Floquet engineering of multifold fermions.

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Main achievement:- They found that the threefold degeneracy of fermions remain symmetry protected even after applying light if the original band structure is rotationally symmetric around the degeneracy, otherwise, light can lift the degeneracy and open up a gap.

⇒ Further investigation on topological fermi arcs.

- topological semimetals are a class of materials which harbor topologically stable energy bands crossing near the fermi-surface.

- The low-energy behaviour around such degeneracies resembles the relativistic ~~degen~~ Dirac equation

  So, it can be basis for discovery of Majorana fermions, Dirac fermions and weyl ~~fermions~~ fermions in condensed matter system.

- Free-fermionic excitation in topological semimetals with no high-energy counterparts, commonly called multifold semi-metals, are characterized by higher order (larger than 2) band crossing at the degenerate points.

- Multifold fermions have an enhanced linear response compared to weyl fermions due to their higher topological charge.

- Floquet engineering → Controlling of topological transitions using periodic drive such as light.

> they have shown that elliptically polarized light can cause a band gap to open up and/or shift the three fold degeneracy depending on the intrinsic symmetries of the system.

Effective Low-energy model

$$H_{3f}(\vec{k}) = E_0 + \hbar v_f \begin{pmatrix} 0 & e^{i\phi} k_x & e^{-i\phi} k_y \\ e^{-i\phi} k_x & 0 & e^{i\phi} k_z \\ e^{i\phi} k_y & e^{-i\phi} k_z & 0 \end{pmatrix} \quad \text{--- (1)}$$

E_0: energy offset

$\hbar v_f$: effective velocity around $\vec{k} = 0$

ϕ > material dependent parameter.

Consider the three band touching point (3-BTP) to be at fermi energy then set $E_0 = 0$

take $\hbar = 1$, $v_f = 1$, $e = 1$ for simplicity.

for spin-1 representation of SU(2)

S^x, S^y, S^z are given by

$$S^x = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \qquad S^y = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}$$

$$S^z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$\therefore\ \vec{K}\cdot\vec{S}$

$$= \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & k_x & 0 \\ k_x & 0 & k_x \\ 0 & k_x & 0 \end{pmatrix} + \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -ik_y & 0 \\ ik_y & 0 & -ik_y \\ 0 & ik_y & 0 \end{pmatrix} + \begin{pmatrix} k_z & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -k_z \end{pmatrix}$$

$$= \begin{pmatrix} k_z & \frac{1}{\sqrt{2}}(k_x - ik_y) & 0 \\ \frac{1}{\sqrt{2}}(k_x + ik_y) & 0 & \frac{1}{\sqrt{2}}(k_x - ik_y) \\ 0 & \frac{1}{\sqrt{2}}(k_x + ik_y) & -k_z \end{pmatrix} \longrightarrow$$

Can we get the same results using this as the $\vec{K}\cdot\vec{S}$, if not then can it give some new physics or same physics but we have to interpret differently.

use, $\vec{S} = i \begin{bmatrix} 0 & \hat{e}_x & -\hat{e}_y \\ -\hat{e}_x & 0 & \hat{e}_z \\ \hat{e}_y & -\hat{e}_z & 0 \end{bmatrix}$

then $\vec{K}\cdot\vec{S} = i\begin{pmatrix} 0 & k_x & -k_y \\ -k_x & 0 & k_z \\ k_y & -k_z & 0 \end{pmatrix}$

[for $\phi = \frac{\pi}{2}$

$H_{3f}(\vec{k}) = \vec{K}\cdot\vec{S}$

but I am not getting how for $\phi = \pi/6$ also it is true]

> After diagonalization the Hamiltonian will give three eigenvalues $E = 0, \pm k$, for $\phi = \frac{\pi}{6}, \frac{\pi}{2}$

So, the band structure is completely centrosymmetric, i.e., have complete rotational symmetry about the degeneracy at $\vec{k} = 0$.

for $\phi = \frac{\pi}{6} \pmod{\pi/3}$

Away from these ϕ values the conical bands ~~had~~ a tilt and the centrosymmetry about the degeneracy vanishes.

The tilt is maximum for

$\phi = 0 \pmod{\pi/3}$

Floquet analysis for the low-energy model :-

Shining the light on the material with threefold crossing.

apply time depended periodic perturbation.

$$H(t+T) = H(t)$$

Using Magnus expansion in floquet theory in the high frequency limit

$$H_{floq}(\vec{k}) = H_0(\vec{k}) + \frac{[H_{+1}(\vec{k}), H_{-1}(\vec{k})]}{\omega} + O\left(\frac{1}{\omega^2}\right)$$

$$\omega = 2\pi/T \qquad H_m(\vec{k}) = \frac{1}{T}\int_0^T H(\vec{k},t)\, e^{-im\omega t}\, dt$$

if we can break the time dependent and independent part of the Hamiltonian then,

$$H_{floq}(\vec{k}) = H_0(\vec{k}) + \frac{[V_{+1}(\vec{k}), V_{-1}(\vec{k})]}{\omega} + O((V/\hbar\omega)^2)$$

if $\omega \gg V$

for low-energy model, various terms in increasing powers of $(1/\omega)$ have the form

$H_0,\ V\frac{V}{\hbar\omega},\ V\left(\frac{V}{\hbar\omega}\right)^2 \ldots$

but as $\omega \gg V$

$$\frac{V}{\hbar\omega} \gg \left(\frac{V}{\hbar\omega}\right)^2$$

(so, we can ignore the 2nd order terms in $(V/\hbar\omega)$)

$$\omega \gg \frac{V}{\hbar}.$$

$k \sim k + A\cdot\frac{e}{\hbar}$ ('A' is vector potential)

$V = H_{perturbed} \sim \hbar v_f \cdot \frac{Ae}{\hbar}$

$$\therefore \frac{V}{\hbar} \sim \frac{e v_f A}{\hbar}$$

$\therefore \omega >> \frac{e v_f A}{\hbar}$

$\therefore \omega >> \sqrt{\frac{e v_f A}{\hbar}}$

$E \sim A\omega$ → r.m.s value of the electric field

if R is the reflectivity of a material.

$(1-R) I$ = energy density $\times c$

$\downarrow$ Intensity

$(1-R) I = \frac{1}{2} \epsilon E^2 c$

$\Rightarrow E = \sqrt{\frac{2I(1-R)}{\epsilon c}}$

$\Rightarrow E \sim \sqrt{\frac{2I(1-R)}{n \epsilon_0 c}}$

n → refractive index

For non-cavity modes, light is plane - polarized which allows to choose $A_z = 0$

take some phase difference θ, b/w the x & y component

$$\vec{A} = [A_x \cos(\omega t), A_y \cos(\omega t + \theta), 0]$$

using peierls substitution

$$k \to k - \frac{qA}{\hbar}$$

$$\to k - \frac{(-e)A}{\hbar} \to k + \frac{eA}{\hbar}$$

$$\to (k + A)$$ taking $e = 1$, $\hbar = 1$

$$\therefore\ H_{3f}(\vec{K}) = E_0 + \hbar v_f \begin{pmatrix} 0 & e^{i\phi}(k_x + \vec{A}_x) & e^{-i\phi}(k_y + \vec{A}_y) \\ e^{-i\phi}(k_x + \vec{A}_x) & 0 & e^{i\phi}(k_z + \vec{A}_z) \\ e^{i\phi}(k_y + \vec{A}_y) & e^{-i\phi}(k_z + \vec{A}_z) & 0 \end{pmatrix}$$

$$= E_0 + \hbar v_f \begin{pmatrix} 0 & e^{i\phi} k_x & e^{-i\phi} k_y \\ e^{-i\phi} \cancel{A_x} & 0 & e^{i\phi} k_z \\ e^{i\phi} k_y & e^{-i\phi} k_z & 0 \end{pmatrix} + \underbrace{\hbar v_f \begin{pmatrix} 0 & e^{i\phi} A_x \cos\omega t & e^{-i\phi} A_y \cos(\omega t+\theta) \\ e^{-i\phi} A_x \cos\omega t & \cdot & \vdots \\ e^{i\phi} A_y \cos(\omega t+\theta) & \vdots & \vdots \end{pmatrix}}_{V(t)}$$

$$V(t) = \hbar v_f \begin{pmatrix} 0 & e^{i\phi} A_x \cos\omega t & e^{-i\phi} A_y \cos(\omega t+\theta) \\ e^{-i\phi} A_x \cos(\omega t) & 0 & 0 \\ e^{i\phi} A_y \cos(\omega t+\theta) & 0 & 0 \end{pmatrix}$$

$\hbar = 1$
$v_f = 1$

$$V_{+1}(k) = \frac{1}{T}\int_0^T V(t, k)\, e^{-i\omega t}\, dt$$

$$\frac{1}{T}\int_0^T e^{i\phi} A_y \cos(\omega t+\theta)\, e^{-i\omega t}\, dt$$

$$= \frac{A_y e^{i\phi}}{T}\left[\int_0^T \frac{e^{i(\omega t+\theta)} + e^{-i(\omega t+\theta)}}{2}\, e^{-i\omega t}\, dt\right]$$

$$= \frac{A_y e^{i\phi}}{2T}\left[e^{i\theta} T + \left[\frac{e^{-i(2\omega t+\theta)}}{-2i\omega}\right]_0^T\right]$$

$$= \frac{A_y e^{i\phi}}{2T}\left[e^{i\theta} T + \frac{e^{-i\theta} - e^{-i\theta}}{-2i\omega}\right]$$

$$= \frac{A_y e^{i\phi} e^{i\theta}}{2}$$

$$= \frac{1}{2}\begin{pmatrix} 0 & e^{i\phi} A_x & e^{-i\phi} A_y e^{i\theta} \\ e^{-i\phi} A_x & 0 & 0 \\ A_y e^{i\phi} e^{i\theta} & 0 & 0 \end{pmatrix}$$

$$V_{-1}(\vec{k}) = \frac{1}{T}\int_0^T H(\vec{k},t)\, e^{+i\omega t}\, dt$$

$$\frac{1}{T}\int_0^T \cos(\omega t+\theta)\, e^{i\omega t}\, dt$$

$$= \frac{1}{2T}\int_0^T dt\, \cancel{e^{i(\omega t+\theta)}} \left(e^{i(\omega t+\theta)}\, e^{i\omega t} + e^{-i(\omega t+\theta)}\, e^{i\omega t}\right)$$

$$= \frac{1}{2T}\int_0^T dt\; e^{-i\theta} = \frac{e^{-i\theta}}{2}$$

$$V_{-1}(\vec{k}) = \frac{1}{2}\begin{pmatrix} 0 & e^{i\phi}A_x & e^{-i\phi}A_y e^{-i\theta} \\ e^{-i\phi}A_x & 0 & 0 \\ e^{i\phi}A_y e^{-i\theta} & 0 & 0 \end{pmatrix}$$

$$\frac{[V_{+1}, V_{-1}]}{\hbar\omega} = \frac{i A_x A_y \sin\theta}{2\omega}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -e^{-i2\phi} \\ 0 & e^{i2\phi} & 0 \end{pmatrix}$$

$$= i\gamma \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -e^{-i2\phi} \\ 0 & e^{i2\phi} & 0 \end{pmatrix}$$

$$\boxed{\gamma = \frac{A_x A_y \sin\theta}{2\omega}}$$

Changes in the band structure :-

effective floquet Hamiltonian -

$$H_{floq} = \begin{pmatrix} 0 & e^{i\phi}k_x & e^{-i\phi}k_y \\ e^{-i\phi}k_x & 0 & e^{i\phi}k_z - i\gamma e^{-2i\phi} \\ e^{i\phi}k_y & e^{-i\phi}k_z + i\gamma e^{2i\phi} & 0 \end{pmatrix}$$

$$\begin{vmatrix} -\lambda & e^{i\phi}k_x & e^{-i\phi}k_y \\ e^{-i\phi}k_x & -\lambda & e^{i\phi}k_z - i\gamma e^{-2i\phi} \\ e^{i\phi}k_y & e^{-i\phi}k_z + i\gamma e^{2i\phi} & -\lambda \end{vmatrix} = 0$$

$$\Rightarrow -\lambda\left(\lambda^2 - \left(e^{-i\phi}k_z + i\gamma e^{2i\phi}\right)\left(e^{i\phi}k_z - i\gamma e^{-2i\phi}\right)\right)$$
$$- e^{i\phi}k_x\left(-\lambda e^{-i\phi}k_x - e^{i\phi}k_y\left(e^{i\phi}k_z - i\gamma e^{-2i\phi}\right)\right)$$
$$+ e^{-i\phi}k_y\left(e^{-i\phi}k_x\left(e^{-i\phi}k_z + i\gamma e^{2i\phi}\right) + \lambda e^{i\phi}k_y\right) = 0$$

$$\Rightarrow -\lambda\left(\lambda^2 - k_z^2 + i\gamma e^{-3i\phi}k_z - i\gamma k_z e^{3i\phi} - \gamma^2\right)$$
$$\cancel{+ \lambda k_x^2 + k_x k_y \gamma e^{2i\phi}} - e^{i\phi}k_x\left(-\lambda e^{-i\phi}k_x - k_y k_z e^{2i\phi} + i\gamma k_y e^{-i\phi}\right)$$
$$+ e^{-i\phi}k_y\left(k_x k_z e^{-2i\phi} + i\gamma e^{i\phi}k_x + \lambda e^{i\phi}k_y\right) = 0$$

$$\Rightarrow -\lambda^3 + \lambda k_z^2 - i\gamma\lambda e^{-i3\phi}k_z + i\gamma\lambda k_z e^{3i\phi} + \lambda\gamma^2$$
$$+ \lambda k_x^2 + k_x k_y k_z e^{3i\phi} - i\gamma \cancel{k_x k_y} + k_x k_y k_z e^{-3i\phi}$$
$$+ i\gamma \cancel{k_y} k_x + \lambda k_y^2 = 0.$$

$$\Rightarrow -\lambda^3 + \lambda k_z^2 + i\gamma \lambda k_z \left(e^{3i\phi} - e^{-3i\phi}\right)$$
$$+ \lambda\gamma^2 + \lambda k_x^2 + \lambda k_y^2 + k_x k_y k_z \left(e^{3i\phi} + e^{-3i\phi}\right) = 0$$

$$\Rightarrow \boxed{\begin{aligned} &-\lambda^3 + \lambda k_z^2 - 2\gamma\lambda k_z \sin(3\phi) \\ &+ \lambda\gamma^2 + \lambda k_x^2 + \lambda k_y^2 + 2k_x k_y k_z \cos(3\phi) = 0 \end{aligned}}$$

for $\phi = \frac{\pi}{6} \left(\bmod \frac{\pi}{3}\right)$

$$\Rightarrow -\lambda^3 + \lambda k_z^2 - 2\gamma\lambda k_z \sin(3\phi) + \lambda\gamma^2 + \lambda k_x^2 + \lambda k_y^2 = 0$$

$$\Rightarrow \underline{\lambda = 0},$$

$$\lambda^2 - k_z^2 + 2\gamma k_z \sin(3\phi) - \gamma^2 - k_x^2 - k_y^2 = 0$$

$$\Rightarrow \lambda^2 = k_x^2 + k_y^2 + k_z^2 - 2\gamma k_z \sin 3\phi + \gamma^2$$

$$\lambda^2 = k_x^2 + k_y^2 + k_z^2 - 2\gamma k_z \sin 3\phi + \gamma^2 \sin^2 3\phi$$
$$+ \gamma^2 - \gamma^2 \sin^2 3\phi$$

$$\Rightarrow \lambda = \pm\sqrt{k_x^2 + k_y^2 + (k_z - \gamma \sin 3\phi)^2 + \gamma^2 \cos^2 3\phi}$$

for $\phi = \frac{\pi}{6} \left(\bmod \frac{\pi}{3}\right)$ $\cos 3\phi = 0$ always.

$$\lambda = \pm\sqrt{k_x^2 + k_y^2 + (k_z - \gamma \sin 3\phi)^2}$$

$$\lambda = 0$$

$\therefore$ for $\phi = \frac{\pi}{6} \pmod{\frac{\pi}{3}}$

$$E = 0, \pm\sqrt{k_x^2 + k_y^2 + (k_z - \gamma\sin 3\phi)^2}$$

which are degenerate at $\vec{k} = (0, 0, \gamma\sin 3\phi)$

Again for $\phi = 0 \pmod{\pi/3}$

$$-\lambda^3 + \lambda k_z^2 + \lambda\gamma^2 + \lambda k_x^2 + \lambda k_y^2 + 2k_x k_y k_z \cos(3\phi) = 0$$

$$\Rightarrow \lambda^3 - \lambda(k_x^2 + k_y^2 + k_z^2 + \gamma^2) - 2k_x k_y k_z \cos 3\phi = 0$$

at $\vec{k} = 0$

$$\lambda^3 - \lambda\gamma^2 = 0$$

$\lambda = 0, \quad \lambda = \pm\gamma, \quad \Delta E\big|_{k=0} = 2\gamma$, for $\phi = 0 \pmod{\frac{\pi}{3}}$

Band gap opens up.

The eigenvalues of H_{floq} satisfy the following equation,

$$E^3 - E\left(\gamma^2 + \kappa^2 - 2\gamma k_z \sin 3\phi\right) - 2\kappa_x \kappa_y \kappa_z \cos 3\phi = 0$$

$$\Rightarrow \quad E^3 - \lambda_1 E - C = 0$$

Not necessary.

$$(E-\gamma_1)(E-\gamma_2)(E-\gamma_3) = 0.$$

$$E^3 - (\gamma_1+\gamma_2+\gamma_3)E^2$$
$$+ (\gamma_1\gamma_2 + \gamma_2\gamma_3 + \gamma_3\gamma_1)E$$
$$- \gamma_1\gamma_2\gamma_3 = 0.$$

$$\gamma_1 + \gamma_2 + \gamma_3 = 0.$$

$$\gamma_1\gamma_2 + \gamma_2\gamma_3 + \gamma_3\gamma_1 = \lambda_1$$

$$\gamma_1\gamma_2\gamma_3 = C$$

$$\gamma_1 + \gamma_2 + \frac{C}{\gamma_1\gamma_2} = 0.$$

$$\gamma_1\gamma_2 + (\gamma_1+\gamma_2)\frac{C}{\gamma_1\gamma_2} = \lambda_1$$

$$\Rightarrow \quad \gamma_1\gamma_2 - (\gamma_1+\gamma_2)^2 = \lambda_1$$

$$\Rightarrow \quad \cancel{-\frac{(\gamma_1+\gamma_2)}{C} - (\gamma_1+\gamma_2)^2} = \lambda_1$$

$$x^3 + ax^2 + bx + c = 0.$$

1st step, calculate

$$Q = \frac{a^2 - 3b}{9} \quad \text{and} \quad R = \frac{2a^3 - 9ab + 27c}{54}$$

let $M = R^2 - Q^3$ — the discriminant.

1) If $M < 0$ (i.e, $R^2 < Q^3$) the polynomial has three real roots,

compute $\theta = \arccos\left(\frac{R}{\sqrt{Q^3}}\right)$

three distinct real roots are,

$$x_1 = -\left(2\sqrt{Q}\cos\frac{\theta}{3}\right) - \frac{a}{3}$$

$$x_2 = -\left(2\sqrt{Q}\cos\frac{\theta + 2\pi}{3}\right) - \frac{a}{3}$$

$$x_3 = -\left(2\sqrt{Q}\cos\frac{\theta - 2\pi}{3}\right) - \frac{a}{3}$$

2) if $M > 0$ (i.e, $R^2 > Q^3$) the polynomial has only one real root.

compute,

$$S = \sqrt[3]{-R + \sqrt{M}}$$

$$T = \sqrt[3]{-R - \sqrt{M}}$$

the real root will be,

$$x_1 = S + T - \frac{a}{3}$$

(the formula for two complex conjugate is not given in the ref. I pick, find somewhere else)

For our case,

$$E^3 - \lambda_1 E - c = 0$$

$$x^3 + ax^2 + bx + c' = 0$$

$$a = 0, \quad b = -\lambda_1 \quad c' = -c$$

Solving these equation in Mathematica we obtained

$$\boxed{\Delta_g = |2\gamma \cos(3\phi)| \text{ and, } k_z^0 = \gamma \sin 3\phi}$$

> So, the $\cos 3\phi$, $\sin 3\phi$ nature of variation of the band gap and shift, respectively, also captures the inherent $(\pi/3)$ periodicity in the response of the system.

> From weyl semimetal studies it has been shown that the lifting of degeneracy in a fully centrosymmetric weyl semimetal is difficult. It has also been shown that tilted weyl semimetal have a better response to light,

which matches with this our cases.

Anamalous Hall conductivity

for $\phi = \pi/6 \pmod{\pi/3}$

$$H_{flog}(\vec{k}) = H_{3f}(\vec{k} - \delta\vec{k}) \quad \text{where} \quad \delta\vec{k} = (0, 0, \gamma \sin 3\phi)$$

at these values of ϕ the three BTP does not open up a gap, it continues to behave line a source or sink of Berry curvature with monopole charge ± 2.

the Hall conductivity $\Delta\sigma_{xy}$ is given by.

$$\Delta\sigma_{xy} = n \frac{e^2}{h} \frac{\nu_z}{2\pi}$$

'n' is chern number of the lower band and ν_z is the shift of the 3-BTP along the k_z direction after applying light.

$$\Delta\sigma_{xy} = 2 \cdot \frac{e^2}{h} \frac{\gamma \sin 3\phi}{2\pi} = \frac{e^2 \gamma \sin 3\phi}{h\pi} = \pm \frac{e^2 \gamma}{\pi h}$$

Hall voltage V_y (when current I_x is applied along x-dirn)

$$V_y = \frac{\sigma_{xy} \delta/d}{\sigma_{xx}^2 + (\sigma_{xy} \delta/d)^2} \frac{I_x}{d}$$

as $\sigma_{xx} \gg \sigma_{xy}$

$$\Delta V_y \approx \frac{\Delta\sigma_{xy}}{\sigma_{xx}^2 d} \frac{\delta I_x}{d}$$

given, $\delta = \dfrac{n(\omega) c \epsilon_0}{R\, \sigma_{xx}(\omega)}$

$$\gamma = \frac{e^2 v_f A^2}{2\hbar^2 \omega} = \frac{e^2 \hbar v_f E^2}{2(\hbar\omega)^3} = \frac{e^2 \hbar v_f}{2(\hbar\omega)^3} \frac{2P(1-R)}{I_x I_y n(\omega) c \epsilon_0}.$$

[for circularly polarized light. $A_x = A_y = A_z = A$, $\sin\theta = 1$