CSIC
CONSEJO SUPERIOR DE INVESTIGACIONES CIENTÍFICAS

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

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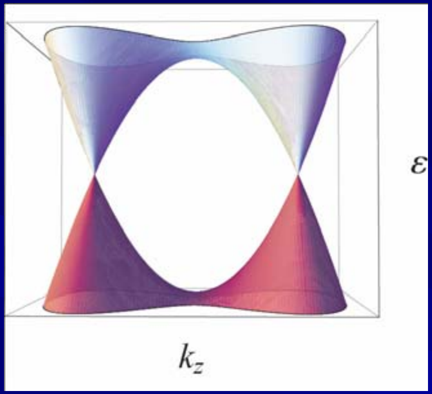
3D SEMIMETALS

We start with a model of 3D Dirac semimetal

$$H_0 = M(\mathbf{k})\,\sigma_z + \hbar v\left(\zeta\, k_x\sigma_x + k_y\sigma_y\right) \qquad \zeta = \pm 1$$

$$M(\mathbf{k}) = m_0 - m_1 k_z^2 - m_2(k_x^2 + k_y^2)$$

The low-energy spectrum has two Dirac points at $\mathbf{k}_c = \left(0, 0, \pm\sqrt{m_0 / m_1}\right)$



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

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

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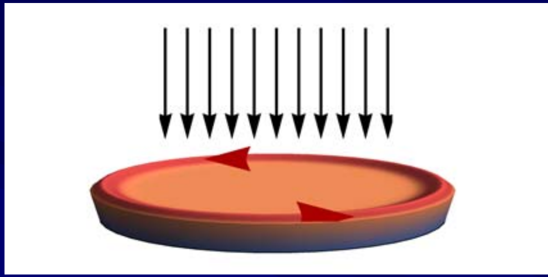
2D AND 3D SEMIMETALS UNDER CIRCULARLY POLARIZED RADIATION



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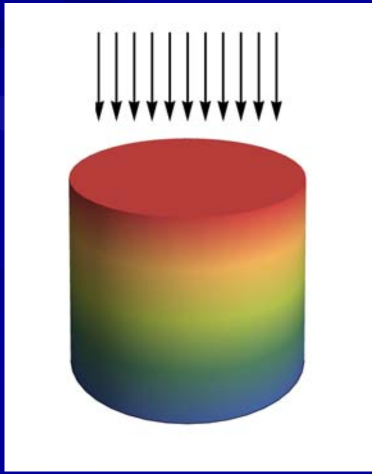

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3D DIRAC SEMIMETALS UNDER RADIATION

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

$$\mathbf{A}(t) = A\big(\eta \sin(\Omega t), \cos(\Omega t), 0\big) \qquad\qquad \eta = \pm 1$$

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

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

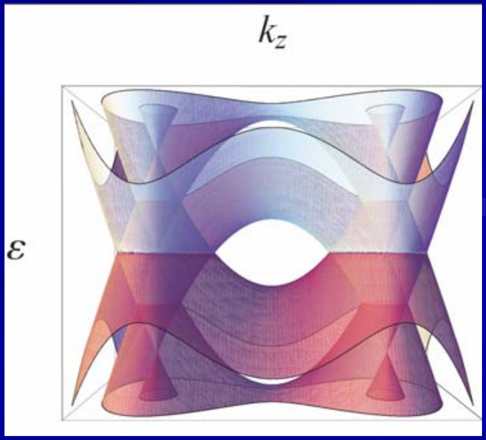
$$\left|\Psi(t)\right\rangle = e^{-i\varepsilon\, t/\hbar}\left|\Phi(t)\right\rangle \;\;,\;\; \left|\Phi(t+T)\right\rangle = \left|\Phi(t)\right\rangle \qquad T = 2\pi/\Omega$$

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

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

$$\sum_n H_{mn}\left|\chi_n^{(\alpha)}\right\rangle = (\varepsilon_\alpha + m\hbar\Omega)\left|\chi_m^{(\alpha)}\right\rangle$$

$$H_{mn} = (1/T)\int_0^T dt\, H(t)\, e^{i(m-n)\Omega t}$$



3D DIRAC SEMIMETALS UNDER RADIATION

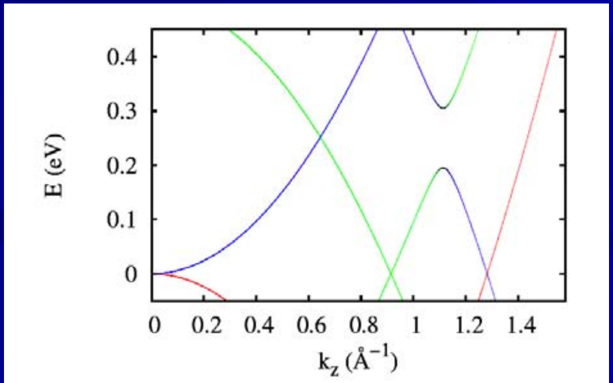
$$\sum_n H_{mn} \left| \chi_n^{(\alpha)} \right\rangle = (\varepsilon_\alpha + m\hbar\Omega) \left| \chi_m^{(\alpha)} \right\rangle$$

In our model we have

$$H_{nn} = H_0 + n\hbar\Omega\,\mathbf{1} - m_2 A^2 \sigma_z$$
$$H_{n+1,n} = (\hbar v/2) A (i\sigma_x - \sigma_y) \; + \; m_2 A(-ik_x - k_y)\sigma_z$$
$$H_{n-1,n} = (\hbar v/2) A (-i\sigma_x - \sigma_y) \; + \; m_2 A(ik_x - k_y)\sigma_z$$

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 $n = 1$



$k_x = 0\,,\, k_y = 0$

$\hbar v = 1.1$ eV Å

$\hbar\Omega = 0.5$ eV

$A = 0.05$ Å^{-1}

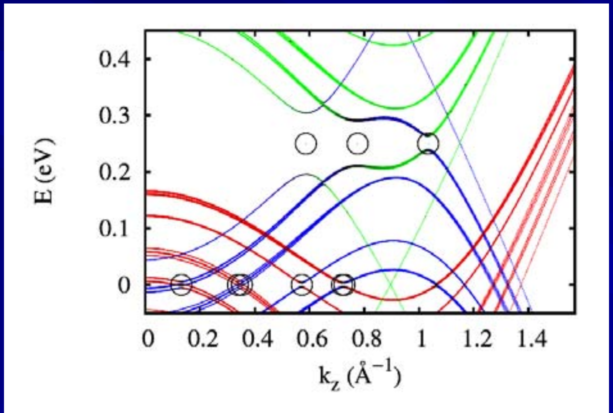
3D DIRAC SEMIMETALS UNDER RADIATION

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

These states come as solutions with real quasi-energy ε_α for complex momenta k_z

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

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



$\hbar v$ = 1.1 eV Å

$\hbar\Omega$ = 0.5 eV

A = 0.05 Å^{-1}

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

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WEYL SEMIMETALS UNDER RADIATION

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

$$H_W = -i\hbar\left(v\sigma_x\partial_x + v\sigma_y\partial_y + v_z\sigma_z\partial_z\right) + \hbar v\, A\left(\sigma_x\cos(\Omega t) + \sigma_y\sin(\Omega t)\right)$$

H_W can be translated to time-independent form by making a unitary transformation

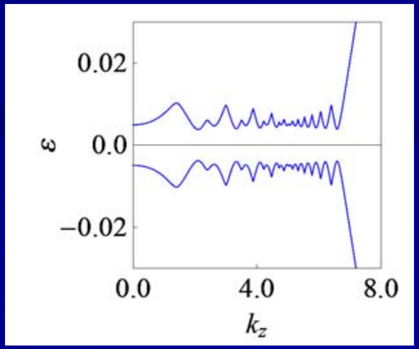
$$\tilde{H}_W = U^+ H_W U - i\hbar U^+\partial_t U = -i\hbar\left(v\sigma_x\partial_x + v\sigma_y\partial_y + v_z\sigma_z\partial_z\right) - \Omega J_z + \hbar v A\sigma_x \qquad U = e^{-iJ_z\Omega t/\hbar}$$

and transforming again we obtain

$$\tilde{H}'_W = P^+\tilde{H}_W P = -i\hbar v\sum e^{\mp i\theta}\left(\partial_r \mp (i/r)\partial_\theta\right)\sigma_\pm - i\hbar v_z\sigma_z\partial_z - \Omega J_z - \hbar\Omega\, Ar\sin(\theta) \qquad P = e^{-iAx}$$

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

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



$\hbar v = 1.1$ eV Å

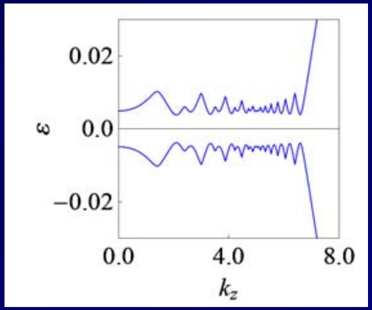
$\hbar\Omega = 0.5$ eV

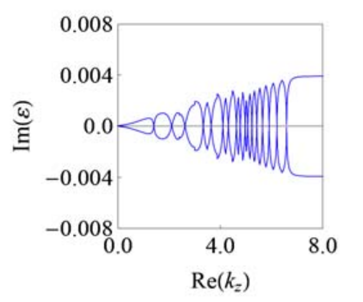
$A = 0.005$ Å^{-1}

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

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





$\hbar v = 1.1$ eV Å

$\hbar\Omega = 0.5$ eV

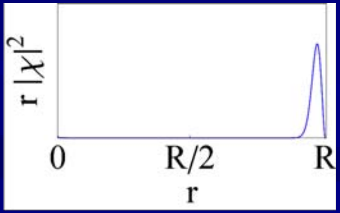
$A = 0.005$ Å^{-1}

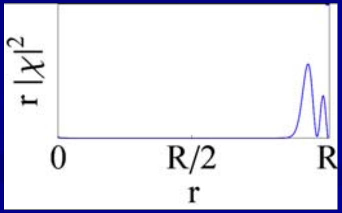
$\mathrm{Im}(k_z) = 0.08$ Å^{-1}

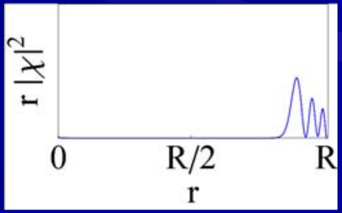
k_i , $\bar{k}_i$ are exceptional points at which $\varepsilon(k_z) = 0$, leading to a segment of real values of ε for

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

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







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

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WEYL SEMIMETALS UNDER RADIATION

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

$$\partial_t\left(\psi^+\psi\right) \approx \partial_\theta j^\theta$$

j^θ can be computed in the space spanned by the states with $j_z = \pm\hbar/2$

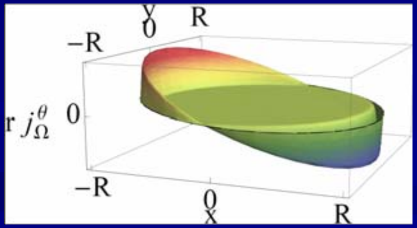
$$\chi = \begin{pmatrix} \phi_1(r) \\ e^{i\theta}\phi_2(r) \end{pmatrix} e^{ik_z z} + \begin{pmatrix} e^{-i\theta}\phi_3(r) \\ \phi_4(r) \end{pmatrix} e^{ik_z z}$$

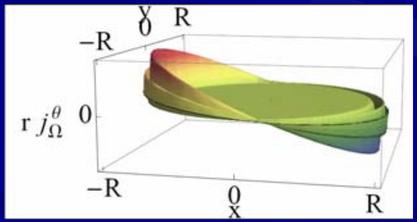
The angular current has a uniform component, which is in general negligible,

$$j^\theta_{\text{static}} = -i\frac{v}{r}\left(\phi_1^*(r)\,\phi_2(r) + \phi_3^*(r)\,\phi_4(r)\right) + \text{h.c.}$$

and a time-dependent component

$$j^\theta_\Omega = -i\frac{v}{r}\left(\phi_1^*(r)\,\phi_4(r)\,e^{-i(\theta-\Omega t)} + \phi_3^*(r)\,\phi_2(r)\,e^{i(\theta-\Omega t)}\right) + \text{h.c.}$$





The corresponding current intensities have magnitudes $\int dr\, r\, j^\theta_\Omega \sim 10^{-3}\, v/a - 10^{-2}\, v/a$

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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

$$e\int dr\, r\, j_{\Omega}^{\theta} \sim 10^{-1}\,\mu\mathrm{A} - 1\,\mu\mathrm{A}$$

- 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