Optical response of graphene under intense terahertz fields

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Optical responses of graphene in the presence of intense circularly and linearly polarized terahertz fields are investigated based on the Floquet theory. We examine the energy spectrum and density of states. It is found that gaps open in the quasi-energy spectrum due to the single-photon/multi-photon resonances. These quasi-energy gaps are pronounced at small momentum, but decrease dramatically with the increase of momentum and finally tend to be closed when the momentum is large enough. Due to the contribution from the states at large momentum, the gaps in the density of states are effectively closed, in contrast to the prediction in the previous work by Oka and Aoki [Phys. Rev. B 79, 081406(R) (2009)]. We also investigate the optical conductivity for different field strengths and Fermi energies, and show the main features of the dynamical Franz-Keldysh effect in graphene. It is discovered that the optical conductivity exhibits a multi-step-like structure due to the sideband-modulated optical transition. It is also shown that dips appear at frequencies being the integer numbers of the applied terahertz field frequency in the case of low Fermi energy, originating from the quasi-energy gaps at small momentums. Moreover, under a circularly polarized terahertz field, we predict peaks in the middle of the “steps” and peaks induced by the contribution from the states around zero momentum in the optical conductivity.

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I. INTRODUCTION

Since the experimental realization of graphene, a monolayer of carbon atoms arranged in a honeycomb lattice, this material has aroused enormous interest due to its unique physical characteristics. Among different works in this field, the linear optical property of graphene is one of the main focuses of attention. The theoretical works based on the Dirac Hamiltonian show that the optical conductivity at high frequency is dominated by the interband optical conductivity, which takes a constant value of \( \sigma_0 = \frac{e^2}{\pi m^*} \) for frequency larger than twice of the Fermi energy \( E_F \) and approaches to zero for frequency below \( 2E_F \) due to the Pauli blocking. The universal value of \( \sigma_0 \) of optical conductivity has been demonstrated to be valid not only in the noninteracting limit but also in the presence of the disorder and the electron-electron interaction as long as the Dirac-cone approximation remains valid. The constant optical conductivity in a wide range of frequency has also been observed in the optical experiments. On the other hand, the optical conductivity at low frequency is determined by the intraband optical conductivity, which presents a Drude peak centred at zero frequency and is strongly influenced by the sample-dependent scattering behavior.

Recently, influence of an intense ac field on electrical and optical properties in graphene has also attracted much attention. It has been found that the application of an intense ac field can dramatically modify the band structure and hence the density of states (DOS). Their results also showed that a stationary energy gap appears around the Dirac point under a circularly polarized ac field. Oka and Aoki calculated the dc and ac conductivities in graphene irradiated by an intense circularly polarized light via the extended Kubo formula, and proposed the photovoltaic Hall effect, which is a novel Hall effect occurring in the absence of uniform magnetic fields. The dc transport properties of graphene-based p-n junctions under an intense ac field were also investigated theoretically. However, contribution in the optical spectra in graphene from the optical sidebands has not yet been well investigated.

In semiconductors, the contribution from the sidebands has been demonstrated to be important for the optical and transport properties. Many interesting phenomena, such as the photon-assisted tunneling, the sideband generation of exciton, the ac Stark effect, and the dynamical Franz-Keldysh (DFK) effect, as well as spin generation and manipulation utilized by the intense terahertz (THz) field are related to the formation of sidebands. Among these effects, the DFK effect describes the influence on optical spectra from the sidebands of the expanded states, which includes finite absorption below the band edge from the contribution of the sidebands below the bottom of the conduction band and the step-like behavior above the band edge due to the sideband-modulated generalized DOS. Just as the DFK effect in semiconductors, the formation of optical sidebands should also influence the optical spectra near the absorption edge around \( 2E_F \) in graphene. Nevertheless, the band structure of graphene is gapless and the energy dispersion is linear, which is quite distinct from semiconductors. Thus the DFK effect in graphene is expected to present some unique behaviors. This makes the investigation on this problem become very interesting and important. It is also noted...
that in previous investigation only the optical conductivity with $E_F$ much smaller than the frequency of the ac field was discussed and thus the contribution from the optical sidebands is difficult to identify. In the present work, we calculate the optical conductivity of graphene under the intense THz field for various Fermi energies and field strengths in order to gain a complete view of the DFK effect in graphene.

In order to include the contribution from the optical sidebands explicitly, we solve the time-dependent Schrödinger equation by using the Floquet theory and obtain the optical conductivity in graphene under an intense THz field via the nonequilibrium Green functions. In this paper, we focus on the optical conductivity at high frequency, which is known to be insensitive to the scattering strength. This allows us to ignore the detail of the scattering and only discuss the optical conductivity in the noninteracting limit. We first examine the energy spectrum and DOS. It is found that gaps appear in the quasi-energy spectrum due to the single-photon/multi-photon resonances. These quasi-energy gaps are pronounced at small momentum, in contrast to the prediction by Oka and Aoki. Our results of the optical conductivity reveal the main features of the DFK effect in graphene.

This paper is organized as follows. In Sec. IIA, we obtain the energy spectrum by exploiting the Floquet theory. Then in Sec. IIB, we derive the optical conductivity via the nonequilibrium Green functions. The numerical results of the DOS and optical conductivity are presented in Sec. III. Finally, we summarize in Sec. IV.

II. MODEL AND FORMALISM

A. Hamiltonian

We consider a graphene layer placed in the $x$-$y$ plane. In the vicinity of the Dirac point, the effective Hamiltonian of graphene can be written as ($\hbar=1$) \[ \hat{H}_{\text{eff}}^\mu(k) = v_F(\mu \sigma_x k_x + \sigma_y k_y). \] (1) Here $\mu = 1(-1)$ for $K(K')$ valley; $v_F$ is the Fermi velocity; $k$ represents the two-dimensional wave vector relative to $K(K')$ point; $\sigma$ is the Pauli matrix in the pseudospin space formed by the A and B sublattices of the honeycomb lattice. Here and hereafter, symbols with present the $2 \times 2$ matrices in the pseudospin space. The eigenvalue and eigenvector of $\hat{H}_{\text{eff}}^\mu$ are $E_{\text{eff}}^\mu = v_F|k|$ and $\psi^\mu_{k\sigma} = 1/\sqrt{2}(\mu e^{-i\theta_k} e^{i\theta_k}, 1)^T$, respectively, with $\nu$ being 1 ($-1$) for electron (hole) band and $\theta_k$ representing the polar angle of $k$. Substituting $k$ by $k + eA(t)$, one obtains the effective Hamiltonian in the presence of a THz field \[ \hat{H}_{\text{eff}}^\mu(k, t) = \hat{H}_{\text{eff}}^\mu(k) + \hat{H}^\mu_{\text{THz}}(t), \] (2) \[ \hat{H}^\mu_{\text{THz}}(t) = e^{i\nu}[\mu \sigma_x A_x(t) + \sigma_y A_y(t)]. \] (3)

For convenience, we choose the THz field as $E(t) = E_0(e_x \cos \theta_E \cos \Omega t + e_y \sin \theta_E \sin \Omega t)$. Thus the vector potential $A(t)$ reads $A(t) = \frac{e}{\hbar}(e_x \cos \theta_E \sin \Omega t + e_y \sin \theta_E \cos \Omega t)$. For $\theta_E = 0, \pi/4$ and $\pi/2$, the THz fields are linearly polarized along the $x$-axis, circularly polarized and linearly polarized along the $y$-axis, respectively. Without loss of generality, we set the THz field linearly polarized along the $x$-axis when discussing the case for a linearly polarized THz field.

By exploiting the Floquet theory, \[ \psi_{k\alpha}(t) = e^{-i\nu \frac{E_{\text{eff}}^\mu}{\Omega} t} \psi_{k\alpha}(0), \] (4) in which $\alpha$ represents the branch index of the solution; $\psi_{k\alpha}^\mu$ and $\psi_{k\alpha}$ are the eigenvalue (quasi-energy) and eigenvector determined by \[ \left( \frac{E_{\text{eff}}^\mu}{\Omega} - n \right) \psi_{k\alpha}^\mu = \frac{i}{2} \left[ \mu \cos \theta_E - \sigma \sin \theta_E \right] \psi_{k\alpha}^{\mu-1-\sigma} - \left( \mu \cos \theta_E + \sigma \sin \theta_E \right) \psi_{k\alpha}^{\mu+1-\sigma} + \frac{v_F k}{\Omega} \mu e^{-i\theta_k} \psi_{k\alpha}^{\mu-1-\sigma} \psi_{k\alpha}^{\mu-1-\sigma} \] (5) with $\beta = v_F e E_0/\Omega^2$. The above equation shows that the relation between the normalized quasi-energy $E_{\text{eff}}^\mu/\Omega$ and the normalized momentum $v_F k/\Omega$ is only determined by the dimensionless quantity $\beta$. Due to the periodicity of $\hat{H}_{\text{eff}}^\mu(k, t)$, the eigenvalues are also periodic, i.e., if $E_{\text{eff}}^\mu_{k_0}$ is a solution of Eq. (5), then $E_{\text{eff}}^\mu_{k_0 + \Omega t}$ is also a solution. It is evident that the eigenvectors of $E_{\text{eff}}^\mu_{k_0 + \Omega t}$ and $E_{\text{eff}}^\mu_{k_0 - \Omega t}$ satisfy $\psi_{k\alpha}^{\mu+1-\sigma} = \psi_{k\alpha}^{\mu-1-\sigma}$, thus $E_{\text{eff}}^\mu_{k_0 + \Omega t}$ and $E_{\text{eff}}^\mu_{k_0 - \Omega t}$ correspond to the same physical solution of the Schrödinger equation. Namely, the quasi-energies is a multi-valued quantity of the Floquet state. Nevertheless, for each momentum and each valley, the number of the independent quasi-energies is 2, which is determined by the dimension of the Hilbert space. For convenience, we choose the independent quasi-energies $E_{\text{eff}}^\mu_{k_0}$ in the reduced Floquet zone $(-\Omega/2, \Omega/2)$, with $\eta = \pm$ representing the index of independent solutions. These quasi-energies are referred to as the reduced quasi-energies in the following. The corresponding eigenvectors are labelled as $|\phi_{k\mu\eta}^\mu\rangle$. Therefore, by choosing the proper integer $l$, arbitrary quasi-energy $E_{\text{eff}}^\mu_{k_0}$ and the corresponding eigenvectors $\psi_{k\mu}^{\mu+1-\sigma}$ can be written into the form \[ E_{\text{eff}}^\mu_{k_0} = E_{\text{eff}}^\mu_{k_0 + \Omega \eta}, \] (6) \[ \psi_{k\mu}^{\mu+1-\sigma} = \psi_{k\mu}^{\mu-1-\sigma}. \] (7)
In addition, for the reduced quasi-energies with different $\eta$, one has
\[ \varepsilon_{k+}^{\mu,n} = -\varepsilon_{k-}^{\mu,n} - (n + m)\Omega, \]
and the corresponding weights are
\[ W_{k+}^{\mu,n} = \langle \phi_{\mu k+}^n | \phi_{\mu k+}^{\eta} \rangle. \]

From Eqs. (8) and (9), one can see that the quasi-energies and weights of the sidebands satisfy
\[ \varepsilon_{k+}^{\mu,n} = -\varepsilon_{k-}^{\mu,n} - (n + m)\Omega, \]
\[ W_{k+}^{\mu,n} = W_{k-}^{\mu,n}. \]

Besides the quasi-energy, another important quantity of the Floquet state is the mean energy,
\[ \overline{\varepsilon_{k+}^{\mu}} = \frac{1}{T_0} \int_{0}^{T_0} dt \langle \Phi_{k+}^{\mu}(t) | \hat{H}_{\mu}^{n} | \Phi_{k+}^{\mu}(t) \rangle = \varepsilon_{k+}^{\mu} - \sum_{\sigma} n\Omega \langle \phi_{\mu k+}^{n\sigma} | \phi_{\mu k+}^{\eta} \rangle, \]
where $T_0 = 2\pi/\Omega$ is the period of the applied THz field. Independent of the choice of the quasi-energy, the mean energy is a single-valued structure quantity of the Floquet state. Thus in previous works, the mean energy was utilized to identify the filled Floquet states, i.e. states with lower mean energy will be occupied at first. In this paper, we also use this ansatz to obtain the distribution function of the Floquet state, which will be discussed in the next subsection. Moreover, the mean energy is used to identify whether the Floquet state is electron- or hole-like. Analogous to the definition of the electron and hole states in the field-free case, we define the quasi-electron ($\eta = +$) and quasi-hole states ($\eta = -$) as the Floquet states satisfying $\overline{\varepsilon_{k+}^{\mu}} > 0$ and $\overline{\varepsilon_{k-}^{\mu}} < 0$, respectively.

**B. Optical conductivity**

It is known that the optical absorption is measured by the real part of optical conductivity. Therefore we focus on the real part of the optical conductivity in the following. For the probing light field of frequency $\omega_\ell$ with the polarization in the $\ell$ ($=x, y$) direction, the linear-response theory yields the real part of optical conductivity:
\[ \text{Re}\sigma_{\ell l}(T, \omega_\ell) = -\frac{g_\ell g_\ell}{\omega_\ell} \text{Im}\Pi_{\ell l}^T(T, \omega_\ell). \]

Here $g_\ell = 2$ and $g_\ell = 2$ are the valley and spin degeneracies, respectively; $\Pi_{\ell l}^T(T, \omega_\ell)$ is retard current-current correlation function in the $K$ valley. Here and hereafter we only give the correlation function in the $K$ valley and omit the valley index $\mu$ in all symbols, as the contributions to optical conductivity from both valleys are identical. $\Pi_{\ell l}^T(T, \omega_\ell)$ can be written as
\[ \Pi_{\ell l}^T(T, \omega_\ell) = \int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} dt' e^{i\omega_\ell t} \Pi_{\ell l}^T(T - \frac{t}{2}, T - \frac{t'}{2}), \]
where
\[ \Pi_{\ell l}^T(t, t') = -i \theta(t - t') \langle [j^\ell(t), j^l(t')] \rangle. \]

with $j^\ell = e_{\ell\ell}^\Pi \sigma_\ell$ presenting the $\ell$ component of the current operator in graphene. Via the nonequilibrium Green function method, we have
\[ \Pi_{\ell l}^T(t, t', T, \omega_\ell) = -i \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega''}{2\pi} \Pi_{\ell l}^T(t, T, \omega) \Pi_{\ell l}^T(t', T, \omega') \Pi_{\ell l}^T(t', T, \omega''), \]
\[ X_{\ell l}^T(t, T, \omega_\ell) = \int_{-\infty}^{\infty} d\omega \int_{-\infty}^{\infty} d\omega' \int_{-\infty}^{\infty} d\omega'' \Pi_{\ell l}^T(t, T, \omega) \Pi_{\ell l}^T(t', T, \omega') \Pi_{\ell l}^T(t', T, \omega''), \]
\[ \Pi_{\ell l}^T(t, t', T, \omega_\ell) = -i \theta(t - t') \langle [j^\ell(t), j^l(t')] \rangle. \]

with $G^\alpha_{\ell l}^\sigma_\ell (T, t', t')$ representing the retarded (advanced, lesser) single-particle Green function. Substituting Eq. (18) into Eq. (19), one has
\[ \Pi_{\ell l}^T(t, t', T, \omega_\ell) = -i \sum_{k_{\ell,1} \sigma_{\ell 1}} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega''}{2\pi} \Pi_{\ell l}^T(t, T, \omega) \Pi_{\ell l}^T(t', T, \omega') \Pi_{\ell l}^T(t', T, \omega'') \]
\[ \times \left[ G^\alpha_{\ell l}^\sigma_\ell (T, \omega + \omega') + G^\alpha_{\ell l}^\sigma_\ell (T, \omega - \omega') \right]. \]

Since
\[ \left[ G^\sigma_{\ell l}^\alpha_\ell (T, \omega_\ell) \right]^* = -G^\sigma_{\ell l}^\alpha_\ell (T, \omega_\ell) \] and \[ \left[ G^\sigma_{\ell l}^\alpha_\ell (T, \omega_\ell) \right]^* = -G^\sigma_{\ell l}^\alpha_\ell (T, \omega_\ell), \] one obtains
\[ \Pi_{\ell l}^T(t, t', T, \omega_\ell) = -i \sum_{k_{\ell,1} \sigma_{\ell 1}} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega''}{2\pi} \Pi_{\ell l}^T(t, T, \omega) \Pi_{\ell l}^T(t', T, \omega') \Pi_{\ell l}^T(t', T, \omega'') \]
\[ \times \left[ G^\sigma_{\ell l}^\alpha_\ell (T, \omega + \omega') + G^\sigma_{\ell l}^\alpha_\ell (T, \omega - \omega') \right] G^\sigma_{\ell l}^\alpha_\ell (T, \omega). \]

In above equations, we have used the relation \[ A_{\ell l}^\alpha_\ell (T, \omega) = i[G^\sigma_{\ell l}^\alpha_\ell (T, \omega) - G^\sigma_{\ell l}^\alpha_\ell (T, \omega)]. \] In the noninteracting limit, the retarded Green function is given by
\[ \hat{G}^\sigma_{\ell l} (t_1, t_2) = -i\theta(t_1 - t_2) \sum_{\eta} \langle \Phi_{k\eta}(t_1) | \Phi_{k\eta}(t_2) \rangle. \]
Thus the spectral function in the frequency space can be written as

\[
\hat{A}_k(T, \omega) = \int_{-\infty}^{\infty} d\tau e^{i\omega \tau} \sum_\eta |\Phi_{k\eta}(T + \frac{\tau}{2})\rangle\langle \Phi_{k\eta}(T - \frac{\tau}{2})|
\]

\[
= 2\pi \sum_{n,m} \epsilon(n-m)\Omega T \phi_{k\eta}^\dagger \phi_{k\eta}^m \delta(\omega - \varepsilon_{k\eta} + (n + m)\frac{\Omega}{2}),
\]

(22)

The next step is to calculate \( \hat{G}_k^{<}(T, \omega) \). The equal-time lesser function can be expressed in the form

\[
\hat{G}_k^{<}(t, t) = i \sum_{\eta_1\eta_2} \rho_{k\eta_1\eta_2} \langle \Phi_{k\eta_1}(t) | \Phi_{k\eta_2}(t) \rangle.
\]

(23)

Here \( \rho_{k\eta_1\eta_2}(t) \) is the nonequilibrium density matrix in the Floquet picture which can be determined by the kinetic equation including the electron-impurity, electron-phonon and electron-electron scatterings. This approach is very complicated and left as the subject of our future work. Here we obtain the lesser function based on a simple ansatz following the previous works of Oka and Aoki, the steady-state density matrix is diagonal with the diagonal term \( f_{k\eta} \) being the Fermi distribution on the mean energy of the Floquet state,

\[
\rho_{k\eta_1\eta_2}(t) = f_{k\eta} \delta_{\eta_1\eta_2} = n_F(\overline{\varepsilon}_{k\eta}) \delta_{\eta_1\eta_2}.
\]

(24)

In the present paper, we focus on the case at zero temperature, and then

\[
f_{k\eta} = \theta(\overline{\varepsilon}_{k\eta} - E_F),
\]

(25)

where the Fermi energy \( E_F \) can be obtained from

\[
N_e = g_s g_v \sum_{k\eta} \theta(E_F - \overline{\varepsilon}_{k\eta}).
\]

(26)

Substituting Eq. (24) into Eq. (23), one gets

\[
\hat{G}_k^{<}(t, t) = i \sum_\eta \rho_{k\eta} |\Phi_{k\eta}(t)\rangle \langle \Phi_{k\eta}(t)|,
\]

(27)

By further exploiting the generalized Kadanoff-Baym Ansatz, the two-time lesser function can be obtained as

\[
\hat{G}_k^{<}(t, t') = i \hat{G}_k^{<}(t, t') \hat{G}_k^{<}(t', t) - i \hat{G}_k^{<}(t, t') \hat{G}_k^{<}(t', t')
\]

\[
= i \sum_\eta f_{k\eta} |\Phi_{k\eta}(t)\rangle \langle \Phi_{k\eta}(t')|.
\]

(28)

Then we have

\[
\hat{G}_k^{<}(T, \omega_l) = i \sum_\eta f_{k\eta} \hat{A}_{k\eta}(T, \omega),
\]

(29)

with \( \hat{A}_{k\eta}(T, \omega) = \int_{-\infty}^{\infty} d\tau e^{i\omega \tau} |\Phi_{k\eta}(T + \frac{\tau}{2})\rangle\langle \Phi_{k\eta}(T - \frac{\tau}{2})| \). Using the above equations, one obtains the optical conductivity

\[
\sigma^{\text{ll}}(T, \omega_l) = \frac{g_s g_v \pi}{\omega_l} \sum_{k\eta_1\eta_2} \langle \phi_{k\eta_1}^{n_1} | j_k^l | \phi_{k\eta_2}^{n_2} \rangle \langle \phi_{k\eta_1}^{n_1} | j_k^l | \phi_{k\eta_2}^{n_2} \rangle
\]

\[
\times (f_{k\eta_1} - f_{k\eta_2}) e^{i(n_1 - n_2 + n_2 - n_1)\Omega T} \delta(\varepsilon_{k\eta_1} - \varepsilon_{k\eta_2} - (n_1 + n_2 - n_2 - n_1)\frac{\Omega}{2} + \omega_l).\]

(30)

The time-averaged optical conductivity can be written as

\[
\Sigma^{\text{ll}}(T, \omega_l) = \frac{1}{T_0} \int_{0}^{T_0} dT \sigma^{\text{ll}}(T, \omega_l)
\]

\[
= \frac{g_s g_v \pi}{\omega_l} \sum_{k\eta_1\eta_2} \langle \phi_{k\eta_1}^{n_1-N} | j_k^l | \phi_{k\eta_2}^{n_2-N} \rangle \langle \phi_{k\eta_1}^{n_1-N} | j_k^l | \phi_{k\eta_2}^{n_2-N} \rangle
\]

\[
\times (f_{k\eta_1} - f_{k\eta_2}) \delta(\varepsilon_{k\eta_1} - \varepsilon_{k\eta_2} - N\Omega + \omega_l).\]

(31)

It is found that the time-averaged optical conductivity from the nonequilibrium Green functions agrees with that from the extended Kubo formula used in Ref. [26] (see also Appendix A). However, it is noted that our method not only gives the time-averaged optical conductivity but also the time-dependent one, and thus can provide the dynamical information of optical response, which can be observed via the time-resolved measurements. It is also noted the distribution used by Oka and Aoki, i.e., \( f_{k\eta}^{\text{int}} = \sum_{l\nu} n_{F}(E_{k\nu}) |\langle \kappa_{k\nu} | \phi_{k\eta}^{n_l} \rangle|^2 \), is obtained by projecting the equilibrium Fermi distribution in the field-free case to the basis set formed by the Floquet eigenvectors, corresponding to the “sudden approximation”. Obviously, this distribution, referred to as the projected distribution in the following, is quite different from the mean-energy-determined distribution used in this paper. The comparison of the optical conductivities obtained from these two distributions will be addressed in next section.

### III. NUMERICAL RESULTS

In this section, we discuss the numerical results of the energy spectrum, DOS and optical conductivity of graphene under an intense THz field. The typical parameters used in the computation are \( \Omega = 5 \) THz, \( E_0 = 15 \) kV/cm (corresponding to \( \beta = 2.3 \)), \( N_e = 1.5 \times 10^{12} \text{ cm}^{-2} (E_F = 6\Omega) \) and \( 2.5 \times 10^{11} \text{ cm}^{-2} (E_F = 2.7\Omega) \). It is noted that our results can be generalized to the other \( \Omega \) regime as long as Eq. (24) remains valid, since the behaviors of the energy spectrum and the DOS are only determined by \( \beta \) and the behavior of the optical conductivity is only determined by \( \beta \) and \( E_F/\Omega \). We also restrict our investigation of optical conductivity in the frequency regime \( \omega_l > \Omega \), since the scattering process is not considered in our model and the optical conductivity at low frequency is known to be strongly dependent on the scattering strength [39–41].
A. Energy spectrum

Although the energy spectrum in this system has been investigated by many works, a complete investigation on this problem is still lacking. In particular, the energy spectrum at large momentum has not been well investigated in previous works. In this section, we investigate the energy spectrum under a circularly polarized THz field in a wide range of momentum. Pronounced quasi-energy gaps appear at small momentum in both cases with low and high field strengths. We also discuss the case with a linearly polarized THz field and show that the energy spectrum becomes anisotropic.

We first concentrate on the case for a circularly polarized THz field with low field strength (small $\beta$). In Fig. 1(a), the quasi-energies of the sidebands $\xi_{k\eta}^n$ [Eq. (10)] for $\beta = 0.4$ are plotted as function of momentum. Here the color coding represents the weight $W_{nk\eta}^n$ [Eq. (11)] of the corresponding sideband. Since the quasi-energy spectrum is isotropic under a circularly polarized field, we only present the results with $\theta_k = 0$. The most interesting feature seen in this figure is the appearance of gaps at small momentum in the quasi-energy spectrum, in consistence with the previous investigations. These gaps appear around the momentums $m\Omega/2\nu_F$ and the quasi-energies $m\Omega/2 + \Omega l$, with $m$ and $l$ being integers. All gaps at the same momentum share the identical magnitude due to the periodicity of the quasi-energy spectrum. These quasi-energy gaps can be attributed to the ac Stark splittings induced by the single-photon/multi-photon resonances.

FIG. 1: (Color online) Circularly polarized THz field with $\beta = 0.4$. (a) Quasi-energies $\xi_{k\eta}^n$ against the normalized momentum. The color coding represents the weight $W_{nk\eta}^n$ of the corresponding sideband. The blue crosses represent the selected quasi-energies of the quasi-electron states. (b) Quasi-energy $\epsilon_{k+}$ (red solid curve) and mean energy $\tau_{k+}$ (blue dashed curve) of the quasi-electron state as well as the field-free electron energy (green dotted curve) against the normalized momentum. In the inset of (b), we plot the quasi-energy around the gap at $k = 0.5\Omega/v_F$ and $\epsilon_{k\eta} = 0.5\Omega$ [the region labelled by the box in (a)] as well as the corresponding mean energy as function of momentum. The solid (dashed) curves with and without crosses represent the quasi-energies (mean energies) of the quasi-electron ($\eta = +$) and quasi-hole ($\eta = -$) states, respectively. The black chain line indicates the momentum of the crossover point $k_0$. Note the scale of mean energy is on the right-hand side of the frame.

FIG. 2: (Color online) Circularly polarized THz field with $\beta = 2.3$. (a) Quasi-energies $\xi_{k\eta}^n$ against the normalized momentum. The color coding represents the weight $W_{nk\eta}^n$ of the corresponding sideband. The blue crosses represent the selected quasi-energies of the quasi-electron states. (b) Quasi-energy $\epsilon_{k+}$ (red solid curve) and mean energy $\tau_{k+}$ (blue dashed curve) of the quasi-electron state as well as the field-free electron energy (green dotted curve) versus the normalized momentum. The thin black lines mark the mean energies being $1.5\Omega$, $1.8\Omega$, $2.3\Omega$ and $2.7\Omega$, which are used in the Fig. 1(c). Note the scale of mean energy is on the right-hand side of the frame.
The physics is that if a pair of states are coupled by an electromagnetic field with frequency $\Omega$ and the energy difference between these two states equals to $m\Omega$, then an ac Stark splitting appears unless the corresponding transition is forbidden. Specifically, in the present case, the gaps around the momentum satisfying $2v_F k = m\Omega$ are induced by the $m$-photon resonances.

Nevertheless, the behaviour of the quasi-energy spectrum in large momentum regime becomes very different. From Fig. 1(a), one can see that the energy gaps decrease dramatically with the increase of $k$ and finally tend to be closed when the momentum is large enough. This effect can be understood via Eq. (32) under the rotating-wave approximation (the derivation is presented in Appendix B), which shows that the quasi-energy gap around the momentum $m\Omega /2v_F$ is determined by the effective coupling parameter $|y_m(\theta_k)|$, given by [see also Eq. (B11)]

$$|y_m(\theta_k)| = \frac{1}{\sqrt{2}}|J_{m+1}(\sqrt{2}\beta) - J_{m-1}(\sqrt{2}\beta)|, \quad (32)$$

with $J_m(\sqrt{2}\beta)$ being the Bessel function. Due to the $m$-dependence of $J_m(\sqrt{2}\beta)$, the effective coupling parameter $|y_m(\theta_k)|$ decreases dramatically with the increase of $m$ when $m$ is large enough. Thus the quasi-energy gaps become negligible at large momentum. Our calculations also show that, associated with the absence of the gaps, the band-mixing, i.e., the hole (electron) component of the quasi-electron (quasi-hole) state, becomes negligible, and the wave function becomes very close to the one without the interband term of $H_{THz}$.

In Fig. 1(b), we plot the mean energy $\bar{\epsilon}_{k+}$ [Eq. (14)] and the quasi-energy $\epsilon_{k+}$ of the quasi-electron state ($\epsilon_{k+} > 0$) as well as the field-free electron energy for $\beta = 0.4$ as function of momentum. In order to compare the above three energies directly, we choose the quasi-energy $\epsilon_{k+}$ according to the following rules: 1) the continuity of the quasi-energy is kept as far as possible; 2) the quasi-energy at large momentum is closest to the field-free electron energy. We also plot these selected quasi-energies in Fig. 1(a) (blue crosses). From Fig. 1(b), it is shown that the mean energy and the quasi-energy are far away from (very close to) the field-free energy at small (large) momentum, in consistence with the behaviour of the quasi-energy gap. Moreover, it is also seen that the mean energy reaches zero at a momentum somewhere inside the quasi-energy gap, except the one at zero momentum. In order to reveal the underlying physics, we plot the quasi-energy around the gap at $k = 0.5\Omega /v_F$ and $\epsilon_{k0} = 0.5\Omega$ [the region labelled by the box in Fig. 1(a)] as well as the corresponding mean energy as function of momentum in the inset of Fig. 1(b). It shows that there is a crossover point (labelled as $K_0$) between the quasi-hole state (blue solid curve) and the quasi-electron state (red solid curve with crosses) in the quasi-energy above the gap. Since the quasi-energy varies continuously with $k$ at this point, the corresponding mean energy also varies continuously, i.e., $\bar{\epsilon}_{K_0+} = \bar{\epsilon}_{K_0-}$. Also, from Eqs. (13) and (32), one can see that $\bar{\epsilon}_{K_0+} = -\bar{\epsilon}_{K_0-}$. Consequently, the mean energies at this point must be zero. The finite mean energy at $k = 0$ is based on the similar reason. As shown in Fig. 1(a), the quasi-energy above the gap at zero momentum always belongs to the quasi-electron state [blue crosses in Fig. 1(a)], hence no crossover appears.

Now we turn to the case for a circularly polarized THz field with high field strength (Fig. 2). From Fig. 2(a), it is seen that pronounced quasi-energy gaps appear in a wider range of $k$. However, unlike the previous case, the momentums of the gaps markedly deviate from $m\Omega /2v_F$. This is because the effect of the rapidly varying terms in the resonance equations [Eqs. (15) and (16)] cannot be neglected for strong field, i.e., the rotating-wave approximation is not valid. The joint effect of the terms with different oscillating frequencies leads to

![Image of linearly polarized THz field with $\beta = 2.3$. Quasi-energies $\epsilon_{k0}^{\alpha}$ against the normalized momentum for different polar angles $\theta_k$. The color coding represents the weight $W_{k0}^{\alpha}$ of the corresponding sideband. $k_{n}$ in (c) stands for $k \cdot \hat{n}$ with $\hat{n}$ being the unit vector at an angle $\pi/6$ with respect to the $x$-axis.](image-url)
the complicated behaviour of the quasi-energy spectrum. However, the quasi-energies where the gaps appear are still around $\Omega/2$, determined by the symmetry of the quasi-energies of the sidebands [Eq. (13)]. Figure 2 also shows that the quasi-energy gaps become extremely small and the quasi-energy and mean energy become very close to the field-free energy at large momentum. The physics is similar to the weak-field case. When the photon number involved in the resonance becomes too large, the effective resonant coupling becomes extremely weak. Thus the influence of the THz field on the energy spectrum becomes negligible.

Finally we address the case for a linearly polarized THz field (Fig. 3). Here we only present the results with high field strength as they are sufficient for showing the main features in this case. Recall that the linearly polarized THz field is set along the $x$-axis throughout this paper, thus $\theta_k$ equals to the angle between the momentum and the THz field. From Fig. 3 it is seen that quasi-energy gaps are closed at zero momentum. This effect can be understood from the exact analytical solution

$$\Phi_{k=0 \pm (t)} = \sum_n J_{n \pm 1}(\beta)e^{in\Omega t}(1, \pm 1)^T. \tag{33}$$

Clearly, the quasi-energy is zero at zero momentum, thus the gap disappears. Another interesting feature is the anisotropy of the quasi-energy spectrum. For momentum along the $x$-axis [Fig. 3(a)], all gaps are closed, since the intraband term of $H_{\text{THz}}$ [Eq. (14)] becomes zero and hence the quasi-energy is exactly the same as the field-free energy, as shown in Eqs. (15) and (16) in Appendix B. For momentum along the $y$-axis [Fig. 3(b)], all gaps except the ones around $k = 0.5\Omega/v_F$ are effectively closed. This is because the intraband term of $H_{\text{THz}}$ [Eq. (14)] becomes zero, and thus the gaps from the multi-photon resonances become extremely small, as shown in Fig. 3 in Appendix B. For other polar angle, e.g., $\theta_k = \pi/6$ [Fig. 3(c)], pronounced quasi-energy gaps appear not only around $k = 0.5\Omega/v_F$ but also around the other resonant points at small momentum, similar to the case with a circularly polarized THz field.

### B. DOS

Then we turn to investigate the DOS. By using the spectral function Eq. (22), one obtains the time-averaged DOS

$$D^{\text{ave}}(\omega) = \frac{g_s g_v}{2\pi T} \int_0^{T_0} dT \sum_{k\eta} \text{Tr} A_{k\eta}(T, \omega)$$

$$= \frac{g_s g_v}{2\pi T} \sum_{k\eta n} \langle \phi_{k\eta}^n | \phi_{k\eta}^n \rangle \delta(\omega - \varepsilon_{k\eta} + n\Omega)$$

$$= \frac{g_s g_v}{2\pi T} \sum_{k\alpha} \langle \psi_{k\alpha}^0 | \psi_{k\alpha}^0 \rangle \delta(\omega - \mathcal{E}_{k\alpha}). \tag{34}$$

The last equality is derived from Eqs. (1) and (7). It is noted that the above equation is in the same form as the one reported by Oka and Aoki. In Fig. 4(a), we plot the time-averaged DOS under circularly and linearly polarized THz fields for $\beta = 2.3$. The region close to $\omega \sim 0$ is enlarged in the inset. (b) Time-averaged DOS versus $\omega$ under a circularly polarized THz field for $\beta = 2.3$ with all relevant states (red solid curve), limited in the momentum regimes $v_F k < 2\Omega$ (blue dashed curve) and $v_F k < 0.5\Omega$ (green dotted curve). The yellow chain curve represents the DOS from Ref. 21.

![FIG. 4: (Color online) (a) Time-averaged DOS versus $\omega$ under circularly (red solid curve) and linearly (blue dashed curve) polarized THz fields for $\beta = 2.3$. The region close to $\omega \sim 0$ is enlarged in the inset. (b) Time-averaged DOS versus $\omega$ under a circularly polarized THz field for $\beta = 2.3$ with all relevant states (red solid curve), limited in the momentum regimes $v_F k < 2\Omega$ (blue dashed curve) and $v_F k < 0.5\Omega$ (green dotted curve). The yellow chain curve represents the DOS from Ref. 21.](image-url)
C. Optical conductivity

1. Under a circularly polarized THz field

In this subsection we discuss the optical conductivity under a circularly polarized THz field. Without loss of generality, we restrict ourselves to the $n$-type case, i.e., $E_F > 0$. Thus only the quasi-electron states with $\varepsilon_{k\eta} > E_F$ are not occupied and the corresponding interband transitions are allowed.

We first focus on the case with high Fermi energy. The time-dependent and time-averaged optical conductivities as function of the optical frequency $\omega_l$ are plotted in Figs. 6(a) and (b), respectively. Here $\sigma_0 = e^2/\hbar$ is used as the unit of the optical conductivity. It is shown that the
optical conductivity exhibits a multi-step-like structure at $\omega_l \sim 2E_F$, in contrast to the single-step-like behaviour in the field-free case [yellow curve in Fig. 5(b)].

Similar to the DFK effect in semiconductors, this effect is from the sideband-modulated optical transition, i.e., $n\Omega$ in the delta functions in Eqs. (30) and (31). It is also seen that the number of “step” increases with the increase of the field strength. This can be understood by noticing that the weight of the sideband is distributed in a wider range of frequency for stronger field.

Figure 5 also shows that the optical conductivity varies mildly with the increase of $\omega_l$ in each “step”, which is quite different from the DFK effect in semiconductors, where the optical absorption is strongly dependent on $\omega_l$ in each “step”. This behavior can be understood as follows. Since the effect from the interband term of $H_{\text{THz}}$ becomes negligible at large momentum, the optical conductivity at high Fermi energy can be approximately described by Eq. (C5) (the derivation is presented in Appendix C), which indicates that the frequency dependence of the optical conductivity is only from the factor $1 - N\Omega/\omega_l$ in the optical transition between the sidebands with the energy difference $2\epsilon_{k^+} + N\Omega$. This factor originates from the linear dispersion of graphene. It is also noted that the optical conductivity is dominated by the optical transitions with small $|N|$, and the pronounced “steps” only appear at $\omega_l \sim 2E_F$. Thus the frequency dependence of the optical conductivity becomes very weak in each “step” for high Fermi energy.

Then we turn to the case with low Fermi energy. The time-dependent and time-averaged optical conductivities are plotted as function of the optical frequency in the cases with $E_F = 2.7\Omega$ in Figs. 6(a) and (b), respectively. It is seen that dips appear around the frequencies satisfying $\Omega$ when the applied THz field is strong enough. This is because the states at small momentum, where the quasi-energy gaps become pronounced as shown in Fig. 5(b), can contribute to the optical conductivity in this case. More interesting features are presented in the Fermi energy dependence of optical conductivity [Fig. 6(c)]. It is shown that peaks appear in the middle of the “steps” for $E_F = 2.3\Omega$ (red solid curve). The scenario is as follows. From Fig. 6(b), it is seen that the maximum of the mean energy $\bar{\epsilon}_{k^+}$ at $2.5\Omega/v_F$ is slightly higher than the Fermi energy $2.3\Omega$. Consequently, in this momentum regime only the quasi-electron states around $2.5\Omega/v_F$ can contribute to the optical conductivity and hence induces the peaks in the middle of the “steps”. When the Fermi energy decreases, more and more states in this momentum regime can contribute to the optical conductivity. Consequently the peaks become wider and wider, and finally become the new “steps”, as shown in the case with $E_F = 1.8\Omega$ (yellow chain curve). Moreover, when the Fermi energy decreases to $1.5\Omega$ (blue dashed curve), sharp peaks appear in the optical conductivity. This originates from the contribution around $k = 0$, in which $\bar{\epsilon}_{k^+}$ is slightly higher than $1.5\Omega$ as shown in Fig. 6(b). One also notes that the van Hoff singularities at nonzero momentum have no effect on the optical conductivity with finite Fermi energy, since the mean energy is close to zero at the momentum of the quasi-energy gaps, as shown in Fig. 6(b).

FIG. 7: (Color online) Linearly polarized THz field with $\beta = 2.3$. (a) Time-averaged optical conductivity as function of the optical frequency for different Fermi energies. (b) Time-averaged optical conductivities versus the optical frequency from the states in different polar angle regions $[\theta_{12}^m - \pi/128, \theta_{12}^m + \pi/128]$ as well as the one with all polar angles integrated. $E_F = 2.5\Omega$. (c) Mean energies of the quasi-electron states with different polar angles $\theta_{k'}$ against the normalized momentum. The thin black line indicates the mean energy being $2.5\Omega$. 
We also plot the time-averaged optical conductivity as function of the optical frequency under a linearly polarized THz field in Fig. 7(a). The behavior in this case is simpler than that under a circularly polarized THz field. The multi-step-like behavior and the dips around $\hbar \Omega$ still appear. Nevertheless, the peaks in the middle of the “steps”, which still appear in the optical conductivity at low frequency for $E_F = 2.5\Omega$ and $1.2\Omega$, are much less pronounced than the ones under a circularly polarized THz field. In order to reveal the underlying physics, we plot the time-averaged optical conductivity from the states with different polar angles as function of the optical frequency for $E_F = 2.5\Omega$ in Fig. 7(b). The corresponding mean energies are plotted against the normalized momentum in Fig. 7(c). As mentioned above, the peaks in the middle of the “steps” only appear in the situation satisfying the criteria that a local maximum of the mean energy $\gamma_{k,\eta}$ is slightly higher than the Fermi energy. From Fig. 7(c), one can see that the above criteria is satisfied for the states with $\theta_k = \pi/12$ and $\pi/6$, thus pronounced peaks appear in the optical conductivity from the states with these angles [red solid and blue dashed curves in Fig. 7(b)] and the corresponding angles with the same quasi-energy $\beta$. However, this criteria cannot be satisfied for the states with the other polar angles, e.g., $\theta_k = \pi/8$ and $\theta_k = \pi/4$, so peaks are absent in the corresponding optical conductivity [green dotted and yellow chain curves in Fig. 7(b)]. Therefore, after the summation of the contribution from all polar angles, the peaks in the middle of the “steps” become much less pronounced.

3. Comparison of the optical conductivities calculated with the mean-energy-determined distribution and the projected distribution

In this subsection, we compare the optical conductivities calculated with the distribution determined by the mean energy and the projected distribution. As mentioned above, the projected distribution used in Ref. 26 is described by (see also Appendix A)

$$ f^{\text{ini}}_{k,\eta} = \sum_{\nu l} n_F(E_{k\nu})(\zeta_{k\nu}|\phi^l_{k\eta})^2. \quad (35) $$

Recall that $E_{k\nu}$ and $\zeta_{k\nu}$ are the eigenvalue and eigenvector of $\hat{H}_0$. From Eq. (35), one can recognize the main features of the projected distribution at zero temperature: at $k < k_F = E_F/\hbar \nu$, both the field-free electron and hole states are occupied, thus the corresponding quasi-electron and quasi-hole states are both occupied; at $k > k_F$, only the hole state is occupied, so the distribution of the Floquet state is determined by the hole component of this state. Therefore one can see that only the states with $k > k_F$ can contribute to the optical conductivity, and the contribution decreases with the increase of the band-mixing.

![FIG. 8: (Color online) Time-averaged optical conductivities from the mean-energy-determined distribution (solid curves) and the projected distribution (dashed curves) are plotted as function of the optical frequency under a circularly polarized THz field with $\beta = 2.3$ for different Fermi energies.](image)
photon/multi-photon resonances. Nevertheless, in large momentum regime, where the energy spectrum has not been well investigated in previous works, we find that the quasi-energy gaps decrease dramatically with the increase of momentum and finally tend to be closed when the momentum is large enough. Consequently, taking account of the contribution from the states around zero momentum, the gaps in the DOS are effectively closed, in contrast to the prediction by Oka and Aoki.\textsuperscript{21}

We also investigate the optical conductivity from the mean-energy-determined distribution for different field strengths and Fermi energies. These results reveal the main features of the DFK effect in graphene. In the case with high Fermi energy, we discover that the optical conductivity presents a multi-step-like behavior around the optical frequency $\omega_l$ twice of the Fermi energy $E_F$, in contrast to the single-step-like behaviour in the field-free case. This effect is from the sideband-modulated optical transition, similar to the DFK effect in semiconductors. This effect is from the sideband-modulated optical transition, similar to the DFK effect in semiconductors. This kind of peaks become much less pronounced in the case with a linearly polarized field, owing to the anisotropic energy spectrum. Another interesting finding in the case with a circularly polarized field is that the contribution from the states around zero momentum can induce sharp peaks in the optical conductivity when the Fermi energy is lower than the mean energy at $k = 0$.

Finally, we address the distribution function of the Floquet states. Our calculations are based on the ansatz that the distribution function of the Floquet states is determined by the mean energy, following the works in the literature.\textsuperscript{28,59,60} The project distribution function is also adopted in the literature.\textsuperscript{28} It is noted that the multi-step-like behavior and the dips around frequencies $l\Omega$ exist in optical conductivities from both distributions. This indicates that these two effects do not depend on the details of the distribution function and thus are expected to be observed in the optical absorption measurements subject to intense THz fields. Nevertheless, the peaks in the middle of the “steps” and the peaks from the states around zero momentum appear only in the optical conductivity from the mean-energy-determined distribution. By performing experimental investigation on these peaks in the optical conductivity, one can distinguish which distribution function of the Floquet state is closest to the genuine one. One may also solve the kinetic equations with all the scattering explicitly included\textsuperscript{23} to determine the distribution function.

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**Appendix A: Optical conductivity from extend Kubo formula**

We write Eq. (3) in Ref. \textsuperscript{26} into the form

$$\sigma_{xx}^{\text{ave}}(\omega_l) = \frac{4\pi}{\omega_l} \sum_{\nu \neq \nu_l} \langle \nu_l | \hat{J}_k | \nu \rangle \langle \nu | \hat{J}_k | \nu_l \rangle \times (\hat{f}_{k\alpha} - \hat{f}_{k\beta}) \delta(\varepsilon_{k\alpha} - \varepsilon_{k\beta} + \omega_l)$$

with $\hat{f}_{k\alpha} = \sum_{\nu} |(\zeta_{k\nu} | \nu_l^0) |^2 n_\nu(E_{k\nu})$. Recall that $E_{k\nu}$ and $\zeta_{k\nu}$ are the eigenvalues and eigenvectors of $\hat{H}_0$. By using Eqs. (6) and (7), one obtains

$$\sigma_{xx}^{\text{ave}}(\omega_l) = \frac{4\pi}{\omega_l} \sum_{\nu \neq \nu_l} \langle \nu_l | \hat{J}_k | \nu \rangle \langle \nu | \hat{J}_k | \nu_l \rangle \times (\hat{f}_{k\alpha}^{\text{ini}} - \hat{f}_{k\beta}^{\text{ini}}) \delta(\varepsilon_{k\alpha} - \varepsilon_{k\beta} - N\Omega + \omega_l)$$

with $\hat{f}_{k\alpha}^{\text{ini}} = \sum_{\nu} n_\nu(E_{k\nu}) |(\zeta_{k\nu} | \nu_l^0) |^2$. It is seen that the above equation is in the same form as Eq. \textsuperscript{61}, but the distribution $\hat{f}_{k\alpha}^{\text{ini}}$ is quite different from $\hat{f}_{k\alpha} = n_\nu(\zeta_{k\nu})$ used in the present paper.

**Appendix B: Approximate analytical solution of Schrödinger equation**

We first transform the effective Hamiltonian into the basis set formed by the eigenvectors of $H_0$. Thus the Schrödinger equation can be written as

$$\left[ v_F k \hat{a}_z + \hat{H}_{\text{THz}}(t) \right] |\Psi_{k_\eta}(t)\rangle = \frac{1}{i} \frac{\partial}{\partial t} |\Psi_{k_\eta}(t)\rangle.$$  

(B1)

Here $|\Psi_{k_\eta}(t)\rangle = |\hat{U}_k(t)|\Psi_{k_0}(t)\rangle$, with the transformation matrix

$$U_k = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\theta_k} & -e^{-i\theta_k} \\ 1 & 1 \end{pmatrix};$$

(B2)

$\hat{H}_{\text{THz}}(\theta_k, t)$ can be divided into the intraband $\hat{H}^{\text{intra}}_{\text{THz}}(\theta_k, t)$ and interband $\hat{H}^{\text{inter}}_{\text{THz}}(\theta_k, t)$ terms,
given by
\[
\hat{H}^{\text{intra}}_{\text{THz}}(\theta_k, t) = \beta \Omega \tilde{a}_\omega (-\cos \theta_E \cos \theta_k \sin \Omega t \\
+ \sin \theta_E \sin \theta_k \cos \Omega t), \tag{B3}
\]
\[
\hat{H}^{\text{inter}}_{\text{THz}}(\theta_k, t) = \beta \Omega \tilde{a}_\omega (\cos \theta_E \sin \theta_k \sin \Omega t \\
+ \sin \theta_E \cos \theta_k \cos \Omega t). \tag{B4}
\]

Then we solve the Schrödinger equation without the interband term \(\hat{H}^{\text{inter}}_{\text{THz}}(\theta_k, t)\) and obtain
\[
|\Psi^{(0)}_{\theta_k}(t)\rangle = e^{-iv\cdot k \cdot t} |u^{(0)}(\theta_k, t)(1, 0)\rangle, \tag{B5}
\]
\[
|\Psi^{(0)}_{\theta_k}(t)\rangle = e^{iv\cdot k \cdot t} |u^{(0)}(\theta_k, t)^\dagger(0, 1)\rangle, \tag{B6}
\]
with
\[
u^{(0)}(\theta_k, t) = \exp \left\{ i \beta \cos \theta_E \cos \theta_k [1 - \cos(\Omega t)] \\
- i \beta \sin \theta_E \sin \theta_k \sin(\Omega t) \right\}. \tag{B7}
\]

It is evident that \(\nu^{(0)}(\theta_k, t)\) is a time-periodic function, thus the quasi-energy of \(|\Psi^{(0)}_{\theta_k}(t)\rangle\) is exactly the same as the field-free energy \(\eta v\cdot k\). This indicates that all quasi-
energy gaps disappear without \(\hat{H}^{\text{inter}}_{\text{THz}}(\theta_k, t)\).

The next step is to write the solution of Eq. (B1) into the form
\[
|\Psi_{\theta_k}(t)\rangle = a_{\theta_k, 1}(t)|\Psi^{(0)}_{\theta_k}(t)\rangle + a_{\theta_k, 2}(t)|\Psi^{(0)}_{\theta_k}(t)\rangle. \tag{B8}
\]

Substituting Eq. (B8) into Eq. (B1), one obtains
\[
\frac{\partial}{\partial t} a_{\theta_k, 1}(t) = -\frac{1}{2} \beta \Omega a_{\theta_k, 2}(t) \sum_l y_l^*(\theta_k) e^{-i(2\eta v\cdot k - \Omega)t}, \tag{B9}
\]
\[
\frac{\partial}{\partial t} a_{\theta_k, 2}(t) = \frac{1}{2} \beta \Omega a_{\theta_k, 1}(t) \sum_l y_l(\theta_k) e^{-i(2\eta v\cdot k - \Omega)t}, \tag{B10}
\]
where
\[
y_l(\theta_k) = u_{l-1}^{(1)}(\theta_k)(\sin \theta_E \cos \theta_k - i \cos \theta_E \sin \theta_k) \\
+ u_{l+1}^{(1)}(\theta_k)(\sin \theta_E \cos \theta_k + i \cos \theta_E \sin \theta_k), \tag{B11}
\]
\[
u_1^{(1)}(\theta_k) = \frac{1}{T_0} \int_0^{T_0} dt e^{i\Omega t} [u^{(0)}(\theta_k, t)]^2
\]
\[= e^{i2\beta \cos \theta_E \cos \theta_k} J_1(2 |z(\theta_k)|) \left| \frac{-z(\theta_k)}{|z(\theta_k)|} \right|^l, \tag{B12}
\]
\[z(\theta_k) = \beta (\sin \theta_E \sin \theta_k + i \cos \theta_E \cos \theta_k). \tag{B13}
\]

In above derivation, we have applied the summation rule of the Bessel function
\[
J_l(|Z|) \left( \frac{Z^l}{|Z|^l} \right) = \sum_j e^{i\theta_j} J_j(y) J_{l-j}(x), \tag{B14}
\]
with \(Z = x + e^{i\theta} y \) (\(x \) and \(y \) are real numbers). Since Eqs. (B9) and (B10) cannot be solved in analytical closed form, we solve these equations via the rotating-wave approximation, which is widely used in the weak electromagnetic field related problem. Exploiting this approximation, we neglect the rapidly varying terms with
Thus one has
\[ |\Psi_{k\eta}(t)\rangle = e^{-\frac{1}{2} \frac{\eta v}{\sqrt{2}} (\Delta_m(\theta_k))^2} \left[ \begin{array}{c} \eta \langle 0 | e^{-\frac{1}{2} m \Omega t} u^{(0)}(\theta_k, t), \\ e^{i m \Omega t} [u^{(0)}(\theta_k, t)]^* \end{array} \right] \] (B22)

Evidently, the corresponding quasi-energy is
\[ \varepsilon_{k\eta} = \frac{\eta}{2} \sqrt{\delta_{km}^2 + (\Delta_m(\theta_k))^2}. \] (B23)

Thus the quasi-energy gap at the resonant point \( \delta_{km} = 0 \) reads
\[ \Delta_m(\theta_k) = \beta |y_m(\theta_k)| \Omega \mod \Omega. \] (B24)

It is seen that the magnitude of the gap \( \Delta_m(\theta_k) \) is determined by the effective coupling parameter \( |y_m(\theta_k)| \).

In Fig. 9 we plot the magnitude of the quasi-energy gaps \( \Delta_m \) against the corresponding momentums from the exact calculation (dots) and the approximate formula Eq. (B24) (squares) under circularly polarized THz fields with different field strengths. As shown in Figs. 2(a) and (b), the momentums of the gaps from the calculation markedly deviate from \( m \Omega/(2e\eta v) \) in the strong-field regime. Therefore, we define \( \Delta_0 \) as the gap at \( k = 0 \) and \( \Delta_m \ (m \neq 0) \) as the \( m \)-th gap from the one at \( k = 0 \) for gaps from the exact calculation. The corresponding indices \( m \) are labelled in Fig. 9. In the case with low field strength (red solid curves in Fig. 9), it is seen that the results from the approximate formula agree well with the ones from the exact computation. In the case with high field strength (blue dashed curves), the magnitude of the gaps from these two approaches are comparable, but the corresponding momentums differ significantly, owing to the rotating-wave approximation. In Fig. 9 we also plot the results from the exact calculation without the intraband term \( \hat{H}_{THz}^{\text{intra}} \) (triangles). It is seen that except for the gap with \( m = 1 \), the gaps without \( \hat{H}_{THz}^{\text{intra}} \) are much smaller than the ones with the intraband term. In particular, the gaps with \( m \) being even numbers vanish within the error range of our computation (about \( 10^{-10} \Omega \)). These results indicate that the intraband term \( \hat{H}_{THz}^{\text{intra}} \) plays a significant role in the formation of the quasi-energy gaps induced by the multiphoton resonances.

**Appendix C: Approximate analytical formula of optical conductivity**

Now we discuss the approximate analytical formula of the optical conductivity at high Fermi energy. It is known that the optical conductivity in this case is only from the contribution from the states with large momentum, where the effect from the interband term of \( \hat{H}_{THz} \) becomes negligible. Thus one can neglect the interband term and obtain the eigenvector
\[ |\Phi_{k\gamma}(t)\rangle = \hat{U}_k|\Psi_{k\eta}^{(0)}(t)\rangle \] (C1)

FIG. 10: (Color online) Time-averaged optical conductivities from the exact calculation (solid curves) and the approximate formula Eq. (C5) (dashed curves) as plots as function of the optical frequency under a circularly polarized THz field with \( \beta = 2.3 \) for different Fermi energies.

in which \( \hat{U}_k \) is given by Eq. (B22) and \( |\Psi_{k\eta}^{(0)}(t)\rangle \) is determined by Eqs. (B5) and (B6). Then one has
\[ \varepsilon_{k\gamma} = \varepsilon_{k\eta} = \eta v k, \] (C2)
\[ |\phi_{k \gamma}^{(0)}\rangle = u_n^{(0)}(\theta_k)(e^{-i\theta_k}, 1)^T / \sqrt{2}, \] (C3)
\[ |\phi_{k \gamma}^{(1)}\rangle = [u_n^{(0)}(\theta_k)]^*(-e^{-i\theta_k}, 1)^T / \sqrt{2}, \] (C4)

where
\[ u_n^{(0)}(\theta_k) = e^{i\beta \cos \theta_k \cos \theta_k} J_n(|z(\theta_k)|) \left[ -z(\theta_k) \right]^n \]

with \( z(\theta_k) \) given by Eq. (B13). Substituting Eqs. (C2)- (C5) into Eq. (B11), one obtains
\[ \text{Re} \sigma_\parallel^{\text{av}}(\omega_l) = \frac{\epsilon^2}{4\pi} \sum_N (1 - N \frac{\Omega}{\omega_l}) R_N \theta(\omega_l - 2E_F - N\Omega), \] (C5)

where
\[ R_N = \int_0^{2\pi} d\theta_k A_z^2(\theta_k) J_z^2(2|z(\theta_k)|), \]

with \( A_z(\theta_k) = \sin \theta_k \) and \( A_y(\theta_k) = \cos \theta_k \).

In Fig. 10 we plot the optical conductivities from the exact calculation (solid curves) and the approximate formula Eq. (C5) (dashed curves) as function of the frequency for different Fermi energies. It is seen that the difference between two calculations becomes smaller when the Fermi energy increases. This indicates that the effect from the interband term of \( \hat{H}_{THz} \) becomes negligible for high Fermi energy, in consistence with the discussion in the main text.
For the sake of the convergence, we replace the delta function $\delta(x)$ in the DOS and optical conductivity by a Lorentzian $\frac{\Gamma}{\pi(x^2 + \Gamma^2)}$. The values of $\Gamma$ are set as 0.001Ω and 0.02Ω for the calculation of the DOS and optical conductivity, respectively. It is noted that our main results are independent of the value of $\Gamma$ when $\Gamma$ is small enough.

Note that the so-called 0-photon resonance, which leads to the gap at zero momentum, is corresponding to the multiphoton process which first absorbs a photon and then emits one or vice versa.

Since $\lim_{k \to 0} k/|\nabla_k \varepsilon_k|$ is finite, the van Hoff singularity at $k = 0$ does not induce any divergence in the DOS. However, the states around zero momentum can still significantly enhance the DOS at the frequencies of the sidebands with large weight, as shown in the DOS limited in $k < 0.5\Omega$ [green dotted curve in Fig. 4(b)].

The DOS corresponding to the van Hoff singularities diverges as $\omega^{-1/2}$ in the case with isotropic energy spectrum, and diverges logarithmically in the case with anisotropic energy spectrum. See also [P. Y. Yu and M. Cardona, Fundamentals of Semiconductors (Springer, Berlin, 2005)]

It is easy to prove that the quasi-energies and mean energies for $\pm \theta_k$ and $\pi \pm \theta_k$ are identical.

Comparing the Hamiltonian of the external field in this paper with the one in Ref. 48, one can see $\beta \Omega$ corresponds to $\epsilon/2$ in Ref. 48.

I. S. Gradshteyn and I. M. Ryzhik, Table of Integrals, Series and Products, 5th ed. (Academic, New York, 1994).