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Transport and optical phenomena in two-dimensional Dirac semimetals

G. R. Rakhmanova [1]✉, D. D. Sedov [1], I. V. Iorsh [1]

[1] School of Physics and Engineering, ITMO University, Saint Petersburg, Russia

✉ gulnaz.rahmanova@metalab.ifmo.ru

Abstract. The discovery of graphene with Dirac cones at the Fermi energy attracted intense interest in the field of two-dimensional materials. However, in many two-dimensional materials, including graphene, Dirac points are gapped by spin-orbit coupling. Here we consider two-dimensional Dirac semimetals which have Dirac-like band dispersion in the presence of spin-orbit coupling protected by nonsymmorphic lattice symmetry. This is of interest because it opens a richer spectrum of optical properties than other topological materials. We choose the model of nonsymmorphic Dirac semimetal α-bismuthine containing anisotropic Dirac cones. We calculated interband and intra-band linear optical conductivity within the formalism based on the density matrix approach and Kubo formula. We show that electronic state in conductance band supports plasmons with quasi-linear anisotropic dispersion. The difference in the interband absorption spectrum can only be observed for electronic states on the Femi surface and a width equal to the plasmon energy. The results suggest that such Dirac semimetals can be promising material for studying nonlinear optical properties.

Keywords: Dirac semimetal, plasmon, conductivity, linear response

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Материалы конференции
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Транспортные и оптические свойства двумерных материалов с дираковским спектром носителей заряда

Г. Р. Рахманова [1]✉, Д. Д. Седов [1], И. В. Иорш [1]

[1] Физико-технический мегафакультет, Университет ИТМО, Санкт-Петербург, Россия

✉ gulnaz.rahmanova@metalab.ifmo.ru

Аннотация. Были изучены транспортные и оптические свойства двумерных (2D) полуметаллов Дирака. Исследован пример α-висмутена как 2D несимморфного полуметала, содержащий анизотропные конусы Дирака, с различными скоростями Ферми вдоль направлений x и y. С помощью формализма Кубо были рассчитаны линейная внутризонная и межзонная проводимости. Было показано, что электронные состояния поддерживают 2D плазмоны с анизотропной квазилинейной дисперсией. Результаты позволяют предположить, что 2D полуметаллы Дирака несут в себе потенциал для усиленных квадратичных оптических откликов.

Ключевые слова: полуметаллы Дирака, проводимость, плазмоны, линейный отклик

Финансирование: Численные расчеты выполнены при финансовой поддержке гранта НИРМА ФТ МФ Университета ИТМО. Аналитические расчеты выполнены при финансовой поддержке Фонда развития теоретической физики и математики «БАЗИС» (№ 21-1-5-17-1).

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Introduction

The discovery of graphene with Dirac cones at the Fermi energy attracted intense interest in the field of two-dimensional (2D) materials [1]. However, Dirac points in many 2D materials, including graphene, are vulnerable to spin-orbit coupling (SOC) [2]. Recently, 2D Dirac semimetals with a nonsymmorphic symmetry has been predicted to have Dirac points not gapping by SOC [3]. Despite the long-term discovery of similar three-dimensional SOC-resistant Dirac points in several bulk materials [4], the search for realistic 2D materials that possess Dirac points at low energy remains a challenge. The article [5] discloses a family of monolayer materials of the HfGeTe as the first example of materials that support Dirac fermions robust against SOC close to the Fermi level. In [6] was shown the existence of 2D Dirac fermions in a chemically modified group-VA 2D puckered structure. In the presence of SOC Dirac nodal lines split and form an hourglass-shaped dispersion protected by a nonsymmorphic symmetry. These discoveries open the door to the study of 2D nonsymmorphic Dirac semimetal which may provide a richer spectrum of optical properties than other topological materials.

Dirac-like band dispersions have recently been described in the nonsymmorphic monolayer film, α-bismuthene (α-Bi) [7]. It is centrosymmetric and nonmagnetic material, so the time-reversal and inversion symmetries are preserved. In addition, the lattice is invariant under a glide mirror reflection that leads to protected Dirac points at the high symmetry momentum points of the Brillouin zone. In [8] theoretical analysis of the photon absorption spectrum for the model of α-Bi was investigated. In the absence of a magnetic field, the absorption coefficient is very similar to the absorption coefficient of graphene in that it is independent of frequency. In this paper, we will explore the new properties that nonsymmorphic symmetry brings to the optical conductivity.

Materials and Methods

Consider a quantum system described by the time independent Hamiltonian H_0 in equilibrium. Its eigenenergies are E_n and eigenstates are $|n\rangle$. Suppose now that a weak external perturbation is applied to the system at some time, $t = t_0$, in such a way that the Hamiltonian of the system is now written in the form:

$$\hat{H}(t) = \hat{H}_0 + \theta\left(t - t_0\right)\hat{V}(t) \tag{1}$$

Linear conductivity can be obtained within the formalism based on the density matrix approach, where the average current is given by:

$$\left\langle J(t)\right\rangle = \mathrm{Tr}\left[J\rho(t)\right] = \sum\nolimits_n \frac{e^{-\beta E_n}}{z}\left\langle n(t)\middle|\hat{J}(t)\middle|n(t)\right\rangle, \tag{2}$$

where J is the current operator, $\rho(t)$ is the density matrix operator, E_n and $|n(t)\rangle$ are the eigenvalues and eigenfunctions written in the interaction picture, respectively. The time-dependent eigenstates in the interaction picture are $\left|n(t)\right\rangle = \exp\left(-i/\hbar\int^t dt'\hat{V}(t')\right)\left|n\right\rangle, A$ the interaction term is given by $\hat{V}(t) = J(t,r)A(t,r'), A$ is the vector potential of the perturbing field.

The current operator is introduced as $J = \frac{\partial H}{\partial A}$. The coupling to electromagnetic field is introduced via the gauge transform $k \to k - eA$.

The linear response of the current density j to the electric field E is defined in the frequency domain by

$$j(r,\omega) = \int d^3 r' \sigma(r, r', \omega) E(r', \omega) \tag{3}$$

where σ(r, r', ω) is the conductivity tensor. The corresponding Fourier transform can be taken in order to express the conductivity tensor in the representation σ(q, ω), where q is the wave vector.

Results and Discussion

1. Model

We choose the model of nonsymmorphic Dirac semimetal α-Bi containing anisotropic Dirac cones with different Fermi velocities along the x and y - directions that described by the Hamiltonian in the form [8]:

$$\hat{H} = \nu_x k_x \left(\sigma_x \cos\alpha + \sigma_y \sin\alpha\right) + \nu_y k_y \sigma_z \tag{4}$$

where σ_i are Pauli matrices for the spin degree of freedom, $\nu_y = \nu$ and $\nu_x = \rho\nu$. The anisotropy factor ρ refers to the mismatch in the Fermi velocity along x and y-direction. The angle α is the “mixing angle”, which is an intrinsic parameter of the model.

The eigenvalues are:

$$E = \pm\nu\sqrt{\rho^2 k_x^2 + k_y^2} \tag{5}$$

2. Linear Conductivity

We shall assume that $T \to 0$ and wave vector of plasmons is much smaller than Fermi wave vector.

We calculated x and y – components of the average current using the formula (2) and find the expression for conductivity through the formula (3).

Analytical solution for intra-band absorption coefficient in conductance band is given by:

$$\mathrm{Re}\left(\sigma_x\left(w, \tilde{q}\right)\right) = \frac{\alpha c}{\rho^2} \frac{2k_F \omega^2}{\nu q^2} \frac{1}{\sqrt{\nu^2 \tilde{q}^2 - \omega^{2'}}} \tag{6}$$

where $\alpha = e^2 / \hbar c$ standing for the fine structure constant and $\tilde{q} = \sqrt{\rho^2 q_x^2 + q_y^2}$.

The result of eq. (6) describes 2D plasmons with anisotropic quasi-linear dispersion $\omega = \nu\tilde{q}$. Such plasmons are characterized by extremely long lifetimes. The (Fig. 1, *a*) shows the isofrequency diagram of absorption in the space of a quasi-wave vector in a 2D semimetal with a finite relaxation time, where it can be seen that the plasmons has an anisotropic dispersion. The Figure 1 (*b*) shows that plasmons have quasi-linear dispersion.

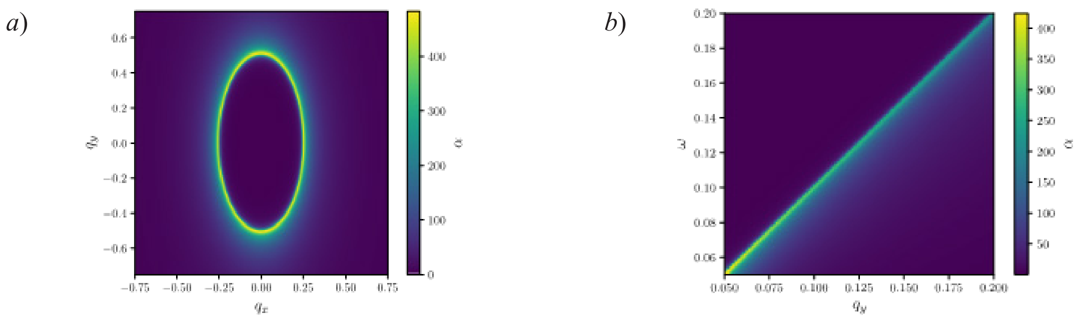

Fig. 1. The isofrequency diagram of absorption in the space of a quasi-wave vector in a 2D semimetal with a finite relaxation time (*a*). Absorption diagram in q,ω-space for q_x=0 (*b*)

Consider the interband conductivity. At zero temperature, plasmons, the collective oscillations of electrons, can only be excited at the Fermi surface. Therefore, the difference in the interband absorption spectrum can only be in the electronic states with the wave vector k_F. In terms of energy, the width of this region will be $2\nu q$, because it cannot be greater than the energy of the plasmon due to the conservation of energy and momentum. For electronic states with wave vector bigger than k_F the interband absorption coefficient is frequency-independent as in graphene:

$$\mathrm{Re}\left(\sigma_x\right)=\frac{\pi\alpha\nu c}{2\rho^2}. \tag{7}$$

Conclusion

In conclusion, we demonstrate that 2D Dirac semimetals with nonsymmorphic symmetry have Dirac-like band dispersion in the presence of spin-orbit coupling that provides richer spectrum of optical properties. The electronic states in conductance band supports plasmons with quasi-linear anisotropic dispersion. The difference in the interband absorption spectrum can only be observed for electronic states on the Fermi surface and a width equal to the plasmon energy. These results suggest that 2D nonsymmorphic Dirac semimetals can be promising material for studying nonlinear optical properties. Also, such materials can be promising for tunable magneto-optical devices.

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THE AUTHORS

RAKHMANOVA Gulnaz R.
gulnaz.rahmanova@metalab.ifmo.ru
ORCID: 0000-0001-8750-4065

IORSH Ivan V.
i.iorsh@metalab.ifmo.ru
ORCID: 0000-0003-4992-6122

SEDOV Denis D.
denis.sedov@metalab.ifmo.ru
ORCID: 0000-0002-7241-7572

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