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Floquet engineering of 2D materials

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Abstract. We demonstrate theoretically that the interaction of electrons in the 2D materials (gapped graphene and transition metal dichalcogenide monolayer) with a strong off-resonant electromagnetic field substantially renormalizes their band structure, including the band gaps and the spin-orbit splitting. Moreover, the renormalized electronic parameters drastically depend on the field polarization. Namely, a linearly polarized 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 field can serve an effective tool to control spin and valley properties of the 2D materials and be potentially exploited in optoelectronic applications.

1. Introduction

Advances in laser physics and microwave technique 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 well-known Floquet theory of periodically driven quantum systems [1]). As a consequence, the electronic properties of various nanostructures driven by oscillating fields are actively studied to exploit unique features of composite states of field and matter (see, e.g., Refs. [2, 3, 4] and references therein).

The discovery of graphene [5] initiated studies of the new class of artificial 2D nanomaterials. While graphene by itself is characterized by the gapless electron energy spectrum, many efforts have been dedicated towards fabrication 2D materials with the band gap between the valence and conduction bands. In the present study, we focused on the two 2D materials: gapped graphene [5] and transition metal dichalcogenide (TMDC) monolayer [6]. Below, we present the recently elaborated theory of Floquet engineering for these actively studied 2D materials.

2. Model

Electronic properties of both discussed 2D materials near the band edge can be described by the same two-band Hamiltonian

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

where $\mathbf{k} = (k_x, k_y)$ is the electron wave vector in the layer plane, γ is the parameter describing electron dispersion, $\varepsilon_{\tau s}^c = \Delta_g/2 + \tau s \Delta_{so}^c/2$ is the energy of the conduction band edge,



$\varepsilon_{\tau s}^v = -\Delta_g/2 - \tau s \Delta_{so}^v/2$ 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 and the K and $-K$ valleys in TMDC monolayers). If $\Delta_g \neq 0$ and $\Delta_{so}^{c,v} \neq 0$, the Hamiltonian (1) describes TMDC monolayer. In the case of zero spin-orbit splitting, $\Delta_{so}^{c,v} = 0$, the Hamiltonian (1) describes gapped graphene, whereas the case of $\Delta_g = \Delta_{so}^{c,v} = 0$ corresponds to usual gapless graphene.

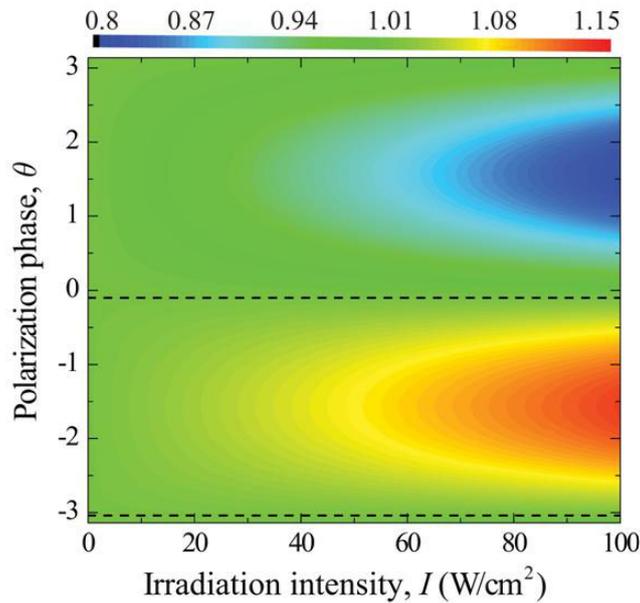


Figure 1. Dependence of the band gap in irradiated gapped graphene ($\Delta_g = 2$ meV, $\gamma/\hbar = 10^6$ m/s) on the irradiation intensity, I , and the polarization, θ , for the photon energy $\hbar\omega = 10$ meV [2]. The dashed lines correspond to the polarizations, θ , which do not change the band gap.

3. Results and conclusions

Let us consider a 2D material with the Hamiltonian (1), which is subjected to a monochromatic electromagnetic wave propagating perpendicularly to its plane. Considering the electron-field interaction within the minimal coupling scheme, the Hamiltonian of the periodically driven 2D material, $\hat{\mathcal{H}}(t)$, results from the Hamiltonian (1) with the replacement $\mathbf{k} \rightarrow \mathbf{k} - (e/\hbar)\mathbf{A}(t)$, where $\mathbf{A}(t)$ is the time-dependent vector potential of the wave. Solving the Floquet problem corresponding to the time-dependent Hamiltonian, $\hat{\mathcal{H}}(t)$, we can reduce it to the effective time-independent Hamiltonian, $\hat{\mathcal{H}}_{\text{eff}}$, which describes stationary electronic properties renormalized by the field. The stationary Hamiltonian, $\hat{\mathcal{H}}_{\text{eff}}$, formally coincides with the Hamiltonian (1), where the band parameters of “bare” electrons should be replaced with the renormalized band

parameters depending on the field intensity, I , and the field frequency, ω : $\gamma_{x,y} \rightarrow \tilde{\gamma}_{x,y}(I, \omega)$, $\Delta_g \rightarrow \tilde{\Delta}_g(I, \omega)$, $\Delta_{s_0}^{c,v} \rightarrow \tilde{\Delta}_{s_0}^{c,v}(I, \omega)$. As a consequence, the dependence of the band structure on the field appears. Solving the stationary Schrödinger problem with the effective Hamiltonian $\hat{\mathcal{H}}_{\text{eff}}$, we arrive at the renormalized band structure of gapped 2D materials.

It follows from analysis of the renormalized band structure that an irradiation can be used as an effective tool to control various electronic properties of 2D materials, including the band gap in gapped graphene and the spin splitting in TMDC monolayers (see Fig. 1). Particularly, both the band gap and the spin splitting can be closed by the irradiation. 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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