difference between $A_x$ and $A_y$ is introduced $A = A[\cos(\omega t), \pm \sin(\omega t)]$ where the plus (minus) sign refers to right (left)-handed polarization.

Here we are only interested in the circularly polarized light and focus on the resonance region, i.e, $\hbar \omega > 2\lambda$. In this region, photon absorption take place on the resonance circles $E_{\pm}(k_0) = \pm \hbar \omega/2$ where $E_{\pm}(k)$ is the eigenvalue of the intrinsic silicene without radiation. When the strength of radiation is increased, dynamic gaps first appear on this resonance circles. It is well known that the coupling between the circularly polarized light and silicene is strongly valley dependent, spin-valley physics [4,7] are developing rapidly. In our case, we find that the values of dynamical gaps are also valley dependent. In the following, we will calculate the values of these gaps numerically using Floquet theorem, and we find that the gaps for different valley are quite asymmetric.

III. NUMERICAL RESULTS USING FLOQUET THEOREM

We employ the Floquet theorem[17] to solve the time-dependent problem numerically. The full time-dependent wave function $\Psi(k, t)$ as the product of a periodic function $\Phi(k, t)$ (with period $T = 2\pi/\omega$) and a time evolution factor

$$\Psi_k(x, t) = e^{-i\epsilon_k t} \Phi_k(x, t)$$  \hspace{1cm} (2)

where $\Phi(t + T) = \Phi(t)$. By defining the Floquet operator $F_k(t) = H_k(t) - i \hbar \frac{\partial}{\partial t}$, the Schrödinger equation can be written as $F_k(t)\Psi_k(x, t) = 0$. Substituting equation (2) into the Schrödinger equation yields $H_k(t)\Phi_k(x, t) - i\hbar \frac{\partial}{\partial t} \Phi_k(x, t) = \epsilon_k \Phi_k(x, t)$. The periodic wavefunctions $\Phi$ are called ‘Floquet states’, and $\epsilon_k$ is called the quasienergy.

In order to solve the Schrödinger equation for $\epsilon_k$ and $\Phi_k(x, t)$, the expanded Hilbert space $\mathcal{R} \otimes \mathcal{T}$ of squareintegrable function of space and function of time with period $T$ is needed. In this space, the inner product is defined as the usual spatial inner product with the average over one period:

$$\langle\langle n|m \rangle\rangle = \frac{1}{T} \int_0^T \langle n|m \rangle dt$$  \hspace{1cm} (3)

where $n$ and $m$ represent states in $\mathcal{R} \otimes \mathcal{T}$ [17]. Hence the wavefunction $\Phi$ satisfy that

$$\langle\langle \Phi_{\alpha}(t)|\Phi_{\beta}(t) \rangle\rangle = \delta_{\alpha \beta}$$  \hspace{1cm} (4)
FIG. 2: We use the left circularly polarized light and set $\hbar \omega = 10 \text{meV}$ and $V_F e A = 1 \text{meV}$. In Fig.(a) we can see that isotropic dynamical gaps are opened at $E = \hbar \omega/2$ and the magnitude of the gaps are asymmetric for two different valleys. In Fig.(b) we compare the difference of the two gaps and find that in our case the gap opened in K valley is a little smaller than the gap opened in K' valley.

Since the functions $\Phi(k, t)$ are periodic, one can expand $\Phi(k, t)$ with the complete set of eigenfunctions ($\phi$) of the non-radiative Hamiltonian,

$$\Phi_{\alpha}(x, t) = \sum_{\gamma} \sum_{n=\infty}^{\infty} B_{\alpha, \gamma, n} \phi_{\gamma}(x) e^{j\omega t}$$

where $\alpha$ labels the Floquet state and $\gamma$ labels the eigenstates of Hamiltonian $H(k)$. $B$ is the expanding coefficients. The perturbation term does not couple states with different momenta, therefore the momentum is still a good quantum number in the Floquet states. The details of the derivation is discussed in appendix A.

In the numerical calculation, we use a left-circularly-polarized light and we set $\hbar \omega = 10 \text{meV}$ and $V_F e A = 1 \text{meV}$. In Fig. 2(a), we have drawn the 3-dimension dispersion relationship in the vicinity of both K and K’ valley. We can intuitively see that the left circularly-polarized light has opened isotropic gaps at $E = \hbar \omega/2$ in both valleys, however, the magnitude of the gaps are different for K and K’ valleys. In our case, the gap opened in K valley is larger than the gap in K’ valley. If we use a right circularly-polarized light, the conclusion is reversed. In Fig. 2(b), we compare the gap difference more specifically. The gap opened in K valley is about 0.8 meV while the gap in K’ valley is about 1.2 meV. If the fermi energy is higher than 5.4 meV and lower than 5.6 meV (or higher than 4.4 meV and lower than 4.6 meV ), the conducting electrons are only contributed by K valley. In such case we can say that the current is valley polarized.

In Fig. 3, we increase the strength of the polarized light to $V_F e A = 4 \text{meV}$ and we can see that the magnitude of the gaps opened on the resonance circle are also increased. Moreover, the asymmetry of different valleys become much clearer. In Fig. 3(b), we show that the gap opened in K valley is about 2.4 meV while the gap in K’ valley is about 3.8 meV. We can define valley polarization if the fermi energy is higher than 6.1 meV and lower than 6.8 meV (or higher than 3.2 meV and lower than 3.9 meV ). The conducting electrons are only contributed by K valley.

IV. SUMMARIES

In this paper, we have numerically calculated the Floquet band structure of silicene manipulated by the on-resonance light. We find that on the resonance circle, dynamical gaps are asymmetric for K and K’ valleys. Hence, we can define valley polarization.
FIG. 3: We use the left circularly polarized light and set $h\omega = 10\text{meV}$ and $V_F eA = 4\text{meV}$. In Fig.(a) we can see that the isotropic gaps are clearly bigger than the $V_F eA = 1\text{meV}$ case. In Fig.(b) we show that the gap difference between two valleys are also increase.

if Fermi level only penetrate one valley. If the light is left circularly-polarized, we can define $K$ valley polarized current; if the light is right circularly-polarized, we can define $K'$ valley polarized current. We can tune the valley polarization by changing the chirality of the light. Moreover, the advantage of this method is that the frequency of the light is much lower than the off-resonance light. One can safely increase the intensity of the light without burning the material.

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APPENDIX A:

We shall begin with the Schrödinger equation

$$H_k(t)\Phi_k(x, t) - \frac{i\hbar}{\hbar} \frac{\partial}{\partial t} \Phi_k(x, t) = \varepsilon_k \Phi_k(x, t)$$

(A1)

Substituting the expansion (5) into Schrödinger equation, we get

$$\sum_{\gamma} \sum_{n} (H_k - i\hbar \frac{\partial}{\partial t}) B_{k,n}^{\gamma} \varphi_k(x) e^{im\omega t} = \sum_{\gamma} \sum_{n} \varepsilon_n B_{k,n}^{\gamma} \varphi_k(x) e^{im\omega t}$$

(A2)

Multiply equation (A2) with $\varphi_k^{\gamma*}(x) e^{-im\omega t}$ from the left, and after a time-average over one period of driving $T$. Since in terms of the kets $|\varphi_k\rangle$, $\langle x|\varphi_k\rangle = \varphi_k(x)$, the Schrödinger equation becomes

$$\sum_{\gamma} \sum_{n} \langle \varphi_k^{\gamma*} | H_k^{m,n} + \hbar \omega \delta_{mn} | \varphi_k \rangle B_{k,n}^{\gamma} e^{im\omega t} = \varepsilon_n B_{k,n}^{\gamma}$$

(A3)

with definition

$$H_k^{m,n} = \frac{1}{T} \int_0^T dt e^{-i(m-n)\omega t} H_k(t)$$

$$H_k^{m,n}(k) = H_k^{m,n} + \hbar \omega \delta_{mn}$$

(A4)
Hence, the matrix form of the Schrödinger equation (A3) has a block-triangular structure with only the number of angular frequencies $\omega$ in the diagonal varying from block to block. And the quasienergies $\varepsilon_\alpha$ can be obtained as the eigenvalues of the secular equation

$$det[H_F(k) - \varepsilon 1] = 0$$

(A5)

Although the summation over $n$ in Eqn. (A3) is from $-\infty$ to $\infty$, in real calculation, we only need to truncate the matrix $H_F(k)$ into finite dimension, the bigger the dimension of the matrix, the more accurate results one would gets.

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