Tutorial QDev Summer School

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1 Gap opening in circularly driven Dirac fermions I: Discrete time evolution

Consider the two-dimensional Dirac Hamiltonian

$$\mathcal{H}(\boldsymbol{k}) = \hbar v_F (k_x \sigma_x + k_y \sigma_y), \tag{1}$$

with Fermi velocity v_F and the Pauli matrices

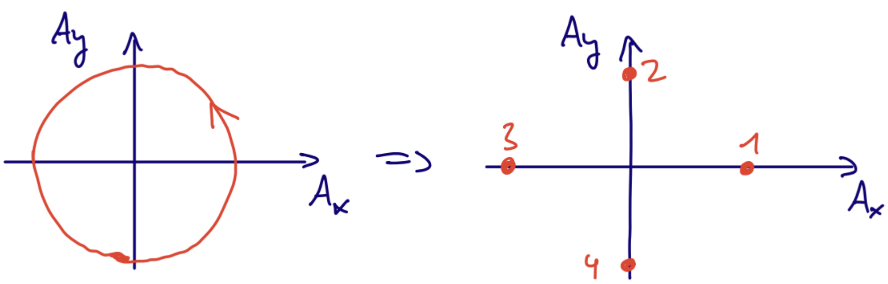
$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}.$$

The Dirac fermions are minimally coupled to a time-dependent vector potential $\boldsymbol{A}(t)$ via

$$\boldsymbol{k} \rightarrow \boldsymbol{k}(t) = \boldsymbol{k} - \boldsymbol{A}(t). \tag{2}$$

To mimick the effect of time-reversal symmetry breaking through a circularly polarized field, we employ the following simplified field:



That is, we assume that the field is kept constant over quarters $T/4$ of the driving period T, and points along positive and negative x and y directions as sketched, with an amplitude A_0.

1. Compute the time evolution operator $\mathcal{U}(\boldsymbol{k}, T)$ for one driving period. To this end, write down $\mathcal{U}_n(\boldsymbol{k})$, $n = 1, 2, 3, 4$ as the sub-period evolution operators, then string them together for the full-period evolution. *Hint:* It is sufficient to keep this as a product of four exponentials at this stage. For temporally constant Hamiltonian H the time evolution operator is given by $\mathcal{U} = \exp(-i\mathcal{H}t/\hbar)$.

2. Focus on the Dirac point, $\boldsymbol{k} = 0$. Take the high-frequency (small T) limit by a Taylor expansion of $\mathcal{U}(\boldsymbol{k}, T)$ to second order in A_0. Then re-exponentiate the resulting Taylor series to obtain an effective Hamiltonian at the Dirac point that generates the time evolution over the entire period. *Hint:* If you know the matrix exponentials of Pauli matrices, this step is not strictly necessary, and you can also obtain $\mathcal{U}(\boldsymbol{k}, T)$ as a closed-form expression, without Taylor expansion.

3. Discuss the result. What is the spectrum of the effective Hamiltonian that results from adding the Dirac-point result to the original Hamiltonian given in Eq. (1)? What are the eigenstates $|u_{v/c,\boldsymbol{k}}\rangle$ of negative/positive energy (valence/conduction, v/c, band)? Compute the Berry phase

$$\phi_v = -i \oint_{\mathcal{C}} \langle u_{v,\boldsymbol{k}} | \nabla_{\boldsymbol{k}} | u_{v,\boldsymbol{k}} \rangle \tag{3}$$

($\phi \in [-\pi, \pi]$) of the quasiparticle in the valence band for a closed clockwise loop $\mathcal{C}$ around the Dirac point (e.g., a circle of fixed radius). How does it change when the circular polarization of $\boldsymbol{A}(t)$ is reversed (i.e., the ordering is $1-4-3-2$ in the above sketch)?

4. Bonus task: write a short code to compute the Berry phase around a closed loop numerically. Question: Why does it not matter whether the eigenstates at individual k points acquire "random" phases?

2 Gap opening in circularly driven Dirac fermions II: Floquet

Now consider the same Dirac model of Eq. 1, $\mathcal{H}(\boldsymbol{k})$, but this time minimally coupled (Eq. 2) to a continuous circularly polarized drive with vector potential

$$\boldsymbol{A}(t) = A_0(\cos(\omega t)\hat{x} + \sin(\omega t)\hat{y}), \tag{4}$$

with $\hat{x}$ the unit vector along x, and $\hat{y}$ the unit vector along y direction, respectively, and $\omega = \frac{2\pi}{T}$ is the driving frequency.

1. Determine the Floquet Hamiltonian

$$\mathcal{H}^F_{mn}(\boldsymbol{k}) = \frac{1}{T}\int_0^T dt\; \mathcal{H}(\boldsymbol{k}(t)) \exp(i(m-n)\omega t) + m\delta_{mn}\hbar\omega\mathcal{I}, \tag{5}$$

where $\mathcal{I}$ is the 2×2 identity matrix. You can restrict m, n to take values $-1, 0, 1$ for display.

2. In the high-frequency and weak-driving limit and at the Dirac point at $\boldsymbol{k} = 0$, you can determine an effective Hamiltonian for the original 2×2 subspace by second-order perturbation theory:

$$\mathcal{H}^F_{\text{eff}} \approx \mathcal{H}^F_{00} + \frac{[\mathcal{H}^F_{0,1}, \mathcal{H}^F_{0,-1}]}{\hbar\omega}, \tag{6}$$

involving the commutator $[\mathcal{H}^F_{0,1}, \mathcal{H}^F_{0,-1}]$ of Floquet blocks that bridge the 0-photon sector with the ±1-photon sectors. What is the resulting $\mathcal{H}^F_{\text{eff}}$? Compare to the result from Exercise 1.

3. Why is there no "dynamical localization effect" in the infinite-frequency limit? That is, why is $\mathcal{H}^F_{00}(\boldsymbol{k})$ identical to the original Dirac Hamiltonian?

4. Bonus task: Write code to diagonalize the full Floquet matrix, Eq. 5, truncated at appropriate values of the m, n (try different truncations), and for a path along k_x at $k_y = 0$ (e.g., $-1 < k_x < 1$). You can set $\hbar = 1$, $v_F = 1$. Play around with your code to see if you can confirm the scaling of the light-induced gap at the Dirac point with A_0 and ω found in perturbation theory. When does the perturbative result break down? What happens when the gap becomes so large that sideband crossings occur at the Dirac point?

5. Homework: What happens under linearly polarized light (along x)? What do the Floquet bands look like along k_x versus k_y? Can you recognize some of the features discussed in Y. H. Wang et al., Science 342, 453–457 (2013)?