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Discussion

Topologically trivial and nontrivial edge bands in graphene induced by irradiation

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ABSTRACT

We proposed a minimal model to describe the Floquet band structure of two-dimensional materials with light-induced resonant inter-band transition. We applied it to graphene to study the band features caused by the light irradiation. Linearly polarized light induces pseudo gaps (gaps are functions of wavevector), and circularly polarized light causes real gaps on the quasi-energy spectrum. If the polarization of light is linear and along the longitudinal direction of zigzag ribbons, flat edge bands appear in the pseudo gaps, and if it is in the lateral direction of armchair ribbons, curved edge bands can be found. For the circularly polarized cases, edge bands arise and intersect in the gaps of both types of ribbons. The edge bands induced by the circularly polarized light are helical and those by linearly polarized light are topologically trivial ones. The Chern number of the Floquet band, which reflects the number of pairs of helical edge bands in graphene ribbons, can be reduced into the winding number at resonance.

1. Introduction

Graphene has drawn much attention since it was discovered in the laboratory [1,2]. Graphene has a number of interesting physical properties and has a great potential for application. Pristine graphene is a gapless Dirac material, while the energy gap is needed for the fabrication of switching devices. There are a few causes, such as staggered substrate influence [3–5] and the spin–orbit coupling [6–8], to open a gap on the spectrum of graphene. The latter is more attractive because it makes graphene a topologic insulator and leads to helical edge bands which are topologically protected by the time-reversal symmetry [6]. However, the spin–orbit coupling in graphene is proven to be too weak to detect [2]. Recent researches implied that the time dependent driving may have the similar effects as the spin–orbit coupling in graphene: it generates gaps and turns a normal material into a special topologic insulator called Floquet topologic insulator [9–13]. Besides in condensed matters, the interest of the novel effects of driving is increasing in cold atoms [14–17] and other fields. Recently, the Floquet topologic phase was realized in a photonic crystal [18], which indicated the validity of the theoretical prediction. Light irradiation is an important periodically driving source, and the irradiation induced energy gaps in a topological insulator were observed recently [19]. These experiments provide the probability to generate gaps and change the topologic property of graphene by light irradiation [20–23].

Light irradiation generates energy gaps in graphene by two mechanisms. First, under the affection of light, the electron near the Dirac point emits a photon and re-absorbs it to renormalize the band structure, and a gap is generated at the Dirac point to separate the conduction and valence bands [24–27], which is the effect of second order perturbation. Second, light induces resonant transition between conduction band and valence band states, and produces dynamic gaps on the quasi-energy spectrum at $E = \pm\hbar\omega/2$, where ω is the angular frequency of light [28–31]. The latter is more attractive because it is a first order process.

Typically, periodically driven system is treated in frequency space [32–34], also called Floquet space. The whole space is divided into infinite subspaces according to the number of photons absorbed and emitted. The system is solved by truncating the Floquet space at a finite dimension. For the weak driven cases, the main physics is determined by the one-photon processes that can be well understood. It is possible to develop a short theory to handle the driven system by only taking the one-photon processes into account. The theory should simplify the calculation, reproduce the results of other more complicated methods, and more importantly, give more insight on the physics of driven systems.

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In this paper, we proposed a minimal model to describe the Floquet band structure of two-dimensional materials with light-induced resonant inter-band transition and applied the theory to graphene. Linearly polarized light induces pseudo gaps, and circular polarized light causes real gaps on the Floquet quasi-energy spectrum of graphene. For the circular polarization cases, edge bands arise in the gaps and intersect for both zigzag and armchair ribbons. Interestingly, linear polarized illumination can also lead to edge bands, depending on the type of ribbon and the polarization orientation. If the polarization is longitudinal along zigzag ribbons, flat edge bands appear in the pseudo gaps, and if it is in the lateral direction of armchair ribbons, curved edge bands arise. The topologic property of the Floquet bands is reflected by the Chern number, and we found it can be reduced into the winding number at resonance. The edge bands induced by the circular polarized light are helical and those by linear polarized light are topologically trivial ones.

2. Floquet theory of inter-band optic transition

We consider a two-band system consisting of one conduction band and one valence band. When a laser normally irradiates on the graphene sheet, a time-dependent vector potential $\boldsymbol{\mathcal{A}}(t) = \boldsymbol{A}\cos\omega t$ is introduced, where $\boldsymbol{A}$ is the amplitude vector of $\boldsymbol{\mathcal{A}}$, ω is the angular frequency, and t is the time. If the system is weakly perturbed, in the frame of $A\cdot p$ approximation, the time-dependent Hamiltonian reads

$$H_0(t) = H_{\boldsymbol{k}} - \boldsymbol{\mathcal{A}}(t)\cdot\boldsymbol{p}, \tag{1}$$

where $H_{\boldsymbol{k}}$ is the Hamiltonian without light irradiating, and $\boldsymbol{p}$ is the momentum operator. The eigenvalues of $H_{\boldsymbol{k}}$ are the conduction and valence band energies denoted by ϵ_c and ϵ_v, and the corresponding eigenstates are $|c\rangle$ and $|v\rangle$, respectively. In Eq. (1), the electron charge e and the electron effective mass m are set to be 1. In basis of $|c\rangle$ and $|v\rangle$, the time-dependent Hamiltonian (rotating wave approximate is used) can be written as

$$H(t) = \begin{pmatrix} \epsilon_c & \frac{1}{2}g^* e^{-i\omega t} \\ \frac{1}{2}g e^{i\omega t} & \epsilon_v \end{pmatrix}, \tag{2}$$

where g is the transition element defined by

$$g = -\boldsymbol{A}\cdot\langle v|\,\boldsymbol{p}\,|c\rangle. \tag{3}$$

The time-dependent Schrödinger equation $i\partial_t\psi = H(t)\psi$, in which the $\hbar$ is set to be 1, can be reduced into a static one $\mathcal{H}\psi = E\psi$ by introducing the unitary transformation

$$U = \begin{pmatrix} e^{-i(\epsilon_c-\delta/2)t} & 0 \\ 0 & e^{-i(\epsilon_v+\delta/2)t} \end{pmatrix}, \tag{4}$$

where $\delta = (\epsilon_c - \epsilon_v) - \omega$ is the detune. The static Hamiltonian is obtained by

$$\mathcal{H} = UHU^+ + iU\frac{\partial U^+}{\partial t} = \frac{1}{2}\begin{pmatrix} \delta & g^* \\ g & -\delta \end{pmatrix}. \tag{5}$$

Solving the eigen-problem of the static Hamiltonian, we have the eigen-pairs

$$E_\pm = \pm\frac{1}{2}D, \quad \psi_\pm = \frac{1}{\sqrt{2}}\begin{pmatrix} \sqrt{|\pm 1+\delta/D|} \\ \pm e^{i\theta}\sqrt{|\pm 1-\delta/D|} \end{pmatrix}, \tag{6}$$

where $D = \sqrt{|g|^2+\delta^2}$ and $\theta = \arg(g)$ is the complex angle. Go back to the basis of $|c\rangle$ and $|v\rangle$, and we have the quantum states satisfying the time-dependent Schrödinger equation for $H(t)$,

$$U\psi_\pm e^{-iE_\pm t}. \tag{7}$$

According to the Floquet theorem, the solutions of time-dependent Schrödinger equation for periodic time-dependent Hamiltonian must be of the form $\psi = e^{-iE^F t}\psi^F$, where E^F is time independent and ψ^F is of the same period as $H(t)$. The quantities E^F and ψ^F are called as Floquet energy and Floquet state respectively, which are the solution pair of the Floquet equation $H^F\psi^F = E^F\psi^F$, where $H^F = H(t) - i\partial_t$ is the Floquet operator. One can verify that, if E^F and ψ^F satisfy the Floquet equation, $E^F + n\omega$ and $\psi^F e^{in\omega t}$ for arbitrary integer n are also a Floquet pair. To eliminate the non-uniqueness, we choose proper n so that the Floquet energies are recovered to the conduction and valence band energies for infinitesimal weak driven intensity. After doing so, we have the Floquet energies

$$E^F_\pm = \frac{1}{2}(\epsilon_c+\epsilon_v) \pm \frac{1}{2}(\eta D + \omega), \tag{8}$$

where η is the sign of δ. The corresponding Floquet states are

$$\begin{aligned} \psi^F_+ &= a_F|c\rangle + b_F|v\rangle e^{i\omega t}, \\ \psi^F_- &= b^*_F|c\rangle e^{-i\omega t} - a_F|v\rangle, \end{aligned} \tag{9}$$

where the coefficients a_F and b_F are defined as

$$a_F = \frac{1}{\sqrt{2}}\sqrt{1+\left|\frac{\delta}{D}\right|}, \quad b_F = e^{i\theta}\frac{\eta}{\sqrt{2}}\sqrt{1-\left|\frac{\delta}{D}\right|}. \tag{10}$$

In Eqs. (8) and (9), when we set $g\to 0$, the Floquet energies $E^F_\pm$ are reduced into ϵ_c and ϵ_v, and Floquet states $\psi^F_\pm$ are recovered to $|c\rangle$ and $|v\rangle$, respectively.

The above derivations are based on linearly polarized irradiation, but also valid for circular polarization by regarding the vector potential amplitude $\boldsymbol{A}$ as a complex quantity. The irradiation has two known effects. (1) It generates resonant gaps on the Floquet spectrum. (2) It can change the topologic property of band structure and create new edge bands, depending on the polarization of irradiation. In the following, we will apply the above theory to graphene and investigate how the two effects act on graphene.

3. Resonant gaps of bulk graphene

There are two non-equivalent valleys in graphene. The low-energy Hamiltonian of valley K reads

$$H_{\boldsymbol{k}} = \boldsymbol{\sigma}\cdot\boldsymbol{k} = \begin{pmatrix} 0 & k_x - ik_y \\ k_x + ik_y & 0 \end{pmatrix}, \tag{11}$$

where $\boldsymbol{\sigma} = (\sigma_x, \sigma_y)$ is the Pauli matrix set, $\boldsymbol{k} = (k_x, k_y)$ is the wavevector, and the Fermi velocity v_F is set to be 1. The band energies and band states are

$$\epsilon_{c/v} = \pm k, \quad |c,v\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \pm e^{i\varphi} \end{pmatrix}, \tag{12}$$

where $k = (k_x^2+k_y^2)^{1/2}$ and $\varphi = \arg(k_x + ik_y)$ reflect the amplitude and orientation of $\boldsymbol{k}$. When the graphene is under illumination, the Peierls substitution $\boldsymbol{k}\to\boldsymbol{k}-\boldsymbol{\mathcal{A}}$ should be applied, and this leads to $H_{\boldsymbol{k}}$ which is replaced with $H_{\boldsymbol{k}} - \boldsymbol{\sigma}\cdot\boldsymbol{\mathcal{A}}$. Because the momentum is defined by $\boldsymbol{p} = \nabla_{\boldsymbol{k}}H_{\boldsymbol{k}} = \boldsymbol{\sigma}$, we have substitution Hamiltonian $H_{\boldsymbol{k}} - \boldsymbol{\mathcal{A}}\cdot\boldsymbol{p}$, which is just the Hamiltonian in Eq. (1) [35]. So, the $A\cdot P$ approximation can also be applied to graphene [35], and the detailed discussion about this can be found in the Appendix. According to Eq. (3), the transition element is calculated as

$$g = i\,(A_x\sin\varphi - A_y\cos\varphi), \tag{13}$$