Photon-mediated electronic correlation effects in irradiated two-dimensional Dirac systems

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Abstract
Periodically driven systems can host many interesting phenomena. Two-dimensional Dirac systems irradiated by circularly polarized light are especially attractive thanks to the special absorption and emission of photons near Dirac cones. Here, letting the light travel in the two-dimensional plane, we treat the light-driven Dirac systems by using a unitary transformation, instead of usual Floquet theory, to capture the photon-mediated electronic correlation effects. In this approach, the direct electron–photon interaction terms can be removed and the resulting effective electron–electron interactions can produce important effects. The effective interactions can produce topological band structure in the case of irradiated 2D Dirac fermion system, and can lift the energy degeneracy of the Dirac cones for irradiated graphene. This method can be applied to other light-driven Dirac systems to investigate their photon-mediated electronic effects. These phenomena would be observed with ultraviolet light in some effective two-dimensional Dirac systems of honeycomb long-period superstructures.

Keywords: Dirac system, 2D, light driving

(Some figures may appear in colour only in the online journal)

1. Introduction
Periodically driven systems attract more and more attention because of emerging novel phenomena which are absent in the corresponding equilibrium states [1–18]. The periodic driving can be realized by applying periodic external electric and/or magnetic fields, through adjusting the amplitude and frequency of light, and so on. It can produce various interesting phases such as Chern insulators [5, 6, 19], Weyl semimetals [11, 16, 18], the photovoltaic Hall effect [1, 3], quantum Floquet anomalous Hall states and quantized ratchet effect [20], and large currents in graphene [21].

Floquet theory can be used to describe some of the novel properties in such periodic systems [19, 22–24]. The eigenstates of the time-translation-invariant Hamiltonian $H(x, t) = H(x, t + T)$ can be written as $\{\phi_{\alpha \mathbf{k}}(x, t)\} = e^{i\mathbf{k} \cdot \mathbf{x} + i\lambda \cdot \mathbf{v} t} \{u_{\alpha \mathbf{k}}(x, t)\}$, where $\phi_{\alpha \mathbf{k}}$ stands for the quasi-energy of the Floquet state, $\alpha$ is the band index, and $\{u_{\alpha \mathbf{k}}(x, t)\}$ is periodic in $x$ and $t$. The quasi-energy $\varepsilon_{\alpha \mathbf{k}}$ is a periodic function of period $\omega = 2\pi/T$. Floquet theory can describe the absorption and emission of photons. Actually, Floquet method has been used to study the exotic phenomena in graphene irradiated by circularly polarized light [1, 6, 10, 15, 25]. Nevertheless, Floquet theory essentially is a single-electron theory although it captures the effects of incident light on single electrons [1, 6, 10, 22–24]. Beyond Floquet theory, photons can mediate many-electron interactions and even remote electron–electron interactions [26–28]. Therefore, it is highly desirable to explore photon-mediated electron–electron interactions and resulting effects, especially in fermion systems including Dirac cones.

Because virtual photon processes of absorption and emission can cause effective second-order electron–electron interactions, we shall show that the photon-mediated electronic correlation can cause interesting band structures near...
the Fermi level. To show such key effects clearly, we choose the external field traveling in the 2D plane, and use the second quantization form of photon–electron interaction and study effective two-electron interactions, as one has treated the electron–phonon interaction in superconductors. For an irradiated 2D fermion system with one Dirac cone, the effective interactions will produce a topologically-nontrivial band structure with unavoidable band crossing [29]. For the irradiated graphene, we find that the Dirac cones remain gapless, but their energy degeneracy can be lifted by adjusting the frequency and amplitude of electromagnetic waves properly. These unexpected interesting results can be attributed to the frequency and amplitude of electromagnetic waves properly.

Figure 1. Schematic of a driven 2D system. The light travels in the y direction in the 2D plane. Before the driving is switched on, the 2D band structure has one Dirac cone.

The starting Hamiltonian that describes a 2D Dirac fermion system can be expressed as

$$\hat{H}_D = \sum_k \hat{c}_k^\dagger \sigma^i \hat{c}_k, \quad i = x, y,$$

where \( \hat{k} \) is the momentum in the 2D plane, \( \sigma^i \) denotes the Pauli matrix, and \( \hat{c}_k \) is the two-component annihilation operator with pseudo-spin. We use \( \hat{H} \) to denote the Hamiltonian including the fermion operators explicitly, keeping the bare \( H \) to the one-body Hamiltonian without the fermion–photon operators. We have set the Fermi velocity as 1 for actual graphene, the Fermi velocity \( v_F \approx 10^6 \text{ m s}^{-1} \). We use the summation convention: the same index means summation over it. We apply light traveling in the y direction on the 2D fermion system, as shown in figure 1. This in-plane light driving is different from those with perpendicular incident light [21]. The vector potential of the light lies in the x-z plane, which means that only the x component distributes to the coupling with the Dirac fermions.

At the high frequency limit, effective Hamiltonian in terms of Floquet theory reads \( H_{\text{eff}} = H_0 + [\hat{H}, H_{\text{ext}}]/\hbar \omega + O(1/\omega^2) \) [3, 6, 11], where \( H_0 = \int_0^T H(t)e^{i\omega t}dt \) and \( H(t) = [k_x + A_x(t)]\sigma_x + i\partial_y \sigma_y \), because we choose \( A = (A_0 \cos(qy - \omega t), 0) \) in the graphene plane. Except \( H_{\text{eff}} \) the other terms in \( H_{\text{eff}} \) vanish in this situation, which leaves the Dirac cones unchanged.

Treating the external field through plane wave expansion, we express the field operators in terms of momentum representation [30]

$$A_i = A_0 \cos(qy - \omega t) \frac{\Delta}{\hbar \omega} + e^{iqx},$$

where \( a (a^\dagger) \) is the annihilation (creation) operator of a photon with momentum \( q \) and energy \( \hbar \omega \). Here, we set \( e = c = 1 \) and define the normalization constant as \( N_q = \frac{A_0}{\sqrt{2q}} \). Then, we can write the full Hamiltonian as

$$\hat{H} = -i \int d\mathbf{r} \hat{\Psi}(r)(\hat{\partial}_x + iA_i)\sigma^i\hat{\Psi}(r) + \omega a^\dagger a = \sum_k \left[ \hat{c}^\dagger_k \sigma^i \hat{c}_k + N_q(a^{\dagger}c_{q-k}^\dagger \sigma^i c_{-q} + a^\dagger c_{q-k} \sigma^i \hat{c}_{-q}) \right] + \omega a^\dagger a,$$

where we use the Fourier transformation \( \hat{\Psi}(r) = \sum_k c_k e^{-ikr} \). The Hamiltonian includes the fermion and photon operators explicitly, which is key to investigating photon-mediated many-fermion interactions. It is similar to the electron–photon interaction in superconductors, if we replace the fermion operator with the two-component spinor.

3. Results and discussion

3.1. Effective interactions of fermions

We shall cancel the first-order fermion-photon interaction by using Nakajima transformation [29], producing effective fermion–fermion interactions. The total Hamiltonian can be expressed as

$$\hat{H} = \hat{H}_0 + \hat{H}_I$$

$$\hat{H}_0 = \sum_k \hat{c}_k^\dagger \sigma^i \hat{c}_k + \hbar \omega a^\dagger a$$

$$\hat{H}_I = \sum_k N_q(\hat{a}^{\dagger}_q \hat{c}_{-q} \sigma^i \hat{c}_k + a^\dagger_k \hat{c}_{q} \sigma^i \hat{c}_{-q})$$

Introducing a Nakajima unitary transformation \( U = e^{-S} \) satisfying \( S^\dagger = -S \), we obtain

$$\hat{H}_5 = e^{-S}\hat{H}_5 e^S = \hat{H} + [\hat{H}, S] + \frac{1}{2}([\hat{H}, S], S) + \cdots$$

$$= \hat{H}_0 + [\hat{H}_I + [\hat{H}_0, S]] + \frac{1}{2}([\hat{H}_I + [\hat{H}_0, S]], S)$$

$$+ \frac{1}{2} [\hat{H}_I, S] + \cdots.$$  

Choosing \( S \) so as to satisfy the condition

$$\hat{H}_I + [\hat{H}_0, S] = 0,$$

the first-order term of \( \hat{H}_I \) will be eliminated, and the effective interaction will begin with the second order,

$$\hat{H}_5 = \hat{H}_0 + \frac{1}{2} [\hat{H}_I, S].$$
For our system, we actually make \( S \) take the form
\[
S = \sum_k (a_{k+q}^\dagger W_{kq} - a_k^\dagger c_{k-q}^\dagger W_{kq})
\]
where \( c_i \) are the Pauli matrix and \( \beta_i \) is its coefficients.

Condition (6) can also be expressed as \( \langle m|S|n \rangle = \frac{(m|Br|n)}{E_m - E_n} \),
with the eigenstates of \( H_0 \), \( |\pm \rangle \), \( N_\alpha \) = \( \frac{1}{\sqrt{2}}(e^{-i\alpha(k)}|\uparrow \rangle \pm |\downarrow \rangle) \times |N_\alpha \rangle \), where \( \uparrow \) and \( \downarrow \) denote pseudo-spins and \( N_{ph} \) is photon number. A key assumption is the high frequency limit, which means that photon energy is much larger than Dirac electron’s energy, \( \hbar \omega \gg \epsilon_k \). In detail, we have
\[
\langle +k + q \rangle, 0|\hat{H}_1| + k, 1 \rangle \sim \frac{1}{2\hbar \omega} N_\epsilon(e^{i\omega(k+q)} + e^{-i\omega(k)})
\]
\[
= \langle +k + q \rangle, 0|S| + k, 1 \rangle
\]
\[
\langle -k - q \rangle, 0|\hat{H}_1| - k, 1 \rangle \sim \frac{1}{2\hbar \omega} N_\epsilon(e^{-i\omega(k+q)} - e^{i\omega(k)})
\]
\[
= \langle -k - q \rangle, 0|S| + k, 1 \rangle
\]

It is easy to find \( \beta_i = \frac{N_\epsilon}{\hbar \omega} \) and others vanish. As a result, we obtain
\[
S = \frac{N_\epsilon}{\hbar \omega} \sum_k (a_{k+q}^\dagger \sigma_i c_k - a_k^\dagger c_{k-q}^\dagger \sigma_i c_k).
\]
Substituting this expression into (7) and neglecting self-energy terms and the higher-order terms of photon operators, we obtain the effective two-body Hamiltonian:
\[
\hat{H}^\text{eff}_1 = -\frac{N_\epsilon^2}{\hbar \omega} \sum_{k,k'} c_{k+q}^\dagger \sigma_i c_{k'}^\dagger c_{k+q}^\dagger \sigma_i c_{k}.
\]

The bands of \( \hat{H}_0(k) \) and \( \hat{H}_D(k + q) \) cross at \( k_y = -q/2 \) and the scattering \( c_{k+q}^\dagger \sigma_i c_{k} \) mainly occurs at this \( k \) point. Letting \( |\pm \rangle = (e^{-i\omega(k)}, \pm 1)^T/\sqrt{2} \) be the eigenvectors of the Dirac fermion Hamiltonian \( \hat{H}_D \) for \( \pm \epsilon \), respectively, where \( \tan \phi = k_y/k_x \), it is reasonable to set the mean field \( \Delta = (\langle -0, q/2 \rangle |\sum_{k} c_{k+q}^\dagger \sigma_i c_{k} | - \langle -0, -q/2 \rangle ) = i \).

Therefore, the final effective one-body Hamiltonian can be expressed as
\[
\hat{H}^\text{eff}_1 = \sum_k c_{k}^\dagger (\mathbf{k} \cdot \sigma c_{k} - \langle N_\epsilon \Delta/\hbar \omega \rangle c_{k+q}^\dagger \sigma_i c_{k} + \text{h.c.})
\]
These are beyond Floquet theory and include the effective electron–electron interactions mediated by photons.

It should be pointed out that this method in essence is a second-order perturbation method and it requires the perturbation condition \( N_\epsilon = \frac{\hbar \omega}{\sqrt{2}E_\epsilon} < 1 \). The fluctuations of the mean-field approximation are negligible near \( k_y = q/2 \), but become rather large when \( k_y \) is far away from \( q/2 \). This implies that the approximation is only valid near \( k_y = q/2 \), and our method is reliable to capture the electronic band structures near \( k_y = q/2 \). Therefore, we will focus on discussing the interesting physics near the \( k \) points.

3.2. Effective band structure and topological property

Noticing that the external field reduces the continuous (infinitesimal) translational symmetry to the discrete translational symmetry \( T : y \rightarrow y + 2\pi/q \), the Brillouin zone will fold from infinity to \( q \). The band structure of the effective Hamiltonian (12) with \( k_y = 0 \) is illustrated in figure 2. The effective scattering in (12) will not make an energy gap at the Dirac point, but will bend the bands at \( k = \pm \frac{q}{2} \). That makes the lowest two bands in the first Brillouin zone have a crossing feature, as illustrated in figure 3. This makes another example of the Mobius twisted band discussed by several groups [31, 32]. The crossing of the bands is a topological property protected by nonsymmorphic symmetry \( G \) and inversion symmetry \( P \) [32], and the effective two-bands Hamiltonian is
\[
H(k) = \sin \left( \frac{2\pi}{q} k_y \right) \sigma_3 + \left( 1 - \cos \left( \frac{2\pi}{q} k_y \right) \right) \sigma_1.
\]
The band crossing for Hamiltonian (13). The two eigenstates (and the energy levels) will interchange after a 2π period, which guarantees the odd times the number of the band crossing in the Brillouin zone.

\[ U = e^{i\alpha(k)\sigma^x} e^{i2\sigma^y} \] to diagonalize the Hamiltonian with the rotational parameter \( \tan 2\alpha(k) = \frac{h_b(k)}{h_a(k)} \). In fact, both \( U \) and \( e^{i2\sigma^y}U \) diagonalize the same Hamiltonian. Thus, one can construct a fiber bundle \( E \) with the base manifold of \( S^1 \) and the fiber of the rotating operator \( e^{i\alpha(k)\sigma^y} \) and the structure group \([I, e^{i2\sigma^y}]\). The unitary matrix \( U(k) \) that diagonalizes the Hamiltonian belongs to one section of this fiber.

To further elucidate the topological property, we can divide \( S^1 \) into two parts, \([−\pi/2, \pi/2]\) and \([\pi/2, 3\pi/2]\), and construct \( U(k) \) respectively, and thereby describe the topology by the homotopy group of the map from the overlapping zone \([−\pi/2, \pi/2]\) to the structure group \([I, e^{i2\sigma^y}]\). Consequently, the topology is characterized by \( Z_2 \). For the Hamiltonian (13), one can easily show that it is topologically nontrivial. Noticing that considering that \( U \) is well defined at \( k = 0 \). If \( k \) changes from \( −\pi/2 \) to \( \pi/2 \), one can make \( 2\alpha \) take values from \( −\pi/4 \) to \( −3\pi/4 \), with \( 2\alpha = −\pi/2 \) at \( k = 0 \); when \( k \) belongs to \([\pi/2, 3\pi/2]\), one can choose \( 2\alpha \) between \( \pi/4 \) and \( −\pi/4 \); and thus we obtain the nontrivial map: \(-\pi/2 \mapsto 1, \pi/2 \mapsto e^{i\pi/2} \). Intuitively speaking, with \( k \) moving in \( S^1 \), \( U(k) \) changes according to \( H(k) \), but when \( k \) comes back to the starting point after a circle, \( U(k) \) accumulates a factor \( e^{i\pi} \), which will switch the two eigenstates of \( H(k) \). This means that the energy levels of the two eigenstates will interchange after a circle of \( k \) movement, and guarantees the odd times of the band-crossings in the Brillouin zone, as illustrated in figure 3.

**3.3. Energy splitting of Dirac cones**

It will become more interesting when we consider a system with two topologically different Dirac points, characterized by the chirality \( W_D = \text{sgn}(|\text{det}(V)|) \) for the Hamiltonian \( H(k) = V_0k_x\sigma^x \) for a Dirac cone. Let us consider a semi-Dirac-point Hamiltonian

\[ H_{SD} = \sum_k c^\dagger_k [k_x\sigma^x + (k_y^2 - b^2)\sigma^y]c_k. \]

This Hamiltonian describes two different Dirac points located at the two points: \((0, \pm b)\). Following similar procedures, we obtain similar effective interaction terms, and the effective Hamiltonian can be expressed as

\[ H_{\text{eff}} = \sum_k \left\{ c^\dagger_k [k_x\sigma^x + (k_y^2 - b^2)\sigma^y]c_k - \left( \frac{N_D^2}{\lambda^2} \right) c^\dagger_k \sigma^\dagger \sigma c^\dagger_k c_k + \text{h.c.} \right\}. \]

It is interesting to study the low-energy physics and the scattering from one Dirac point to the other. Letting \( k_y = -b \) and \( q = 2b \) in equation (15), we obtain the scattering term \(-\left( \frac{N_D^2}{\lambda^2} \right) c^\dagger_k \sigma^\dagger \sigma c^\dagger_k c_k + \text{h.c.} \). Combining with the free Dirac term, one can use a four-component \( \Gamma \) matrix to describe the scattering

\[ H^{(q=2b)}_{\text{eff}} = k_x\sigma^x + 2bk_y\sigma^\tau \sigma^z + \frac{N_D^2}{q}\sigma\tau, \]

where the Pauli matrices \( \tau^{x,z} \) describe the two Dirac points. This Hamiltonian can be bulk diagonalized by the unitary transformation \( U = e^{i\Gamma \sigma^y} \). As a result, we get

\[ H^{(q=2b)}_{\text{eff}} = k_x\sigma^x + 2bk_y\sigma^\tau \sigma^z + \frac{N_D^2}{q}\tau^z. \]

This means that the energy levels of the two Dirac points shift up and down by \( \frac{N_D^2}{q^2} \), respectively, as illustrated in figure 4, with the normalization constant \( N_D = \frac{A_0}{2\sqrt{\pi}} \). The energy spacing is proportional to the square of the light strength \( A_0 \).
Because $q = 2b$ is decided by the irradiated material with two Dirac points, one can control the density of states at the Fermi level by splitting the Dirac points through adjusting the light strength, and thus manipulate the transport property of the interesting fermion systems. Therefore, the radiation with specific frequency $\hat{\omega} \sim 2b$ can make the Dirac cones split in energy, where $2b$ is the separation of Dirac cones in momentum space. This energy-splitting phenomenon provides us a way to control the density of states at the Fermi level by tuning the light strength applied on the Dirac materials.

3.4. Application to graphene and others

It is interesting to study graphene by light irradiation and voltage driving [33–37] and to explore graphene superlattices [38, 39]. For graphene, the experimental lattice constant is $a \approx 1.42$ Å, and the distance between two Dirac cones is around $2b \approx 1.7$ Å$^{-1}$. Because its wave vector is defined as $q = 2\pi/\lambda$ in terms of the wavelength $\lambda$, this implies that the x-ray is needed, with a wavelength of $\lambda \approx 3.7\text{Å}$. Around this $q$, the energy of photon $h\omega \sim 10^3$ eV is much larger than the graphene band width $\sim 10$ eV, satisfying the condition in equations (9). On the other hand, there are some two-dimensional Dirac honeycomb monolayers that have smaller band widths and longer lattice constants [40, 41]. For the CoBr$_2$ and the Be$_3$C$_2$, the honeycomb lattice constants are 3.6 Å and 5.69 Å, and hence the wavelengths of the photon are 5.4 Å and 8.5 Å, respectively. These are at the low end of the x-ray region.

Several recent experiments illustrated some honeycomb-like superstructures, with the spatial period being ten to hundred times the crystal constant, and thus they can create much closer Dirac cones in the first Brillouin zone [42–45]. Furthermore, it is suggested that applying strain on graphene will destroy its $C_3$ symmetry and make its Dirac cones become close to each other [46], and more candidates can be made available. Thus, the wavelength of the photon can be increased to nearly 1000 Å, which implies that only ultraviolet light of lower frequency is needed in such cases.

4. Conclusion

In summary, we treat the irradiated two-dimensional Dirac systems beyond usual Floquet method and thereby capture the photon-mediated electron–electron interactions. This method is especially important when we apply the light in the 2D plane of the Dirac systems. To capture the effective two-electron interactions, we use Nakajima transformation to remove the first-order electron–photon interaction, and then derive the effective electron–electron interactions mediated by photon. The effective interaction can result in interesting phenomena. For an irradiated Dirac system with one Dirac cone, it is found that the photon-mediated electronic interactions lead to the scattering at the Brillouin zone boundary and thus bend the bands there, and thus produce the effective topologically-nontrivial band structure protected by nonsymmorphic symmetry combined with inversion symmetry. For irradiated graphene, we find that the Dirac points at $K$ and $K'$ will scatter from each other when the light wave vector $q$ matches the distance between the Dirac points, which splits them in energy level, i.e. lifts the energy degeneracy of the Dirac points. The energy spacing is equivalent to $\frac{q^2}{2m}$, suggesting that one can control Dirac points through tuning light strength to change the transport property of the Dirac system. These phenomena would be observed with ultraviolet light in some effective two-dimensional Dirac systems of honeycomb long-period superstructures. This method should applicable to other systems, capturing their effective photon-mediated many-electron interactions.

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