Valley-contrastive selection rules of a nonlinear optical transition in graphene with an energy gap

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A valley degree of freedom in graphene has been playing significant roles in novel properties of the material. For graphene whose energy spectrum has a gap, valley-contrastive phenomena in nonlinear optics are theoretically studied. With the use of the Floquet method and the wave vector point group theory, we show that N-photon resonant excitation by circularly polarized light obeys a selection rule that is complementary with respect to the number of the photons involved, handedness of the circularly polarized laser field, and the valley index. In particular, a hallmark of inversion symmetry breaking is clarified in the selection rule. Besides, the band gap renormalization as an influence of the applied laser field is found to be also valley dependent.

I. INTRODUCTION

Enthusiasm for research on graphene is unbounded. Since the discovery of electron dispersion with conical intersection, called Dirac electrons,[1] the physical properties expected in graphene have been important subjects in condensed matter physics for more than half a century, and the recent experimental realization by the Novel laureates has drastically developed the research activity.[2] The electron in graphene behaves in such a fashion that mimics the massless Dirac fermion in quantum electrodynamics. In this respect, the advent of the material has bridged the two branches of physics, relativistic physics and nonrelativistic condensed matter physics, fueling the extensive studies.

In neutral graphene, the chemical potential exactly crosses the Dirac points located at the two nonequivalent Brillouin-zone corner points $K_{\pm}$, and a semimetallic behavior is thus predicted. This observation primarily aroused research interests in electron transport properties, which results in finding novel behaviors in, for instance, cyclotron resonance,[3,4] magnetoresistance,[5,6] and the anomalous integer quantized Hall effect.[7,8] In particular, the report of ultrahigh electron mobility at the room temperature $\sim 15,000\ [\mathrm{cm^2/Vs}]$,[9] which is beyond the conventional figure (e.g., about $1400[\mathrm{cm^2/Vs}]$ in silicon) extends the graphene research for device application. When one intends to use the material in such a device as a field effect transistor, the gapless energy spectrum would be unfavorable since the magnitude of the energy gap of the material measures on-and-off ratio and the threshold of the voltage of the device. Thus a method to open an energy gap in graphene is devised for stable device operation. Nowadays, several schemes are proposed such as imposing Kekúle distortion on the layer[10] and chemical decorations with ammonia[11] and CrO_3 (Ref. 12). Among them, the graphene fabricated on the SiC substrate is found to be a semiconductor that has direct gaps with an identical magnitude at the $K_{\pm}$ points, which are referred to as $K_{\pm}$ valleys.[13–15] Although the detail of the gap-opening mechanism has still been an open question, it is widely believed that the substrate introduces an on-site staggered electron potential into the carbon layer. This effect breaks the spacial inversion symmetry of graphene, resulting in opening energy gaps at the Dirac points.

This interplay between the basic and applied physics brings about another synergy effect. The graphene with an energy gap, in turn, puts optical properties of the material on the list of relevant research subjects. Along this line, a circular dichroism that depends on the valley degree of freedom in a linear optical response was theoretically reported in Ref. 16: When electric dipole transition by a left (right) circularly polarized photon is allowed (forbidden) at one valley, the selection rule at the other valley alternates. From the analogy with the conventional circular dichrolism that originates from an electron spin, the valley indexes should become central degrees of freedom for "valleytronics".[17]

To fully understand the optical properties of gapped graphene it is quite natural to ask whether valley-contrastive selection rules would be expected in nonlinear optics. In spite of the immenseness of the interest, the procedures used in Ref. 16 cannot be straightforwardly applied to the nonlinear regime. In this paper, we take other routes to explore valley-contrastive phenomena in nonlinear optics and clarify a selection rule for circular polarization in N-photon resonant processes. For this purpose, we first apply the Floquet method. Since graphene is well described by a tight binding model on a lattice with two sites in a unit cell (honeycomb lattice), or equivalently by a two-level system at each wave number, one can immediately be reminded of the usefulness of the Floquet method. In addition to the selection rule, the method reveals that the band gap renormalization as an influence of the driving laser field also depends on the valley index. The selection rule obtained by the Floquet method covers the processes where the photons involved have an identical circular polarization. Thus, we also rely on the wave vector point group theory to complete the selection rule. The latter method shows that an experimental observation of the nonlinear optical selection rule enables one to identify the symmetry that has been broken for the gap opening.

II. NONLINEAR OPTICAL SELECTION RULE

A. Floquet method approach

Consider spinless electrons subjected to a monochromatic laser field in graphene with a broken spatial inversion symmetry. The electron dynamics is well described in the tight
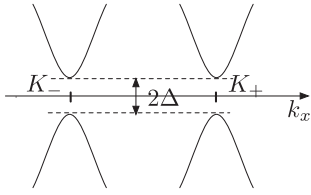
FIG. 1. Energy band structure with $k_y = 0$ around the $K_\pm$ valleys.

binding approximation, whose Hamiltonian is given in the wave number space as ($\hbar = 1$)

$$H = \sum_k \begin{pmatrix} a_k^\dagger & b_k^\dagger \end{pmatrix} \mathcal{H}(t) \begin{pmatrix} a_k \\ b_k \end{pmatrix}, \tag{1}$$

with the 2×2 matrix[18]

$$\mathcal{H}(t) = \begin{pmatrix} \Delta & t_1 \sum_i e^{+i(\vec{k} + e\vec{A}(t)) \cdot \vec{d}_i} \\ t_1 \sum_i e^{-i(\vec{k} + e\vec{A}(t)) \cdot \vec{d}_i} & -\Delta \end{pmatrix}. \tag{2}$$

In this equation, the two components in the row and column vectors $a_k(a_k^\dagger)$ and $b_k(b_k^\dagger)$ are annihilation (creation) operators of an electron residing on the A and B triangular sublattices, respectively, of the honeycomb lattice. The parameters t_1 and Δ each denote the nearest-neighbor hopping integral and staggered on-site electron potential, the latter of which breaks the spacial inversion symmetry. The three vectors connecting the nearest-neighboring sites in the honeycomb lattice, $\vec{d}_i (i = 1,2,3)$, are set as $\vec{d}_1 = a(\sqrt{3}/2, 1/2), \vec{d}_2 = a(-\sqrt{3}/2, 1/2)$, and $\vec{d}_3 = a(0, -1)$ with the lattice constant a. In the present coordinate system, the $K_\pm$ points, at which the two Dirac points appear for an ideal graphene with $\Delta = 0$, are positioned at $(k_x, k_y) = (\pm 4\pi/3\sqrt{3}a, 0)$. When the staggered on-site energy potential is finite, $\Delta > 0$, the degeneracies at the Dirac points are lifted and energy gaps with magnitude 2Δ open [see Fig. 1].

The driving laser field is described by the vector potential $\vec{A}(t)$, whose wave vector is assumed to be normal to the plane. The laser field is also assumed to be circularly polarized to pick up the valley-contrastive phenomena in this system. The vector potential for the laser field with frequency ω and amplitude E_0 then takes the form of $\vec{A}(t) = (E_0/\omega)(-\sin\omega t, \tau\cos\omega t)$, where $\tau = +1(-1)$ indicates the left (right) circularly polarized light. Here and hereafter, the matrix $\mathcal{H}(t)$ is simply referred to as the Hamiltonian.

Our central interest is the selection rules of a nonlinear optical transition by the circularly polarized light in N-photon resonant processes. For this purpose, we apply the Floquet method, which is the powerful tool to tackle sinusoidally time-dependent problems. In the present context, an advantage of this scheme is that a selection rule in nonlinear optics can be obtained on an equal footing with the one in a linear process. The procedure is as follows.[19] For the time-dependent Schrödinger equation $\left[\mathcal{H}(t) - i(\partial/\partial t)\right]|\Psi\rangle = 0$ with temporally periodic Hamiltonian $\mathcal{H}(t) = \mathcal{H}(t + 2\pi/\omega)$, the Floquet theory assumes the solution of this equation in the form of

$$\begin{aligned} |\Psi\rangle &= e^{-i\epsilon t}|\Phi\rangle \\ &= \sum_\alpha \sum_n e^{-i\epsilon t} e^{-in\omega}|\alpha, n\rangle. \end{aligned} \tag{3}$$

The bases used in the expansion in the second line are defined as $|\alpha, n\rangle \equiv |\alpha\rangle \otimes |n\rangle$, which are the composites of the appropriate electronic bases $|\alpha\rangle$ and photonic bases $|n\rangle$. The integer n can be interpreted as the photon numbers involved. Substituting the form of the solution to the Schrödinger equation turns the problem into a (time-independent) eigenvalue problem $H_F|\Phi\rangle = \epsilon|\Phi\rangle$, where ϵ is the quasi-energy and the operator H_F is the Floquet Hamiltonian. In the renewed eigenvalue problem, one has to treat the infinite-dimensional matrix H_F consisting of block matrices H^{mn}

$$H_F = \begin{pmatrix} \ddots & \vdots & \vdots & \vdots & \cdots \\ \cdots & H^{11} & H^{10} & H^{1-1} & \cdots \\ \cdots & H^{01} & H^{00} & H^{0-1} & \cdots \\ \cdots & H^{-11} & H^{-10} & H^{-1-1} & \cdots \\ \ddots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \tag{4}$$

The diagonal block H^{nn} operates on an n-photon sector, which is defined as a Hilbert subspace with a fixed photon number n. The each entry in H_F is the 2×2 matrix $H^{mn} = \{H_{\alpha\beta}^{mn}\}(\alpha, \beta = 1,2)$, where

$$H_{\alpha\beta}^{mn} = \frac{\omega}{2\pi} \int_0^{2\pi/\omega} \mathcal{H}(t)_{\alpha\beta} e^{i(m-n)\omega t} dt + \delta_{mn}\delta_{\alpha\beta}m\omega. \tag{5}$$

The matrix elements are evaluated by the wave numbers of the $K_\pm$ valleys, at which the direct optical transitions are addressed:

$$H_{11}^{mn} = (\Delta + m\omega)\delta_{mn}, \tag{6}$$

$$\begin{aligned} H_{12}^{mn} = t_1 J_N(-\lambda)(-i)^{\tau N} \\ \times \left[2\cos\left\{\frac{\pi}{3}(\tau N \pm 2)\right\} + (-1)^{\tau N} \right], \end{aligned} \tag{7}$$

$$\begin{aligned} H_{21}^{mn} = t_1 J_N(+\lambda)(-i)^{\tau N} \\ \times \left[2\cos\left\{\frac{\pi}{3}(\tau N \mp 2)\right\} + (-1)^{\tau N} \right], \end{aligned} \tag{8}$$

$$H_{22}^{mn} = (-\Delta + m\omega)\delta_{mn}, \tag{9}$$

with $N \equiv n - m$th order Bessel function J_N and $\lambda = eaE/\omega$. Here, the zero-photon sector $n = m = 0$ is found to be diagonal. Thus in the following, the diagonal state with higher (lower) energy is referred to as a conduction (valence) band state at the $K_\pm$ valleys.

In the framework of the Floquet method, the transition probability from a given initial state to a target state is described by an infinite sum of the matrix elements of the time evolution operator determined by H_F. The probability in the present problem is then written as

$$P_{v \to c}(t) = \sum_n |\langle c, n| \exp[-iH_F t]|v, 0\rangle|^2, \tag{10}$$

where the Floquet states $|v, 0\rangle$ and $|c, n\rangle$ denote the initial valence band and conduction band states, respectively. This infinite sum is approximated when the N-photon resonant condition $N\omega = 2\Delta$ is satisfied; Eq. (10) is dominated by the transition between the two Floquet states, $|c, -N\rangle$ and $|v, 0\rangle$

TABLE I. Selection rules at the $K_\pm$ valleys for left/right cocircularly polarized light. The capital letters A/F indicate that the optical transition is "allowed"/"forbidden".

	$N = 1$	$N = 2$	$N = 3$
K_+	A/F	F/A	F/F
K_-	F/A	A/F	F/F

(Ref. 19). Thus the Hamiltonian matrix is reduced from H_F into the 2×2 matrix $H_F^{(N)}$ spanned by the corresponding two Floquet states, and the transition probability can be simplified as $P_{v \to c}^{(N)}(t) = |\langle c, -N| \exp[-i H_F^{(N)} t]|v, 0\rangle|^2$, where

$$H_F^{(N)} = \begin{pmatrix} H_{11}^{00} & H_{21}^{0-N} \\ H_{12}^{-N0} & H_{22}^{-N-N} \end{pmatrix}. \tag{11}$$

We note, in passing, that for below-gap excitation, the influence of the laser field effectively appears in the renormalization of electron hopping integrals.[20] One can now immediately find out the selection rule from the off-diagonal matrix elements in $H_F^{(N)}$; when they are null (finite), the direct optical transition is forbidden (allowed). The selection rule is summarized in Table I. The result in $N = 1$ (i.e., a linear process) is confirmed to be line with that in Ref. 16. One can observe alternation with respect to the polarization direction as well as the valley index. We remark that the result describes the transitions with cocircular photons in nonlinear responses.

B. Wave vector point group approach

Next, the wave vector point group theory is applied to derive a selection rule for nonlinear processes where the left and right circularly polarized photons are simultaneously involved.

The space group that the graphene with broken inversion symmetry belongs to is $P\bar{6}m2$ and the wave vector point group at the $K_\pm$ points is C_{3h} (Refs. 21,22). The irreducible representations of this point group characterize energy eigenfunctions at the $K_\pm$ valleys. From the character table, one finds that three-fold rotations $R(\pm 2\pi/3)$ add a phase factor to the wave functions of valence (conduction) band states at the $K_\pm$ valleys, $|v(c); K_\pm\rangle$, in such a manner that

$$R(2\pi/3)|v(c); K_\pm\rangle = e^{+i2\pi m_{v(c)}^\pm/3}|v(c); K_\pm\rangle, \tag{12}$$

$$R(-2\pi/3)|v(c); K_\pm\rangle = e^{-i2\pi m_{v(c)}^\pm/3}|v(c); K_\pm\rangle, \tag{13}$$

with $m_v^+ = -m_c^+ = -m_v^- = m_c^- = -1$. The azimuthal selection rule for a $N(= n_R + n_L)$-photon process, where $n_R(n_L)$ is the number of the right (left) circularly polarized photon, is determined by a condition that quantity

$$\sum_{\phi = 0, \pm 2\pi/3} (e^{im_c^\pm \phi})^* e^{i(n_R - n_L)\phi} e^{im_v^\pm \phi}, \tag{14}$$

should be finite. This leads to an equality

$$-m_c^\pm + n_R - n_L + m_v^\pm = 3M, \tag{15}$$

with an integer M. This relation obviously includes the results presented in Table I. Moreover, the "mixed" processes involving both polarizations are now covered. For instance, the second order transition with $n_L = n_R = 1$ is found to be forbidden at both the valleys, while the "mixed" third order process with $n_{L(R)} = 2$ and $n_{R(L)} = 1$ is optically active at the $K_{+(-)}$ valley.

Here, we would like to emphasize that the selection rule is nontrivial with respect to the following two aspects. In the field theoretical description, the chiral symmetry is found to be equipped with the graphene system. Since the chiral nature of the system is often related with the helicity (i.e., the projection of a spin degree of freedom along the momentum vector) one might think that left- and right-handedness should appear in a certain form and that the valley-contrastive selection rule is one of the natural manifestations of it. However, it is not straightforward: that is the case in three space dimensional systems, and not valid in two space dimensions (e.g., in graphene). The reason is that in two space dimensions a momentum operator has two components (k_x, k_y), thus the projection of the spin degrees of freedom resides in the plane where the momentum operator is defined. Thus, the in-plane projection does not have a direct relation with the helicity possessed by the laser field, the latter of which is normal to the plane. More precisely, the helicity in two space dimensions is not well defined.[23] Thus, the alternation with respect to the handedness shown in the selection rule should not be ascribed to the chiral nature of the graphene system.

The other aspect that should be remarked is the influence of the three-fold rotation. The period three with respect to N in the selection rule is caused by the phase factor attached to the eigenfunction in the course of the three-fold rotation. The phase factor in the form of $e^{\pm i2\pi/3}$ is not a consequence of the three-fold symmetry of the lattice, as opposed to the appearance. This is obviously understood when one is reminded that the wave vector point group at the $K_\pm$ points in an ideal graphene is D_{3h}[24]. In this system, the phase factor $e^{\pm i\pi}$ is picked up for the $R(\pm 2\pi/3)$ rotations, although the three-fold symmetry remains.

The point group that the $K_\pm$ valleys obey has a tight connection with the mechanism how the degeneracies at the Dirac points are lifted. The key of the present gapped graphene is that the energy gap originates from inversion symmetry breaking. Various physical and chemical methods to open an energy gap in graphene are proposed. All of the means mentioned in Sec. I break the inversion symmetry, and the selection rule is insensitive to further details of the methods to open the gap, as long as the symmetry that is broken for the gap opening is commonly the spacial inversion. When a gap opening mechanism with another symmetry is introduced to graphene, a distinct selection rule should be obtained. For instance, the intrinsic spin-orbit coupling is found to open an energy gap with preserving the graphene lattice symmetry. Thus, for *this* graphene with the energy gap, the wave vector point group at the $K_\pm$ valleys should be D_{3h}, and the selection rule Eq. (15) would not hold. This fact inversely enables one to experimentally identify a relevant symmetry causing an optical gap by observing the selection rule in nonlinear optics. The behavior with the period three with respect to the photon numbers is the hallmark of broken inversion symmetry.

III. VALLEY-DEPENDENT BAND GAP RENORMALIZATION

One might think that the use of the wave vector point group would solely meet the present purpose since the selection rule obtained by the method is more general. When our discussion is limited to qualitative aspects, this would be true. However, when we expand our interest to quantitative issues, the group theoretical approach could not be helpful. Thus, we once again rely on the Floquet method to examine a quantitative valley-dependent phenomenon in one-photon resonant process, and discuss band gap renormalization as an influence of driving the laser field.

The reduced Floquet matrix in the lowest order approximation $H_F^{(N)}$ was sufficient to derive the selection rule, as shown above. However, to discuss quantitative nature we have to move to the next order approximation, where the effects of matrix elements discarded in the course of the matrix-size reduction should be considered. These appear as an energy shift in the second order approximation. Individual couplings of the Floquet states $|c, -1\rangle$ and $|v, 0\rangle$ with remaining Floquet states yield to the relevant correction

$$\delta\bigg|_{K_\pm L(R)} = \sum_{n \neq 0,1} \frac{|H_{12}^{(0n)}|^2}{(n-1)\omega}, \quad (16)$$

at the $K_\pm$ valleys under the shining of left (right) circularly polarized light. Taking these corrections into the diagonal elements of $H_F^{(N=1)}$, electron dynamics at the $K_\pm$ valleys is described by

$$H_{F2}^{(N=1)}\bigg|_{K_+ L} = \left(H_{F2}^{(N=1)}\bigg|_{K_- R}\right)^*$$
$$= \begin{pmatrix} -\omega/2 + \delta_{\pm\pm} & -3it_1 J_{-1}(\lambda) \\ 3it_1 J_1(-\lambda) & -\omega/2 - \delta_{\pm\pm} \end{pmatrix}, \quad (17)$$

$$H_{F2}^{(N=1)}\bigg|_{K_+ R} = H_{F2}^{(N=1)}\bigg|_{K_- L}$$
$$= \begin{pmatrix} -\omega/2 + \delta_{\pm\mp} & 0 \\ 0 & -\omega/2 - \delta_{\pm\mp} \end{pmatrix}, \quad (18)$$

where

$$\delta_{\pm\pm} = 9t_1^2 \sum_{m \neq 0} \frac{|J_{3m+1}(-\lambda)|^2}{3m}, \quad (19)$$

$$\delta_{\pm\mp} = 9t_1^2 \sum_{m \neq 0} \frac{|J_{3m+2}(\lambda)|^2}{3m+1}. \quad (20)$$

While these energy corrections do not alter the optical selection rule, the inequality of $\delta_{\pm\pm}$ with $\delta_{\pm\mp}$ indicates another valley-dependent phenomenon; the amount of the band gap renormalization is different between the two valleys. The transition probability $P(t)$ when the band gap renormalization is taken into account is given as

$$P_{v\to c}^{(N=1)}(t) = \frac{g^2}{\delta_{\pm\pm}^2 + g(\lambda)^2} \sin^2\left(\sqrt{\delta_{\pm\pm}^2 + g(\lambda)^2} t\right), \quad (21)$$

for $H_{F2}^{(N=1)}|_{K_+ L} = H_{F2}^{(N=1)}|_{K_- R}$, where $g(\lambda)^2 = 9t_1^2 J_1^2(\lambda)$. It is also straightforward to obtain the time profile of the Rabi oscillation $R(t)$,

$$R(t) \equiv \left|\langle v0| \exp\left(-i H_{F2}^{(N=1)})t\right)|v0\rangle\right|^2$$
$$= \cos^2\left(\sqrt{\delta_{\pm\pm}^2 + g(\lambda)^2} t\right)$$
$$+ \frac{\delta_+^2}{\delta_{\pm\pm}^2 + g(\lambda)^2} \sin^2\left(\sqrt{\delta_{\pm\pm}^2 + g(\lambda)^2} t\right), \quad (22)$$

where the initial state is assumed to occupy the valence band.

IV. CONCLUSION

We obtained the valley-contrastive selection rules of a nonlinear optical transition by circularly polarized light in graphene with an energy gap. The selection rule is complementary with respect to the photon numbers involved, handedness of the laser field and the valley index. The experimental observation of the rule enables us to identify the dominant symmetry of the mechanism that lifts the degeneracies at the Dirac points in graphene. In particular, the period three with respect to the photon numbers in the selection rule is the hallmark of broken inversion symmetry, which should be understood in term of the wave vector point group symmetry of the $K_\pm$ valley, but not of the three-fold symmetry of the lattice structure. The band gap renormalization is found to be a quantitatively valley-dependent phenomenon.

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