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# Universal absorption of two-dimensional materials within $\mathbf{k} \cdot \mathbf{p}$ method

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## ABSTRACT

The universal optical absorption is a fascinating property existing in certain two-dimensional (2D) materials. By introducing a general two-band  $\mathbf{k} \cdot \mathbf{p}$  effective Hamiltonian, we demonstrate that the absorptance can manifest an universal value at the direct band-edge of 2D materials in three specific cases. However, for general 2D materials, the absorptance becomes nonuniversal. We investigate the dependency of absorptance on the band parameters of general 2D materials. The influences of band-anisotropy and band warping are also considered. Interestingly, we find that the coherent interband coupling and the band warping are responsible for the occurrence of the saddle-point type of Van Hove singularity, which leads to strong light-matter interactions in 2D materials.

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## 1. Introduction

Graphene, the first isolated two-dimensional (2D) material formed by a single layer of honeycomb-arranged carbon atoms, has been demonstrated to possess extraordinary properties compared to its bulk counterpart [1,2]. However, graphene suffers from the weakness of zero band-gap, so that it cannot work as semiconductors in transistor devices. Motivated by finding alternative 2D materials beyond graphene, a variety of atomically thin materials, including silicene, germanene, transition metal dichalcogenides (TMDCs), few-layer black phosphorus and other 2D compounds have been theoretically proposed and experimentally prepared [3–9]. The researches of these 2D materials are now growing at a tremendous rate and are expected to have great impacts on the next-generation electronics and optoelectronics [10,11].

Among the unique properties of 2D materials, the optical absorption is the specially fascinating one. For example, the absorption of graphene is attested to be only determined by the universal value  $\pi\alpha_0 = 2.3\%$  in a wide spectral range, where  $\alpha_0 \approx 1/137$  is the fine structure constant [12,13]. Interestingly, Fang et al. found this universal value also appear (approximately) in the quantized absorption spectra of the free-standing InAs membranes [14], which implies there might be certain universal essence of 2D sys-

tems underlying their optical absorptions [15]. However, we notice that there are exceptional 2D materials such as TMDCs which were reported to possess strong light-matter interactions and complicated spectra other than the universal absorption [16,17]. In addition, the optical conductivity of a hybrid Dirac and Schrödinger 2D system was revealed to be nonuniversal [18]. Therefore, it is of interest to consider from a general point of view that with which features the 2D materials could exhibit the universal absorption, and how the absorptance would depend on the parameters of general 2D materials.

In this paper, we derive a simple expression for the absorption coefficient due to the transition between the first valence band (VB) and conduction band (CB) of direct-gap 2D materials. We find the occurrence of universal absorption can be ascribed to the cancelation of the modular square of the interband velocity matrix element, i.e., denoted by  $\hbar^2 |\mathbf{v}_{cv}(\mathbf{k})|^2$ , and the derivative term  $\left| \frac{\partial(\varepsilon_{cv}^2)}{\partial(k^2)} \right|$ , where  $\varepsilon_{cv}$  is energy difference between CB and VB, and  $k$  is the magnitude of wave vector. For graphene (or isotropic Dirac fermion systems), this cancelation is exact. For other 2D materials with finite band-gap and/or mass terms, this cancelation is generally not hold. So the absorptance usually has light-frequency and band parameters dependency. However, the universal absorption can exist at the direct band-edge for certain kinds of 2D materials. By introducing a general two-band effective Hamiltonian of 2D materials with  $\mathbf{k} \cdot \mathbf{p}$  method, we can analytically derive the conditions for the occurrence of universal absorption at the di-

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rect band-edge. In addition, we also investigate the dependency of the absorptance on the parameters of 2D materials, including the band-gap, remote-bands couplings, band-anisotropies and band-warping. These general considerations are helpful for the understanding of the optical properties of 2D materials.

This paper is organized as follows. In Sec. 2 we describe the general formalism of optical absorption and the low energy effective Hamiltonian of 2D materials. In Sec. 3, we first provide the analytical results of the absorptance at the direct band-edge and the absorptance of the isotropic 2D materials. Then we discuss the influences of the band-anisotropies and band-warping by the numerical calculations. In Sec. 4 we give a brief summary and some conclusions.

2. Theoretical formalism

2.1. General formula of absorption coefficient

We shall start from the Hamiltonian of the light-matter interaction. Under the illumination of a single-color light with frequency  $\omega$ , the total Hamiltonian can be written as

$$\hat{H}_t = \hat{H} + \hat{V}(t), \tag{1}$$

where  $\hat{H}$  is the effective Hamiltonian of the 2D material,  $\hat{V}(t) = \hat{\mathfrak{H}}e^{-i\omega t} + \hat{\mathfrak{H}}^\dagger e^{i\omega t}$  represents the electron-radiation interaction, and

$$\hat{\mathfrak{H}} = \frac{e}{i\omega m_0} \hat{\mathbf{p}} \cdot \mathbf{E}. \tag{2}$$

Here,  $\hat{\mathbf{p}} = m_0 \hat{\mathbf{v}}$  is the momentum operator,  $m_0$  is the free electron mass,  $\hat{\mathbf{v}}$  is the velocity vector operator and  $\mathbf{E}$  is the complex amplitude of the electric field. In this paper, we focus on the optical transition between the first CB and VB in the low energy range, so we can consider a two-band model only consisting of the empty CB states  $|c, \mathbf{k}\rangle$  and the occupied VB states  $|v, \mathbf{k}\rangle$ . Their energies are denoted by  $\varepsilon_{c\mathbf{k}}$  and  $\varepsilon_{v\mathbf{k}}$ , respectively. The optical transition rate between CB and VB is given by the Fermi's golden rule

$$W = \frac{2\pi}{\hbar} |\langle c, \mathbf{k} | \hat{\mathfrak{H}} | v, \mathbf{k} \rangle|^2 \delta(\varepsilon_{c\mathbf{k}} - \hbar\omega), \tag{3}$$

with  $\varepsilon_{cv} [\equiv \varepsilon_{cv}(\mathbf{k})] = \varepsilon_{c\mathbf{k}} - \varepsilon_{v\mathbf{k}}$ . The number of optical transitions per unit volume per unit time is

$$\eta = \frac{1}{AL_z} \sum_{\mathbf{k}} W = \frac{1}{(2\pi)^2 L_z} \int W d^2\mathbf{k}, \tag{4}$$

where  $A$  is area of the 2D material,  $L_z$  is the thickness of the 2D layer, and  $\int_{BZ} d^2\mathbf{k}$  represents the integration over the 2D Brillouin zone. The absorption power is equal to the loss of energy per unit volume per unit time due to the transitions, and can be given by  $\eta\hbar\omega$ . Then the optical absorption coefficient can be defined as

$$\alpha(\omega) = \frac{\text{Absorption power}}{\text{Energy flux density of the light}} = \frac{\eta\hbar\omega}{I}, \tag{5}$$

where  $I = 2cn_r\varepsilon_0(\mathbf{E} \cdot \mathbf{E}^*)$  is the energy flux density of the light,  $c$  is the velocity of light,  $n_r$  is the relative refractive index and  $\varepsilon_0$  is the vacuum permittivity.

For the absorption coefficient of the light linearly polarized along  $\mathbf{e}_\mu$ , i.e.,  $\mathbf{E} = E_0\mathbf{e}_\mu$  ( $\mu = x, y$ ), one obtains

$$\alpha^\mu(\omega) = \frac{e^2}{4cn_r\omega\varepsilon_0\pi L_z} \int_{BZ} |v_{cv}^\mu(\mathbf{k})|^2 \delta(\varepsilon_{cv} - \hbar\omega) d^2\mathbf{k}, \tag{6}$$

where  $v_{nn'}^\mu(\mathbf{k}) = \langle n, \mathbf{k} | \hat{\mathbf{v}} \cdot \mathbf{e}_\mu | n', \mathbf{k} \rangle$  denotes the  $\mu$  component of the velocity matrix element between  $|n, \mathbf{k}\rangle$  and  $|n', \mathbf{k}\rangle$  state. Note in

Eq. (6), the 2D integral containing delta function can be transformed to the integral on the constant-energy contours determined by  $\varepsilon_{cv}(\mathbf{k}) = \hbar\omega$ , as the following

$$\int_{BZ} |v_{cv}^\mu(\mathbf{k})|^2 \delta(\varepsilon_{cv} - \hbar\omega) d^2\mathbf{k} \rightarrow g_s g_v \int_{\varepsilon_{cv}=\hbar\omega} |v_{cv}^\mu(\mathbf{k})|^2 \frac{dl_k}{|\nabla_{\mathbf{k}}\varepsilon_{cv}|}, \tag{7}$$

where  $g_s$  and  $g_v$  are the degrees of spin and valley degeneracy, respectively.  $g_s$  and  $g_v$  appear because they account for the number of identical constant-energy contours due to the degeneracies. If the material is illuminated by the unpolarized light, the unpolarized absorption coefficient can be given by  $\alpha = (\alpha^x + \alpha^y)/2$ . By introducing the fine structure constant  $\alpha_0 \equiv e^2/(4\pi\varepsilon_0 c\hbar)$ , the unpolarized absorption coefficient can be written in a simple form

$$\alpha(\omega) = \frac{1}{n_r L_z} \Phi(\omega) \alpha_0, \tag{8}$$

where  $\Phi(\omega)\alpha_0$  can be viewed as the dimensionless absorptance, and  $\Phi(\omega)$  is the prefactor. It is convenient to perform the integration over the constant-energy contour in the polar coordinates system. Let  $\mathbf{k} \equiv (k, \varphi)$ , where  $k$  and  $\varphi$  are the magnitude and azimuth angle of wave vector, respectively. One can find the relations  $dl_k = \sqrt{k^2 + (\partial k/\partial\varphi)^2} d\varphi$ , and  $|\nabla_{\mathbf{k}}\varepsilon_{cv}| = \sqrt{(\partial\varepsilon_{cv}/\partial k)^2 + (1/k \cdot \partial\varepsilon_{cv}/\partial\varphi)^2}$ . And on the constant-energy contours, one also has  $\partial k/\partial\varphi = -(\partial\varepsilon_{cv}/\partial\varphi)/(\partial\varepsilon_{cv}/\partial k)$ . With these relations, we obtain a simple expression for the prefactor of dimensionless absorptance

$$\begin{aligned} \Phi(\omega) &= \frac{g_s g_v \hbar}{2\omega} \int_{\varepsilon_{cv}=\hbar\omega} |\mathbf{v}_{cv}(\mathbf{k})|^2 \left| \frac{\partial\varepsilon_{cv}}{\partial k} \right|^{-1} k d\varphi \\ &= \frac{g_s g_v}{2} \int_{\varepsilon_{cv}=\hbar\omega} \hbar^2 |\mathbf{v}_{cv}(\mathbf{k})|^2 \left| \frac{\partial(\varepsilon_{cv}^2)}{\partial(k^2)} \right|^{-1} d\varphi, \end{aligned} \tag{9}$$

where  $|\mathbf{v}_{cv}(\mathbf{k})|^2 \equiv |v_{cv}^x(\mathbf{k})|^2 + |v_{cv}^y(\mathbf{k})|^2$ . Obviously, we can see that if  $\hbar^2 |\mathbf{v}_{cv}(\mathbf{k})|^2$  cancels with  $\left| \frac{\partial(\varepsilon_{cv}^2)}{\partial(k^2)} \right|$ , the integral of Eq. (9) will give rise to a simple constant. While for the three-dimensional (3D) bulk materials, the integration over 3D Brillouin zone transforms to the integral on constant-energy surfaces, which leads to a  $k$ -dependent integrand. And the  $k$ -dependent integrand always approaches 0 when  $k \rightarrow 0$ . Therefore, for the 3D systems, one cannot expect an universal value of the absorptance. For the 2D systems, we can define a canceling factor  $\Omega \equiv \hbar^2 |\mathbf{v}_{cv}(\mathbf{k})|^2 \left| \frac{\partial(\varepsilon_{cv}^2)}{\partial(k^2)} \right|^{-1}$ . If  $\Omega$  equals to a simple constant  $C$ , the dimensionless absorptance of 2D material will have the universal value  $Cg_s g_v \pi \alpha_0$ .

In the case of graphene, this condition can be exactly fulfilled in the low energy range. Graphene has a Dirac-cone band structure near the  $K$  ( $K'$ ) point with the CB and VB formed by  $\pi$  and  $\pi^*$  states, respectively. Due to the symmetry of  $\pi$  and  $\pi^*$  states, they approach each other (apart from a phase factor) in the limit  $\mathbf{k} \rightarrow 0$ . So  $|\mathbf{v}_{cv}(\mathbf{k})|^2$  can be approximately replaced by  $|\mathbf{v}_{cc}(\mathbf{k})|^2 = |\nabla_{\mathbf{k}}\varepsilon_{c\mathbf{k}}/\hbar|^2$ . With the linear dispersion of Dirac cone, i.e.,  $\varepsilon_{c(v)\mathbf{k}} = \pm\hbar v_F k$ , one can get

$$\Omega = \hbar^2 |\nabla_{\mathbf{k}}\varepsilon_{c\mathbf{k}}/\hbar|^2 \left| \frac{\partial(\varepsilon_{cv}^2)}{\partial(k^2)} \right|^{-1} = \frac{1}{4}. \tag{10}$$

Therefore, for graphene ( $g_s = g_v = 2$ ), it can be shown that  $\Phi = g_s g_v \cdot \frac{1}{4} \cdot \pi = \pi$ , which produces the well-known universal absorptance  $\pi\alpha_0$  of graphene.

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