Exploring the Optical States for Black Phosphorus: Anisotropy and Bandgap Tuning

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The dressed states arising from the interaction between electrons and holes, and off-resonant electromagnetic radiation have been investigated for recently fabricated gapped and anisotropic black phosphorus. Our calculations were carried out for the low-energy electronic subbands near the $\Gamma$ point. States for both linear and circular polarizations of the incoming radiation have been computed. However, our principal emphasis is on linearly polarized light with arbitrary polarization since this case has not been given much attention for dressing fields imposed on anisotropic structures. We have considered various cases for one- and few-layer phosphorus, including massless Dirac fermions with tunable in-plane anisotropy. Initial Hamiltonian parameters are renormalized in a largely different way compared to those for previously reported for gapped Dirac structures and, most importantly, existing anisotropy which could be modified in every direction.

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I. INTRODUCTION

Black phosphorus (BP) is a layered structure of buckled atomic phosphorus for which the layers are connected by weak van der Waals forces. This is the most stable phosphorus-based crystal at room temperature and for a wide range of pressure values. Crystalline BP is a semiconductor, for which $P$ atoms are covalently bonded with three adjacent atoms. Such a structure exhibits strong anisotropy for an arbitrary number of layers, as well as hybrid electron and hole states in the vicinity of the band edge in phosphorene featuring both Dirac cone and a conventional Schrödinger electron behavior. While bulk BP is a semiconductor with a small bandgap of $0.3\,eV$, its monolayer counterpart is a semiconductor with a large direct bandgap ($\sim 2\,eV$) and is referred to as phosphorene in analogy to graphene and could be exfoliated in a mechanical way.

It is not surprising that reliable information for the band structure of BP with a specified number of layers has been appreciated as being extremely important for device applications, including a field-effect transistor. This has stimulated a large number of first-principles calculations based on the density functional theory as well as the tight-binding model, group-theoretical calculations and the continuum model of BP structures, which recently received a significant amount of attention for their success in analyzing experimental data. The quality of all such models depends on the accuracy of the exchange-correlation approximation. Over time, we are going to witness numerous attempts to engineer new types of anisotropic electronic band structure of BP-based devices using various mechanisms such as electron-photon interaction with a dressing field. The corresponding effect from an imposed electrostatic field was addressed in Ref. 12.

The possibility of an electronic topological transition and electrically-tunable Dirac cone was theoretically predicted for multi-layer BP. The fact that the bandgap of BP is mainly determined by the number of layers was confirmed in experiment, i.e., the energy gap is strongly decreased for a larger number of layers and could be effectively neglected for $N_L > 5$. Yet demonstrating a Dirac cone with no effective mass or energy bandgap, such electrons still possess strong anisotropic properties for pristine black phosphorus. Consequently, non-symmetric Klein tunneling
FIG. 1: (Color online) Schematics of a phosphorene layer(s) irradiated by external dressing light with either linear or circular polarization is shown in (a). Panel (b) presents electron and hole energy bands $\varepsilon_{\pm}(k)$ given by Eq.(3) along the $x$ ($\phi_0 = 0$, solid black lines) and $y$ ($\phi_0 = \pi/2$, blue and short-dashed) directions, and also for the ($\phi_0 = \pi/4$, the red and long-dashed curve). Negative (reflected) electron dispersion $-\varepsilon_{\Delta}(k_x)$ is also presented for comparison to highlight the electron-hole asymmetry in phosphorene.

could be observed with a shifted transmission peaks similar to electron tunneling for graphene in the presence of magnetic field.

Phosphorene is one of the most recently discovered members of a sizable group of low-dimensional structures with great potential for nanoelectronics applications. The most famous part of this family is graphene, fabricated in 2004. Because of its unique properties, graphene has initiated a new direction in electronic devices. A subsequent crucial advance was the discovery of the buckled honeycomb lattices such as silicene and germanene. Their most distinguished feature is the existence and tunability of two non-equivalent spin-orbit and sublattice-asymmetry bandgaps. The latter one, $\Delta_z$ is directly modified by an external electrostatic field. This is a result of the out-of plane buckling, which is due to a larger radius of $Si$ and $Ge$ atoms compared to carbon and $sp^3$ hybridization. The most recently fabricated germanene possesses similar buckling features but with different bandgaps and Fermi velocity.

Another important class of such materials are the transition metal dichalcogenides (TMDC’s) structures such as $MC_2$, where $M$ denotes a metal such as $Mo$, $W$, and $C$ is a chalcogen atom ($S$, $Se$, or $Te$). Molybdenum disulfide $MoS_2$, a typical representative of TMDC’s, has exhibited a large energy bandgap $\simeq 1.9\,eV$, and broken symmetry between the electron and hole subbands so that for all experimentally accessible electron density values only one hole subband is doped. As a result, all the electronic, collective and transport properties vary significantly for the electron and hole types of doping. However, all these low-dimensional materials exhibit almost complete (with a slight deviation for $MoS_2$) isotropy in the $x-y$ plane. Consequently, phosphorene is a totally new material with its very unusual properties, so that complete and thorough studies of these characteristics open a new important chapter in low-dimensional science and technology.

With the newest achievements in laser and microwave science, it has become possible to achieve substantial control and tunability of the electronic properties of low-dimensional condensed-matter materials by subjecting them to strong off-resonant high-frequency periodic fields (so-called “Floquet engineering“, schematically shown in Fig. refFIG:1 (a)). If the electron-phonon coupling strength is high, such a bound system could be considered as a single, holistic object and has been investigated using quantum optics and mechanics. These electrons with substantially modified energy dispersions, referred to as “dressed states”, became a commonly used model in present-day low-dimensional physics. One of the first significant achievements has been the demonstration of a metal-insulator transition in graphene, which drastically affected the electron tunneling and the Klein paradox. Important collective properties such as exchange and correlation energies are also affected by the presence of an energy gap and spin dynamics on the surface of a three-dimensional topological insulator is also modified.

The rest of our paper is organized in the following way. In Sec. II we present our model, the low-energy Hamiltonian and the energy dispersions for phosphorene, i.e., single-layer black phosphorus with strong in-plane anisotropy and a large energy bandgap. The electron-photon dressed states for phosphorene are presented and discussed in Sec. III. Section IV is devoted to calculating the dressed states for few-layer phosphorus, in which the electrons are anisotropic massless Dirac fermions without a gap. Mathematical generalizations of such a model with both on- and off-diagonal bandgaps is considered, and the corresponding dressed states are also obtained. Concluding remarks are provided in Sec. V.
II. LOW-ENERGY MODEL FOR PHOSPHORENE

Our calculations utilize the model for BP presented in Refs. [5,6]. Being somewhat similar to the truly two-dimensional hexagon structure of graphene, the atomic arrangement for single layer BP results in a packed surface due to the sp$^3$ hybridization composed of the 3s and 3p orbitals. For silicene, such hybridization is responsible for out-of-plane “buckling” displacement of the Si atoms.

The continuum $k$–dependent Hamiltonian is usually based on the tight-binding model. Close to the Γ point, approximated up to second order in the wave vector components, it is given as

\[ \mathbb{H}^{Δ}_{ph}(k) = \left( E_i + \sum_{i=x,y} \eta_i k_i^2 \right) \hat{I}_{2\times2} + \left( \Delta_O + \sum_{i=x,y} \gamma_i k_i^2 \right) \hat{Σ}_x - \chi k_y \hat{Σ}_y , \]

or in the matrix form,

\[ \mathbb{H}^{Δ}_{ph}(k) = \begin{bmatrix} E_i + \sum_{i=x,y} \eta_i k_i^2 & \Delta_O + \sum_{i=x,y} \gamma_i k_i^2 - i\chi k_y \\ \Delta_O + \sum_{i=x,y} \gamma_i k_i^2 + i\chi k_y & E_i + \sum_{i=x,y} \eta_i k_i^2 \end{bmatrix} . \] (2)

This Hamiltonian clearly displays significantly different structure and properties, compared to that for graphene. First, there are no linear $k$–terms, except $\pm i\chi k_y$. Furthermore, there are no linear $k_x$ elements. As one of the most evident consequences of this structure, we note that circularly polarized irradiation with $x$- and $y$-components being equally important, couples to such electrons only in the $\sim A^2$ level.

Secondly, the energy bandgap is presented in a $\hat{Σ}_x$, off-diagonal form, contributing to the asymmetry between the electron and hole states in contrast to the $\hat{Σ}_z$-type gap. These properties, coming directly from the Hamiltonian structure, are new and have not been encountered previously. The energy dispersions are

\[ \varepsilon^\pm_Δ(k) = E_i + \sum_{i=x,y} \eta_i k_i^2 \pm \left[ \left( \Delta_O + \sum_{i=x,y} \gamma_i k_i^2 \right)^2 + \chi^2 k_y^2 \right]^{1/2} , \] (3)

where $\gamma_{e,h} = \pm 1$ corresponds to the electron or hole solution. For small values of the wave vector, these dispersions are approximated as

\[ \varepsilon^\pm_Δ(k) \simeq E_i \pm \Delta_O + (\eta_x \pm \gamma_x) k_x^2 + \left[ \eta_y \pm \left( \gamma_y + \frac{\chi^2}{2\Delta_O} \right) \right] k_y^2 . \] (4)

The effective masses given by [5]

\[ m^{(e,h)}_x = \frac{\hbar^2}{2(\eta_x \pm \gamma_x)} , \]

\[ m^{(e,h)}_y = \frac{\hbar^2/2}{\eta_y \pm (\gamma_y + \chi^2/(2\Delta_O))} \]

are anisotropic, and this anisotropy is different for the electron and hole states as $\sim \chi^2/\Delta_O$.

III. ELECTRON DRESSED STATES FOR IN SINGLE LAYER

In this Section, we calculate electron-light dressed states for phosphorene. As far as circularly polarized irradiation is concerned, one must consider second order coupling in order to see how both components of the wave vector are modified. Such consideration is critical for the vector potential given by Eq. (37), but is clearly beyond the scope of conventional analytical methods. The mere presence of an off-diagonal energy gap $\Delta_O$ means that there is no electron/hole symmetric solution, obtained in Refs. [41,47]. This situation also leads us to conclude that the Hamiltonian parameters, such as the energy gap, are affected at lower order than such parameters for Dirac fermions. Consequently, for monolayer BP, we focus on the case for linearly polarized irradiation.
A. Linear polarization of the dressing field and induced anisotropy

Since electron energy dispersion relations and their effective masses are intrinsically anisotropic for phosphorenes, the direction of the dressing field polarization now plays a substantial role. We define this direction by an arbitrary angle \( \theta_0 \) from the \( x \)-axis and generalize the vector potential used in Ref. [47] so that it now has both \( x \)- and \( y \)- non-zero components

\[
\mathbf{A}_L(t) = \begin{cases} 
\frac{E_0}{\omega} \cos \omega t \cos \theta_0; & \frac{E_0}{\omega} \cos \omega t \sin \theta_0 
\end{cases}
\] (6)

The renormalized Hamiltonian for the dressed states is obtained by the canonical substitution \( k_{x,y} \Rightarrow k_{x,y} - e/\hbar A_{x,y} \), where \( e \) stands for the electron charge, yielding

\[
\hat{H}(k) = \hat{H}_{ph}^\Delta + \hat{h}_0 + \hat{h}_{int},
\] (7)

where \( \hat{H}_{ph}^\Delta \) is the “bare”, non-interacting electron Hamiltonian, given by Eq. (2). The zeroth-order, \( k \)-independent interaction Hamiltonian may be expressed as

\[
\hat{h}_0 = \chi E_0 e \frac{\sin \omega t \cos \omega t}{\hbar} \hat{\Sigma}_y = c_0 \left( \begin{array}{cc} 0 & -i \cos \omega t \\ i \cos \omega t & 0 \end{array} \right),
\] (8)

where \( c_0 = \chi \sin \theta_0 E_0 \epsilon/(\hbar \omega), \epsilon = |e| \). We conclude that the vector potential of linearly polarized light \( \hat{A}_L \) must have a non-zero \( y \)-component in order to enable \( \sim \mathbf{A}_L \) coupling. We now turn our attention to the interaction term which is linear in \( \mathbf{k} \) and given by

\[
\hat{h}_{int} = 2 \frac{e}{\hbar} \left( \sum_{i=x,y} \eta_i k_i A_i^L(t) \mathbb{I}_{2 \times 2} + \sum_{i=x,y} \gamma_i k_i A_i^L(t) \hat{\Sigma}_x \right),
\] (9)

or, introducing the following simplifying notations \( \epsilon_\alpha = \sqrt{\alpha_x^2 k_x^2 + \alpha_y^2 k_y^2}, \phi(\alpha) = \tan^{-1}[\alpha_y k_y/(\alpha_x k_x)] \) for \( \alpha = \eta, \gamma \) and \( c(2) = (2\epsilon E_0)/(\hbar \omega) \), we express it as

\[
\hat{h}_{int} = c(2) \cos \omega t \left( \begin{array}{cc} \epsilon_\eta \cos(\phi(\eta) - \theta_0) & \epsilon_\gamma \cos(\phi(\gamma) - \theta_0) \\ \epsilon_\gamma \cos(\phi(\gamma) - \theta_0) & \epsilon_\eta \cos(\phi(\eta) - \theta_0) \end{array} \right).
\] (10)

As the first step, we solve a time-dependent Schrödinger equation for \( k = 0 \):

\[
i\hbar \frac{\partial \Psi_0(t)}{\partial t} = \hat{h}_0 \Psi_0(t).
\] (11)

We obtain the solution in a straightforward way to be

\[
\Psi_0^{\beta=\pm 1}(t) = \frac{1}{\sqrt{2}} \left[ \begin{array}{c} 1 \\ \beta i \end{array} \right] \exp \left\{ -i \beta \frac{c_0}{\hbar \omega} \sin \omega t \right\}.
\] (12)

It is noteworthy that even if both energy bandgaps \( \Delta_O \) and the initial energy shift \( E_i \) are included so that the Hamiltonian takes the form

\[
h_0 = E_i \mathbb{I}_{2 \times 2} + \Delta_O \hat{\Sigma}_x + c_0 \cos \omega t \hat{\Sigma}_y = c_0 \left( \begin{array}{cc} E_i & \Delta_O - i \cos \omega t \\ \Delta_O + i \cos \omega t & E_i \end{array} \right),
\] (13)

the solution could still be determined analytically as
\[ \Psi_0^{\beta=\pm 1}(t) = \frac{1}{\sqrt{2}} \left[ \frac{1}{\beta i} \exp \left\{ -\beta i \left[ \frac{c_0}{\omega} \sin \omega t - (\Delta_O - \beta \Xi_i) t \right] \right\} \right]. \]  

(14)

We note that such a trivial solution could only be obtained for equal diagonal energies \( \Xi_0 \), i.e., for an introduced non-\( \Sigma_z \) type of energy gap. If the diagonal energies are not equivalent, given by \( \Xi_{1,2} = \Xi_i \pm \Delta_D \), complete symmetry between the two components of the wave function no longer exists and such a solution could not be determined analytically. Consequently, we will use basic set in Eq. (12) for the rest of the present calculation. Such a situation (non-zero diagonal gap \( \Delta_D \)) appears if there is a relatively small non-zero vertical electrostatic field component and the symmetry between the vertically displaced phosphorus atoms is broken similar to silicene. We will often use this mathematical generalization in the rest of our work.

For finite wave vector, we present the eigenfunction as an expansion in terms of a basis set [12]

\[ \Psi_k(t) = \mathcal{F}^\uparrow \Psi_0^+(t) + \mathcal{F}^\downarrow \Psi_0^-(t), \]  

(15)

where \( \mathcal{F}^\uparrow, \mathcal{F}^\downarrow = \mathcal{F}^\uparrow \gamma, (k_x, k_y | t) \) are scalar, time-dependent coefficients with anisotropic \( k \)-dependence. This equation immediately results in the two following identities

\[ i \hbar \frac{d\mathcal{F}^{\uparrow, \downarrow}}{dt} = \langle \Psi_0^+(t) | \delta \mathcal{H}_{ph}^\gamma (k) | \Psi_0^+(t) \rangle \mathcal{F}^{\uparrow} + \langle \Psi_0^-(t) | \delta \mathcal{H}_{ph}^\gamma (k) | \Psi_0^-(t) \rangle \mathcal{F}^{\downarrow}, \]  

(16)

where

\[ \delta \mathcal{H}_{ph}^\gamma (k) = \mathcal{H}_{ph}^\gamma + \hat{h}_{int} \]  

(17)

is the bandgap and wave vector dependent portion of the total Hamiltonian [7]. This system becomes

\[ i \frac{d\mathcal{F}^{\uparrow, \downarrow}}{dt} = \left[ \Xi_i + \eta_z k_x^2 + (\eta_y k_y \pm \chi) k_y + c^{(2)} \epsilon_\gamma \cos(\phi(\gamma) - \theta_0) \cos \omega t \right] \mathcal{F}^{\uparrow, \downarrow} \pm \]

\[ \pm i \left[ \mp i \Delta_D + \Delta_O + \gamma_z k_x^2 + \gamma_y k_y^2 + c^{(2)} \epsilon_\gamma \cos(\phi(\gamma) - \theta_0) \cos \omega t \right] \mathcal{F}^{\uparrow, \downarrow} \exp \left[ \pm 2i \frac{c_0}{\hbar \omega} \sin \omega t \right] \]  

The quasiparticle energy dispersion relations \( \varepsilon_d(k) \) are calculated by using the Floquet theorem from the following substitution

\[ \mathcal{F}^{\uparrow, \downarrow}(t) = \exp \left[ -i \frac{\varepsilon_d(k)}{\hbar} t \right] \sum_{\lambda=-\infty}^{\infty} f^{\uparrow, \downarrow}_{\lambda} \exp \left[ i \lambda \omega t \right], \]  

(19)

where \( f^{\uparrow, \downarrow}(t) = f^{\uparrow, \downarrow}(t + 2\pi/\omega) \) are time-dependent periodic functions. The nested exponential dependence is usually simplified using the Jacobi-Anger identity

\[ \exp \left[ \pm 2i \frac{c_0}{\hbar \omega} \sin \omega t \right] = \sum_{\nu=-\infty}^{\infty} \exp \left[ i \nu \omega t \right] J_{\nu} \left( \frac{\pm 2c_0}{\hbar \omega} \right). \]  

(20)

The orthonormality of Fourier expansions results in the following system of \( 2\mu, \mu \Rightarrow \infty \) equations

\[ \varepsilon_d(k) f^{\uparrow, \downarrow}_{\mu} = \left[ \mu \hbar \omega + \Xi_i \pm \eta_z k_x^2 + (\eta_y k_y \pm \chi) k_y \right] f^{\uparrow, \downarrow}_{\mu} + \left[ \frac{c^{(2)}}{2} \epsilon_\gamma \cos(\phi(\gamma) - \theta_0) \right] \left( f^{\uparrow, \downarrow}_{\mu+1} + f^{\uparrow, \downarrow}_{\mu-1} \right) \sum_{\lambda=-\infty}^{\infty} f^{\uparrow, \downarrow}_{\lambda} \times \]

\[ \times \left\{ \left[ \Delta_D \pm i \left( \Delta_O + \gamma_z k_x^2 + \gamma_y k_y^2 \right) \right] J_{\mu-\lambda} \left( \frac{\pm 2c_0}{\hbar \omega} \right) + \left[ \frac{c^{(2)}}{2} \epsilon_\gamma \cos(\phi(\gamma) - \theta_0) \right] \sum_{\alpha=\pm 1} J_{\mu+\alpha-\lambda} \left( \frac{\pm 2c_0}{\hbar \omega} \right) \right\}. \]  

(21)
FIG. 2: (Color online) Energy dispersions of electron dressed states in phosphorene interacting with linearly-polarized light. The two panels correspond to the $x-$ and $y-$components of the wave vector. For each plot, the chosen dimensional electron-photon coupling constant is $\alpha_c = 0.0$ (black solid line), $\alpha_c = 0.15$, red and dashed, and $\alpha_c = 0.4$ (blue small-dashed curve).

In our consideration, the frequency of the off-resonant dressing field is high enough so that only diagonal elements in the eigenvalue equation (21) are retained. However, if we need to include the first-order electron-field coupling terms $\sim \tilde{c}^2$, we must keep the summations with $\lambda = \mu \pm 1$.

In the simplest case, where only diagonal elements are kept, the quasiparticle energy dispersion relations are

$$\varepsilon_d(k) = E_i + \sum_{i=x,y} \eta_i k_i^2 \pm \left\{ \left[ \frac{\Delta_D^2 + \Delta_O^2}{\Delta_D^2 + \Delta_O^2} - \alpha_c^2 \right] \left[ \Delta_D^2 + \Delta_O^2 \right] \right\}^{1/2} k_i^2 + \left[ \eta_i \pm \frac{\gamma_i \Delta_O (1 - \alpha_c^2)}{\sqrt{(1 - \alpha_c^2) \Delta_D^2 + \Delta_O^2}} \right] k_i^2,$$

where $\alpha_c = 2c_0/(\hbar \omega)$ is a dimensionless coupling coefficient. The electron effective masses are now readily obtained. If there is no $\Sigma_z$-type energy bandgap $\Delta_D$, the expressions are simplified as

$$m_{(e,h)}^{(x)} = \frac{\hbar^2}{2 (\eta_x \pm \tilde{\alpha}_c \gamma_x)},$$

$$m_{(e,h)}^{(y)} = \frac{\hbar^2/2}{\eta_y \pm \tilde{\alpha}_c \gamma_y + \chi^2/(2\Delta_D \tilde{\alpha}_c)},$$

where $\tilde{\alpha}_c = \sqrt{1 - \alpha_c^2} \sim 1 - \alpha_c^2/2$. The obtained energy dispersion relations are presented in Fig. 2. It is interesting to note that both energy bandgaps are renormalized by the electron-photon interaction, showing a substantial decrease, while the diagonal terms for the initial effective masses of a “bare” electron $\eta_{x,y}$ are unchanged.

IV. ANISOTROPIC MASSLESS FERMIONS IN FEW-LAYER PHOSPHORUS

The central property, as well as the research focus of phosphorene, is the electron dispersion relation and effective mass anisotropy. At the same time, BP-based materials have a band gap which is determined by the number of layers, which varies from 0.6 eV for five layers to 1.5 eV for a single layer. Specifically, we consider anisotropic massless Dirac particles, which could be observed in special few-layer ($N_L > 5$) black phosphorus superlattices for a narrow range of energies.

This anisotropic Dirac Hamiltonian

$$\mathcal{H}^{70}_{nl} = \hbar v_F \left( k_x \tilde{\Sigma}_x + \gamma_0 k_y \tilde{\Sigma}_y \right)$$

(25)
The energy eigenvalues are given by
\[ \varepsilon_{\pm m}(k) = \pm \hbar v_F \sqrt{k_x^2 + (\gamma_0 k_y)^2}. \] (26)

For such fermions interacting with light having linear polarization in arbitrary direction \( \theta_0 \) described by Eq. (6), we obtain the following Hamiltonian
\[ \hat{H}(k) = \hat{H}_{\text{mt}}^0(k) + \hat{h}_0, \] (27)
where
\[ \hat{h}_0 = \epsilon v_F \mathbf{\Sigma} \cdot \mathbf{A}^\prime(t) = \frac{\epsilon v_F E_0}{\omega} \begin{pmatrix} 0 & e^{-i\theta} \cos \omega t \\ e^{i\theta} \cos \omega t & 0 \end{pmatrix} \] (28)
is the \( k = 0 \) portion of the total Hamiltonian. Here, we also introduced \( \theta_s = \tan^{-1}[\gamma_0 \tan(\theta_0)] \) so that \( e^{\pm i\theta_s} = \cos \theta_0 \pm i\gamma_0 \sin \theta_0 \). We define \( c_0 = \epsilon v_F E_0 / \omega \) to be the electron-photon interaction coefficient with the dimension of energy and for a given range of frequency \( c_0 \ll \hbar \omega \) - dressing field which cannot be absorbed by electrons. Traditionally, we first need to solve the time-dependent Schrödinger equation for \( k = 0 \) and Hamiltonian \( \hat{h}_0 \). The eigenfunction is obtained in a straightforward way as
\[ \Psi_{0,\pm1}^\beta(t) = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ \beta e^{i\theta_0} \end{bmatrix} \exp \left\{ -i\beta \frac{c_0}{\hbar \omega} \sin \omega t \right\}. \] (29)

In order to determine the solution for a finite wave vector we once again employ the expansion (15) and solve Eq. (16) for the time-dependent coefficients \( \mathcal{F}_{\beta,\gamma} = \mathcal{F}_{\beta,\gamma}(k_x, k_y | t) \). In our case, this leads to
\[ i \frac{d \mathcal{F}_{\beta,\gamma}}{dt} = \pm v'_F k_y \cos(\phi(\gamma) - \theta_0) \mathcal{F}_{\beta,\gamma} + \pm i v'_F k_y \sin(\phi(\gamma) - \theta_0) \mathcal{F}_{\beta,\gamma} \exp \left\{ \pm 2i \frac{c_0}{\hbar \omega} \sin \omega t \right\}, \] (30)
where \( \phi(\gamma) = \tan^{-1}[\gamma_0 k_y / k_x] \) or \( \phi(\gamma) = \tan^{-1}[\gamma_0 \tan(\phi_0)] \) and \( \tan \phi_0 = k_y / k_x \). We also denote \( k_\gamma = \sqrt{k_x^2 + (\gamma_0 k_y)^2} \).

Now we also use the Floquet theorem to extract the quasiparticle energy \( \varepsilon_d(k) \) and expand the remaining time-periodic functions as a Fourier series. The result is again a system of \( 2\mu, \mu \Rightarrow \infty \) equations
\[ \varepsilon_d(k) f_{\mu,\gamma}^{\beta,\psi} = \sum_{\lambda=-\infty}^{\infty} \delta_{\mu,\lambda} \begin{pmatrix} \mu \omega \pm \hbar v'_F k_y \cos(\phi(\gamma) - \theta_0) \\ \pm i \hbar v'_F k_y \sin(\phi(\gamma) - \theta_0) \end{pmatrix} J_{\mu,\lambda} \left( \begin{pmatrix} \pm 2c_0/\hbar \omega \\ -v'_F k_x \cos(\phi(\gamma) - \theta_0) \end{pmatrix} f_{\lambda,\gamma}^{\beta,\psi} \right). \] (31)

In the region of interest, i.e., for large frequency \( \omega \gg v'_F k \) and \( \omega \gg \epsilon(k) \) we approximate \( f_{\mu,\gamma}^{\beta,\psi} \approx 0 \). Finally, the eigenvalue equation becomes \( \varepsilon_d(k) f_{\mu,\gamma}^{\beta,\psi} = \tilde{K}(\beta, \gamma | \gamma_0, k) \times f_{\mu,\gamma}^{\beta,\psi} \), where
\[ \tilde{K}(\beta, \gamma | \gamma_0, k) = \begin{bmatrix} h v'_F k_x \cos(\phi(\gamma) - \theta_0) & i v_0 h v'_F k_y \sin(\phi(\gamma) - \theta_0) J_0[2c_0/(\hbar \omega)] \\ -i v_0 h v'_F k_y \sin(\phi(\gamma) - \theta_0) J_0[-2c_0/(\hbar \omega)] & -h v'_F k_y \cos(\phi(\gamma) - \theta_0) \end{bmatrix}. \] (32)
The energy eigenvalues are given by
\[ \varepsilon_d(k) = \pm \hbar v'_F \sqrt{k_x^2 + (\gamma_0 k_y)^2} \left\{ \cos^2(\phi(\gamma) - \theta_0) + \sin^2(\phi(\gamma) - \theta_0) J_0 \left( \frac{2c_0}{\hbar \omega} \right)^2 \right\}^{1/2}. \] (33)
For small light intensity \( c_0 \ll \hbar \omega \) the zeroth-order Bessel function of the first kind behaves as
\[ J_{0,\hbar \omega}^{2c_0} \left( \frac{2c_0}{\hbar \omega} \right) \approx 1 - \frac{c_0^2}{(\hbar \omega)^2} + \frac{c_0^4}{4(\hbar \omega)^4} - \ldots \] (34)
FIG. 3: (Color online) Angular dependence of the energy dispersion for anisotropic mass fermions (AMF’s) subjected to the linearly polarized dressing field for chosen $|k| = 1.0 \, nm$, shown as polar plots. Each panel corresponds to different polarization directions $\theta_0$ and Dirac cone anisotropy parameter $\gamma_0$. Plot (a) shows the case when $\theta_0 = 0$ (x-axis linear polarization) and $\gamma_0 = 1/3$, while the inset (i1) demonstrates the way in which the electron-field interation affects the dispersion relations as a zeroth-order Bessel function. Panels (b) and (c) represent angular dispersion for $\gamma_0 = 1$ (isotropic Dirac cone) and $\theta_0 = 0$ and $\pi/6$, respectively. Panel (d) describes the situation for $\theta_0 = \pi/6$ and $\gamma_0 = 0.6$ for the main plot, and $\gamma_0 = 0.3$ in inset (i2). For each panel, the electron-photon coupling parameter $\alpha = 2c_0/(\hbar \omega) = 0.0$ (no irradiation), 0.8, 1.2 and 1.6.

and we have approximately for the energy dispersion

$$\varepsilon_d(k) = \pm \hbar v_f \left\{ \left[ 1 - \frac{2c_0^2}{(\hbar \omega)^2} \sin^2 \theta_\gamma \right] k_x^2 + \gamma_0^2 \left[ 1 - \frac{2c_0^2}{(\hbar \omega)^2} \cos^2 \theta_\gamma \right] k_y^2 + \frac{2\gamma_0c_0}{(\hbar \omega)^2} k_x k_y \sin(2\theta_\gamma) \right\}^{1/2}.$$  \hspace{1cm} (35)

If the light polarization is directed along the x-axis, then $\theta_0 = \theta_\gamma = 0$ and

$$\varepsilon_d(k) = \hbar v_f \sqrt{k_x^2 + \gamma_0^2 \left[ 1 - \frac{2c_0^2}{(\hbar \omega)^2} \right]^2 k_y^2}.$$  \hspace{1cm} (36)

Angular dependence of the dressed states dispersions is shown in Fig. 3. We notice that initially existing in-plane anisotropy is affected for all in-plane angles, depending on the dressing field polarization direction. For small intensity of the incoming radiation, polarized along the x-axis, the anisotropy coefficient is simply renormalized.

A. Circular Polarization

For circular polarization of the dressing radiation, the vector potential is

$$\mathbf{A}^C(t) = \{A_{0,x}, A_{0,y}\} = \frac{E_0}{\omega} \{\cos \omega t, \ sin \omega t\}.$$  \hspace{1cm} (37)

Being completely isotropic, this type of field is known to induce the metal-insulator transition in graphene, resulting in the creation of a non-zero energy bandgap. If such a gap already exists, it could be increased or decreased depending on its initial value. At the same time, the slope of the Dirac dispersions, known as Fermi velocity and the in-plane isotropy are not changed. The situation cannot be the same for an initially anisotropic Dirac cone for AMF’s.
The total Hamiltonian for the interacting quasiparticle now becomes
\[ \hat{H}(k) = H^\gamma_{ml}(k) + \hat{h}_0^{(c)}, \]
where the \( k = 0 \) interaction term is
\[ \hat{h}_0^{(c)} = \frac{e v_F E_0}{\omega} \hat{\Sigma} \cdot \mathbf{A}^C(t) = \frac{c_0}{2} \left[ \frac{1}{\omega} \sum_{\alpha = \pm 1} (1 + \alpha \gamma) e^{i \alpha \gamma \omega t} \right]. \]

It seems rather surprising, although physically justified, that this problem is mathematically identical to the isotropic Dirac cone interacting with elliptically polarized light addressed in Refs. \[47,48\]. The interaction term also could be presented as
\[ \hat{h}_0^{(c)} = \hat{\Sigma}_x e^{i \omega t} + \hat{\Sigma}_y e^{-i \omega t}, \]
where \( \hat{\Sigma}_\pm = 1/2 \left( \hat{\Sigma}_x \pm i \hat{\Sigma}_y \right) \). This Hamiltonian represents an example of a wide class of periodically driven quantum systems\[35\]. Such problems are generally solved perturbatively, in powers of \( c_0/(\hbar \omega) \), if the electron-field coupling is weak. The effective Hamiltonian for such problem has been shown to be
\[ \hat{H}_{eff}(k) \simeq H^\gamma_{ml}(k) + 1/(\hbar \omega) \left[ \hat{\Sigma}_x \hat{\Sigma}_y \right] + \frac{1}{2(\hbar \omega)^2} \left\{ \left[ \hat{\Sigma}_y, H^\gamma_{ml}(k) \right] \hat{\Sigma}_y + h.c. \right\} + \cdots \]
Evaluating this expression, we obtain
\[ \hat{H}_{eff}(k) = \hbar v_F k_x \left( 1 - \frac{\gamma_0 c_0^2}{2(\hbar \omega)^2} \right) \hat{\Sigma}_x + \hbar v_F \gamma_0 k_y \left( 1 - \frac{c_0^2}{2(\gamma_0 \hbar \omega)^2} \right) \hat{\Sigma}_y - \frac{c_0^2}{\hbar \omega} \gamma_0 \hat{\Sigma}_z. \]
Finally, the energy dispersion is given by
\[ \varepsilon_d(k) = \pm \left( \frac{\gamma_0 c_0^2}{\hbar \omega} \right) + \hbar^2 v_F^2 \left( \left( 1 - \frac{\gamma_0 c_0^2}{2(\hbar \omega)^2} \right) k_x^2 + \gamma_0^2 \left( 1 - \frac{c_0^2}{2(\gamma_0 \hbar \omega)^2} \right) k_y^2 \right)^{1/2}. \]
This result is an approximation. As we mentioned, in the case of an isotropic Dirac cone, electrons in graphene interacting with a circularly-polarized dressing field, the energy gap was found to be \[41,42\]
\[ \Delta_g/2 = \sqrt{\hbar^2 \omega^2 + 2 c_0^2 - \hbar \omega} \simeq \frac{c_0}{\hbar \omega} - \frac{1}{4} \left( \frac{c_0}{\hbar \omega} \right)^2 + \cdots, \]
while the Fermi velocity \( v_F \) is unaffected.

### B. Gapped anisotropic fermions

We now present a generalization of previously considered massless Dirac particles with a finite energy bandgap. Two different gaps added to both on- \( (\Delta_D) \) and off-diagonal terms \( (\Delta_O) \) of the Hamiltonian. Here, an anisotropic Dirac cone is combined with the energy gaps attributed to phosphorene, a single-layer structure. Even though this model does not exactly describe any of the fabricated black phosphorus structures, we consider it as an interesting mathematical generalization of the anisotropic Dirac fermions case, which may become relevant from a physical point of view. Apart from that, this is an intermediate case between phosphorene and few-layer gapless materials, which is expected to approximate the electronic properties of a system with a small number of phosphorus layers. We have
\( \mathcal{H}_g = E_i \hat{\mathbf{i}} \times \mathbf{x} + (\hbar v_F k_x + \Delta_O) \hat{\mathbf{y}} + \hbar v_F k_y \hat{\mathbf{y}} + \Delta_D \hat{\mathbf{z}} = \)

\[
= \begin{bmatrix}
E_i + \Delta_D & 0 \\
0 & E_i - \Delta_D
\end{bmatrix} + \Delta_O \begin{bmatrix}
0 & 1 \\
1 & 0
\end{bmatrix} + \hbar v_F \begin{bmatrix}
0 & k_x + i \gamma_0 k_y \\
k_x - i \gamma_0 k_y & 0
\end{bmatrix}.
\]

The corresponding energy dispersion is given by

\[
\epsilon_{\pm}(k) = E_0 \pm \left\{ \Delta_D^2 + [\Delta_O + \hbar v_F k_x]^2 + (\gamma_0 \hbar v_F k_y)^2 \right\}^{1/2}.
\]

We now address the interaction of these gapped Dirac electrons with the dressing linearly polarized field. The vector potential here is again specified by Eq. (6) and the new Hamiltonian is

\[
\hat{\mathcal{H}}(k) = \mathcal{H}_g(k) + \hat{h}_0,
\]

where \( \hat{h}_0 \) is identical to Eq. (28) since both equations share similar \( k \)-dependent terms. Following this approach, we expand the wave function for a finite wave vector \( \Psi_k(t) \) over the basis and obtain the following equations for the expansion coefficients \( \mathcal{F}^{\pm\gamma}(k_x, k_y | t) \)

\[
i\mathcal{F}^{\pm\gamma} = \pm \left\{ E_i + (\hbar v_F k_x + \Delta_O) \cos \theta_c + \gamma_0 \hbar v_F k_y \sin \theta_c \right\} \mathcal{F}^{\pm\gamma} +
+ i \left\{ -i\Delta_D \pm \gamma_0 \hbar v_F k_y \cos \theta_c \mp (\hbar v_F k_x + \Delta_O) \sin \theta_c \right\} \mathcal{F}^{\pm\gamma} \exp \left[ \pm 2i \frac{c_0}{\hbar \omega} \sin \omega t \right].
\]

Similar to our previous case, we introduce the following simplifying notation

\[
\phi^{(O)} = \tan^{-1} \left\{ \frac{\gamma_0 \hbar v_F k_y}{\hbar v_F k_x + \Delta_O} \right\},
\]

\[
\epsilon_O = \sqrt{(\hbar v_F k_x + \Delta_O)^2 + (\gamma_0 \hbar v_F k_y)^2}.
\]

After performing the Floquet theorem substitution and the expansions similar to the previously adopted procedure and we obtain

\[
\epsilon_d(k) \mathcal{F}^{\pm\gamma} = \left[ \mu \omega + E_i \pm \epsilon_O \cos(\phi^{(O)} - \theta_c) \right] \mathcal{F}^{\pm\gamma} +
+ \sum_{\lambda=-\infty}^{\infty} \left[ \Delta_D \pm i\epsilon_O \sin(\phi^{(O)} - \theta_c) \right] J_{\mu-\lambda} \left( \frac{\pm 2c_0}{\hbar \omega} \right) \mathcal{F}^{\pm\gamma}.
\]

It is interesting to note that the diagonal bandgap \( \Delta_D \) is now on the main diagonal and is affected by the Bessel function. The energy dispersions are now given by

\[
\epsilon_d(k) = E_i \pm \left\{ \epsilon_O \cos(\phi^{(O)} - \theta_c) \right\}^2 + \left[ \Delta_D^2 + \epsilon_O^2 \sin^2(\phi^{(O)} - \theta_c) \right] J_0^2 \left( \frac{2c_0}{\hbar \omega} \right) \right\}^{1/2},
\]

\[
\epsilon_O = \sqrt{(\hbar v_F k_x + \Delta_O)^2 + (\gamma_0 \hbar v_F k_y)^2}.
\]

If the electron-photon interaction is small, then \( \alpha_c = 2c_0/(\hbar \omega) \ll 1 \), the energy dispersion relation is approximated by

\[
(\epsilon_d(k) - E_i)^2 \approx (1 - \alpha_c^2) \Delta_D^2 + [1 - \alpha_c^2 \sin^2 \theta_c \gamma_0^2] (\hbar v_F k_x + \Delta_O)^2 + (\hbar v_F)^2 \gamma_0^2 [1 - \alpha_c^2 \cos^2 \theta_c \gamma_0^2]^2 k_y^2 +
+ 2 \gamma_0 \alpha_c \hbar v_F (\hbar v_F k_x + \Delta_O) k_y \sin(2\theta_c).
\]

From Eqs. (51) and (52) we note that the diagonal \( \Delta_D \) bandgap is decreased as \( \sim \alpha_c^2 \), similar to that for gapped graphene or the transition metal dichalcogenides, while the off-diagonal gap modification drastically depends on the direction of the radiation polarization. This behavior has no analogy in the previously considered structures. At the same time, the Fermi velocity components are modified similarly to that for anisotropic massless fermions.
V. CONCLUDING REMARKS

We have derived closed-form analytic expressions for electron-photon dressed states in one- and few layer black phosphorus. The energy gap is determined by the number of layers comprising the system, reaching its largest value for a single layer (phosphrene) and effectively vanishes for a few-layer structure. The latter case gives rise to anisotropic massless fermions, which exhibits an anisotropic Dirac cone. Since the anisotropy is the most significant and common property of all cases of BP, we focused on linearly polarized dressing field in an arbitrary direction. As a result, we demonstrated the Hamiltonian parameters are modified in an essentially different way compared to all isotropic Dirac systems. Anisotropy of the energy dispersion is modified in all directions, as well as all the electron effective masses. If both diagonal and off-diagonal gaps are present, the latter one remains unaffected, but only for a specific light polarization direction. For AMF’s interacting with circularly polarized light, the problem is mathematically identical with Dirac electrons irradiated by the field with elliptical polarization. In that case we found that initially absent energy bandgap is created and the non-equivalent Fermi velocities in various directions are renormalized. These results are expected to be of high importance for electronic device applications based on recently discovered and fabricated black phosphorus.

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1 J. C. Jamieson, Science 139, 1291 (1963).
2 L. Li, Y. Yu, G. J. Ye, Q. Ge, X. Ou, H. Wu, D. Feng, X. H. Chen, and Y. Zhang, Nat Nano 9, 372 (2014).
3 A. N. Rudenko and M. I. Katsnelson, Phys. Rev. B 89, 201408 (2014).
4 P. Li and I. Appelbaum, Phys. Rev. B 90, 115439 (2014).
5 J. Pereira Jr and M. Katsnelson, Physical Review B 92, 075437 (2015).
6 A. Rodin, A. Carvalho, and A. C. Neto, Physical review letters 112, 176801 (2014).
7 J. Qiao, X. Kong, Z.-X. Hu, F. Yang, and W. Ji, Nature communications 5 (2014).
8 X. Ling, H. Wang, S. Huang, F. Xia, and M. S. Dresselhaus, Proceedings of the National Academy of Sciences 112, 4523 (2015).
9 R. A. Doganov, E. C. O’Farrell, S. P. Koenig, Y. Yeo, A. Ziletti, A. Carvalho, D. K. Campbell, D. F. Coker, K. Watanabe, T. Taniguchi, et al., Nature communications 6 (2015).
10 O. Prytz and E. Flage-Larsen, Journal of Physics: Condensed Matter 22, 015502 (2009).
11 Y. Du, C. Ouyang, S. Shi, and M. Lei, Journal of Applied Physics 107, 093718 (2010).
12 S. P. Koenig, R. A. Doganov, H. Schmidt, A. Castro Neto, and B. Ozyilmaz, Applied Physics Letters 104, 103106 (2014).
13 K. Dolui and S. Y. Quek, Scientific Reports 5, 11699 (2015).
14 Q. Liu, X. Zhang, L. B. Abdalla, A. Fazzio, and A. Zunger, Nano Letters 15, 1222 (2015).
15 M. Buscema, D. J. Groenendijk, S. I. Blanter, G. A. Steele, H. S. van der Zant, and A. Castellanos-Gomez, Nano letters 14, 3347 (2014).
16 Z. Li, T. Cao, M. Wu, and S. G. Louie, arXiv preprint arXiv:1609.06030 (2016).
17 M. R. Masir, P. Vasilopoulos, A. Matulis, and F. Peeters, Physical Review B 77, 235443 (2008).
18 G. Gumbs, A. Iurov, D. Huang, P. Fekete, L. Zhemchuzhina, and M. R. Singh, in AIP Conference Proceedings (AIP, 2014), vol. 1590, pp. 134–142.
19 K. Novoselov, A. K. Geim, S. Morozov, D. Jiang, M. Katsnelson, I. Grigorieva, S. Dubonos, and A. Firsov, nature 438, 197 (2005).
20 A. K. Geim and K. S. Novoselov, Nature materials 6, 183 (2007).
21 A. C. Neto, F. Guinea, N. Peres, K. S. Novoselov, and A. K. Geim, Reviews of modern physics 81, 109 (2009).
22 M. Ezawa, Phys. Rev. Lett. 109, 055502 (2012).
23 C.-C. Liu, W. Feng, and Y. Yao, Phys. Rev. Lett. 107, 076802 (2011).
24 M. Ezawa, New Journal of Physics 14, 033003 (2012).
25 C. J. Tabert and E. J. Nicol, Phys. Rev. B 89, 195410 (2014).
26 A. Acun, L. Zhang, P. Bampoulis, M. Farmanbar, A. van Houselt, A. Rudenko, M. Lingenfelder, G. Brooks, B. Poelsema, M. Katsnelson, et al., J.J. Phys.: Condens. Matt. 27, 443002 (2015).
27 L. Li, S.-Z. Lu, J. Pan, Z. Qin, Y.-Q. Wang, Y. Wang, G.-y. Cao, S. Du, and H.-J. Gao, Adv. Mater. 26, 4820 (2014).
28 M. Dávila, L. Xian, S. Cahangirov, A. Rubio, and G. Le Lay, New J. Phys. 16, 095002 (2014).
29 P. Bampoulis, L. Zhang, A. Safaei, R. Van Gastel, B. Poelsema, and H. J. W. Zandvliet, J. Phys.: Condens. Matt. 26, 442001 (2014).
30 A. Kormányos, V. Zólyomi, N. D. Drummond, P. Rakyta, G. Burkard, and V. I. Fal’ko, Phys. Rev. B 88, 045416 (2013).
31 B. Radisavljevic, A. Radenovic, J. Brivio, i. V. Giacometti, and A. Kis, Nature nanotechnology 6, 147 (2011).
32 L. F. Torres, P. Perez-Piskunow, C. Balseiro, and G. Usaj, Physical review letters 113, 266801 (2014).
33 G. Usaj, P. Perez-Piskunow, L. F. Torres, and C. Balseiro, Physical Review B 90, 115423 (2014).
34 T. Mikami, S. Kitamura, K. Yasuda, N. Tsuji, T. Oka, and H. Aoki, Physical Review B 93, 144307 (2016).
35 H. L. Calvo, H. M. Pastawski, S. Roche, and L. E. F. Torres, Applied Physics Letters 98, 232103 (2011).
36 S. Morina, O. V. Kibis, A. Pervishko, and I. A. Shelykh, Physical Review B 91, 155312 (2015).
37 A. Pervishko, O. V. Kibis, S. Morina, and I. A. Shelykh, Physical Review B 92, 205403 (2015).
38 K. Dini, O. Kibis, and I. Shelykh, Physical Review B 93, 235411 (2016).
39 O. Kibis, O. Kyriienko, and I. Shelykh, Physical Review B 84, 195413 (2011).
40 O. Kibis, S. Morina, K. Dini, and I. Shelykh, Physical Review B 93, 115420 (2016).
41 K. Kristinsson, O. Kibis, S. Morina, and I. Shelykh, Scientific reports 6 (2016).
42 O. Kibis, Physical Review B 81, 165433 (2010).
43 A. Iurov, G. Gumbs, O. Roslyak, and D. Huang, Journal of Physics: Condensed Matter 24, 015303 (2011).
44 A. Iurov, G. Gumbs, O. Roslyak, and D. Huang, Journal of Physics: Condensed Matter 25, 135502 (2013).
45 A. Iurov, G. Gumbs, and D. Huang, Journal of Modern Optics pp. 1–8 (2016).
46 D. Yudin, O. Kibis, and I. Shelykh, New Journal of Physics 18, 103014 (2016).
47 O. Kibis, K. Dini, I. Iorsh, and I. Shelykh, arXiv preprint arXiv:1612.01000 (2016).
48 N. Goldman and J. Dalibard, Physical Review X 4, 031027 (2014).