Assignment - 8:

Berry phase, ballistic transport & Klein tunneling in graphene

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Given the free particle Hamiltonian of a generic 2D Dirac material,

$$\hat{H} = v_F \left[\sigma_x \hat{p}_x + \sigma_y \hat{p}_y + \sigma_z m \right],$$

A] Calculate its (i) eigenvalues $\{E_+, E_-\}$ and

(ii) eigenvectors $\{|E_+\rangle, |E_-\rangle\}$

B] Find the Berry curvature and compare the berry phase for eigenvector $\{|E_+\rangle, |E_-\rangle\}$.

Solution:

A] $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

$$\hat{H} = v_F \begin{pmatrix} m & p_x - ip_y \\ p_x + ip_y & -m \end{pmatrix}$$

In polar coordinates,

$$p_x = p \cos\theta$$

$$p_y = p \sin\theta$$

where, $p = \sqrt{(p_x^2 + p_y^2)}$ $\qquad \theta = \tan^{-1}\left(\frac{p_y}{p_x}\right)$

$$\Rightarrow \quad \hat{H} = v_F \begin{pmatrix} m & pe^{-i\theta} \\ pe^{i\theta} & -m \end{pmatrix}$$

The eigenvalues of $\hat{H}$ are given by

$\det(\hat{H} - E\hat{I}) = 0$, where E is the energy eigenvalue.

$$\Rightarrow \quad (E - v_F m)(E + v_F m) - v_F^2 p^2 = 0$$

$$\Rightarrow \quad E^2 = v_F^2 (p^2 + m^2) \quad \Rightarrow E = \pm v_F \sqrt{p^2 + m^2}$$

$$\therefore \boxed{\text{Set of eigenvalues} = \left\{ v_F \sqrt{p^2+m^2}, -v_F \sqrt{p^2+m^2} \right\}}$$

To solve for the eigenvalues, we take a general 2×1 vector $|E_+\rangle = \begin{pmatrix} a \\ b \end{pmatrix}$, $|E_-\rangle = \begin{pmatrix} c \\ d \end{pmatrix}$

$$\cancel{v_F}\begin{pmatrix} m & pe^{-i\theta} \\ pe^{i\theta} & m \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = \cancel{v_F}\sqrt{p^2+m^2}\begin{pmatrix} a \\ b \end{pmatrix}$$

$$\Rightarrow ma + pe^{-i\theta} b = \sqrt{p^2+m^2}\, a \Rightarrow a = \frac{pe^{-i\theta}}{(\lambda - m)}\, b, \quad \lambda = \sqrt{p^2+m^2}$$

1

$$\Rightarrow b = k\sqrt{\lambda - m} \Rightarrow a = e^{-i\theta}\frac{\sqrt{\lambda^2 - m^2}}{(\lambda - m)}\sqrt{\lambda - m}\, k = k\, e^{-i\theta}\sqrt{\lambda + m}$$

Since $\langle E_+ | E_+ \rangle = 1 \Rightarrow |a|^2 + |b|^2 = 1 \Rightarrow k^2(\lambda + m + \lambda - m) = 1$

$$\Rightarrow |E_+\rangle = k\begin{pmatrix} \sqrt{(\lambda+m)}\, e^{-i\theta} \\ \sqrt{(\lambda - m)} \end{pmatrix} = \frac{1}{\sqrt{2\lambda}}\begin{pmatrix} \sqrt{(\lambda+m)}\, e^{-i\theta} \\ \sqrt{(\lambda - m)} \end{pmatrix}$$

$$\cancel{v_F}\begin{pmatrix} m & pe^{-i\theta} \\ pe^{i\theta} & m \end{pmatrix}\begin{pmatrix} c \\ d \end{pmatrix} = -\cancel{v_F}\sqrt{p^2+m^2}\begin{pmatrix} c \\ d \end{pmatrix} = E_-|E_-\rangle$$

Thus,

$$mc + pe^{-i\theta} d = -\sqrt{p^2+m^2}\, a \quad , \qquad c = \frac{-pe^{-i\theta}}{(\lambda+m)}\, d$$

$$\Rightarrow c = k\sqrt{\lambda+m} \quad \Rightarrow d = -e^{-i\theta}\frac{\sqrt{\lambda^2-m^2}}{(\lambda+m)}\left(\sqrt{\lambda+m}\right)k = -ke^{i\theta}\sqrt{(\lambda-m)}$$

$$\langle E_-|E_-\rangle = 1 \quad \Rightarrow \quad k^2(\lambda+m+\lambda-m) = 1 \quad \Rightarrow k = \frac{1}{\sqrt{2\lambda}}$$

$$|E_-\rangle = \frac{1}{\sqrt{2\lambda}}\begin{pmatrix} -\sqrt{(\lambda-m)}\,e^{-i\theta} \\ \sqrt{(\lambda+m)} \end{pmatrix}$$

$\boxed{\text{The set of eigenvectors are: } \left\{ \frac{1}{\sqrt{2\lambda}} \begin{pmatrix} \sqrt{(\lambda+m)}\, e^{-i\theta} \\ \sqrt{(\lambda-m)} \end{pmatrix}, \frac{1}{\sqrt{2\lambda}} \begin{pmatrix} -\sqrt{(\lambda-m)}\, e^{-i\theta} \\ \sqrt{(\lambda+m)} \end{pmatrix} \right\}}$

B] The Berry phase for an eigenstate $|E_\pm\rangle$ over closed path $\mathcal{C}$ in momentum space:

$$\gamma_\pm = i \oint \langle E_\pm | \vec{\nabla}_{\vec{p}} | E_\pm \rangle \cdot d\vec{p}$$

In polar coordinates, we can take

$$\vec{p} = \begin{pmatrix} p\cos\theta \\ p\sin\theta \end{pmatrix}, \quad \vec{\nabla}_p = \frac{\partial}{\partial p}\hat{p} + \frac{1}{p}\frac{\partial}{\partial\theta}\hat{\theta}.$$

For a circular path (fixed p): $d\vec{p} = p\,d\theta\,\hat{\theta}$

Thus, we only need to calculate $\frac{\partial}{\partial\theta}|E_\pm\rangle$ and take inner product with $\langle E_\pm|$ and integrate θ from 0 to 2π.

$$\frac{\partial}{\partial\theta}|E_+\rangle = \frac{1}{\sqrt{2\lambda}}\begin{pmatrix} -i\sqrt{\lambda+m}\, e^{-i\theta} \\ 0 \end{pmatrix}$$

$$\Rightarrow A_{\theta,+} = i\langle E_+|\frac{1}{\rho}\frac{\partial}{\partial\theta}|E_+\rangle = \frac{i}{2\lambda}\frac{\sqrt{(\lambda+m)}}{\rho}\cancel{e^{i\theta}}\cdot(-i)\sqrt{(\lambda+m)}\,\cancel{e^{-i\theta}} = \frac{1}{\rho}\frac{\lambda+m}{2\lambda}$$

$$\boxed{\Rightarrow \gamma_+\Big|_{\substack{\text{circular}\\ \text{loop}}} = \int_0^{2\pi}\frac{1}{\cancel{\rho}}\left(\frac{\lambda+m}{2\lambda}\right)\cancel{\rho}\,d\theta = \pi\left(\frac{\lambda+m}{\lambda}\right)}$$

$$\frac{\partial}{\partial \theta}|E_-\rangle = \frac{1}{\sqrt{2\lambda}}\begin{pmatrix} -i\sqrt{(\lambda-m)}\, e^{-i\theta} \\ 0 \end{pmatrix}$$

$$\Rightarrow A_{\theta,-} = i\langle E_-|\frac{1}{p}\frac{\partial}{\partial\theta}|E_-\rangle = i\,\frac{1}{2\lambda}\left(-\sqrt{(\lambda-m)}\, e^{i\theta}\right)\begin{pmatrix}\frac{\pm i}{p}\sqrt{(\lambda-m)}\, e^{-i\theta}\end{pmatrix}$$

$$= \frac{i(-i)}{p}\left(\frac{\lambda-m}{2\lambda}\right) = \frac{1}{p}\left(\frac{\lambda-m}{2\lambda}\right)$$

$$\boxed{\Rightarrow \gamma_-\Big|_{\text{circular loop}} = \int_0^{2\pi} \frac{1}{\cancel{p}}\left(\frac{\lambda-m}{2\lambda}\right)\cancel{p}\, d\theta = \pi\left(\frac{\lambda-m}{\lambda}\right)}$$

The berry curvature for a state $|E_\pm\rangle$ is given by:

$$\Omega_z = \frac{\partial}{\partial p_x} A_{p_y,\pm} - \frac{\partial}{\partial p_y} A_{p_x,\pm} = \left(\vec{\nabla}\times\vec{A}_\pm\right)_z, \text{ where } \vec{A}_\pm = \begin{pmatrix} A_{p_x,\pm} \\ A_{p_y,\pm} \end{pmatrix}$$

In polar coordinates,

$$\Omega_{z\pm} = \left[\frac{\partial}{\partial p}\left(p A_{\theta,\pm}\right) - \frac{\partial}{\partial \theta}\left(A_{p,\pm}\right)\right] \qquad \left(\vec{\nabla} \times \vec{A}_{\pm} = \begin{vmatrix} \hat{p} & p\hat{\Theta} & \hat{p}_z \\ \frac{\partial}{\partial p} & \frac{\partial}{\partial \theta} & \frac{\partial}{\partial z} \\ A_{p\pm} & A_{\theta\pm} & \underbrace{A_{z\pm}}_{=0} \end{vmatrix} \right)$$

In the calculation of berry phase, we calculated A_θ, we now calculate A_p.

$$\partial_p|E_+\rangle = \begin{pmatrix} \partial_p(a) \\ \partial_p(b) \end{pmatrix} \qquad \partial_p|E_-\rangle = \begin{pmatrix} \partial_p(c) \\ \partial_p(d) \end{pmatrix}$$

$$\frac{\partial}{\partial p} = \frac{\partial \lambda}{\partial p}\frac{\partial}{\partial \lambda} = \frac{\partial\left(\sqrt{p^2+m^2}\right)}{\partial p}\frac{\partial}{\partial \lambda} = \frac{p}{\lambda}\frac{\partial}{\partial \lambda}$$

$$\Rightarrow \partial_p a = \frac{p}{\lambda}\frac{\partial}{\partial \lambda}\left(\sqrt{\frac{\lambda+m}{2\lambda}}\, e^{-i\theta}\right) = \frac{p}{\lambda}\left(\frac{\sqrt{2\lambda}\big/ 2\sqrt{\lambda+m} - \sqrt{\lambda+m}\big/\sqrt{2\lambda}\left(\frac{2}{2}\right)}{2\lambda}\right)e^{-i\theta}$$

looking at this, we can get the other constants:

For E_+

$$\partial_p a = \frac{p}{\lambda}\left(\frac{\frac{1}{2}\sqrt{\frac{2\lambda}{\lambda+m}} - \sqrt{\frac{\lambda+m}{2\lambda}}}{2\lambda}\right)e^{-i\theta}$$

$$\Rightarrow \partial_p b = \frac{p}{\lambda}\left(\frac{\frac{1}{2}\sqrt{\frac{2\lambda}{\lambda-m}} - \sqrt{\frac{\lambda-m}{2\lambda}}}{2\lambda}\right)$$

$$\partial_p c = \frac{-p}{\lambda}\left(\frac{\frac{1}{2}\sqrt{\frac{2\lambda}{\lambda-m}} - \sqrt{\frac{\lambda-m}{2\lambda}}}{2\lambda}\right)e^{-i\theta}$$

$$\Rightarrow \partial_p d = \frac{p}{\lambda}\left(\frac{\frac{1}{2}\sqrt{\frac{2\lambda}{\lambda+m}} - \sqrt{\frac{\lambda+m}{2\lambda}}}{2\lambda}\right)$$

$$A_{p,+} = \frac{1}{2\lambda}\left[\sqrt{\frac{\lambda+m}{2\lambda}}\,\cancel{e^{+i\theta}} \cdot p\left(\frac{\frac{1}{2}\sqrt{\frac{2\lambda}{\lambda+m}} - \sqrt{\frac{\lambda+m}{2\lambda}}}{\lambda}\right)\cancel{e^{-i\theta}} + \sqrt{\frac{\lambda-m}{2\lambda}} \cdot p\left(\frac{1/2\sqrt{\frac{2\lambda}{\lambda-m}} - \sqrt{\frac{\lambda-m}{2\lambda}}}{\lambda}\right)\right] = \frac{p}{2\lambda}\left(\frac{1}{\lambda} - \left(\lambda+m/2\lambda^2\right) - \left(\frac{\lambda-m}{2\lambda^2}\right)\right)$$

$$= \frac{p}{2\lambda}\left(\cancel{\frac{1}{\lambda}} - \cancel{\frac{1}{\lambda}}\right) = 0$$

$$\Rightarrow \quad A_{p,+} = 0$$

$$A_{p,-} = \frac{1}{2\lambda}\left[-\sqrt{\frac{\lambda-m}{2\lambda}}\,\cancel{e^{i\theta}} \cdot p\left(\frac{\frac{1}{2}\sqrt{\frac{2\lambda}{\lambda-m}} - \sqrt{\frac{\lambda-m}{2\lambda}}}{\lambda}\right)\cancel{e^{-i\theta}} \quad \sqrt{\frac{\lambda+m}{2\lambda}} \cdot p \cdot \left(\frac{1/2\sqrt{\frac{2\lambda}{\lambda+m}} - \sqrt{\frac{\lambda+m}{2\lambda}}}{\lambda}\right)\right] = \frac{1}{2\lambda}\left(\frac{1}{\lambda} - \left(\frac{\lambda-m}{2\lambda^2}\right) - \left(\frac{\lambda+m}{2\lambda^2}\right)\right) = 0$$

$$\Rightarrow \quad A_{p-} = 0$$

Therefore we have:

$$\Omega_{z\pm} = \frac{\partial}{\partial p}\left(p A_{\theta,\pm}\right)$$

$$\Omega_{z+} = \frac{\partial}{\partial p}\left(\cancel{p}\cdot\frac{1}{\cancel{p}}\left(\frac{\lambda+m}{2\lambda}\right)\right) = \frac{p}{2\lambda}\frac{\partial}{\partial\lambda}\left(\frac{\lambda+m}{\lambda}\right) = \frac{p}{2}\left(\frac{\lambda-(\lambda+m)}{\lambda^3}\right)$$

$$\boxed{\Omega_{z+} = \frac{-p\,m}{2\lambda^3} = \frac{-p\,m}{2\,(p^2+m^2)^{3/2}}}$$

$$\left(\because \partial_p = \frac{p}{\lambda}\partial_\lambda\right)$$

$$\Omega_{z,-} = \frac{\partial}{\partial p}\left(\cancel{p}\cdot\frac{1}{\cancel{p}}\left(\frac{\lambda-m}{2\lambda}\right)\right) = \frac{p}{2\lambda}\left(\frac{\lambda-(\lambda-m)}{\lambda^2}\right)$$

$$\boxed{\Omega_{z,-} = \frac{p\,m}{2\,(p^2+m^2)^{3/2}}}$$

Thus, the sum of the Berry phases is 2π over circular loop
sum of berry curvature $= 0$.

The Berry phase over the Brillouin zone (in case of free particle, over all space):

$$\gamma_{\pm}\Big|_{BZ} = \iint_{BZ} \Omega_{\gamma,\pm\infty}\, d^2p = \int_0^{2\pi}\int_0^{\infty} \Omega_{\gamma,\pm}\, p\, dp\, d\theta$$

$$\gamma_{+}\Big|_{BZ} = \frac{m}{\cancel{2}}\cdot \cancel{2}\pi \int_0^{\infty} \frac{-p\, dp}{(p^2+m^2)^{3/2}} = -m\frac{\pi}{2}\int_{|m|^2} t^{-3/2}\, dt = +\frac{m\pi}{\cancel{2}\times\frac{+1}{\cancel{2}}}\left(\frac{-1}{((|m|^2)^{1/2}}\right)$$

$$\Rightarrow \boxed{\gamma_{+}\Big|_{BZ} = -\,\mathrm{sgn}(m)\,\pi}$$

$$\gamma_{-}\Big|_{BZ} = \frac{m}{2}\cdot 2\pi \int_0^{\infty} \frac{p\, dp}{(p^2+m^2)^{3/2}} = \frac{m\pi}{2}\int_{|m|^2}^{\infty} t^{-3/2}\, dt = \mathrm{sgn}(m)\,\pi$$

$$\Rightarrow \boxed{\gamma_{-}\Big|_{BZ} = \mathrm{sgn}(m)\,\pi}$$

Thus, sum of Berry phases over BZ (all space for free particle) $= 0$.