PAPER

Highly anisotropic physics in phosphorene

To cite this article: Motohiko Ezawa 2015 J. Phys.: Conf. Ser. 603 012006

View the article online for updates and enhancements.

You may also like

- <u>Two-dimensional electron bound hole</u> <u>photoluminescence in GaAs in</u> <u>perpendicular magnetic fields</u> J Schuster, T Y Kim, E Batke et al.
- Quantum Hall effects in graphene-based two-dimensional electron systems Yafis Barlas, Kun Yang and A H MacDonald
- Exchange effect and magneto-plasmon mode dispersion in an anisotropic twodimensional electronic system Xiaoguang Wu and





DISCOVER how sustainability intersects with electrochemistry & solid state science research



This content was downloaded from IP address 3.128.94.171 on 07/05/2024 at 20:30

Highly anisotropic physics in phosphorene

Motohiko Ezawa

Department of Applied Physics, University of Tokyo, Hongo 7-3-1, 113-8656, Japan

E-mail: ezawa@ap.t.u-tokyo.ac.jp

Abstract. Phosphorene, monolayer black phosphorus, is a highly anistropic material, where the band structure is Dirac like in one direction and Schrödinger like in the other direction. We present several analytic formulas to demonstrate the electronic properties. The conductance is highly anisotropic reflecting the anisotropy of the band structure. We also detemine the cyclotron motion in phosphorene and Landau level quantization by using the Bohr-Sommerfeld quantization. We show that the Landau-level energy behaves as $B^{2/3}$ as a function of external magnetic field, which is highly contrasted to the case of graphene where the Landau-level energy behaves as \sqrt{B} .

1. Introduction

Monolayer materials are one of the most active fields in condensed matter physics. Graphene, a monolayer carbon atom system, has various fascinating physics since its low-energy band structure is described by the Dirac theory[1]. The success in graphene excites a further search of monolayer materials. Silicene, germanene and stanene, which are monolayers of silicon, germanium and tin, respectively, are among the most remarkable materials since they are expected to be topological insulators in nature[2]. Transition-metal dichalcogenides also attract much attention in the context of the valleytronics[3], which uses the valley degree of freedom.

Recently, phosphorene, monolayer black phosphorus, has been experimentally manufactured by exfoliation method, which has activated a rapid growth of experimental and theoretical studies[4]. Phosphorene is a direct-gap semiconductor with the gap in the region of visible light, which will be suitable for future applications to light-emitting diodes and solar cells. Field-effect transistor made of phosphorene has already been realized experimentally[5]. It is intriguing that the band structure in the low-energy theory is highly anisotropic, where the one direction is Dirac like and the other direction is Schrödinger like[6, 7, 8]. It differentiates the other monolayer materials, where the basic physics is described by the Dirac theory. Recent experiments show highly angle-dependent conductance[9].

In this paper, we investigate the electronic properties of phosphorene which arise from the highly anisotropic energy dispersion. We derive several analytic formulas on the conductivity and the cyclotron motion. We have derived the Landau level energy, which behaves $B^{2/3}$ as a function of external magnetic field. We also show the results on the case of the gapless limit since the physical quantity shows an extremely simple scaling relation due to the scale free structure of the band structure.

2. Hamiltonian

Phosphorene is a direct-gap semiconductor, where the gap exists at the Γ point. The low-energy Hamiltonian for phosphorene is given by the Hamiltonian[6, 7, 8],

$$H_{2D} = \left(uk_y^2 + m\right)\tau_x + v_{\rm F}k_x\tau_y,\tag{1}$$

Content from this work may be used under the terms of the Creative Commons Attribution 3.0 licence. Any further distribution of this work must maintain attribution to the author(s) and the title of the work, journal citation and DOI.

Published under licence by IOP Publishing Ltd

where τ is the Pauli matrices and m is the gap acting as the Dirac mass. The Hamiltonian is linear in the k_x direction, while parabolic in the k_y direction, which produce highly anisotropic physics. This Hamiltonian emerges quite in general when two Dirac cones with the opposite chiralities merge into one cone. It is originally discussed in highly strained graphene[10, 11, 12], where the transfer integral is different over 2 times along the x and y directions. However this scenario is unrealistic since we cannot realize such a strong anisotropy in graphene by applying strain. Later the mimic of this energy is realized in optical lattice[13], where the transfer integral can be tuned arbitrarily. Phosphorene is the first materialization of the Hamiltonian, where the lattice structure is highly anisotropic along the x and y directions, and called the puckered structure. The energy spectrum reads

$$\varepsilon = \pm \sqrt{v_{\rm F}^2 k_x^2 + \left(u k_y^2 + m\right)^2}.$$
(2)

The energy dispersion is Dirac like in the k_y direction, but Schrödinger like in the k_y direction. This anisotropy leads to a highly anisotropic physics in phosphorene such as conductance.

The DOS is given by

$$\rho\left(\mu\right) = \frac{4}{v_{\rm F}\sqrt{u}} \operatorname{Re}\left[i\frac{|\mu|}{\sqrt{|\mu|+m}} K\left(\frac{2\mu}{|\mu|+m}\right)\right],\tag{3}$$

where μ is the chemical potential, K(x) is the complete elliptic integrals of the first kind. In the massless limit, the DOS is given by

$$\lim_{m/\mu\to 0} \rho\left(\mu\right) = \frac{4}{v_{\rm F}\sqrt{u}} \operatorname{Re}\left[iK\left(2\right)\right] \sqrt{|\mu|}.\tag{4}$$

We show the DOS in Fig. 1 both in the massive and massless cases for comparison. It has a good agreement with the previous theoretical results based on the tight-binding Hamiltonian[14]. The DOS is exactly zero within the gap, while the DOS is finite at the band edge $|\mu| = m$. The DOS for the massive Hamiltonian approaches that of the massless Hamiltonian and behaves proportional to the square of the chemical potential for $|\mu| > m$.

The behavior is significantly different from the one in the massive Dirac system,

$$\rho(\mu) = \frac{4}{2\pi v^2} |\mu| \theta(|\mu| - m),$$
(5)

where the DOS is linear as a function of μ



Figure 1. (a) DOS $\rho(\mu)$ as a function of the chemichal potential μ . (b) $\langle v_x^2 \rangle$ and $\langle v_y^2 \rangle$ as a function of the chemical potential μ . (c) σ_{xx} and σ_{yy} as a function of the chemical potential μ . Magenta (Cyan) curves represent the value along the x (y) direction. Solid (dotted) curves represent the massive (massless) case.

3. Velocity

We calculate the average of the Fermi surface velocity defined by

$$\langle v_x v_y \rangle = \frac{\int v_x v_y \delta\left(\varepsilon - \mu\right) dk}{\int \delta\left(\varepsilon - \mu\right) dk},\tag{6}$$

where the velocity is given by differentiating the Hamiltonian with the corresponding momentum,

$$v_x = \frac{\partial \varepsilon}{\partial k_x} = \frac{v_F^2 k_x}{\varepsilon}, \qquad v_y = \frac{\partial \varepsilon}{\partial k_y} = \frac{2uk_y \left(uk_y^2 + m\right)}{\varepsilon}.$$
 (7)

Explicitly we have

$$\left\langle v_x^2 \right\rangle = \frac{2}{\rho\left(\mu\right)} \frac{4v_{\rm F}}{3\left|\mu\right|} \sqrt{\frac{\left|\mu\right| + m}{u}} \left[\left|\mu\right| K\left(\frac{m - \left|\mu\right|}{m + \left|\mu\right|}\right) - mE\left(\frac{m - \left|\mu\right|}{m + \left|\mu\right|}\right) \right],\tag{8}$$

where E(x) is the complete elliptic integrals of the second kind, and

$$\langle v_y^2 \rangle = \frac{2}{\rho(\mu)} \left[\frac{8\sqrt{u}\sqrt{m+|\mu|}}{15v_F|\mu|} \left[\left(9\mu^2 - 2m^2 \right) E\left(\frac{m-|\mu|}{m+|\mu|}\right) + \left(2m-9\,|\mu|\right)\sqrt{u}\sqrt{m+|\mu|}\mu K\left(\frac{m-|\mu|}{m+|\mu|}\right) \right].$$

$$(9)$$

Their massless limit reads

$$\lim_{m \to 0} \left\langle v_x^2 \right\rangle = \frac{2}{\rho(\mu)} \frac{4v_{\rm F}}{3} K(-1) \sqrt{|\mu|} \propto |\mu|^0, \tag{10}$$

and

$$\lim_{m \to 0} \left\langle v_y^2 \right\rangle = \frac{2}{\rho(\mu)} \frac{24}{5gv_F} \left[E\left(-1\right) - K\left(-1\right) \right] |\mu|^{3/2} \propto |\mu|.$$
(11)

Thus, $\lim_{m\to 0} \langle v_x^2 \rangle$ is independent of the chemical potential, while $\lim_{m\to 0} \langle v_y^2 \rangle$ is proportional to the absolute value of the chemical potential. We show the average of the velocity in Fig. 1(b). The velocity is highly anisotropic. This is highly contrasted to the case of graphene, where the average velocity $\langle v_x^2 \rangle = \langle v_y^2 \rangle$ is constant and has no anisotropy.

4. DC Conductivity

Recent experiments have observed a strongly anisotropic conducting behavior[9]. Anisotropic transport behavior along different directions is a unique property of phosphorene. We now derive the analytic results on the conductance as a function of the chemical potential. The DC conductivity is obtained by solving the Boltzmann equation. The semiclassical conductivity tensor is given by using the average of the Fermi surface velocity

$$\sigma_{\alpha\beta} = e^2 \int dk \tau v_{\alpha} v_{\beta} \left(-\frac{\partial f}{\partial \varepsilon} \right) = e^2 \tau \rho \left(\mu \right) \left\langle v_{\alpha} v_{\beta} \right\rangle, \tag{12}$$

where τ is the life time due to the scattering. By substituting the mean velocity, we have

$$\sigma_{xx} = 2e^2 \tau \frac{4v_{\rm F}}{3\,|\mu|} \sqrt{\frac{|\mu|+m}{u}} \left[\mu K \left(\frac{m-|\mu|}{m+|\mu|} \right) - m E \left(\frac{m-|\mu|}{m+|\mu|} \right) \right],\tag{13}$$

and

$$\sigma_{yy} = 2e^{2}\tau \frac{8\sqrt{u}\sqrt{m+|\mu|}}{15v_{\rm F}|\mu|} [\left(9\mu^{2}-2m^{2}\right)E\left(\frac{m-|\mu|}{m+|\mu|}\right) + (2m-9|\mu|)\sqrt{u}\sqrt{m+|\mu|}|\mu|K\left(\frac{m-|\mu|}{m+|\mu|}\right).$$
(14)

We show the conductance in Fig. 1(c). The conductance is highly anisotropic reflecting the anisotropy of the band structure. This is also highly contrasted with the case of graphene, where the conductance is isotropic and proportional to the chemical potential $\sigma \propto |\mu|$.

The Hall conductance σ_{xy} is zero since $\langle v_x v_y \rangle = 0$. We calculate the conductance along the general direction θ

$$\sigma_{\theta\theta} = e^2 \tau \rho \left(\mu \right) \left\langle (v_x \cos \theta + v_y \sin \theta)^2 \right\rangle = \sigma_{xx} \cos^2 \theta + \sigma_{yy} \sin^2 \theta.$$
(15)

The angle dependence of the conductance has a good agreement with the experimental results[9].

5. Cyclotron motion

To describe qualitatively the effect of weak magnetic field, we start with a simple semiclassical argument. Energy levels are quantized according to the Bohr-Sommerfeld quantization condition.

The equation of motion of an electron in magnetic field B is given by the Lorentz equation,

$$\frac{d\mathbf{k}}{dt} = -\frac{e}{c}\mathbf{v} \times \mathbf{B}.$$
(16)

Since the magnetic field does not affect the velocity, an electron performs a cyclotron motion along an equi-energy curve with ε given by (2), which is a quartic curve

$$v_{\rm F}^2 k_x^2 + \left(u k_y^2 + m\right)^2 = \varepsilon^2.$$
 (17)

We show the cyclotron orbits in Fig. 2(b). The period is given as follows. Substituting the form of the velocity Eq. (7) into Eq. (16), we obtain

$$\frac{dk_x}{dt} = -2u\omega_0 k_y \left(m + uk_y^2\right), \qquad \frac{dk_y}{dt} = \omega_0 v_{\rm F}^2 k_x, \tag{18}$$

with $\omega_0 = eB/c\varepsilon$. Eliminating k_x in the above equation, we obtain

$$\frac{d^2k_y}{dt^2} = -2uv_{\rm F}^2\omega_0^2k_y\left(m+uk_y^2\right).$$
(19)

Hence the period is given by

$$T = 2 \int_{-k_{y,\max}}^{k_{y,\max}} dk_y \frac{dk_y}{\sqrt{-uv_F^2 \omega_0^2 k_y^2 \left(2m + uk_y^2\right) + C}},$$
(20)

where the constant C is determined from the condition that $k_y = 0$ when $k_y = k_{y,\text{max}}$ as

$$C = u v_{\rm F}^2 \omega_0^2 k_{y,\rm max}^2 \left(2m + u k_{y,\rm max}^2 \right),$$
(21)

with

$$k_{y,\max} = \sqrt{\frac{|\varepsilon| - m}{u}} \tag{22}$$



Figure 2. (a) Area of cyclotron motion as a function of the chemichal potential μ . The magenta curve represents the exact area Eq. (25), while the cyan curve represents the approximation given by Eq. (29). (b) Contours of cyclotron motion with the equal area. (c) Fan diagram representing the Landau level energy as a function of the magnetic field *B*.

for |E| > m. It is explicitly given as

$$T(\varepsilon) = \frac{4}{\sqrt{uv_{\rm F}^2\omega_0^2(m+|\varepsilon|)}} K\left(\frac{m-|\varepsilon|}{m+|\varepsilon|}\right).$$
(23)

In the massless limit, it reads

$$\lim_{m \to 0} T\left(\varepsilon\right) = \frac{2K(-1)}{\sqrt{uv_{\rm F}^2 \omega_0^2}} \sqrt{\frac{1}{|\varepsilon|}}.$$
(24)

The cyclotron frequency is given by inverting the cyclotron time period, $\Omega_c = 2\pi/T$.

The area of the cyclotron orbit is given by

$$S(\varepsilon) = \int_{-k_{y,\max}}^{k_{y,\max}} \frac{\sqrt{E^2 - (uk_y^2 + m)^2}}{v_F} dk_y$$

= $\frac{4}{3v_F} \sqrt{\frac{|\varepsilon| + m}{u}} \left[\mu K \left(\frac{m - |\varepsilon|}{m + |\varepsilon|} \right) - m E \left(\frac{m - |\varepsilon|}{m + |\varepsilon|} \right) \right].$ (25)

We show the area $S(\varepsilon)$ in Fig. 2(a). The area of the cyclotron orbit will be observed by the de Haas van Alphen effect or the Shubnikov-de Haas effect[15]. The circumference of the cyclotron orbit is given by

$$\frac{dS}{d\varepsilon} = \frac{2|\varepsilon|}{v_{\rm F}\sqrt{u\left(m+|\varepsilon|\right)}} K\left(\frac{m-|\varepsilon|}{m+|\varepsilon|}\right).$$
(26)

The cyclotron mass is defined by[16]

$$m_c = \frac{1}{2\pi} \frac{dS}{d\varepsilon} \tag{27}$$

which can be observed by the cyclotron resonance.

The Landau level is derived by the Bohr-Sommerfeld quantization along one period of the cyclotron motion,

$$S(\varepsilon_n) = 2\pi (n+1/2)eB.$$
(28)

The energy of the Landau level is obtained by solving $S(\varepsilon_n)$ for ε_n . This is in general not possible. However, Eq. (25) is well approximated by

$$S\left(\varepsilon\right) \simeq \frac{4}{3v_{\rm F}\sqrt{u}}K\left(-1\right)\left(\left|\varepsilon\right|^{3/2} - \left|m\right|^{3/2}\right).$$
(29)

By inverting this approximation formula, we obtain the Landau level energy

$$|\varepsilon_n| = \left(\frac{3v_{\rm F}\pi\sqrt{u}}{2}(n+1/2)eB + |m|^{3/2}\right)^{2/3}.$$
(30)

We show the Landau level energy as a function of B in Fig. 2(c). The 2/3 dependence is highly contrasted to the case of the QHE in massive Dirac system, where

$$|\varepsilon_n| = \sqrt{\omega_c^2(n+1) + |m|^2},\tag{31}$$

with ω_c being the cyclotron frequency in graphene. The difference will be checked experimentally in phosphorene.

We consider the massless limit $(m \rightarrow 0)$. The area of the cyclotron orbit reads

$$\lim_{m \to 0} S\left(\varepsilon\right) = \frac{4}{3v_{\rm F}\sqrt{u}} K\left(-1\right) \left|\varepsilon\right|^{3/2},\tag{32}$$

and hence the cyclotron mass is

$$m_c = \frac{1}{2\pi} \lim_{m \to 0} \frac{dS}{d\varepsilon} = \frac{1}{v_{\rm F} \pi \sqrt{u}} K (-1) \sqrt{|\varepsilon|}.$$
(33)

We may solve Eq. (28) to obtain

$$|\varepsilon_n| = \left(\frac{3v_{\rm F}\pi\sqrt{u}}{2}(n+1/2)eB\right)^{2/3},\tag{34}$$

which agrees with Eq. (30) with m = 0[10].

6. Discussion

We have derived several analytic formula of conductivity and quantum Hall effects in phosphorene. They are highly anisotropic reflecting the fact that the band structure is anisotropic. Especially 2/3 dependence in the Landau-level energy is different from that in the case of graphene, which will be detected experimentally.

References

- [1] Katsnelson M I Graphene: Carbon in Two Dimensions (Cambridge Univ. Press, Cambridge, 2012).
- [2] Liu C-C, Feng W and Yao Y 2011 Phys. Rev. Lett. 107 076802
- [3] Xu X, Yao W, Xiao D and Heinz T F 2014 Nat. Phys. 10 343
- [4] Reich E G 2014 Nature 506 19
- [5] Li L, Yu Y, Ye G J, Ge Q, Ou X, Wu H, Feng D, Chen X H and Zhang Y 2014 Nature Nanotech. 9 372
- [6] Rodin A S, Carvalho A and Castro Neto A H 2014 Phys. Rev. Lett. 112 176801
- [7] Low T, Rodin A S, Carvalho A, Jiang Y, Wang H, Xia F and Castro Neto A H 2014 Phys. Rev. B90 075434
- [8] Ezawa M 2014 New J. Phys. 16 065015
- [9] Liu H, Neal A T, Zhu Z, Xu X, Tomanek D and Ye P D 2014 ACS Nano 8 4033
- [10] Dietl P, Piechon F and Montambaux G 2008 Phys. Rev. Lett. 100 236405
- [11] Banerjee S and Pickett W E, Phys. Rev. B86 075124
- [12] Montambaux G, Piechon F, Fuchs J-N and Goerbig M O 2009 Eur. Phys. J. B 73 509
- [13] Tarruell L, Greif D, Uehlinger T, Jotzu G and Esslinger T 2012 Nature 483 302
- [14] Yuan S, Rudenko A N and Katsnelson M I 2014 Transport and Optical Properties of Single- and Bilayer Black Phosphorus with Defects *Preprint* cond-mat/arXiv:1411.1681
- [15] Li L, Ye G J, Tran V, Fei R, Chen G, Wang H, Wang J, Watanabe K, Taniguchi T, Yang L, Chen X H and Zhang Y 2014 Quantum Oscillations in Black Phosphorus Two-dimensional Electron Gas *Preprint* cond-mat/arXiv:1411.6572
- [16] Falkovsky L A 2013 JETP Letters 97 429