FLAT BAND OF MIDGAP ROTATING SURFACE STATES IN 3D DIRAC AND WEYL SEMIMETALS UNDER RADIATION

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3D SEMIMETALS

We start with a model of 3D Dirac semimetal

\[ H_0 = M(k) \sigma_z + \hbar v (\zeta k_x \sigma_x + k_y \sigma_y) \quad \zeta = \pm 1 \]
\[ M(k) = m_0 - m_1 k_z^2 - m_2 (k_x^2 + k_y^2) \]

The low-energy spectrum has two Dirac points at \( k_c = (0, 0, \pm \sqrt{m_0 / m_1}) \)

Near the Dirac points, the dispersion becomes linear in all directions in momentum space

\[ \varepsilon_0(k) = \pm \sqrt{\hbar^2 v^2 (k_x^2 + k_y^2) + 4m_0 m_1 (k_z - k_c)^2} \]

2D AND 3D SEMIMETALS UNDER CIRCULARLY POLARIZED RADIATION


3D DIRAC SEMIMETALS UNDER RADIATION

We investigate the changes in the spectrum when illuminating with circularly polarized light, corresponding to a vector potential

\[ \mathbf{A}(t) = A(\eta \sin(\Omega t), \cos(\Omega t), 0) \quad \eta = \pm 1 \]

We use Floquet theory to find the solutions of the time-dependent Schrödinger equation

\[ -i\hbar \partial_t \left| \Psi(t) \right\rangle = H(t) \left| \Psi(t) \right\rangle \]

\[ \left| \Psi(t) \right\rangle = e^{-i\epsilon t/\hbar} \left| \Phi(t) \right\rangle , \quad \left| \Phi(t + T) \right\rangle = \left| \Phi(t) \right\rangle \quad T = 2\pi / \Omega \]

which amounts to find the result of hybridizing a number of Floquet subbands

\[ \left| \Phi(t) \right\rangle = \sum_m e^{-im\Omega t} \left| \chi_m^{(\alpha)} \right\rangle , \]

\[ \sum_n H_{mn} \left| \chi_n^{(\alpha)} \right\rangle = (\mathcal{E}_\alpha + m\hbar\Omega) \left| \chi_m^{(\alpha)} \right\rangle \]

\[ H_{mn} = \frac{1}{T} \int_0^T dt \ H(t) \ e^{i(m-n)\Omega t} \]
3D DIRAC SEMIMETALS UNDER RADIATION

\[ \sum_n H_{mn} \chi_n^{(\alpha)} = (\varepsilon_\alpha + m\hbar\Omega) \chi_n^{(\alpha)} \]

In our model we have

\[ H_{mn} = H_0 + n\hbar\Omega \mathbf{1} - m_2 A^2 \sigma_z \]

\[ H_{n+1,n} = (\hbar v / 2) A(i\sigma_x - \sigma_y) + m_2 A(-ik_x - k_y)\sigma_z \]

\[ H_{n-1,n} = (\hbar v / 2) A(-i\sigma_x - \sigma_y) + m_2 A(i k_x - k_y)\sigma_z \]

The hybridization of the Floquet subbands gives rise to a gap over an extended ring in momentum space:
- proportional to \( A \) between subbands \( n = 0 \) and \( n = \pm 1 \)
- proportional to \( A^2 \) between subbands \( n = -1 \) and \( n = 1 \)

\[ \hbar v = 1.1 \text{ eV} \text{ Å} \]

\[ \hbar \Omega = 0.5 \text{ eV} \]

\[ A = 0.05 \text{ Å}^{-1} \]

\[ k_x = 0, k_y = 0 \]
3D DIRAC SEMIMETALS UNDER RADIATION

But most interestingly, we can have evanescent states localized at the irradiated surface.

These states come as solutions with real quasi-energy $\varepsilon_\alpha$ for complex momenta $k_z$

$$\chi^{(\alpha)} \sim e^{i k_z z}, \quad k_z = k_R + i k_I$$

Computing for a wire with finite section in the x-y plane (150 $\times$ 150 Å$^2$)

we find evanescent states (for $\text{Im}(k_z) \approx 0.01 \text{ Å}^{-1}$) at the position of the dots within the gap between Floquet subbands in the figure.

WEYL SEMIMETALS UNDER RADIATION

We can have a deeper insight by solving for a single Weyl quasiparticle

\[ H_w = -i\hbar \left( v \sigma_x \partial_x + v \sigma_y \partial_y + v_z \sigma_z \partial_z \right) \]

+ \hbar \nu A \left( \sigma_x \cos(\Omega t) + \sigma_y \sin(\Omega t) \right) \]

\( H_w \) can be translated to time-independent form by making a unitary transformation

\[ \tilde{H}_w = U^* H_w U - i\hbar U^* \partial_z U \]

\( U = e^{-iJ_z \Omega t/\hbar} \)

and transforming again we obtain

\[ \tilde{H}_w' = P^+ \tilde{H}_w P \]

\[ = -i\hbar v \sum e^{\mp i d} (\partial_r \mp (i/r) \partial_\theta) \sigma_z - i\hbar v_z \sigma_z \partial_z \]

\[ - \Omega J_z - \hbar \Omega A r \sin(\theta) \]

\( J_z = -i\hbar \partial_\theta + \hbar \sigma_z / 2 \)

We find that the spectrum has a gap between Floquet subbands with \( j_z = \hbar/2 \) and \( j_z = -\hbar/2 \)

\[ \hbar \nu = 1.1 \text{ eV \ A} \]

\[ \hbar \Omega = 0.5 \text{ eV} \]

\[ A = 0.005 \text{ Å}^{-1} \]
WEYL SEMIMETALS UNDER RADIATION

The gap has oscillations as a function of $k_z$ which are the signature of branch points in the complex plane

$$\varepsilon(k_z) \sim \sqrt{k_i - k_z} \sqrt{\bar{k}_i - k_z}$$

$k_i$, $\bar{k}_i$ are exceptional points at which $\varepsilon(k_z) = 0$, leading to a segment of real values of $\varepsilon$ for

$$|\text{Im}(k_z)| \leq |\text{Im}(k_i)|$$

The set of exceptional points corresponds to a sequence of evanescent states localized at the irradiated surface, with a peculiar quantization pattern

$$\text{Re}(k_1) > \text{Re}(k_2) > \text{Re}(k_3) \ldots$$

WEYL SEMIMETALS UNDER RADIATION

The most important feature of the evanescent states is that they carry an angular current \( j^\theta \) corresponding to the flow of probability density

\[
\partial_z (\varphi^+ \varphi) \approx \partial_\theta j^\theta
\]

\( j^\theta \) can be computed in the space spanned by the states with \( j_z = \pm h/2 \)

\[
\chi = \left( \begin{array}{c} \phi_1(r) \\ e^{i\theta} \phi_2(r) \\ e^{-i\theta} \phi_3(r) \\ \phi_4(r) \end{array} \right) e^{ik_z z}
\]

The angular current has a uniform component, which is in general negligible,

\[
j_{\text{static}}^\theta = -i \frac{\nu}{r} \left( \phi_1^*(r) \phi_2(r) + \phi_3^*(r) \phi_4(r) \right) + \text{h.c.}
\]

and a time-dependent component

\[
j_{\Omega}^\theta = -i \frac{\nu}{r} \left( \phi_1^*(r) \phi_4(r) e^{-i(\Omega - \Omega r)} + \phi_3^*(r) \phi_2(r) e^{i(\Omega - \Omega r)} \right) + \text{h.c.}
\]

The corresponding current intensities have magnitudes

\[
\int dr \, r \, j_{\Omega}^\theta \sim 10^{-3} \nu / a - 10^{-2} \nu / a
\]

3D SEMIMETALS UNDER CIRCULARLY POLARIZED RADIATION

In conclusion,

The irradiation of the surface of 3D semimetals must lead to the observation of evanescent states carrying a non negligible angular current. The feasibility of this observation may be supported by several facts:

- the limited screening in the 3D semimetals, which has to allow the infrared radiation to penetrate sufficiently deep (∼1 µm at Ω ~ 100 THz)
- the magnitude of the angular current of individual states, which have associated a current intensity
  \[ e \int dr r j^0_\Omega \sim 10^{-1} \mu A - 1 \mu A \]
- the possibility of devising an experimental setup to work as a rectenna, benefiting from recent advances to rectify currents oscillating at the frequency of visible light