

All-optical band engineering of gapped Dirac materialsO. V. Kibis,^{1,2,3,*} K. Dini,² I. V. Iorsh,^{3,4} and I. A. Shelykh^{2,4}¹*Department of Applied and Theoretical Physics, Novosibirsk State Technical University, Karl Marx Avenue 20, Novosibirsk 630073, Russia*²*Science Institute, University of Iceland, Dunhagi 3, IS-107 Reykjavik, Iceland*³*Division of Physics and Applied Physics, Nanyang Technological University 637371, Singapore*⁴*ITMO University, Saint Petersburg 197101, Russia*

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We demonstrate theoretically that the interaction of electrons in gapped Dirac materials (gapped graphene and transition-metal dichalcogenide monolayers) with a strong off-resonant electromagnetic field (dressing field) substantially renormalizes the band gaps and the spin-orbit splitting. Moreover, the renormalized electronic parameters drastically depend on the field polarization. Namely, a linearly polarized dressing field always decreases the band gap (and, particularly, can turn the gap into zero), whereas a circularly polarized field breaks the equivalence of valleys in different points of the Brillouin zone and can both increase and decrease corresponding band gaps. As a consequence, the dressing field can serve as an effective tool to control spin and valley properties of the materials and be potentially exploited in optoelectronic applications.

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I. INTRODUCTION

Advances in laser physics and microwave techniques achieved in recent decades have made possible the use of high-frequency fields as tools of flexible control of various atomic and condensed-matter structures (so-called “Floquet engineering” based on the Floquet theory of periodically driven quantum systems [1–5]). As a consequence, the properties of electronic systems driven by oscillating fields are actively studied to exploit unique features of composite states of field and matter. Particularly, an electron strongly coupled to an electromagnetic field—also known as “electron dressed by field” (dressed electron)—has become a commonly used model in modern physics [6,7]. Recently, the physical properties of dressed electrons were studied in various nanostructures, including quantum wells [8–13], quantum rings [14–17], graphene [18–25], and topological insulators [26–30]. Developing this excited scientific trend in the present paper, we elaborated the theory of dressed electrons for gapped Dirac materials.

The discovery of graphene—a monolayer of carbon atoms with linear (Dirac) dispersion of electrons [31–33]—initiated studies of the new class of artificial nanostructures known as Dirac materials. While graphene by itself is characterized by the gapless electron energy spectrum, many efforts have been dedicated towards fabrication Dirac materials with the band gap between the valence and conduction bands (gapped Dirac materials). The electron energy spectrum of the materials is parabolic near band edges but turns into the linear Dirac dispersion if the band gap vanishes. Therefore, electronic properties of gapped Dirac materials substantially depend on the value of the gap and, consequently, are prospective for nanoelectronic applications [34–36]. Although dressed condensed-matter structures have been the focus of attention for a long time, a consistent quantum theory of the gapped Dirac materials strongly coupled to light was not elaborated before. Since the electronic structure of Dirac materials differs

crucially from conventional condensed-matter structures, the known theory of light-matter coupling cannot be directly applied to the gapped Dirac materials. Moreover, it should be noted that gapped Dirac materials are currently considered as a basis for new generation of optoelectronic devices. Therefore, their optical properties deserve special consideration. This motivated us to fill this gap in the theory. To solve this problem in the present study, we will focus on the two gapped Dirac materials pictured schematically in Fig. 1. The first of them is the graphene layer grown on a hexagonal boron nitride substrate [37,38], where the band gap can be tuned in the broad range with an external gate voltage [39] [see Fig. 1(a)]. The second is a transition-metal dichalcogenide (TMDC) which is a monolayer of an atomically thin semiconductor of the type MX_2 , where M is a transition-metal atom (Mo, W, etc.) and X is a chalcogen atom (S, Se, or Te) [40,41] [see Fig. 1(b)]. The specific feature of the TMDC compounds is the giant spin-orbit coupling [42,43] which is attractive for use in novel spintronic and valleytronic devices [44].

Formally, electronic properties of these materials near the band edge can be described by the same two-band Hamiltonian

$$\hat{H} = \begin{pmatrix} \varepsilon_{\tau s}^c & \gamma(\tau k_x - ik_y) \\ \gamma(\tau k_x + ik_y) & \varepsilon_{\tau s}^v \end{pmatrix}, \quad (1)$$

where $\mathbf{k} = (k_x, k_y)$ is the electron wave vector in the layer plane, γ is the parameter describing electron dispersion,

$$\varepsilon_{\tau s}^c = \frac{\Delta_g}{2} + \frac{\tau s \Delta_{so}^c}{2} \quad (2)$$

is the energy of the conduction band edge,

$$\varepsilon_{\tau s}^v = -\frac{\Delta_g}{2} - \frac{\tau s \Delta_{so}^v}{2} \quad (3)$$

is the energy of the valence band edge, Δ_g is the band gap between the conduction band and the valence band, $\Delta_{so}^{c,v}$ is the spin-orbit splitting of the conduction (valence) band, $s = \pm 1$ is the spin index describing the different spin orientations, and $\tau = \pm 1$ is the valley index which corresponds to the two valleys in the different points of the Brillouin zone (the K and K' valleys in graphene [32] and the K and $-K$ valleys

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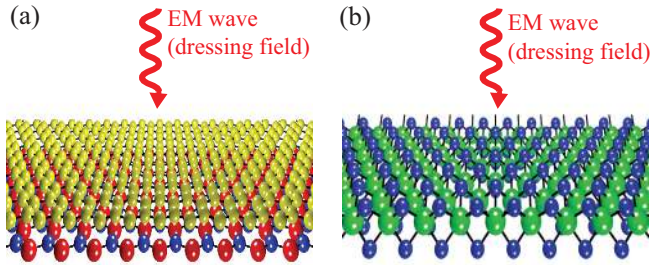


FIG. 1. Sketch of the considered gapped Dirac materials subject to an electromagnetic wave (dressing field): (a) Graphene grown on the substrate of hexagonal boron nitride; (b) transition-metal dichalcogenide monolayer MoS₂.

in TMDC monolayers [43]). If $\Delta_g \neq 0$ and $\Delta_{so}^{c,v} \neq 0$, the Hamiltonian (4) describes TMDC monolayer [43]. In the case of zero spin-orbit splitting, $\Delta_{so}^{c,v} = 0$, the Hamiltonian (4) describes gapped graphene [37], whereas the case of $\Delta_g = \Delta_{so}^{c,v} = 0$ corresponds to usual gapless graphene [32]. It should be noted that the two-band Hamiltonian (1) describes successfully low-energy electron states near the band edge. As to omitted terms corresponding to the trigonal-warping deformation of electron bands in monolayer graphene, they can be neglected if the Rashba spin-orbit coupling is stronger than the intrinsic spin-orbit coupling [45]. In the present paper, we elaborate the theory of electromagnetic dressing for electronic systems described by the low-energy Hamiltonian (1) and demonstrate that both the band gap and the spin splitting can be effectively controlled with the dressing field.

The paper is organized as follows. In Sec. II, we apply the conventional Floquet theory to derive the effective Hamiltonian describing stationary properties of dressed electrons. In Sec. III, we discuss the dependence of renormalized electronic characteristics of the dressed materials on parameters of the dressing field. The last two sections contain the Conclusion and Acknowledgments.

II. MODEL

Let us consider a gapped Dirac material with the Hamiltonian (1), which lies in the plane (x, y) at $z = 0$ and is subjected to an electromagnetic wave propagating along the z axis (see Fig. 1). The frequency of the wave, ω , is assumed to be far from all resonant frequencies of the electron system. Therefore, the electromagnetic wave cannot be absorbed by electrons near band edge and should be considered as a dressing field for the states around $\mathbf{k} = 0$. Considering the electron-field interaction within the minimal coupling approach, properties of dressed electrons can be described by the Hamiltonian

$$\hat{H}(\mathbf{k}) = \begin{pmatrix} 0 & |e|\gamma(\tau A_x - i A_y)/\hbar \\ |e|\gamma(\tau A_x + i A_y)/\hbar & 0 \end{pmatrix} + \begin{pmatrix} \varepsilon_{\tau s}^c & \gamma(\tau k_x - i k_y) \\ \gamma(\tau k_x + i k_y) & \varepsilon_{\tau s}^v \end{pmatrix}, \quad (4)$$

which can be easily obtained from the Hamiltonian of “bare” electrons (1) with the replacement $\mathbf{k} \rightarrow \mathbf{k} - (e/\hbar)\mathbf{A}$, where $\mathbf{A} = (A_x, A_y)$ is the vector potential of the dressing field, and e is the electron charge. It should be noted that the

quantum electrodynamics predicts the quadratic (in the vector potential) additions to the Hamiltonian (4) [46,47]. To avoid complication of the model, we will assume that the considered dressing field is classically strong and can be described successfully with the minimal coupling. In what follows, we will show that the properties of dressed electrons strongly depend on the polarization of the dressing field. Therefore, we have to discuss the solution of the corresponding Schrödinger problem for different polarizations successively.

Linearly polarized dressing field. Assuming the dressing field to be linearly polarized along the x axis, the vector potential can be written as

$$\mathbf{A} = \left(\frac{E_0}{\omega} \cos \omega t, 0 \right), \quad (5)$$

where E_0 is the electric field amplitude, and ω is the wave frequency. Correspondingly, the Hamiltonian of the dressed electron system (4) can be rewritten formally as

$$\hat{H}(\mathbf{k}) = \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_k, \quad (6)$$

where

$$\hat{\mathcal{H}}_0 = \begin{pmatrix} 0 & \Omega \tau \hbar \omega / 2 \\ \Omega \tau \hbar \omega / 2 & 0 \end{pmatrix} \cos \omega t \quad (7)$$

is the Hamiltonian of electron-field interaction,

$$\hat{\mathcal{H}}_k = \begin{pmatrix} \Delta_g/2 + \tau s \Delta_{so}^c/2 & \gamma(\tau k_x - i k_y) \\ \gamma(\tau k_x + i k_y) & -\Delta_g/2 - \tau s \Delta_{so}^v/2 \end{pmatrix} \quad (8)$$

is the Hamiltonian of “bare” electron, and

$$\Omega = \frac{2\gamma|e|E_0}{(\hbar\omega)^2} \quad (9)$$

is the dimensionless parameter describing the strength of electron coupling to the dressing field. The nonstationary Schrödinger equation with the Hamiltonian (7),

$$i\hbar \frac{\partial \psi_0}{\partial t} = \hat{\mathcal{H}}_0 \psi_0, \quad (10)$$

describes the time evolution of electron states at the band edge ($\mathbf{k} = 0$). The two exact solutions of the Schrödinger problem (10) read as

$$\psi_0^\pm = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix} \exp \left[\mp \frac{i\Omega\tau \sin \omega t}{2} \right]. \quad (11)$$

Since the two wave functions (11) form a complete basis at any fixed time t , we can seek solutions of the nonstationary Schrödinger equation with the full Hamiltonian (6) as an expansion

$$\psi_{\mathbf{k}} = a_1(t)\psi_0^+ + a_2(t)\psi_0^-. \quad (12)$$

Substituting the expansion (12) into the Schrödinger equation,

$$i\hbar \frac{\partial \psi_{\mathbf{k}}}{\partial t} = \hat{H}(\mathbf{k})\psi_{\mathbf{k}}, \quad (13)$$

we arrive at the expressions

$$i\hbar \dot{a}_1(t) = \left[\frac{\varepsilon_{\tau s}^c + \varepsilon_{\tau s}^v}{2} + \gamma \tau k_x \right] a_1(t) + \left[\frac{\varepsilon_{\tau s}^c - \varepsilon_{\tau s}^v}{2} + i\gamma k_y \right] e^{i\Omega\tau \sin \omega t} a_2(t),$$

$$i\hbar\dot{a}_2(t) = \left[\frac{\varepsilon_{\tau s}^c + \varepsilon_{\tau s}^v}{2} - \gamma\tau k_x \right] a_2(t) + \left[\frac{\varepsilon_{\tau s}^c - \varepsilon_{\tau s}^v}{2} - i\gamma k_y \right] e^{-i\Omega\tau \sin\omega t} a_1(t). \quad (14)$$

It follows from the conventional Floquet theory of quantum systems driven by an oscillating field [1–3] that the sought wave function (12) must have the form $\Psi(\mathbf{r}, t) = e^{-i\tilde{\varepsilon}(\mathbf{k})t/\hbar} \phi(\mathbf{r}, t)$, where the function $\phi(\mathbf{r}, t)$ periodically depends on time, $\phi(\mathbf{r}, t) = \phi(\mathbf{r}, t + 2\pi/\omega)$, and $\tilde{\varepsilon}(\mathbf{k})$ is the quasienergy of an electron. Since the quasienergy (the energy of dressed electrons) is the physical quantity which plays the same role in quantum systems driven by an oscillating field as the usual energy in stationary ones, the present analysis of the Schrödinger problem (13) should be aimed to find the energy spectrum, $\tilde{\varepsilon}(\mathbf{k})$. It follows from the periodicity of the function $\phi(\mathbf{r}, t)$ that one can seek the coefficients $a_{1,2}(t)$ in Eq. (12) as a Fourier expansion,

$$a_{1,2}(t) = e^{-i\tilde{\varepsilon}(\mathbf{k})t/\hbar} \sum_{n=-\infty}^{\infty} a_{1,2}^{(n)} e^{in\omega t}. \quad (15)$$

Substituting the expansion (15) into Eq. (14) and applying the Jacobi-Anger expansion,

$$e^{iz \sin\theta} = \sum_{n=-\infty}^{\infty} J_n(z) e^{in\theta},$$

one can rewrite the equations of quantum dynamics (14) in the time-independent form,

$$\sum_{n'=-\infty}^{\infty} \sum_{j=1}^2 \mathcal{H}_{ij}^{(nn')} a_j^{(n')} = \tilde{\varepsilon}(\mathbf{k}) a_i^{(n)}, \quad (16)$$

where $J_n(z)$ is the Bessel function of the first kind, and $\mathcal{H}_{ij}^{(nn')}$ is the stationary Hamiltonian of a dressed electron in the Floquet space with the matrix elements

$$\begin{aligned} \mathcal{H}_{12}^{(nn')} &= \left[\frac{\varepsilon_{\tau s}^c - \varepsilon_{\tau s}^v}{2} + i\gamma k_y \right] J_{n'-n}(\Omega\tau), \\ \mathcal{H}_{21}^{(nn')} &= \left[\frac{\varepsilon_{\tau s}^c - \varepsilon_{\tau s}^v}{2} - i\gamma k_y \right] J_{n'-n}(\Omega\tau), \\ \mathcal{H}_{11}^{(nn')} &= \left[\frac{\varepsilon_{\tau s}^c + \varepsilon_{\tau s}^v}{2} + \gamma\tau k_x + n\hbar\omega \right] \delta_{nn'}, \\ \mathcal{H}_{22}^{(nn')} &= \left[\frac{\varepsilon_{\tau s}^c + \varepsilon_{\tau s}^v}{2} - \gamma\tau k_x + n\hbar\omega \right] \delta_{nn'}, \end{aligned} \quad (17)$$

where $\delta_{nn'}$ is the Kronecker delta. It should be noted that the Schrödinger equation (16) describes still exactly the initial Schrödinger problem (13). Next we will make some approximations.

In what follows, let us assume that the field frequency, ω , is high enough to satisfy the condition

$$\left| \frac{\mathcal{H}_{ij}^{(0n)}}{\mathcal{H}_{ii}^{(00)} - \mathcal{H}_{jj}^{(nn)}} \right| \ll 1 \quad (18)$$

for $n \neq 0$ and $i \neq j$. Mathematically, the condition (18) makes it possible to treat nondiagonal matrix elements of

the Hamiltonian (17) with $n \neq n'$ as a small perturbation which can be omitted in the first-order approximation of the conventional perturbation theory for matrix Hamiltonians (see, e.g., Ref. [48]). Since the condition (18) corresponds to an off-resonant field, the field can be neither absorbed nor emitted by the electrons. As a consequence, the main contribution to the Schrödinger equation (16) under the condition (18) stems from terms with $n, n' = 0$, which describe the elastic interaction between an electron and the field. Neglecting the small terms with $n, n' \neq 0$, the Schrödinger equation (16) can be rewritten in the simple form

$$\sum_{j=1}^2 \mathcal{H}_{ij}^{(00)} a_j^{(0)} = \tilde{\varepsilon}(\mathbf{k}) a_i^{(0)}, \quad (19)$$

where $\mathcal{H}_{ij}^{(00)}$ is the 2×2 Hamiltonian with the matrix elements (17). Subjecting this Hamiltonian to the unitary transformation

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix},$$

we arrive at the effective stationary Hamiltonian of electrons dressed by a linearly polarized field, $\hat{\mathcal{H}}_{\text{eff}} = U^\dagger \mathcal{H}^{(00)} U$, which is given by the matrix

$$\hat{\mathcal{H}}_{\text{eff}}(\mathbf{k}) = \begin{pmatrix} \tilde{\Delta}_g/2 + \tau s \tilde{\Delta}_{so}^c/2 & \tau \tilde{\gamma}_x k_x - i \tilde{\gamma}_y k_y \\ \tau \tilde{\gamma}_x k_x + i \tilde{\gamma}_y k_y & -\tilde{\Delta}_g/2 - \tau s \tilde{\Delta}_{so}^v/2 \end{pmatrix}, \quad (20)$$

where

$$\tilde{\Delta}_g = \Delta_g J_0(\Omega) \quad (21)$$

is the effective band gap,

$$\tilde{\Delta}_{so}^c = \frac{\Delta_{so}^c - \Delta_{so}^v}{2} + \frac{\Delta_{so}^c + \Delta_{so}^v}{2} J_0(\Omega) \quad (22)$$

is the effective spin splitting of the conduction band,

$$\tilde{\Delta}_{so}^v = \frac{\Delta_{so}^v - \Delta_{so}^c}{2} + \frac{\Delta_{so}^c + \Delta_{so}^v}{2} J_0(\Omega) \quad (23)$$

is the effective spin splitting of the valence band, and

$$\tilde{\gamma}_x = \gamma, \quad \tilde{\gamma}_y = \gamma J_0(\Omega) \quad (24)$$

are the effective parameters of electron dispersion along the x, y axes. The eigenenergy of the effective Hamiltonian (20),

$$\begin{aligned} \tilde{\varepsilon}_{\tau s}^{\pm}(\mathbf{k}) &= \frac{\tau s (\tilde{\Delta}_{so}^c - \tilde{\Delta}_{so}^v)}{4} \\ &\pm \sqrt{\left[\frac{2\tilde{\Delta}_g + \tau s (\tilde{\Delta}_{so}^c + \tilde{\Delta}_{so}^v)}{4} \right]^2 + \tilde{\gamma}_x^2 k_x^2 + \tilde{\gamma}_y^2 k_y^2}, \end{aligned} \quad (25)$$

is the sought energy spectrum of electrons dressed by the linearly polarized field. Mathematically, the unperturbed Hamiltonian (1) is equal to the effective Hamiltonian (20) with the formal replacements $\Delta_g \rightarrow \tilde{\Delta}_g$, $\Delta_{so}^{c,v} \rightarrow \tilde{\Delta}_{so}^{c,v}$, and $\gamma_{x,y} \rightarrow \tilde{\gamma}_{x,y}$. Therefore, the behavior of a dressed electron is similar to the behavior of a “bare” electron with the renormalized band parameters (21)–(24). It should be noted that the effective Hamiltonian (20) is derived under the condition (18). Taking into account Eq. (17), the condition (18)

can be rewritten as $\gamma k, \Delta_g \ll \hbar\omega$. Therefore, the effective Hamiltonian is applicable to describe the dynamics of a dressed electron near the band edge if the photon energy of the dressed field, $\hbar\omega$, substantially exceeds the band gap, Δ_g . It should be noted that such high-energy photons will lead to direct electron transitions between the valence band and the conduction band. However, the transitions take place very far from the band edge and do not affect the considered renormalization of low-energy electron states.

Circularly polarized dressing field. For the case of a circularly polarized electromagnetic wave, the vector potential $\mathbf{A} = (A_x, A_y)$ can be written as

$$\mathbf{A} = \left(\frac{E_0}{\omega} \cos \xi \omega t, \frac{E_0}{\omega} \sin \xi \omega t \right), \quad (26)$$

where the different chirality indices $\xi = \pm 1$ correspond to the clockwise/counterclockwise circular polarizations. First of all, let us consider electron states at the wave vector $\mathbf{k} = 0$, where the Hamiltonian (4) can be written in the form

$$\hat{\mathcal{H}}(0) = \begin{pmatrix} \varepsilon_{\tau s}^c & -(\hbar\omega\Omega\tau/2)e^{-i\tau\xi\omega t} \\ -(\hbar\omega\Omega\tau/2)e^{i\tau\xi\omega t} & \varepsilon_{\tau s}^v \end{pmatrix}, \quad (27)$$

which is similar to the well-known Hamiltonian of magnetic resonance. The corresponding nonstationary Schrödinger equation,

$$i\hbar \frac{\partial \psi_{\tau s}(0)}{\partial t} = \hat{\mathcal{H}}(0)\psi_{\tau s}(0), \quad (28)$$

describes the time evolution of electron states at the wave vector $\mathbf{k} = 0$. Solutions of Eq. (28) can be sought as

$$\psi_{\tau s}^{\pm}(0) = e^{-i\tilde{\varepsilon}_{\tau s}^{\pm}(0)t/\hbar} \begin{pmatrix} A_{\pm} e^{-i\tau\xi\omega t/2} \\ B_{\pm} e^{i\tau\xi\omega t/2} \end{pmatrix}, \quad (29)$$

where $\tilde{\varepsilon}_{\tau s}^{\pm}(0)$, A_{\pm} , and B_{\pm} are the undefined constants. Substituting the wave function (29) into the Schrödinger equation (28) with the Hamiltonian (27), we arrive at the system of two algebraic equations,

$$\begin{aligned} A_{\pm} \left[\varepsilon_{\tau s}^c - \tau\xi \frac{\hbar\omega}{2} (1 \mp 1) - \tilde{\varepsilon}_{\tau s}^{\pm}(0) \right] - B_{\pm} \frac{\hbar\omega\Omega\tau}{2} &= 0, \\ A_{\pm} \frac{\hbar\omega\Omega\tau}{2} - B_{\pm} \left[\varepsilon_{\tau s}^v + \tau\xi \frac{\hbar\omega}{2} (1 \pm 1) - \tilde{\varepsilon}_{\tau s}^{\pm}(0) \right] &= 0, \end{aligned} \quad (30)$$

which can be easily solved. As a result, the two orthonormal exact solutions of the Schrödinger problem (28) are

$$\begin{aligned} \psi_{\tau s}^{\pm}(0) &= e^{-i\tilde{\varepsilon}_{\tau s}^{\pm}(0)t/\hbar} e^{\pm i\tau\xi\omega t/2} \\ &\times \begin{pmatrix} \mp \left[\frac{\sqrt{\Omega^2 + \delta^2 \pm |\delta|}}{2\sqrt{\Omega^2 + \delta^2}} \right]^{1/2} e^{-i\tau\xi\omega t/2} \\ \text{sgn}(\delta) \left[\frac{\sqrt{\Omega^2 + \delta^2 \mp |\delta|}}{2\sqrt{\Omega^2 + \delta^2}} \right]^{1/2} e^{i\tau\xi\omega t/2} \end{pmatrix}, \end{aligned} \quad (31)$$

where

$$\tilde{\varepsilon}_{\tau s}^{\pm}(0) = \frac{\varepsilon_{\tau s}^c + \varepsilon_{\tau s}^v}{2} \pm \tau\xi \frac{\hbar\omega}{2} \pm \text{sgn}(\delta) \frac{\hbar\omega}{2} \sqrt{\Omega^2 + \delta^2} \quad (32)$$

is the quasienergy (energy of a dressed electron in the conduction/valence band) at $\mathbf{k} = 0$, and

$$\delta = \frac{\varepsilon_{\tau s}^c - \varepsilon_{\tau s}^v - \tau\xi\hbar\omega}{\hbar\omega}$$

is the resonance detuning assumed to be nonzero in order to avoid the field absorption near the band edge. Correspondingly, the effective stationary Hamiltonian of dressed electron states at $\mathbf{k} = 0$ can be written in the basis (31) as

$$\hat{\mathcal{H}}_{\text{eff}}(0) = \begin{pmatrix} \tilde{\varepsilon}_{\tau s}^+(0) & 0 \\ 0 & \tilde{\varepsilon}_{\tau s}^-(0) \end{pmatrix}. \quad (33)$$

In order to find the energy spectrum of a dressed electron at the wave vector $\mathbf{k} \neq 0$, let us restrict the consideration by the case of $\Omega \ll 1$, which corresponds physically to high frequencies ω [see Eq. (9)]. Expanding the electron wave function, $\psi_{\tau s}(\mathbf{k})$, on the basis (31),

$$\psi_{\tau s}(\mathbf{k}) = a^+(t) e^{i\tilde{\varepsilon}_{\tau s}^+(0)t/\hbar} \psi_{\tau s}^+(0) + a^-(t) e^{i\tilde{\varepsilon}_{\tau s}^-(0)t/\hbar} \psi_{\tau s}^-(0), \quad (34)$$

and substituting the expansion (34) into the Schrödinger equation with the total Hamiltonian (4), we arrive at the system of equations

$$\begin{aligned} i\hbar \dot{a}^+(t) &\approx \tilde{\varepsilon}_{\tau s}^+(0) a^+(t) - \text{sgn}(\delta) \gamma (\tau k_x - i k_y) a^-(t), \\ i\hbar \dot{a}^-(t) &\approx \tilde{\varepsilon}_{\tau s}^-(0) a^-(t) - \text{sgn}(\delta) \gamma (\tau k_x + i k_y) a^+(t). \end{aligned} \quad (35)$$

The quantum dynamics equations (35) are equal to the stationary Schrödinger equation,

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} a^+(t) \\ a^-(t) \end{pmatrix} = \hat{\mathcal{H}}_{\text{eff}}(\mathbf{k}) \begin{pmatrix} a^+(t) \\ a^-(t) \end{pmatrix},$$

where

$$\hat{\mathcal{H}}_{\text{eff}}(\mathbf{k}) = \begin{pmatrix} \tilde{\varepsilon}_{\tau s}^+(0) & -\text{sgn}(\delta) \gamma (\tau k_x - i k_y) \\ -\text{sgn}(\delta) \gamma (\tau k_x + i k_y) & \tilde{\varepsilon}_{\tau s}^-(0) \end{pmatrix} \quad (36)$$

is the effective stationary Hamiltonian of the considered system. The eigenenergy of the Hamiltonian,

$$\tilde{\varepsilon}_{\tau s}^{\pm}(\mathbf{k}) = \frac{\tilde{\varepsilon}_{\tau s}^+(0) + \tilde{\varepsilon}_{\tau s}^-(0)}{2} \pm \sqrt{\left[\frac{\tilde{\varepsilon}_{\tau s}^+(0) - \tilde{\varepsilon}_{\tau s}^-(0)}{2} \right]^2 + (\gamma k)^2}, \quad (37)$$

presents the sought energy spectrum of dressed electrons. If $\Delta_g = \Delta_{so}^{c,v} = 0$, Eq. (37) exactly coincides with the known spectrum of electrons in gapless graphene irradiated by a circularly polarized light [25]. It follows from Eq. (37) that the renormalized band gap is

$$\begin{aligned} \tilde{\Delta}_g &= \tau\xi\hbar\omega + \text{sgn}(\Delta_g - \tau\xi\hbar\omega) \hbar\omega \sqrt{\Omega^2 + \left[\frac{\Delta_g - \tau\xi\hbar\omega}{\hbar\omega} \right]^2} \\ &\approx \tau\xi\hbar\omega - \sqrt{\Omega^2 + 1} \left(\tau\xi\hbar\omega - \frac{\Delta_g}{\Omega^2 + 1} \right), \end{aligned} \quad (38)$$

where the last equality holds under condition $\hbar\omega \gg \Delta_g$. The spin splittings in the conduction and valence bands can be written in simple form for the two limiting cases:

$$\tilde{\Delta}_{so}^{c,v} = \pm \frac{\Delta_{so}^c - \Delta_{so}^v}{2} + \frac{\Delta_{so}^c + \Delta_{so}^v}{2\sqrt{1 + \Omega^2}}, \quad \hbar\omega \gg \Delta_g, \quad (39)$$

and

$$\begin{aligned} \tilde{\Delta}_{so}^{c,v} &= \pm \frac{\Delta_{so}^c - \Delta_{so}^v}{2} + \frac{\Delta_{so}^c + \Delta_{so}^v}{2} \left[1 - \frac{\Omega^2 (\hbar\omega)^2}{2 \Delta_g^2} \right], \\ \hbar\omega &\ll \Delta_g. \end{aligned} \quad (40)$$

As expected, the renormalized band gap (38) and spin splittings (39)–(40) turn into their “bare” values, Δ_g and $\Delta_{so}^{c,v}$, if the dressing field is absent ($E_0 \rightarrow 0$).

Elliptically polarized dressing field. Assuming the large axis of polarization ellipse to be oriented along the x axis, the vector potential of arbitrary polarized electromagnetic wave, $\mathbf{A} = (A_x, A_y)$, can be written as

$$\mathbf{A} = \frac{E_0}{\omega} (\cos \omega t, \sin \theta \sin \omega t), \quad (41)$$

where $\theta \in [-\pi/2, \pi/2]$ is the polarization phase: the polarization is linear for $\theta = 0$, circular for $\theta = \pm\pi/2$, and elliptical for other phases θ . Substituting the vector potential (41) into Eq. (4), we can write the total Hamiltonian (4) as

$$\hat{\mathcal{H}}(\mathbf{k}) = \hat{\mathcal{H}}_{\mathbf{k}} + (\hat{V} e^{i\omega t} + \hat{V}^\dagger e^{-i\omega t}), \quad (42)$$

where the Hamiltonian $\hat{\mathcal{H}}_{\mathbf{k}}$ is given by Eq. (8) and

$$\hat{V} = \frac{\hbar\omega\Omega}{4} \begin{pmatrix} 0 & \tau - \sin \theta \\ \tau + \sin \theta & 0 \end{pmatrix} \quad (43)$$

is the operator of electron interaction with the dressing field (41). Generally, the effective stationary Hamiltonian of an electron driven by an oscillating field can be sought in the form [3]

$$\hat{\mathcal{H}}_{\text{eff}}(\mathbf{k}) = e^{i\hat{F}(t)} \hat{\mathcal{H}}(\mathbf{k}) e^{-i\hat{F}(t)} + i \left(\frac{\partial e^{i\hat{F}(t)}}{\partial t} \right) e^{-i\hat{F}(t)}, \quad (44)$$

where $\hat{F}(t)$ is the anti-Hermitian operator which is periodical with the period of the oscillating field, $\hat{F}(t) = \hat{F}(t + 2\pi/\omega)$. In the particular case of weak electron-field coupling, $\Omega \ll 1$, this operator and the effective Hamiltonian (44) can be easily found as power series expansions,

$$\hat{F}(t) = \sum_{n=1}^{\infty} \frac{F^{(n)}(t)}{\omega^n}, \quad \hat{\mathcal{H}}_{\text{eff}}(\mathbf{k}) = \sum_{n=0}^{\infty} \frac{\hat{\mathcal{H}}_{\text{eff}}^{(n)}(\mathbf{k})}{\omega^n}, \quad (45)$$

where $F^{(n)}(t) \sim \Omega^n$ (the Floquet-Magnus expansion [3]). Substituting the expansions (45) into Eq. (44) and restricting the accuracy by terms $\sim \Omega^2$, we arrive at the effective Hamiltonian

$$\hat{\mathcal{H}}_{\text{eff}}(\mathbf{k}) = \hat{\mathcal{H}}_{\mathbf{k}} + \frac{[\hat{V}, \hat{V}^\dagger]}{\hbar\omega} + \frac{[[\hat{V}, \hat{\mathcal{H}}_{\mathbf{k}}], \hat{V}^\dagger] + \text{H.c.}}{2(\hbar\omega)^2}. \quad (46)$$

Taking into account Eqs. (8) and (43), the effective stationary Hamiltonian (46) can be written as a matrix (20), where

$$\tilde{\Delta}_g = \Delta_g \left[1 - \frac{\Omega^2}{4} (1 + \sin^2 \theta) \right] - \frac{\tau \hbar \omega \Omega^2}{2} \sin \theta, \quad (47)$$

$$\tilde{\Delta}_{so}^{c,v} = \pm \frac{\Delta_{so}^c - \Delta_{so}^v}{2} + \frac{\Delta_{so}^c + \Delta_{so}^v}{2} \times \left[1 - \frac{\Omega^2}{4} (1 + \sin^2 \theta) \right], \quad (48)$$

$$\tilde{\gamma}_x = \gamma \left[1 - \frac{\Omega^2}{4} \sin^2 \theta \right], \quad \tilde{\gamma}_y = \gamma \left[1 - \frac{\Omega^2}{4} \right] \quad (49)$$

are the band parameters renormalized by an elliptically polarized dressing field. Correspondingly, the eigenenergy of the effective Hamiltonian (46) represents the sought energy

spectrum of dressed electrons,

$$\tilde{\epsilon}_{\tau s}^{\pm}(\mathbf{k}) = \frac{\tau s (\tilde{\Delta}_{so}^c - \tilde{\Delta}_{so}^v)}{4} \pm \sqrt{\left[\frac{2\tilde{\Delta}_g + \tau s (\tilde{\Delta}_{so}^c + \tilde{\Delta}_{so}^v)}{4} \right]^2 + \tilde{\gamma}_x^2 k_x^2 + \tilde{\gamma}_y^2 k_y^2}, \quad (50)$$

with the renormalized band parameters (47)–(49). It should be stressed that the effective Hamiltonian (20) with the band parameters (47)–(49), which describes electrons dressed by an arbitrary polarized weak field, is derived under the assumption of small coupling constant (9) and high frequency, ω . On the contrary, the effective Hamiltonian (20) with the band parameters (21)–(24) and the effective Hamiltonian (33) are suitable to describe electrons dressed by linearly and circularly polarized dressing fields of arbitrary intensity. As a consequence, the band parameters (21)–(24) and (38)–(39) turn into the band parameters (47)–(49) for $\Omega \ll 1, \hbar\omega \gg \Delta_g$, and $\theta = 0, \pm\pi/2$.

III. RESULTS AND DISCUSSION

First of all, let us apply the developed theory to gapped graphene, assuming $\tilde{\Delta}_{so}^{c,v} = 0$ in all derived expressions. The electron dispersion in gapped graphene, $\tilde{\epsilon}(\mathbf{k})$, is plotted in Fig. 2 for the particular cases of linearly and circularly polarized dressing fields. In the absence of the dressing field, the electron dispersion is isotropic in the graphene plane [see the solid lines in Figs. 2(a) and 2(b)]. However, a linearly polarized field breaks the equivalence of the x, y axes [see Eq. (25)]. As a consequence, the anisotropy of the electron dispersion along the wave vectors k_x and k_y appears [see the dashed and dotted lines in Figs. 2(a) and 2(b)]. In contrast to the linear polarization, a circularly polarized dressing field does not induce the in-plane anisotropy [see Eq. (37)]. However, the electron dispersion is substantially different for clockwise and counterclockwise polarizations [see the dashed and dotted lines in Fig. 2(c)]. Moreover, both linearly and circularly polarized fields renormalize the band gap (see Fig. 3). Mathematically, the dependence of the renormalized band gap, $|\tilde{\Delta}_g|$, on the irradiation intensity, $I \sim E_0^2$, is given by Eqs. (21) and (38) [which are plotted in Fig. 3(a)] and Eq. (47) [which is plotted in Fig. 3(b)]. It should be noted that Eq. (38) correctly describes the gap for any off-resonant frequencies ω , whereas Eqs. (21) and (47) are derived under the condition $\hbar\omega \gg \Delta_g$ and, therefore, applicable only to small gaps. However, the gap can be gate-tunable in the broad range, $\Delta_g = 1\text{--}60$ meV [37–39]. Assuming the gap to be of meV scale and the field frequency to be in the terahertz range, we can easily satisfy this condition. It follows from Eqs. (21), (32), and (47) that the renormalized gap, $\tilde{\Delta}_g$, crucially depends on the field polarization. Particularly, the clockwise/counterclockwise circularly polarized field (polarization indices $\xi = \pm 1$) differently interacts with electrons from different valleys of the Brillouin zone (valley indices $\tau = \pm 1$). Namely, for the case of $\tau\xi = -1$, the value of the gap monotonously increases with intensity [see the dashed line in Fig. 3(a)]. On the contrary, for the case of $\tau\xi = 1$, the gap first decreases to zero and then starts to grow [see the solid

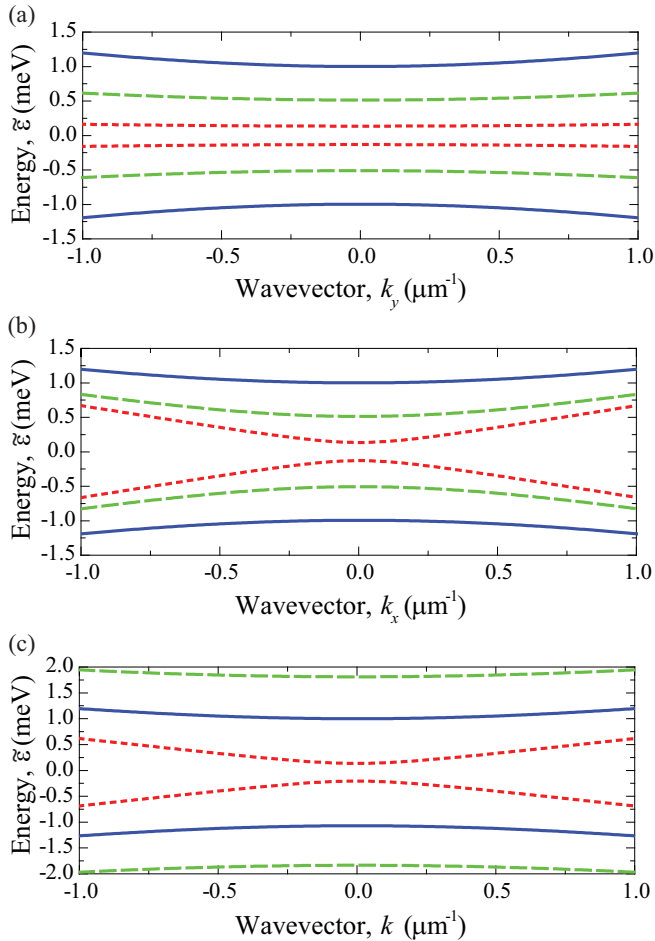


FIG. 2. The energy spectrum of dressed electron, $\tilde{\varepsilon}(\mathbf{k})$, near the band edge of gapped graphene ($\Delta_g = 2$ meV, $\gamma/\hbar = 10^6$ m/s) irradiated by a dressing field with the photon energy $\hbar\omega = 10$ meV and the different intensities, I . In parts (a) and (b) the dressing field is linearly polarized along the x axis; the irradiation intensities are $I = 0$ (solid lines), $I = 7.5$ kW/cm² (dashed lines), and $I = 15$ kW/cm² (dotted lines). In part (c) the dressing field is circularly polarized; the solid line describes the energy spectrum of “bare” electron ($I = 0$), whereas the dotted and dashed lines correspond to the different circular polarizations ($\tau\xi = -1$ and $\tau\xi = 1$, respectively) with the same irradiation intensity $I = 300$ W/cm².

line in Fig. 3(a)]. This light-induced difference in the band gaps for the two different valleys is formally equivalent to the appearance of an effective magnetic field acting on the valley pseudospin and, therefore, can be potentially used in valleytronics applications. It should be noted that this optically induced lifting of valley degeneracy has been observed for TMDC in recent experiments [49] which are in reasonable agreement with the present theory. As to linearly polarized dressing field, it always quenches the band gap and can even turn it into zero [see the dotted line in Fig. 3(a)]. Formally, the collapse of the band gap originates from zeros of the Bessel function in Eq. (21). Since the linearly and circularly polarized fields change the gap value oppositely, there are field polarizations which do not change the gap. The polarization phases, θ , corresponding to such polarizations are marked by the dashed lines in Fig. 3(b).

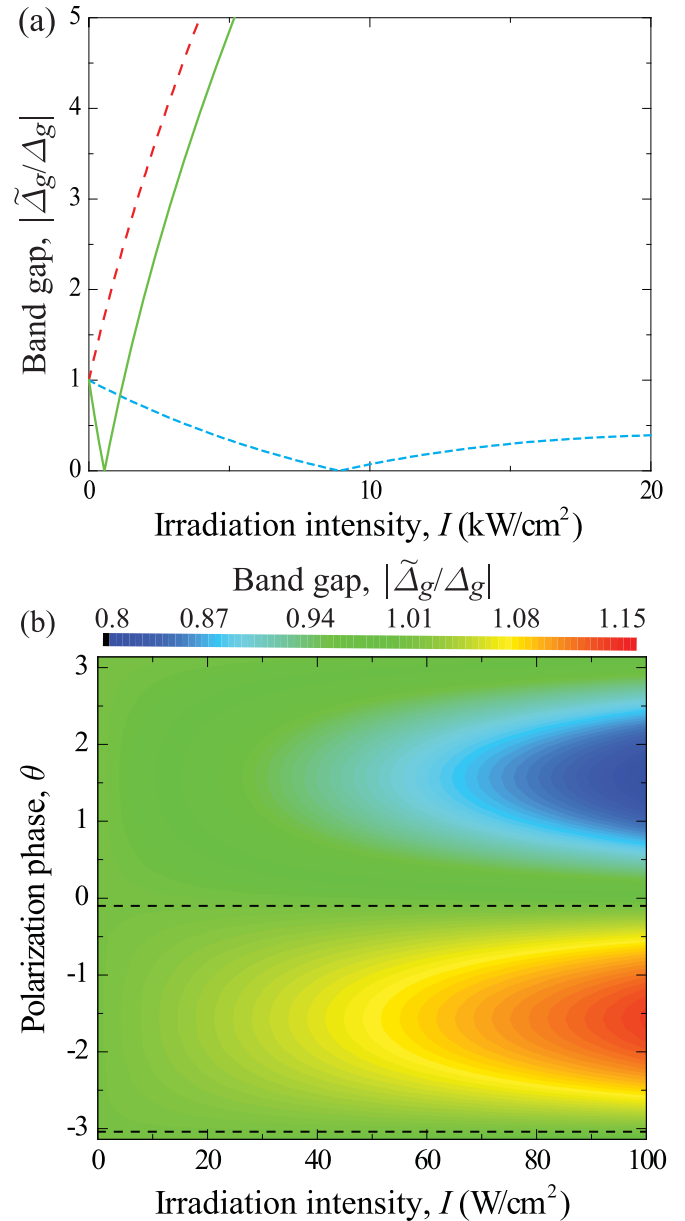


FIG. 3. Dependence of the band gap in irradiated gapped graphene ($\Delta_g = 2$ meV, $\gamma/\hbar = 10^6$ m/s) on the irradiation intensity, I , and the polarization, θ , for the photon energy $\hbar\omega = 10$ meV. In part (a) the dotted line corresponds to the linearly polarized dressing field, whereas the dashed and solid lines correspond to the different circular polarizations ($\tau\xi = -1$ and $\tau\xi = 1$, respectively). In part (b) the dashed lines correspond to the polarizations, θ , which do not change the band gap.

Applying the elaborated theory to analyze the renormalized spin splitting in TMDC monolayers, let us restrict the consideration by the most examined TMDC monolayer MoS₂. The dependence of the spin splitting on the dressing field is described by Eqs. (22) and (23) for the case of a linearly polarized field, Eqs. (39) and (40) for the case of a circularly polarized field, and Eq. (48) for an arbitrary polarized field. It follows from analysis of these expressions that the most pronounced renormalization of the splitting takes place for a circularly polarized field. The dependence of the field-induced

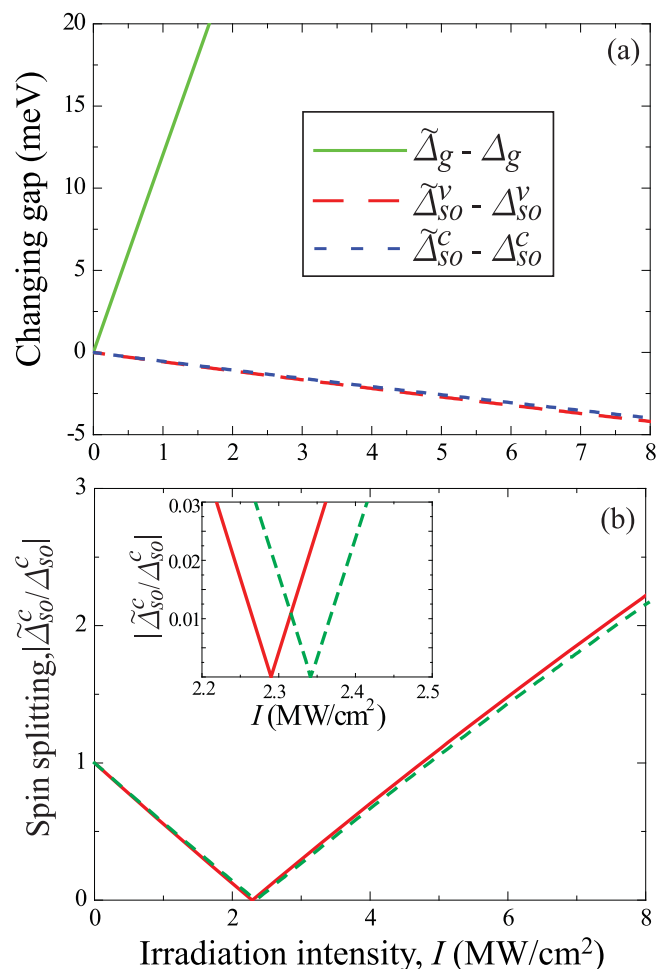


FIG. 4. Dependence of the band gap, $\tilde{\Delta}_g$, and the spin splitting of conduction and valence bands, $\tilde{\Delta}_{so}^{c,v}$, on the irradiation intensity for MoS₂ monolayer ($\Delta_g = 1.58$ eV, $\Delta_{so}^c = 3$ meV, $\Delta_{so}^v = 147$ meV, $\gamma/\hbar = 7.7 \times 10^5$ m/s) irradiated by a circularly polarized field with the photon energy $\hbar\omega = 10$ meV: (a) The field-induced changing of the band gap and the spin splitting for the circularly polarized field with $\tau\xi = -1$; (b) The renormalized spin-splitting of conduction band for different field polarizations (the solid and dashed lines correspond to $\tau\xi = -1$ and $\tau\xi = 1$, respectively).

renormalization of the band gap, $\tilde{\Delta}_g$, and the spin splitting, $\tilde{\Delta}_{so}^{c,v}$, in MoS₂ monolayer on the field intensity, $I \sim E_0^2$, is plotted in Fig. 4 for such a field. It is seen in Fig. 4(a) that absolute values of the field-induced renormalization are of the same order for both the band gap, $\tilde{\Delta}_g - \Delta_g$, and the spin splitting, $\tilde{\Delta}_{so}^{c,v} - \Delta_{so}^{c,v}$. However, the unperturbed spin splitting of the conduction band, Δ_{so}^c , is small as compared to both the unperturbed band gap, Δ_g , and the unperturbed spin splitting of the valence band, Δ_{so}^v (see Ref. [43]). Therefore, the relative field-induced renormalization, $|\tilde{\Delta}_{so}^c/\Delta_{so}^c|$, is most pronounced for the spin splitting of the conduction band [see Fig. 4(b)]. It should be stressed that the renormalized splitting depends on the product of the polarization and valley indices, $\tau\xi = \pm 1$, and can be turned into zero by a dressing field [see Fig. 4(b)]. It should be noted also that the renormalization of both band gap and spin splitting is the result of mixing electron states from the valence and conduction bands by the field. Therefore, the

renormalized band parameters strongly depend on the value of the “bare” band gap, Δ_g . In contrast to gapped graphene with band gaps of meV scale, TMDC monolayers have band gaps of eV scale [43]. As a consequence, the considered terahertz photons effect on the gaps of TMDC is very weak (in contrast to the previously considered case of narrow-gapped graphene). Particularly, it follows from this that the irradiation intensity which collapses the spin splitting in TMDC monolayers [see Fig. 4(b)] is much larger than the intensity collapsing the band gap in gapped graphene [see Fig. 3(a)].

It should be noted that the similar optically induced spin splitting was recently observed experimentally in GaAs [50]. However, the one-band energy spectrum of conduction electrons in GaAs differs crucially from the electron spectrum of gapped Dirac materials described by the two-band Hamiltonian (1). Therefore, the known theory of optically induced spin splitting for electrons with simple parabolic dispersion—including both the recent paper [50] and the classical article [51]—cannot be applied directly to the materials under consideration. One has to also take into account that optical properties of TMDC are dominated by excitons [52,53]. To avoid the influence of excitons on the discussed dressing-field effects, the photon energy, $\hbar\omega$, should be less than the binding exciton energy (which is typically of hundreds of meV in TMDC).

From the viewpoint of experimental observability of the discussed phenomena, it should be noted that all dressing-field effects increase with increasing the intensity of the dressing field. However, an intense irradiation can melt a condensed-matter sample. To avoid the melting, it is reasonable to use narrow pulses of a strong dressing field. This well-known methodology has been elaborated long ago and is commonly used to observe various dressing effects—particularly modifications of energy spectrum of dressed electrons arisen from the optical Stark effect—in semiconductor structures (see, e.g., Refs. [54–56]). Within this approach, giant dressing fields (up to GW/cm²) can be applied to the structures. It should be noted also that we consider the electromagnetic wave as a purely dressing field which cannot be absorbed by electrons. Within the classical Drude theory, the collisional absorption of the oscillating field (5) by conduction electrons is given by the well-known expression

$$Q = \frac{1}{T} \int_0^T \mathbf{j}(t) \mathbf{E}(t) dt = \frac{E_0^2}{2} \frac{\sigma_0}{1 + (\omega\tau_0)^2},$$

where T is the period of the field, Q is the period-averaged field energy absorbed by conduction electrons per unit time and per unit volume, $\mathbf{j}(t)$ is the ohmic current density induced by the oscillating electric field $\mathbf{E}(t) = E_0 \sin \omega t$, σ_0 is the static Drude conductivity, and τ_0 is the electron relaxation time. Evidently, the Drude optical absorption, Q , is negligibly small under the condition $\omega\tau_0 \gg 1$. Thus, an electromagnetic wave can be considered as a purely dressing field in the high-frequency limit (see, e.g., Ref. [10] for more details). It should be stressed that the increasing of temperature decreases the time τ_0 because of the strengthening of the electron-phonon scattering. Therefore, the temperature should be low enough to meet the aforementioned condition.

IV. CONCLUSION

We showed that the electromagnetic dressing can be used as an effective tool to control various electronic properties of gapped Dirac materials, including the band gap in gapped graphene and the spin splitting in TMDC monolayers. Particularly, both the band gap and the spin splitting can be closed by a dressing field. It is demonstrated that the strong polarization dependence of the renormalized band parameters appears. Namely, a linearly polarized field decreases the band gap, whereas a circularly polarized field can both decrease and increase one. It is found also that a circularly polarized field breaks equivalence of valleys in different points of the Brillouin zone, since the renormalized band parameters depend

on the valley index. As a consequence, the elaborated theory creates a physical basis for novel electronic, spintronic, and valleytronic devices operated by light.

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