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Light-modulated electron retroreflection and Klein tunneling in a graphene-based n–p–n junction

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We investigate the electron retroreflection and the Klein tunneling across a graphene-based n–p–n junction irradiated by linearly polarized off-resonant light with the polarization along the x direction. The linearly polarized off-resonant light modifies the band structure of graphene, which leads to the anisotropy of band structure. By adjusting the linearly polarized light and the direction of n–p–n junction simultaneously, the electron retroreflection appears and the anomalous Klein tunneling, the perfect transmission at a nonzero incident angle regardless of the width and height of potential barrier, happens, which arises from the fact that the light-induced anisotropic band structure changes the relation of wavevector and velocity of electron. Our finding provides an alternative and flexible method to modulate electron retroreflection and Klein tunneling.

Keywords: linearly polarized light, electron retroreflection, Klein tunneling, graphene

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1. Introduction

Graphene, experimentally prepared by Novoselov and Geim in 2004,[1] has attracted considerable attention widely due to its peculiar physical properties and potential applications.[2–15] In the real space, graphene is a carbon atom-based two-dimensional hexagonal honeycomb lattice. Similarly, in the momentum space, graphene has the same hexagonal honeycomb structure with two degenerate and inequivalent high symmetry points K and K' at the corners of the first Brillouin zone. In the low energy approximation, its Hamiltonian near the high symmetry points was described by the massless Dirac equation.[9] By applying external fields such as electric field, magnetic field, light, and temperature gradient, a lot of fantastic properties were found in graphene such as half-integer quantum Hall effect,[3] Klein tunneling,[4] and topological phase transition.[2,11,12,15] Recently, the superconductivity was predicted in twisted bilayer graphene in theory and was observed in experiment.[10,16–18]

In the isotropic system, only electron specular reflection happens at the interface of junction because of the same direction of transverse wave vector and velocity component along the interface. In the anisotropic system, the anisotropic band structure will lead to the opposite directions of transverse wave vector and velocity component along the interface, which makes electron retroreflection possible. Electron retroreflection was first reported in the AB-stacked graphene bilayer-based superconducting junction[19] and then was studied in a twisted graphene bilayer-based superconducting junction.[20] We also gave some discussion in an 8-*Pmmn* borophene-based n–p–n junction.[21] Although the electron retroreflection was investigated in the systems mentioned above, it is difficult to realize the superconducting interface in graphene and 8-*Pmmn* borophene in experiment. In addition, electron retroreflection can not be tuned by external fields in the above-mentioned systems. Thus, it is an urgent duty to find a mature and external field-controlled system in experiment for realizing electron retroreflection. In this paper, using the Floquet theory,[22–27] we show that the electron retroreflection can be realized in a graphene-based n–p–n junction irradiated by linearly polarized off-resonant light.

Besides the discussion about the electron retroreflection, we study the Klein tunneling in a graphene-based n–p–n junction irradiated by the linearly polarized off-resonant light. In the region of high energy physics, there is a novel phenomenon that is a perfect tunneling phenomenon of a relativistic electron at the normal incidence regardless of the width and height of potential barriers. This exotic tunneling is called Klein tunneling.[28,29] However, in high energy physics, it is difficult to test Klein tunneling in experiment due to the high energy of the relativistic electron. Fortunately, in 2006, a graphene-based n–p–n junction was designed by Katsnelson to test this unique tunneling phenomenon.[4] After that, Klein tunneling in graphene was discussed widely in

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both theory and experiment.[30–35] Interestingly, the anomalous Klein tunneling, i.e., the perfect tunneling with non-normal incidence of electron, was described in the black phosphorus superlattices-based n–p–n junction,[36] the Dirac–Weyl fermion systems with tilted energy dispersion,[37] and the 8-*Pmmn* borophene-based p-n and n–p–n junctions.[21,38] Although the anomalous Klein tunneling has been investigated in these systems,[21,36–38] the realization of these systems in experiment needs to be explored further in comparison with graphene. Naturally, there appears a question how to modulate the anomalous Klein tunneling in graphene by the external field continuously.

In general, the angle of Klein tunneling in graphene is zero due to the isotropic band structure. The nonzero angle of Klein tunneling happens in black phosphorus, Dirac–Weyl fermion systems with tilted energy dispersion, and 8-*Pmmn* borophene because of the anisotropic band structure. Therefore, if we find an external field-induced anisotropic band structure in graphene, we will solve the above question. Fortunately, we find that the linearly polarized off-resonant light meets our expectation. In fact, graphene, modulated by circularly polarized off-resonant light, has been studied extensively.[12,23,39–41] However, the circularly polarized light-induced gap can damage the Klein tunneling, which does not meet our expectation. The paper is organized as follows. We firstly give the model and basic formalism. Then, the numerical results and theoretical analysis are presented and discussed. Finally, the main results of this work are summarized.

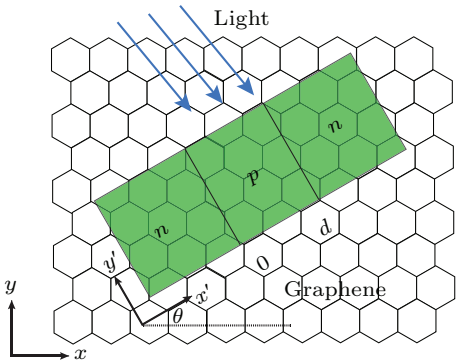


Fig. 1. Top view of the proposed experimental setup for transport measurements. The direction of n–p–n junction irradiated by the linearly polarized off-resonant light is characterized by θ.

2. Models and methods

We consider a graphene-based n–p–n junction shown in Fig. 1. The Hamiltonian of n–p–n junction without irradiated light is

$$H_0 = \hbar v_{\rm F}(k_x\sigma_x + k_y\sigma_y) + V\sigma_0. \tag{1}$$

Here $v_{\rm F} = 10^6$ m/s, $\sigma_{x,y}$ and σ_0 represent the Pauli matrix and unit matrix, respectively, and $V = V_0\Theta(x')\Theta(d-x')$ with the Heaviside step function Θ, the electric potential in the middle region of n–p–n junction, can be adjusted by doping or gate voltage. When the linearly polarized off-resonant light with the vector potential $\boldsymbol{A} = (A_x, 0)$ (i.e., the direction of the polarization along the x direction) is irradiated in the graphene-based n–p–n junction, through the canonical substitution, the wave vector k_x in Eq. (1) is rewritten as $k_x \to k_x - eA_x/\hbar$. Here $A_x = \frac{E_0}{\omega}\cos\omega t$ with the electric field intensity E_0 and the frequency of light ω. Then the Hamiltonian of the light-irradiated junction is modified as $H_{\rm L} = H_0 + H_{\rm int}$ with $H_{\rm int} = -v_{\rm F}\sigma_x eA_x = \widehat{O}{\rm e}^{{\rm i}\omega t} + \widehat{O}^{\dagger}{\rm e}^{-{\rm i}\omega t}$ with $\widehat{O} = \widehat{O}^{\dagger} = -\frac{v_{\rm F}\sigma_x eE_0}{2\omega}$. By using the Floquet theory,[22–27] the effective Hamiltonian is written as

$$H^{\rm eff} \simeq H_0 + \frac{1}{\hbar\omega}[\widehat{O},\widehat{O}^{\dagger}] + \frac{1}{2(\hbar\omega)^2}\{[[\widehat{O},H_0],\widehat{O}^{\dagger}] + {\rm H.c.}\}. \tag{2}$$

By a simple derivation, the effective Hamiltonian above is rewritten as

$$H^{\rm eff} \simeq \hbar v_{\rm F}[k_x\sigma_x + (1-\gamma)k_y\sigma_y] + V\sigma_0. \tag{3}$$

Here $\gamma = (\frac{v_{\rm F}eE_0}{\hbar\omega^2})^2$, which comes from the contribution of the linearly polarized off-resonant light.

The energy dispersion of the effective Hamiltonian is

$$E_{\pm} = V \pm \sqrt{(\hbar v_{\rm F}k_x)^2 + (\hbar v_{\rm F}^{\rm eff}k_y)^2}, \tag{4}$$

where $+$ $(-)$ denotes conduction (valence) band and $v_{\rm F}^{\rm eff} = (1-\gamma)v_{\rm F}$. According to the schematic diagram in Fig. 1, the relations between the wave vector components in coordinate systems x–y and x'–y' are

$$\begin{cases} k_x = k_{x'}\cos\theta - k_{y'}\sin\theta, \\ k_y = k_{x'}\sin\theta + k_{y'}\cos\theta. \end{cases} \tag{5}$$

Then, in coordinate system x'–y', the wavefunctions in left, right, and middle regions are written as

$$\begin{aligned} \Psi_{\rm L} &= \psi_{\rm L}^{\rm i} + r\psi_{\rm L}^{\rm r}, \\ \Psi_{\rm M} &= a\psi_{\rm M}^{\rm i} + b\psi_{\rm M}^{\rm r}, \\ \Psi_{\rm R} &= t\psi_{\rm R}^{\rm t}, \end{aligned} \tag{6}$$

where r (t) is the reflection (transmission) coefficient in the left (right) region and a (b) is the incidence (reflection) coefficient in the middle region. By solving the equation $H_{\rm eff}\psi = \varepsilon\psi$, the incident, reflected, and transmitted wavefunctions in each region are given as follows:

$$\begin{aligned} \psi_{\rm L}^{\rm i(r)} &= \left(1, \frac{\hbar v_{\rm F}k_x^{\rm i(r)} + {\rm i}\hbar v_{\rm F}^{\rm eff}k_y^{\rm i(r)}}{\varepsilon}\right)^{\rm T} {\rm e}^{{\rm i}(k_{x'}^{\rm i(r)}x' + k_{y'}y')}, \\ \psi_{\rm M}^{\rm i(r)} &= \left(1, \frac{\hbar v_{\rm F}q_x^{\rm i(r)} + {\rm i}\hbar v_{\rm F}^{\rm eff}q_y^{\rm i(r)}}{\varepsilon - V_0}\right)^{\rm T} {\rm e}^{{\rm i}(q_{x'}^{\rm i(r)}x' + k_{y'}y')}, \\ \psi_{\rm R}^{\rm t} &= \left(1, \frac{\hbar v_{\rm F}k_x^{\rm t} + {\rm i}\hbar v_{\rm F}^{\rm eff}k_y^{\rm t}}{\varepsilon}\right)^{\rm T} {\rm e}^{{\rm i}(k_{x'}^{\rm t}x' + k_{y'}y')}, \end{aligned} \tag{7}$$

where ε is the incident energy of electron, T represents the transformation of matrix, the values of $k_{x'}^{\rm i(r,t)}$ and $k_{y'}$ meet

$\varepsilon = E_+$ while the values of $q_{x'}^{\mathrm{i(r,t)}}$ and $k_{y'}$ meet $\varepsilon = E_-$, and $k_x^{\mathrm{i(r,t)}}$, $k_y^{\mathrm{i(r,t)}}$, $q_x^{\mathrm{i(r)}}$, and $q_y^{\mathrm{i(r)}}$ can be calculated by Eq. (5). Then, according to the continuity of wavefunction, the wavefunctions at the interface of n–p–n junction meet

$$\Psi_{\mathrm{L}}(0) = \Psi_{\mathrm{M}}(0), \quad \Psi_{\mathrm{M}}(d) = \Psi_{\mathrm{R}}(d), \tag{8}$$

and the corresponding transmission coefficient is written as

$$t = \frac{(M_{\mathrm{i}} - M_{\mathrm{r}})(N_{\mathrm{i}} - N_{\mathrm{r}})}{(M_{\mathrm{i}} - N_{\mathrm{i}})(M_{\mathrm{r}} - N_{\mathrm{r}})\mathrm{e}^{\mathrm{i}q_{x'}^{\mathrm{i}}d} - (M_{\mathrm{r}} - N_{\mathrm{i}})(M_{\mathrm{i}} - N_{\mathrm{r}})\mathrm{e}^{\mathrm{i}q_{x'}^{\mathrm{r}}d}}, \tag{9}$$

where

$$\begin{aligned} M_{\mathrm{i(r)}} &= \frac{\hbar v_{\mathrm{F}} k_x^{\mathrm{i(r)}} + \mathrm{i}\hbar v_{\mathrm{F}}^{\mathrm{eff}} k_y^{\mathrm{i(r)}}}{\varepsilon}, \\ N_{\mathrm{i(r)}} &= \frac{\hbar v_{\mathrm{F}} q_x^{\mathrm{i(r)}} + \mathrm{i}\hbar v_{\mathrm{F}}^{\mathrm{eff}} q_y^{\mathrm{i(r)}}}{\varepsilon - V_0}. \end{aligned} \tag{10}$$

The transmission probability across the n–p–n junction is written as $T = t^* t$. Before the discussion about Klein tunneling, we discus the physical properties of the polarized light. In Floquet theory, the energy of light $\hbar\omega$ is required that its value is much larger than the hopping integral of graphene (about 2.3 eV). We choose $\hbar\omega = 12$ eV, which is about six times larger than the hopping integral. For the convenience of calculation in the following, we set $\gamma \in [0, 0.9]$ and then the value of the electric field intensity E_0 of light varies from 0 to 2.08×10^{11} V/m.

3. Results and discussion

3.1. Electron retroreflection

In the coordinate x'–y' system, the velocity components of incident (reflected) electron are defined as

$$\begin{aligned} u_{x'\mathrm{i(r)}} &= \frac{\partial \varepsilon}{\hbar \partial k_{x'}} = \frac{v_{\mathrm{F}}[k_x \cos\theta + (1-\gamma)^2 k_y \sin\theta]}{\sqrt{k_x^2 + (1-\gamma)^2 k_y^2}}, \\ u_{y'\mathrm{i(r)}} &= \frac{\partial \varepsilon}{\hbar \partial k_{y'}} = \frac{-v_{\mathrm{F}}[k_x \sin\theta - (1-\gamma)^2 k_y \cos\theta]}{\sqrt{k_x^2 + (1-\gamma)^2 k_y^2}}. \end{aligned} \tag{11}$$

We consider the incident energy in the conduction band in all the calculations in this paper, so the incident energy $\varepsilon = E_+$ in Eq. (11). The incident (reflected) angle of electron is defined as $\varphi_{\mathrm{i(r)}} = \arctan(u_{y'\mathrm{i(r)}}/u_{x'\mathrm{i(r)}})$. When the transverse wave vector $k_{y'}$ and the incident energy ε are given, it is easy to obtain the longitudinal wave vector of incident (reflected) electron by solving Eq. (4). Then the incident angle-dependent reflected angle is plotted in Fig. 2 with $\theta = 0$, $\frac{\pi}{4}$, $\frac{\pi}{3}$, and $\frac{\pi}{2}$ in the different optical parameters γ. In Fig. 2(a) with $\theta = 0$, there is only electron specular reflection (SR) regardless of the value of γ. According to the conversation of transverse wave vector $k_{y'}$, we can obtain the incident angle $\varphi_{\mathrm{i}} = \arctan(k_{y'}(1-\gamma)^2/k_{x'\mathrm{i}})$ and the reflected angle $\varphi_{\mathrm{r}} = \arctan(k_{y'}(1-\gamma)^2/k_{x'\mathrm{r}})$ easily. By solving Eq. (4), it is easy to obtain $k_{x'\mathrm{i}} = -k_{x'\mathrm{r}}$, so $\varphi_{\mathrm{i}} = -\varphi_{\mathrm{r}}$, which is consistent with the result in Fig. 2(a). With the change of direction of junction, as shown in Figs. 2(b) and 2(c), electron retroreflection (RR) happens and the proportion of RR increases as optical parameter γ increases. In Fig. 2(d) with $\theta = \frac{\pi}{2}$, it is easy to obtain the incident angle $\varphi_{\mathrm{i}} = \arctan(k_{y'}/[k_{x'\mathrm{i}}(1-\gamma)^2])$ and the reflected angle $\varphi_{\mathrm{r}} = \arctan(k_{y'}/[k_{x'\mathrm{r}}(1-\gamma)^2])$. In the same way, we obtain $k_{x'\mathrm{i}} = -k_{x'\mathrm{r}}$ by solving Eq. (4), and then $\varphi_{\mathrm{i}} = -\varphi_{\mathrm{r}}$, which is consistent with the result in Fig. 2(d).

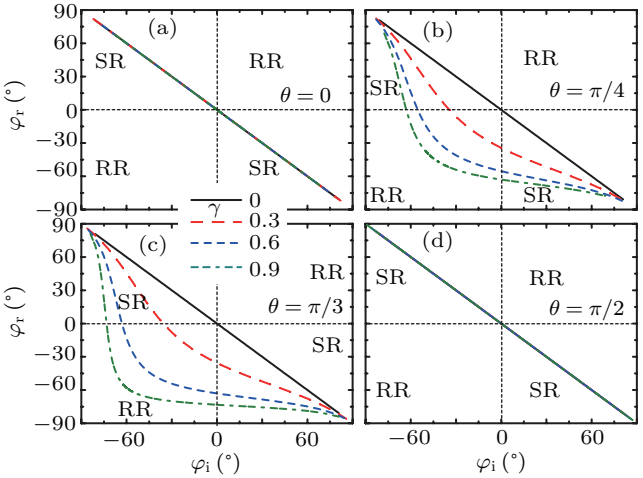


Fig. 2. (a)–(d) Incident angle-dependent reflected angle with the parameters $V_0 = 0.3$ eV, $\varepsilon = 0.05$ eV, and $d = 80$ nm in the different directions of n–p–n junction with different values of optical parameter γ.

3.2. Anomalous Klein tunneling

In the coordinate x'–y' system, the effective Hamiltonian described by Eq. (3) is rewritten as

$$H_{\mathrm{eff}} = \hbar(S_x k_{x'} + S_y k_{y'}) + V\sigma_0, \tag{12}$$

where $S_x = v_{\mathrm{F}}\sigma_x \cos\theta + v_{\mathrm{F}}^{\mathrm{eff}}\sigma_y \sin\theta$ and $S_y = -v_{\mathrm{F}}\sigma_x \sin\theta + v_{\mathrm{F}}^{\mathrm{eff}}\sigma_y \cos\theta$. The velocity operator along the x' direction is $\hat{u}_{x'} = \frac{1}{\mathrm{i}\hbar}[x', H_{\mathrm{eff}}] = S_x$. Its time evolution is given by the Heisenberg equation of motion:

$$\dot{\hat{u}}_{x'} = \frac{1}{\mathrm{i}\hbar}[\hat{u}_{x'}, H_{\mathrm{eff}}] = 2v_{\mathrm{F}}v_{\mathrm{F}}^{\mathrm{eff}}\sigma_z k_{y'}. \tag{13}$$

When $k_{y'} = 0$, we have $\dot{\hat{u}}_{x'} = 0$, which means that the velocity along x' is conserved and the perfect transmission ($T = 1$, i.e., Klein tunneling) happens. In the isotropic system, the incident angle of electron is defined as $\arctan(k_{y'}/k_{x'})$, which indicates that the incident angle must be zero when Klein tunneling happens. However, in our anisotropic system, the incident angle is defined as $\varphi_{\mathrm{i}} = \arctan(u_{y'\mathrm{i}}/u_{x'\mathrm{i}})$. Obviously, we can easily obtain the incident angle of electron from Eq. (11) when Klein tunneling happens

$$\varphi_{\mathrm{i}} = \arctan\left(-\frac{k_x \sin\theta - (1-\gamma)^2 k_y \cos\theta}{k_x \cos\theta + (1-\gamma)^2 k_y \sin\theta}\right). \tag{14}$$

From Eq. (14), we can give a conclusion that the Klein tunneling happens at zero incident angle when $\theta = 0$ ($\frac{\pi}{2}$) or

$\gamma = 0$ by a simple derivation, which is verified in Figs. 3(a)–3(d) by numerical calculations. We also give the incident angle-dependent transmission probability in the case of the different values of θ and γ in Figs. 3(a)–3(d). The nonzero incident angles of Klein tunneling are labeled in Fig. 3 by numerical calculations, which are consistent with the analytic expression (14). In fact, there are other angles for $T = 1$ in Fig. 3, which arises from the resonant tunneling of electron. These resonant angles are sensitive to the incident energy ε, the direction of junction θ, the width of potential barrier d, the height of potential barrier V_0, and the optical parameter γ.

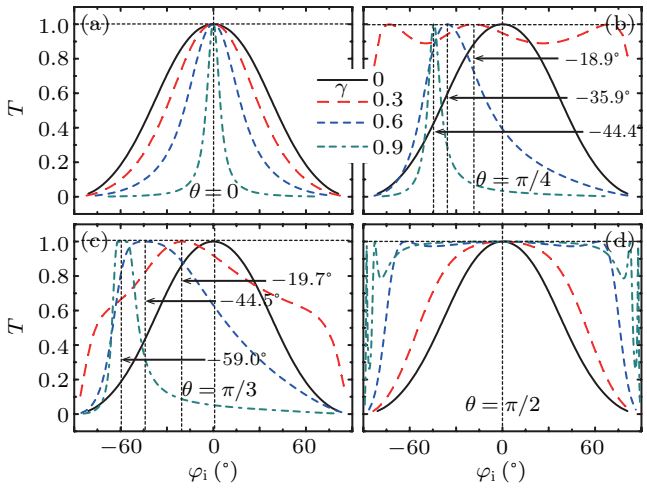


Fig. 3. (a)–(d) Incident angle-dependent transmission probability with the parameters $V_0 = 0.3$ eV, $\varepsilon = 0.05$ eV, and $d = 80$ nm in the different directions of n–p–n junction and optical parameters γ.

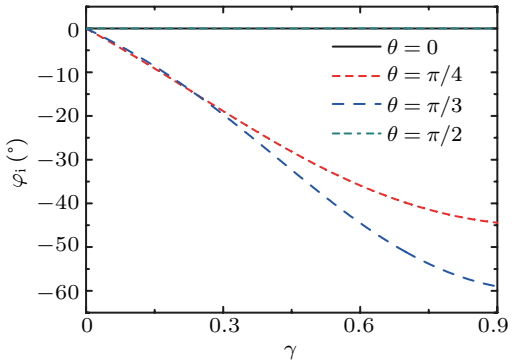


Fig. 4. The optical parameter γ-dependent incident angle of Klein tunneling in the different directions of n–p–n junction. The other parameters are the same as those in Fig. 2.

In Fig. 4, the optical parameter γ-dependent incident angle of Klein tunneling is plotted in the different directions of junction. In the regime of $\theta = 0$ and $\theta = \frac{\pi}{2}$, the incident angle of Klein tunneling keeps zero regardless of the variation of γ, which can be tested by Eq. (14) clearly. In the regime of $\theta = \frac{\pi}{3}$ and $\theta = \frac{\pi}{4}$, the absolute value of incident angle of Klein tunneling increases as γ increases. The maximal value of incident angle of Klein tunneling can reach about $-60°$. In order to understand θ and γ-dependent incident angle of Klein tunneling comprehensively, the contour graph of the two-parameter-dependent incident angle of Klein tunneling is plotted in Fig. 5. The incident angle of Klein tunneling increases as these two parameters increase and the maximal value can reach around $-80°$. In experiment, graphene-based n–p–n junction was constructed to test Klein tunneling.[34,42] The circularly polarized off-resonant light was used to induce anomalous Hall effect in graphene experimentally.[14] Therefore, if the circularly polarized off-resonant light in Ref. [14] is changed with the linearly polarized off-resonant light, combined with the means of preparing graphene-based n–p–n junction in Refs. [34,42], the anomalous Klein tunneling in our work will be tested in experiment.

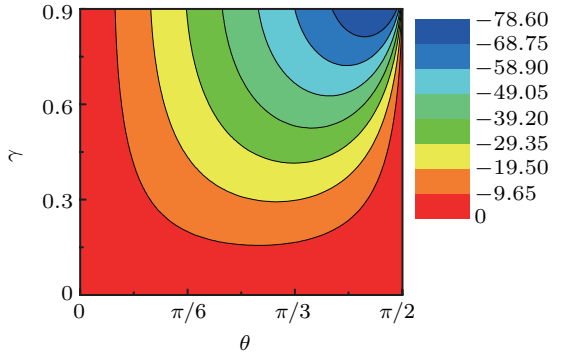


Fig. 5. The contour graph of the direction of n–p–n junction θ and optical parameter γ-dependent incident angle of Klein tunneling. The other parameters are the same as those in Fig. 2.

4. Conclusion

In summary, we have investigated the electron retroreflection and the Klein tunneling in a graphene-based n–p–n junction irradiated by the linearly polarized off-resonant light with the direction of polarization along the x direction. The electron retroreflection and the anomalous Klein tunneling can be realized by adjusting the direction of junction and light due to the linearly polarized off-resonant light-induced anisotropic band structure of graphene. The light-modulated Klein tunneling surpasses the traditional view that there exists the appearance of Klein tunneling at one specific angle in a definite device. Our work gives an alternative and flexible method to modulate electron retroreflection and Klein tunneling.

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