Helical metals and insulators in interacting Dirac matter

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H.R., E. Cappelluti, and A. V. Balatsky,
Phys. Rev. B 98, 245114 (2018)

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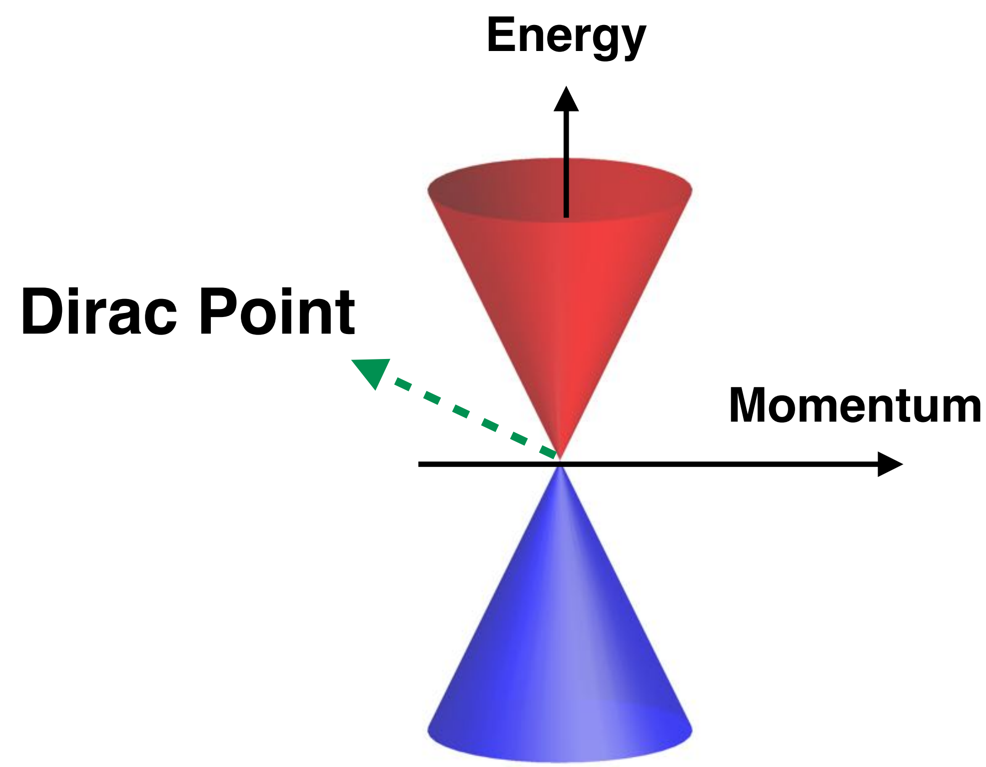
Frascati, Rome

Outline

- **Introduction: theory and experiment**
- **Interaction induced helical insulator and metal**
- **Berry curvature: sheet singularity**
- **Landau level spectrum**

Dirac Matter



$d = 2$ Graphene, TI surface states,…

$$\mathcal{H} = v\sigma \cdot \mathbf{k} = v(k_x\sigma_x + k_y\sigma_y)$$

$d = 3$ Weyl semimetals such as TaAs compounds,…

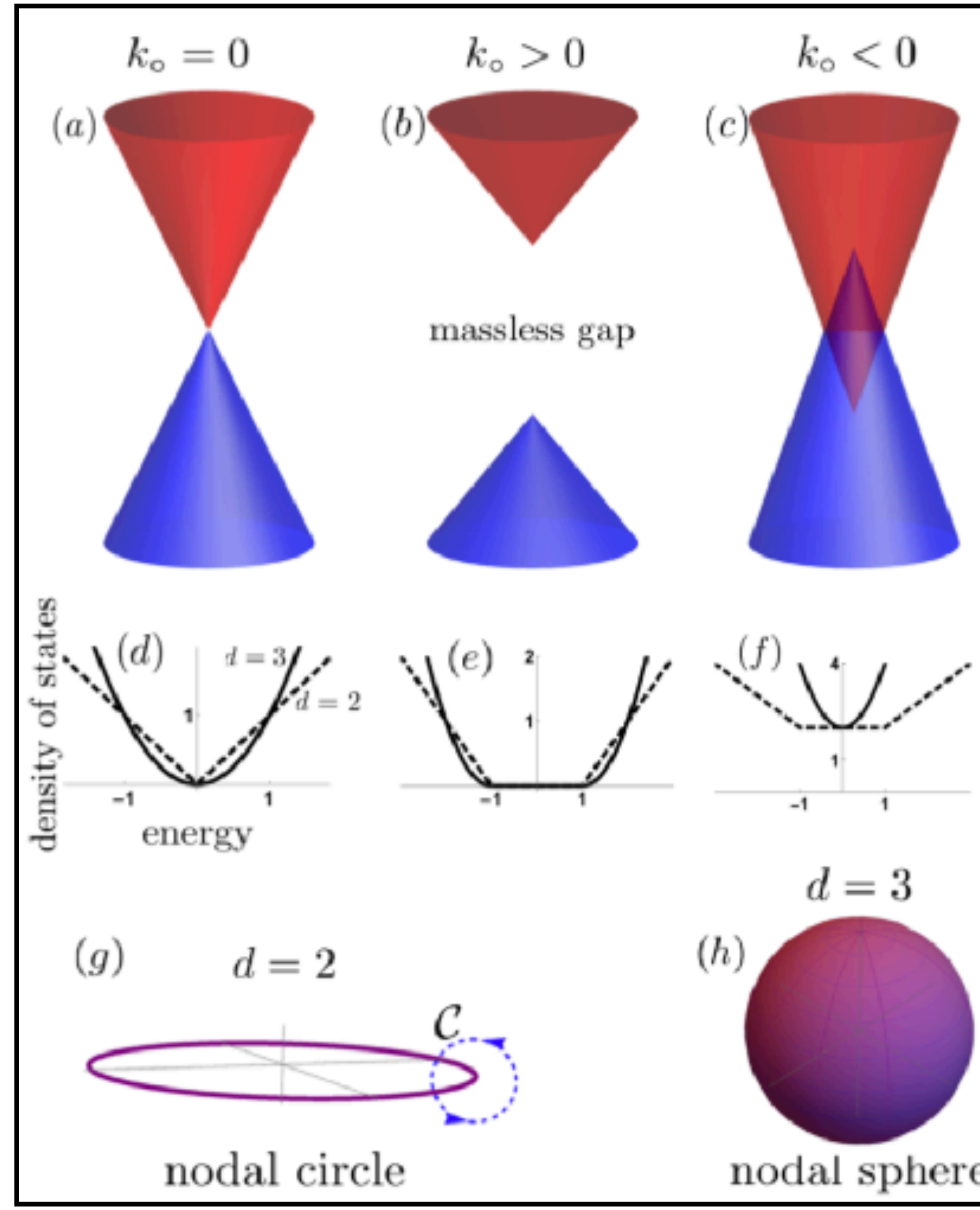
$$\mathcal{H} = v\sigma \cdot \mathbf{k} = v(k_x\sigma_x + k_y\sigma_y + k_z\sigma_z)$$

Helical insulators and metals

$$\hat{\Sigma}(\mathbf{k}) = \Delta \frac{\hat{\sigma}\cdot\mathbf{k}}{k} \qquad\qquad \Delta = \hbar v k_\circ$$

$$\hat{\mathcal{H}}_{\boldsymbol{k}} = \hbar v k \hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{k}} + \Delta \hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{k}},$$

$$\hat{\mathcal{H}}_{\boldsymbol{r}} = \hbar v \hat{\boldsymbol{\sigma}} \cdot \left[-i\boldsymbol{\nabla} + \frac{i k_\circ (d-1)}{2\pi^{d-1}} \int d^d \boldsymbol{s} \, \frac{\boldsymbol{s} \exp\{\boldsymbol{s}\cdot\boldsymbol{\nabla}\}}{s^{d+1}} \right]$$



- **Helicity operator**

$$\hat{h} = \hat{\sigma}\cdot\hat{\mathbf{k}} \qquad [\hat{\mathcal{H}}_k, \hat{h}] = 0$$

- **Lifshitz transition:**

$$\textbf{Dirac point} \rightarrow \begin{cases} \textbf{gapped} \\ \textbf{nodal circle/sphere} \end{cases}$$

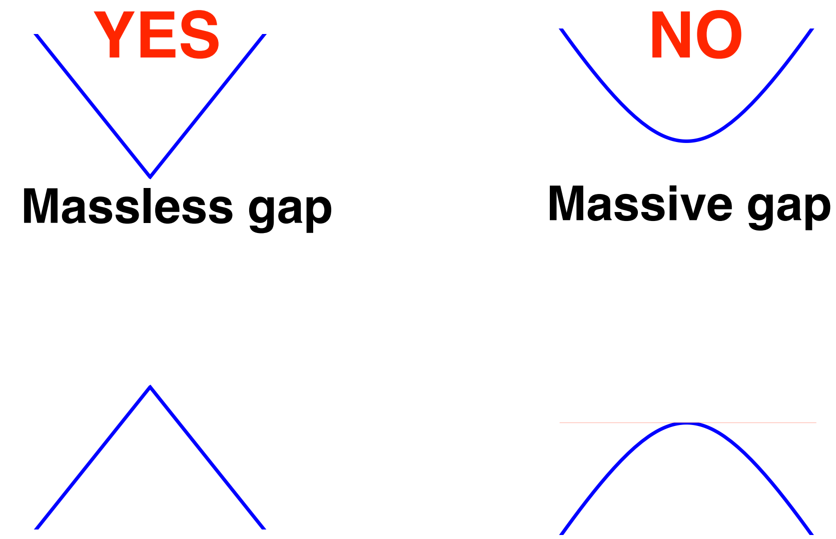
"Fermi surface changes its topology"

$$N_1 = \frac{1}{2\pi i} \oint_{\mathcal{C}} d\ell \,\mathrm{Tr}[\hat{G}(i\omega, \boldsymbol{k}) \partial_\ell \hat{G}^{-1}(i\omega, \boldsymbol{k})],$$

Massless gap opening in graphene

L. Benfatto and E. Cappelluti, PRB **78**, 115434 (2008)

Inversion symmetry:



$$\hat{\Sigma}(\mathbf{k}) = -V \sum_{\mathbf{k}', i\omega_n} F(\mathbf{k}-\mathbf{k}')\hat{G}(\mathbf{k}', i\omega_n) e^{i\omega_n 0^+}$$

Anisotropic scattering

$$F(\phi - \phi') = \Theta(\phi_c - |\phi - \phi'|) \quad , \quad \phi_c < \pi$$

$$\hat{\Sigma}(\mathbf{k}) \propto \Lambda^2 \sin(\phi_c)\hat{\sigma} \cdot \hat{\mathbf{k}}$$

Spontaneously symmetry breaking

$$\hat{H}(\mathbf{k}) = \hat{H}_0(\mathbf{k}) + T \sum_{\mathbf{p},n} \frac{V(\mathbf{k}-\mathbf{p})}{i\omega_n \hat{I} - \hat{H}(\mathbf{k})}.$$

E. Cappelluti et al, AdP, 526, 387(2014)

Linearized gap equation at T=0

$$\hat{\phi}(\mathbf{k}) = \sum_{\mathbf{p}} V(\mathbf{k}-\mathbf{p}) \frac{\hat{\phi}(\mathbf{p})}{2E(\mathbf{p})},$$

Critical coupling constant

$$\alpha = e^2/(\epsilon_0 \hbar v)$$

$$\alpha_{\text{massless}-\text{gap}} \geq 1.76$$

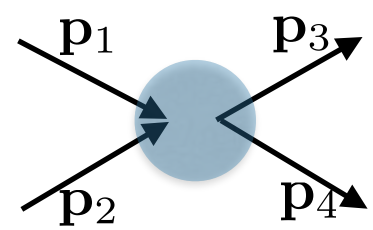
$$\alpha_{\text{masive}-\text{gap}} \geq 0.46$$

Weyl Mott Insulator

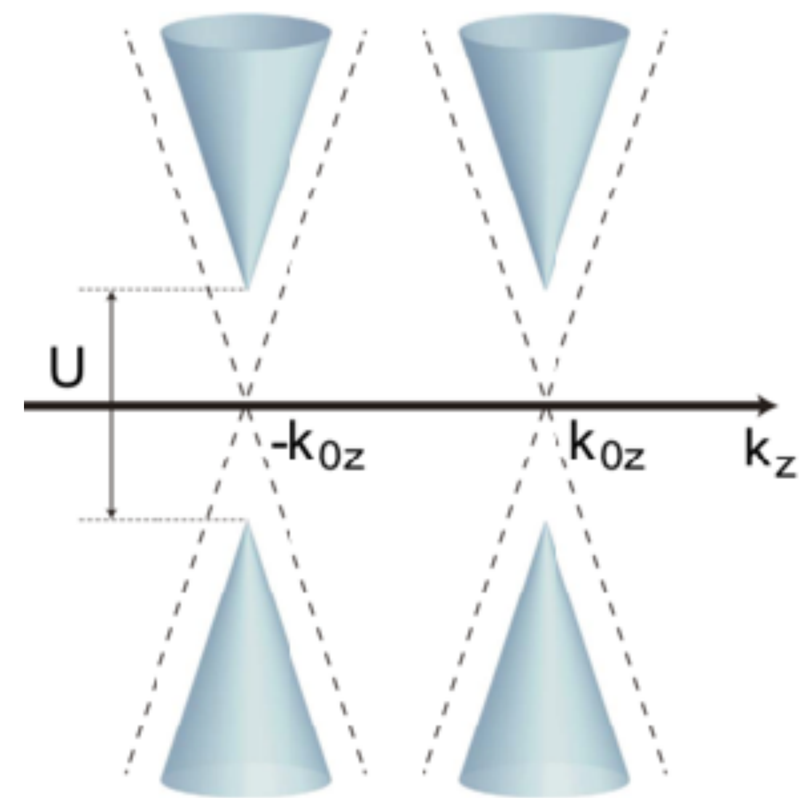
Hatsugai-Kohmoto's model (1992)

$$\hat{V}_{ee} = \frac{V}{2} \sum_{\boldsymbol{k}} \left(\hat{\psi}^\dagger_{\boldsymbol{k}} \hat{\psi}_{\boldsymbol{k}} - 1 \right)^2$$

$$\mathbf{p_1} + \mathbf{p_2} = \mathbf{p_3} + \mathbf{p_4}$$



$$\mathbf{r}_1 + \mathbf{r}_2 = \mathbf{r}_3 + \mathbf{r}_4$$



T. Morimoto and N. Nagaosa, Scientific Reports 6, 19853 (2016)

$$\mathcal{H} = \sum_{\mathbf{k}} \left\{ \hbar v k (n_{\mathbf{k}+} - n_{\mathbf{k}-}) + \frac{V}{2} (n_{\mathbf{k}+} + n_{\mathbf{k}-} - 1)^2 \right\}$$

$n_{\mathbf{k}\pm} = c^\dagger_{\mathbf{k}\pm} c_{\mathbf{k}\pm}$ where $\pm$ corresponds to the cones with opposite helicity.

$$|\Omega\rangle \quad , \quad E_{\text{vac}} = V/2$$

$$|\Psi^{(1)}_{\mathbf{k}\pm}\rangle = c^\dagger_{\mathbf{k}\pm} |\Omega\rangle \quad , \quad E^{\text{single}}_{\pm} = \pm \hbar v k$$

$$|\Psi^{(2)}_{k}\rangle = c^\dagger_{\mathbf{k}+} c^\dagger_{\mathbf{k}-} |\Omega\rangle \quad , \quad E^{\text{double}} = V/2$$

$$V > 0$$

$$\hat{\Sigma}(\boldsymbol{k}) = \frac{V}{2} \hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{k}}$$

Hatsugai-Kohmoto's model as an exactly solvable model

Y. Hatsugai and M. Kohmoto, Journal of the Physical Society of Japan 61, 2056 (1992)

F. S. Nogueira and E. V. Anda, International Journal of Modern Physics B 10 (1996)

$$\hat{G}(i\omega_n, \boldsymbol{k}) = \hat{U}_{\boldsymbol{k}} \begin{bmatrix} \mathcal{G}_{++}(i\omega_n, \boldsymbol{k}) & 0 \\ 0 & \mathcal{G}_{--}(i\omega_n, \boldsymbol{k}) \end{bmatrix} \hat{U}_{\boldsymbol{k}}^{\dagger}$$

$$= \left\{ i\omega_n - \hbar v \hat{\boldsymbol{\sigma}} \cdot \boldsymbol{k} - \hat{\Sigma}(i\omega_n, \boldsymbol{k})) \right\}^{-1}$$

$$\boxed{\mathcal{G}_{\lambda\lambda} = \frac{A_-}{i\omega_n - \lambda\varepsilon_-} + \frac{A_+}{i\omega_n - \lambda\varepsilon_+}} \quad \boxed{A_{\pm} = \frac{\exp\{\pm\beta\varepsilon_{\pm}\} + 1}{2 + \exp\{-\beta\varepsilon_-\} + \exp\{\beta\varepsilon_+\}}}$$

$V > 0$ $\qquad \hat{\Sigma}(\boldsymbol{k}) = \frac{V}{2} \hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{k}}$

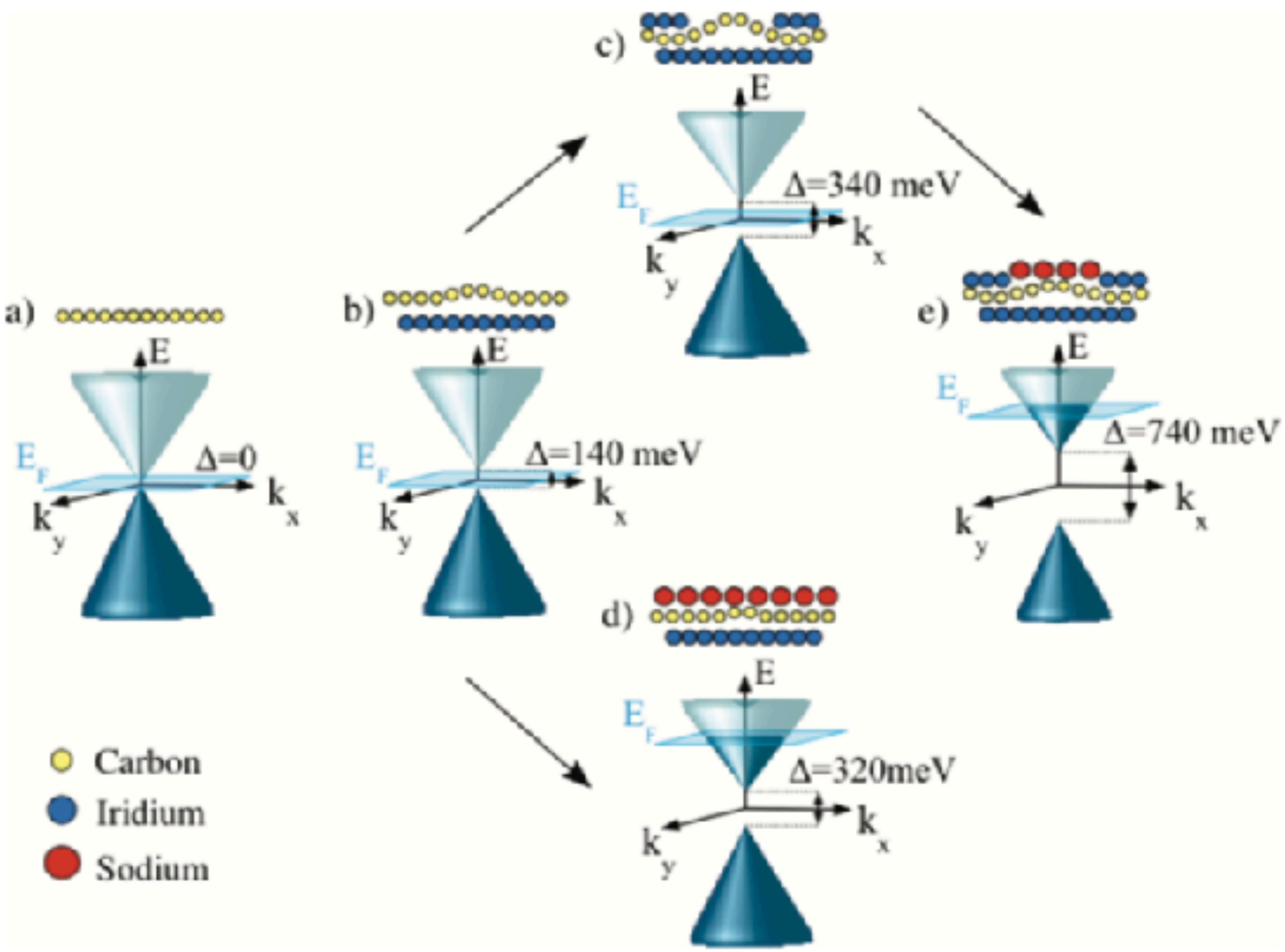
$V < 0 \;\&\; \hbar v k > V/2$ $\qquad \hat{\Sigma}(\boldsymbol{k}) = \frac{V}{2} \hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{k}}$

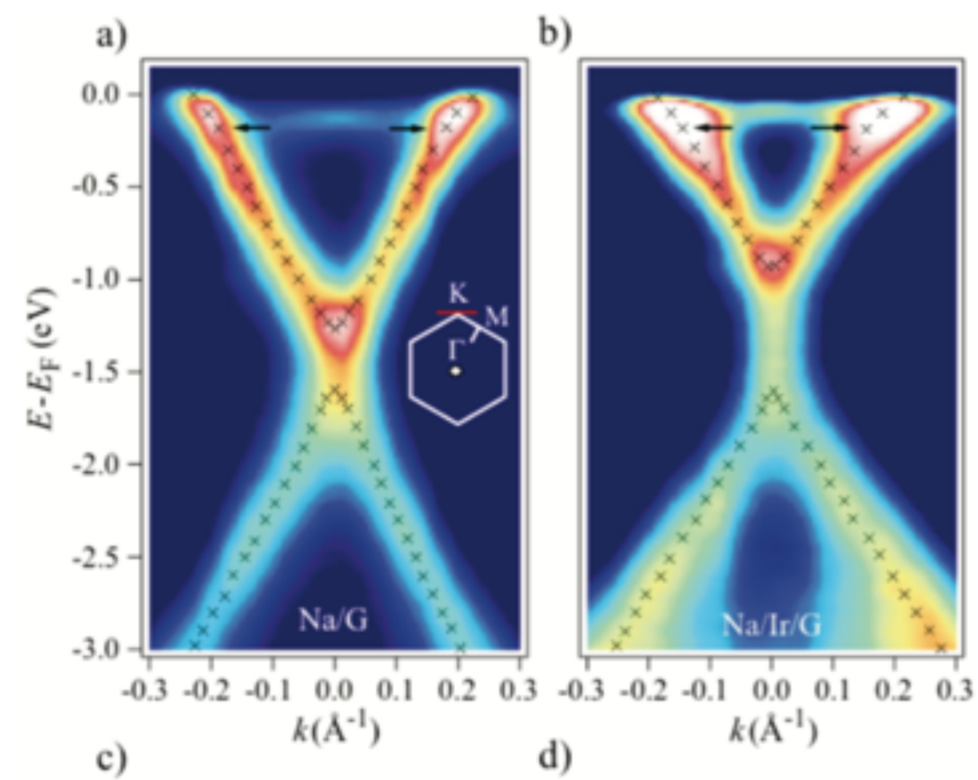
$V < 0 \;\&\; \hbar v k < V/2$ $\qquad \hat{\Sigma}(i\omega_n, \boldsymbol{k}) = \frac{V^2}{4} \frac{i\omega_n + \hat{\boldsymbol{\sigma}} \cdot \boldsymbol{k}}{(i\omega_n)^2 - (\hbar v k)^2}$

T. Morimoto and N. Nagaosa, Scientific Reports 6, 19853 (2016)

H.R., E. Cappelluti, and A. V. Balatsky, Phys. Rev. B 98, 245114 (2018)

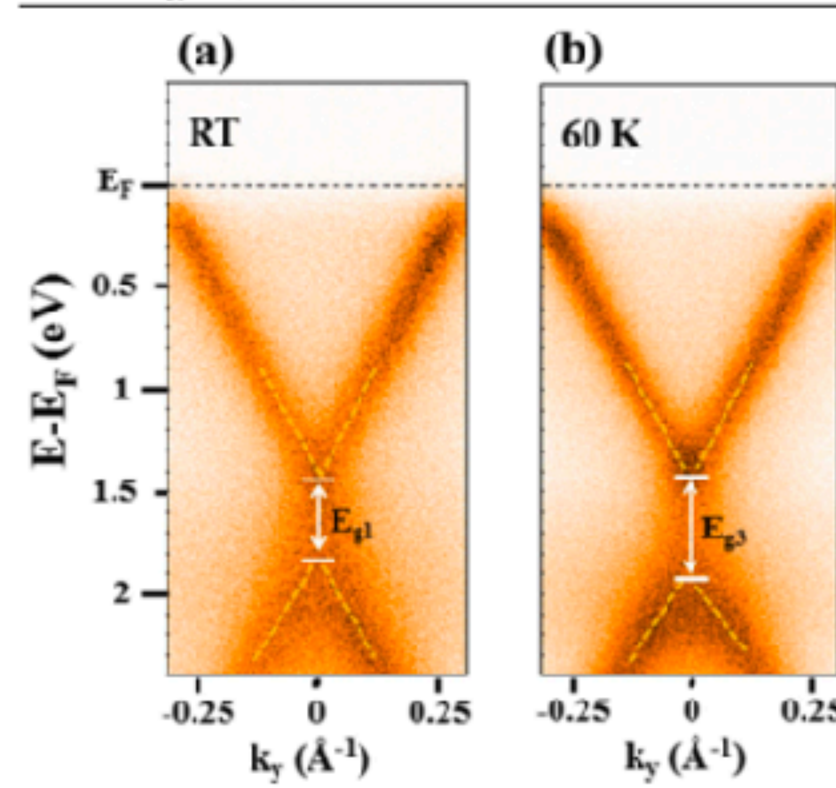
Massless gap opening: experiment





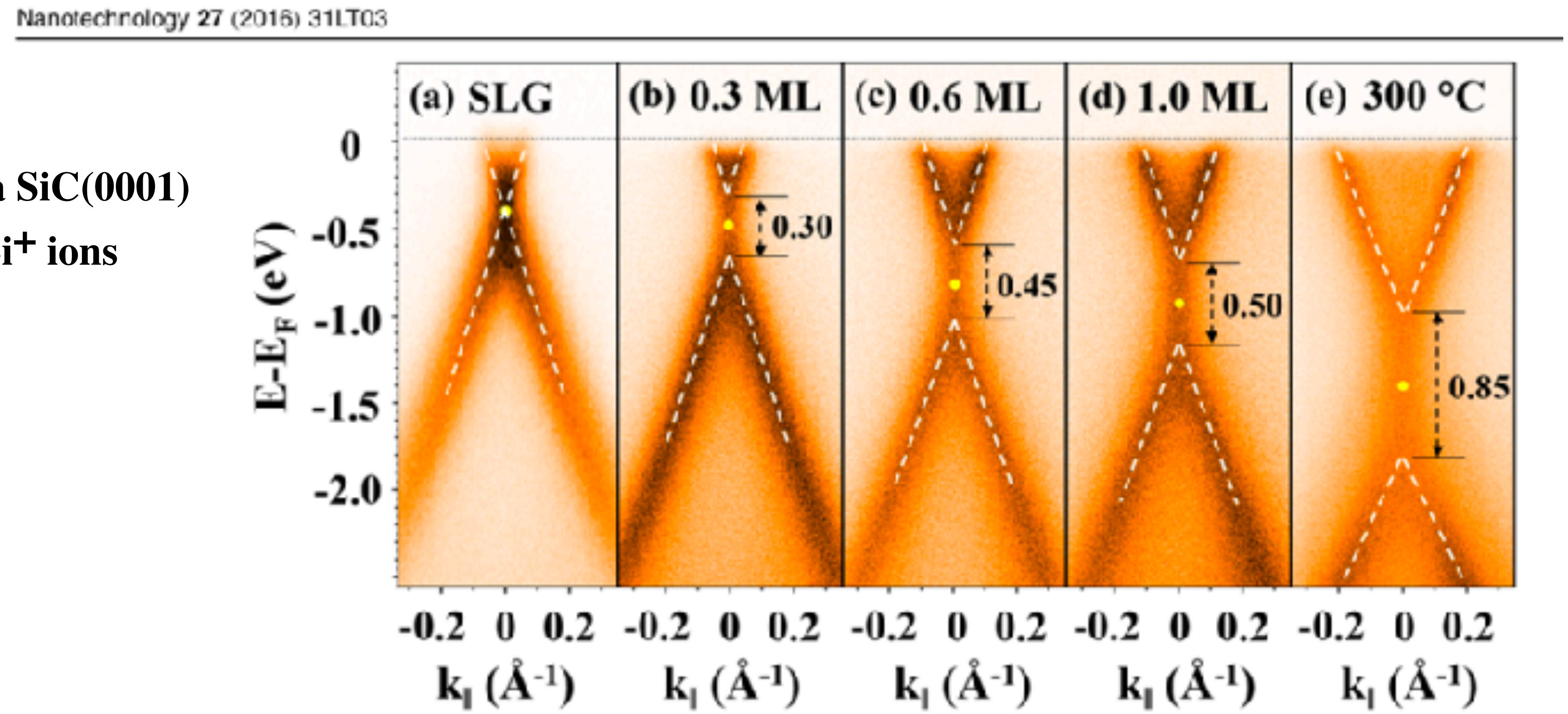
M. Papagno et al, *ACS Nano* ***6*,** 199 (2012).

Nanotechnology **28** (2017) 205201

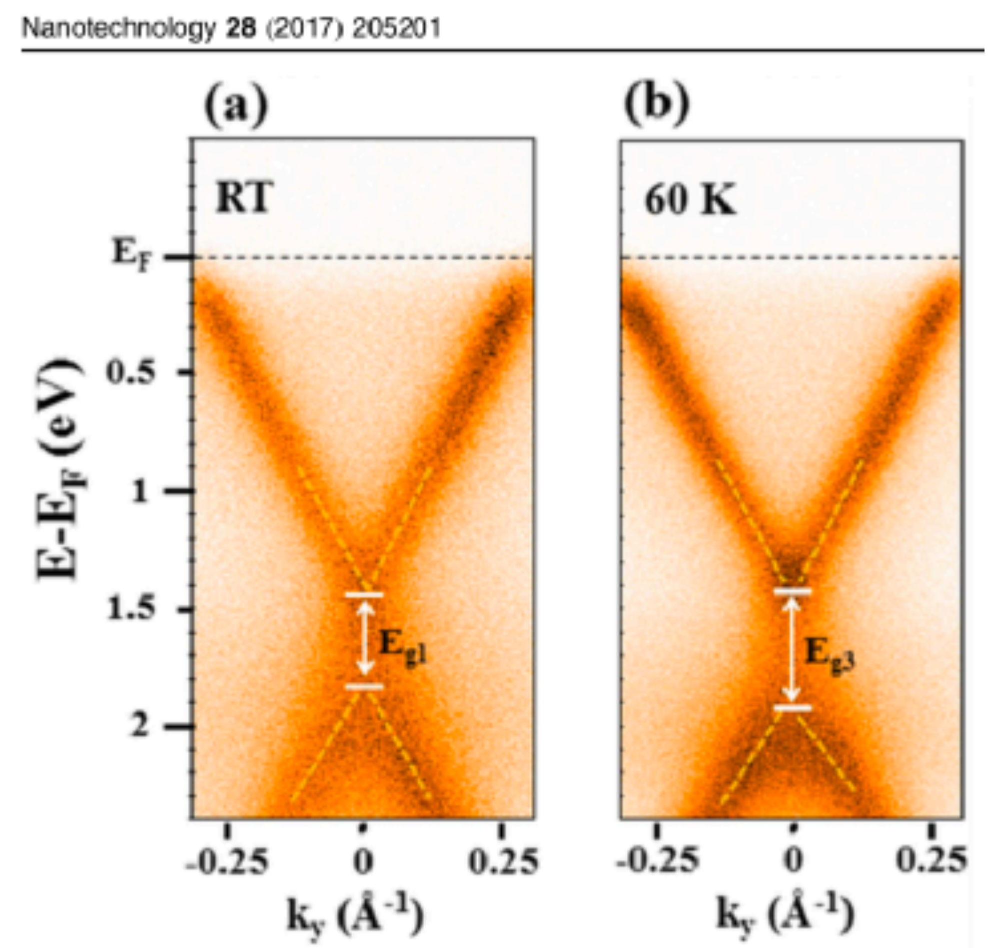


Europium (Eu)-induced changes in the π-band of graphene (G) formed on the 6H-SiC (0001) surface

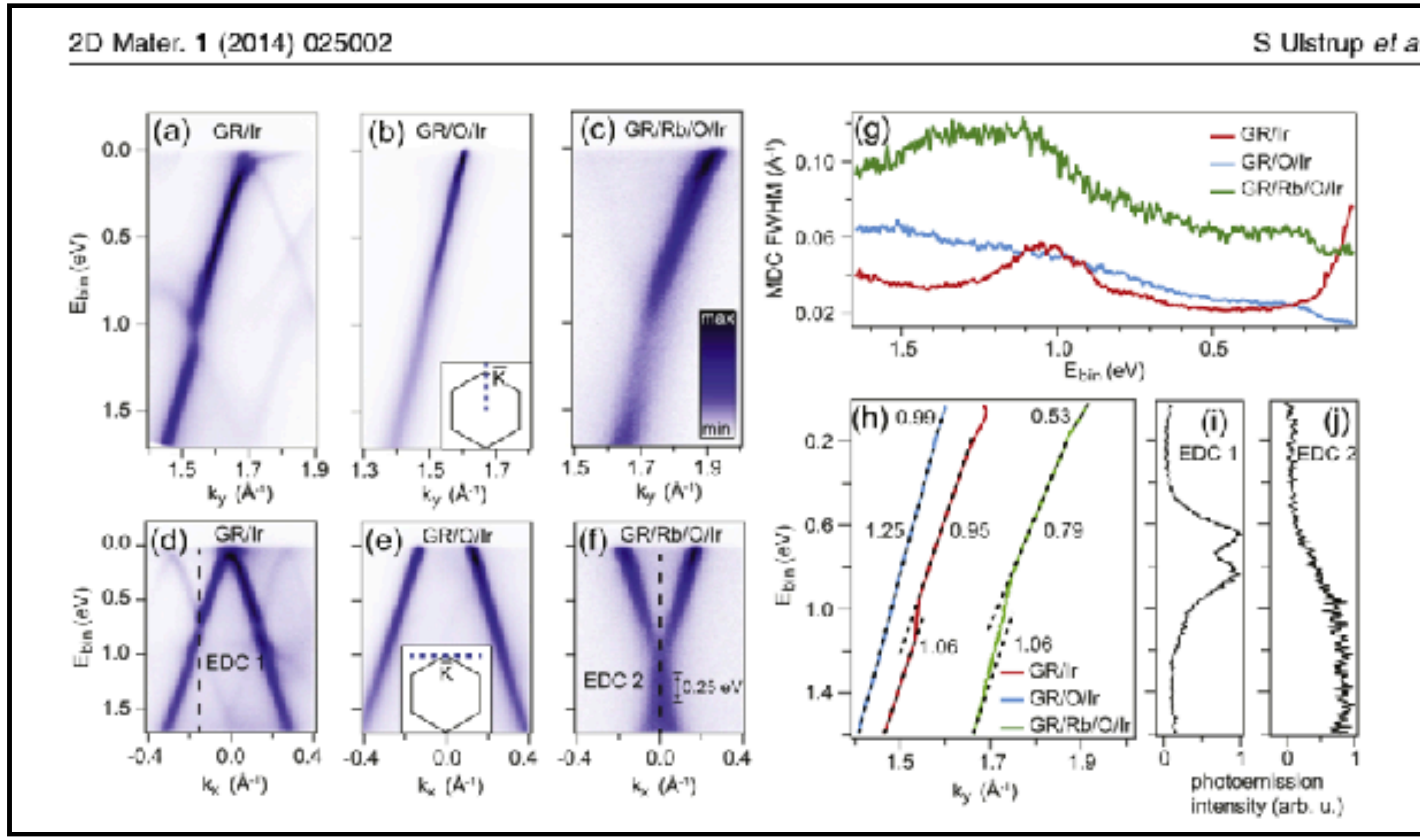
Single-layer graphene (SLG) grown on a SiC(0001) substrate by doping low-energy (5 eV) Li^+ ions



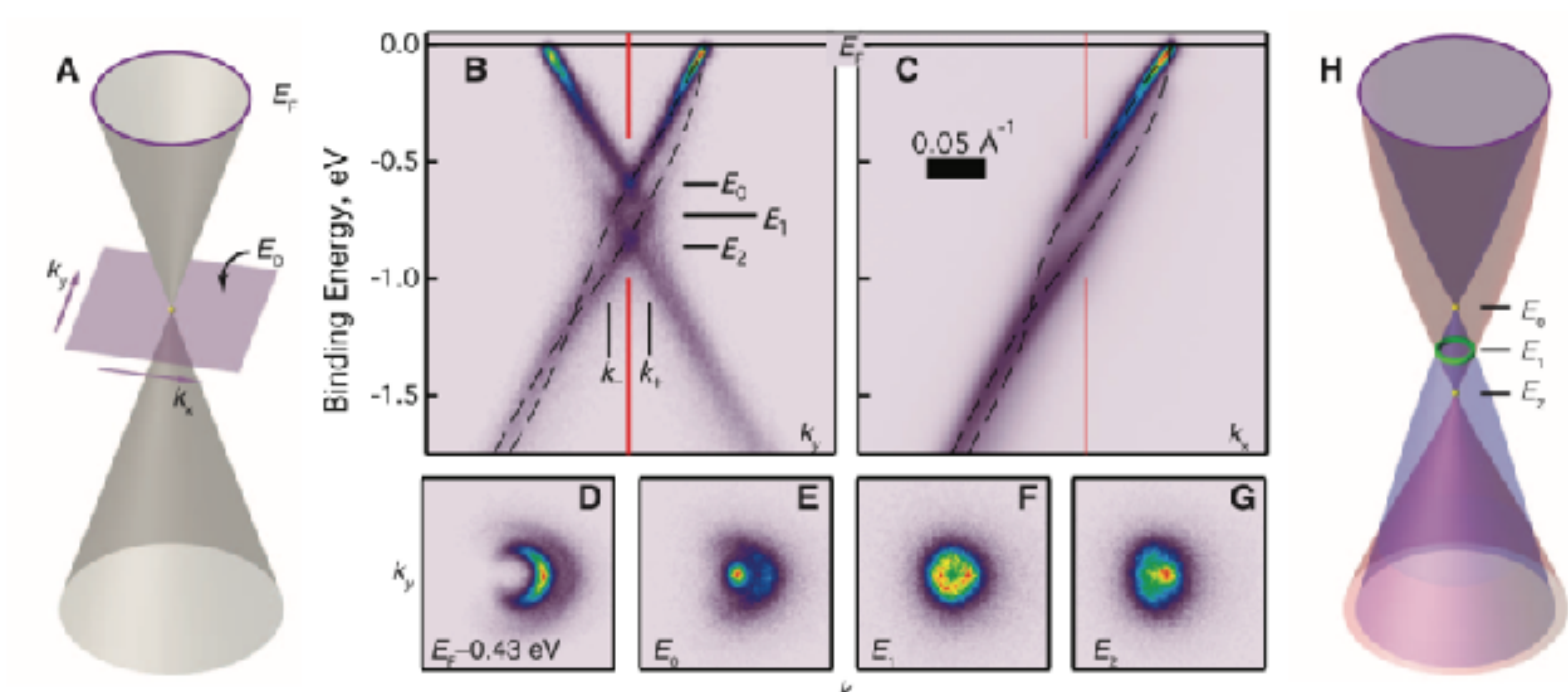
Europium (Eu)-induced changes in the π-band of graphene (G) formed on the 6H-SiC (0001) surface



Maybe Plasmarons!



Observation of Plasmarons in Quasi-Freestanding Doped Graphene
Aaron Bostwick *et al.*
Science **328**, 999 (2010);

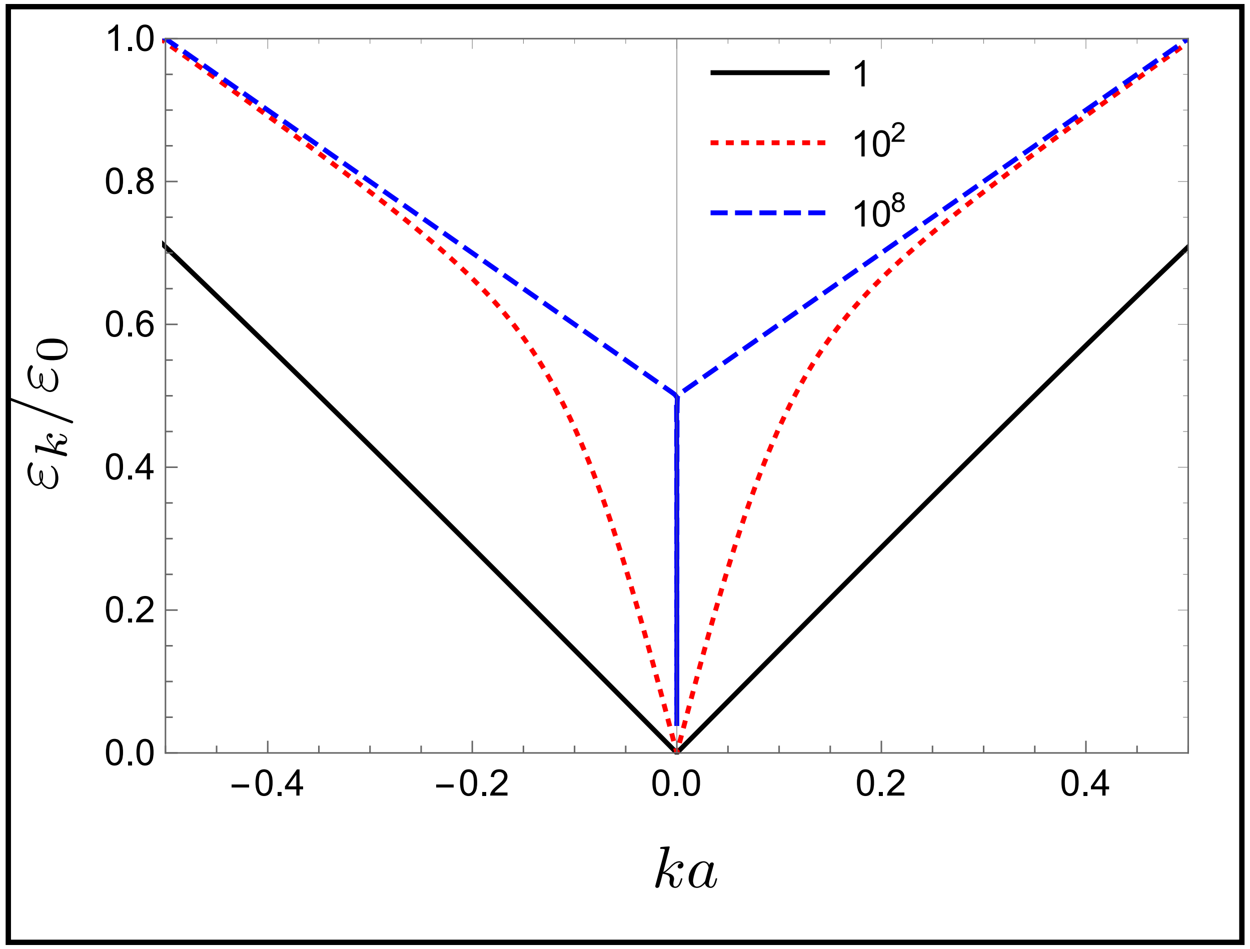


Self-energy for Gaussian interaction profile V(q)

$$\hat{V}_{ee} = \frac{1}{2}\sum_{\boldsymbol{q}} V(\boldsymbol{q})\hat{\rho}(\boldsymbol{q})\hat{\rho}(-q),$$

$$\boxed{V(\boldsymbol{q}) = V(2\pi)^d \frac{e^{-\xi|\boldsymbol{q}|^2}}{(\pi/\xi)^{d/2}},}$$

$$\xi \to \infty \qquad V_{ee} = \frac{V}{2}\left(\sum_{\mathbf{k}} \hat{\psi}^\dagger_{\mathbf{k}}\hat{\psi}_{\mathbf{k}}\right)^2$$



$$\hat{\Sigma}(\boldsymbol{k}) = i\int \frac{d\omega}{2\pi}\int \frac{d^d\boldsymbol{q}}{(2\pi)^d} V(\boldsymbol{k}-\boldsymbol{q})\hat{G}(i\omega,\boldsymbol{q})$$

$$\hat{G}(i\omega,\boldsymbol{q}) = -\frac{i\omega + \hbar v\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{q}}{\omega^2 + (\hbar v q)^2}.$$

$$\boxed{\hat{\Sigma}(\boldsymbol{k}) = V C_d M\left(1/2, 1+d/2, -k^2\xi\right) k\sqrt{\xi}\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{k}},}$$

$$C_{d=2} = 1/16\pi^{\frac{3}{2}},\; C_{d=3} = 1/12\pi^{\frac{7}{2}}$$

H. R, E. Cappelluti, and A. V. Balatsky, Phys. Rev. B 98, 245114 (2018)

Boson-mediated effective interaction

$$\hat{\mathcal{H}} = \hbar v \sum_{\mathbf{k}} \hat{\psi}^{\dagger}_{\mathbf{k}} \hat{\sigma} \cdot \mathbf{k} \hat{\psi}_{\mathbf{k}} + \hbar\omega_0 \hat{a}^{\dagger}_0 \hat{a}_0 + g \sum_{\mathbf{k}} \hat{\psi}^{\dagger}_{\mathbf{k}} \hat{\Gamma}_{\mathbf{k}} \hat{\psi}_{\mathbf{k}} (\hat{a}^{\dagger}_0 + \hat{a}_0),$$

Lang-Firsov transformation

$$\hat{\mathcal{H}}' = e^{\hat{S}} \hat{\mathcal{H}} e^{-\hat{S}} \qquad \hat{S} = \frac{g}{\hbar\omega_0} \hat{\mathcal{N}} (\hat{a}^{\dagger}_0 - \hat{a}_0) \qquad \hat{\mathcal{N}} = \sum_{\boldsymbol{k}} \hat{\psi}^{\dagger}_{\boldsymbol{k}} \hat{\Gamma}_{\boldsymbol{k}} \hat{\psi}_{\boldsymbol{k}}.$$

$$\hat{\psi}'_{\boldsymbol{k}} = e^{\hat{S}} \hat{\psi}_{\boldsymbol{k}} e^{-\hat{S}} = \hat{X}_{\boldsymbol{k}} \hat{\psi}_{\boldsymbol{k}}$$

$$\boxed{\hat{X}_{\boldsymbol{k}} = \exp\left[\frac{g}{\hbar\omega_0} \hat{\Gamma}_{\boldsymbol{k}} (\hat{a}_0 - \hat{a}^{\dagger}_0)\right]}$$

$$\boxed{\hat{\mathcal{H}}' = \hbar v \sum_{\boldsymbol{k}} \hat{\psi}^{\dagger}_{\boldsymbol{k}} \left[\hat{X}^{\dagger}_{\boldsymbol{k}} \hat{\boldsymbol{\sigma}} \cdot \boldsymbol{k} \hat{X}_{\boldsymbol{k}}\right] \hat{\psi}_{\boldsymbol{k}} - U \left[\sum_{\boldsymbol{k}} \hat{\psi}^{\dagger}_{\boldsymbol{k}} \hat{\Gamma}_{\boldsymbol{k}} \hat{\psi}_{\boldsymbol{k}}\right]^2,}$$

$$\boxed{U = g^2/\hbar\omega_0}$$

Boson-mediated effective interaction

$$\boxed{\hat{\mathcal{H}}' = \hbar v \sum_{\boldsymbol{k}} \hat{\psi}^\dagger_{\boldsymbol{k}} \left[\hat{X}^\dagger_{\boldsymbol{k}} \hat{\boldsymbol{\sigma}} \cdot \boldsymbol{k} \hat{X}_{\boldsymbol{k}}\right] \hat{\psi}_{\boldsymbol{k}} - U \left[\sum_{\boldsymbol{k}} \hat{\psi}^\dagger_{\boldsymbol{k}} \hat{\Gamma}_{\boldsymbol{k}} \hat{\psi}_{\boldsymbol{k}}\right]^2,}$$

- $\hat{\Gamma}_{\boldsymbol{k}} \propto \hat{I}$

$$\boxed{\hat{X}^\dagger_{\boldsymbol{k}} \hat{\boldsymbol{\sigma}} \cdot \boldsymbol{k} \hat{X}_{\boldsymbol{k}} = \hat{\boldsymbol{\sigma}} \cdot \boldsymbol{k},}$$

- $\hat{\Gamma}_{\boldsymbol{k}} = \hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{n}}$

$$\boxed{\begin{aligned}\hat{X}^\dagger_{\mathbf{k}} \hat{\sigma} \cdot \mathbf{k} \hat{X}_{\mathbf{k}} &= \cosh(2\hat{B}) \hat{\sigma} \cdot \mathbf{k} + [1 - \cosh(2\hat{B})](\hat{\sigma} \cdot \hat{\mathbf{n}})(\hat{\mathbf{n}} \cdot \mathbf{k}) \\ &\quad - i \sinh(2\hat{B})(\hat{\mathbf{n}} \times \mathbf{k}) \cdot \hat{\sigma}\ .\end{aligned}}$$

$$\hat{B} = [g/\hbar\omega_0](\hat{a}_0 - \hat{a}^\dagger_0)$$

Holstein approximation

$$\hat{\psi}^\dagger_{\mathbf{k}} [\hat{X}^\dagger_{\mathbf{k}} \hat{\sigma} \cdot \mathbf{k} \hat{X}_{\mathbf{k}}] \hat{\psi}_{\mathbf{k}} \to \langle 0 | \hat{\psi}^\dagger_{\mathbf{k}} [\hat{X}^\dagger_{\mathbf{k}} \hat{\sigma} \cdot \mathbf{k} \hat{X}_{\mathbf{k}}] \hat{\psi}_{\mathbf{k}} | 0 \rangle.$$

Self-energy for different electron-boson couplings

- $\hat{\Gamma}_{\boldsymbol{k}} \propto \hat{I}$

$$\hat{\mathcal{H}} = \hbar v \sum_{\mathbf{k}} \hat{\psi}^{\dagger}_{\mathbf{k}} \hat{\sigma} \cdot \mathbf{k} \hat{\psi}_{\mathbf{k}} - U \Big[\sum_{\mathbf{k}} \hat{\psi}^{\dagger}_{\mathbf{k}} \hat{\psi}_{\mathbf{k}} \Big]^2,$$

$$\boxed{\hat{\Sigma}(\mathbf{k}) = -U \frac{\hat{\sigma} \cdot \mathbf{k}}{k}}$$

- $\hat{\Gamma}_{\boldsymbol{k}} = \hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{n}}$

$$\hat{\mathcal{H}} = \hbar v \sum_{\mathbf{k}} \hat{\psi}^{\dagger}_{\mathbf{k}} \left[\gamma \hat{\sigma} \cdot \mathbf{k}_{\perp} + \hat{\sigma} \cdot \mathbf{k}_{\parallel} \right] \hat{\psi}_{\mathbf{k}} - U \Big[\sum_{\mathbf{k}} \hat{\psi}^{\dagger}_{\mathbf{k}} \hat{\sigma} \cdot \hat{\mathbf{n}} \hat{\psi}_{\mathbf{k}} \Big]^2,$$

$\gamma = \exp[-2(g/\hbar\omega_0)^2]$

$$\boxed{\hat{\Sigma}(\boldsymbol{k}) = U \frac{\gamma \hat{\boldsymbol{\sigma}} \cdot \boldsymbol{k}_{\perp} - \hat{\boldsymbol{\sigma}} \cdot \boldsymbol{k}_{\parallel}}{\sqrt{\gamma^2 k_{\perp}^2 + k_{\parallel}^2}}}$$

For $\hat{\mathbf{n}} = \hat{\mathbf{z}}$ in two-dimensions:

$$\boxed{\hat{\Sigma}(\boldsymbol{k}) = U \hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{k}},}$$

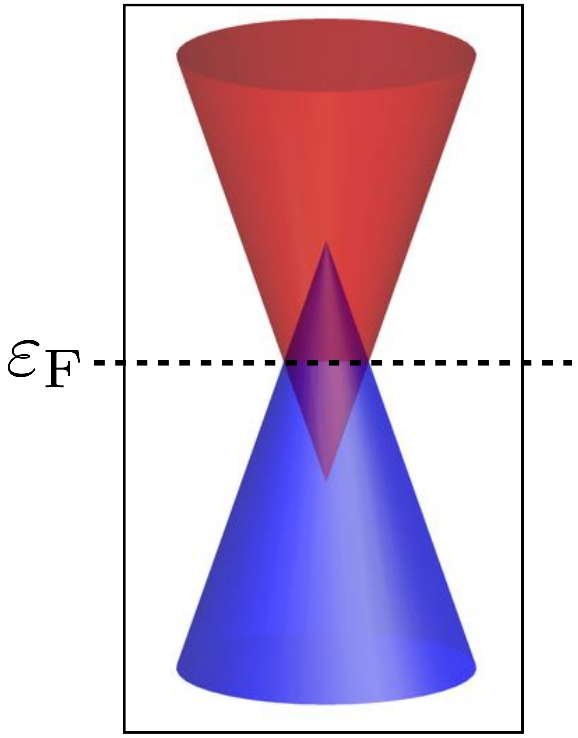
- $\hat{\mathcal{H}}_{\text{int}} = g \sum_{\boldsymbol{k}} \hat{\psi}^{\dagger}_{\boldsymbol{k}} \left[(\hat{a}_0 + \hat{a}^{\dagger}_0) \hat{\Gamma}_a + (\hat{b}_0 + \hat{b}^{\dagger}_0) \hat{\Gamma}_b \right] \hat{\psi}_{\boldsymbol{k}}$ $\quad \hat{\Gamma}_{a,b} = \hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{n}}_{a,b}$ with $\hat{\boldsymbol{n}}_a \cdot \hat{\boldsymbol{n}}_b = 0$

$$\hat{\mathcal{H}} = \gamma \hbar v \sum_{\boldsymbol{k}} \hat{\psi}^{\dagger}_{\boldsymbol{k}} \boldsymbol{k} \cdot \hat{\boldsymbol{\sigma}} \hat{\psi}_{\boldsymbol{k}} - \gamma^2 U \sum_{i=a,b} \Big[\sum_{\boldsymbol{k}} \hat{\psi}^{\dagger}_{\boldsymbol{k}} \hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{n}}_i \hat{\psi}_{\boldsymbol{k}} \Big]^2$$

$$\boxed{\hat{\Sigma}(\mathbf{k}) = 0}$$

Transverse and longitudinal modes cancel each other effects

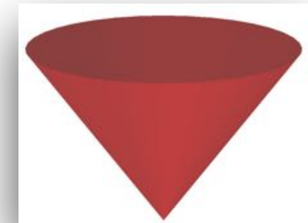
Berry curvature: sheet singularity



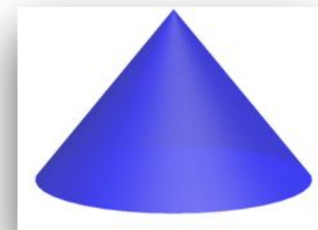
Occupied band Berry curvature

$$\Omega(\mathbf{k}) = \sum_{\lambda} \Omega_\lambda(\mathbf{k}) n_{\mathrm{F}}(\varepsilon_k^\lambda)$$

3D

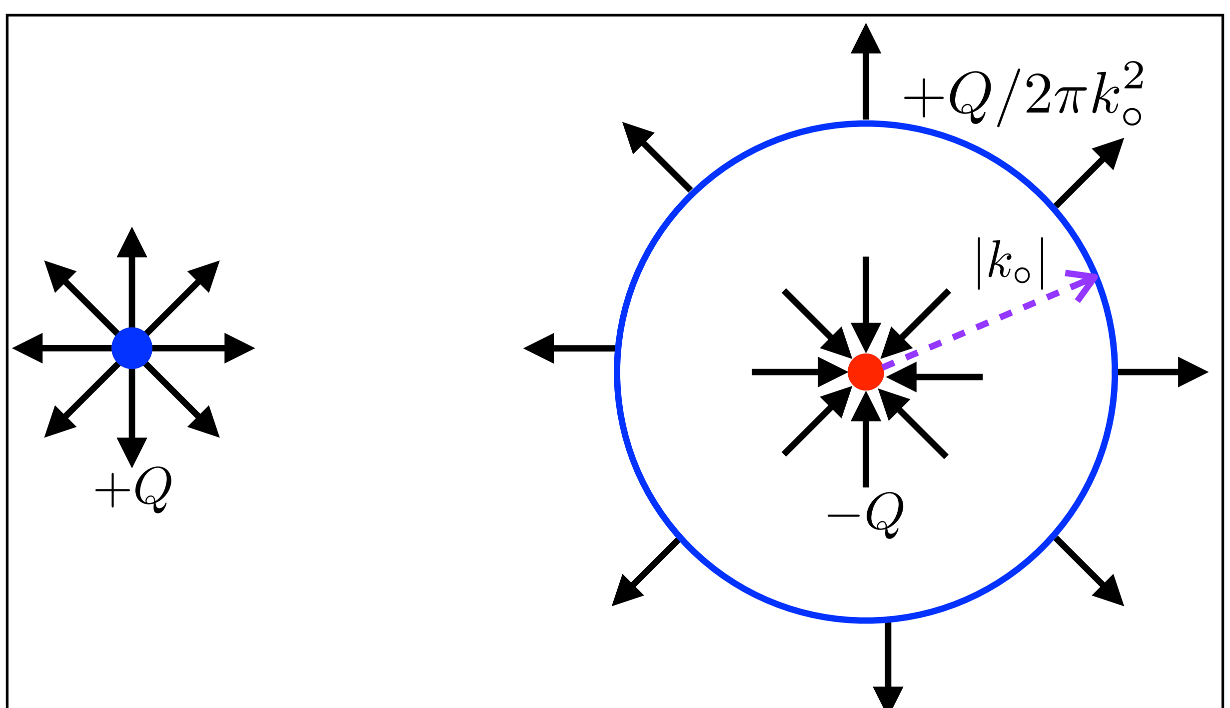


$$\Omega_+(\mathbf{k}) = -\frac{\mathbf{k}}{2k^3}$$



$$\Omega_-(\mathbf{k}) = +\frac{\mathbf{k}}{2k^3}$$

$$\Omega(\mathbf{k}) = \mathrm{sign}(k - |k_\circ|)\frac{\mathbf{k}}{2k^3} \;\Rightarrow\; \nabla \cdot \Omega(\mathbf{k}) = -2\pi\delta^{(3)}(\mathbf{k}) + \frac{\delta(k - |k_\circ|)}{k_\circ^2}$$



Berry curvature measurement :
“time-reversal” protocol

$$\frac{\mathbf{v}(\mathbf{k}, -\mathbf{E}) - \mathbf{v}(\mathbf{k}, \mathbf{E})}{2} = \mathbf{E} \times \mathbf{\Omega}(\mathbf{k})$$

H. M. Price and N. R. Cooper, Phys. Rev. A **85**, 033620 (2012).

Landau level in 2D: zero energy level

$$\boxed{\hat{\mathcal{H}}(\hat{\boldsymbol{\pi}}) = v\left[\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}} + \frac{\hbar k_\circ}{2}\left\{(\hat{\boldsymbol{\pi}}\cdot\hat{\boldsymbol{\pi}})^{-1/2}, \hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\right\}\right]}$$

$$\hat{\boldsymbol{\pi}} = \hbar\boldsymbol{k} + e\boldsymbol{A}$$

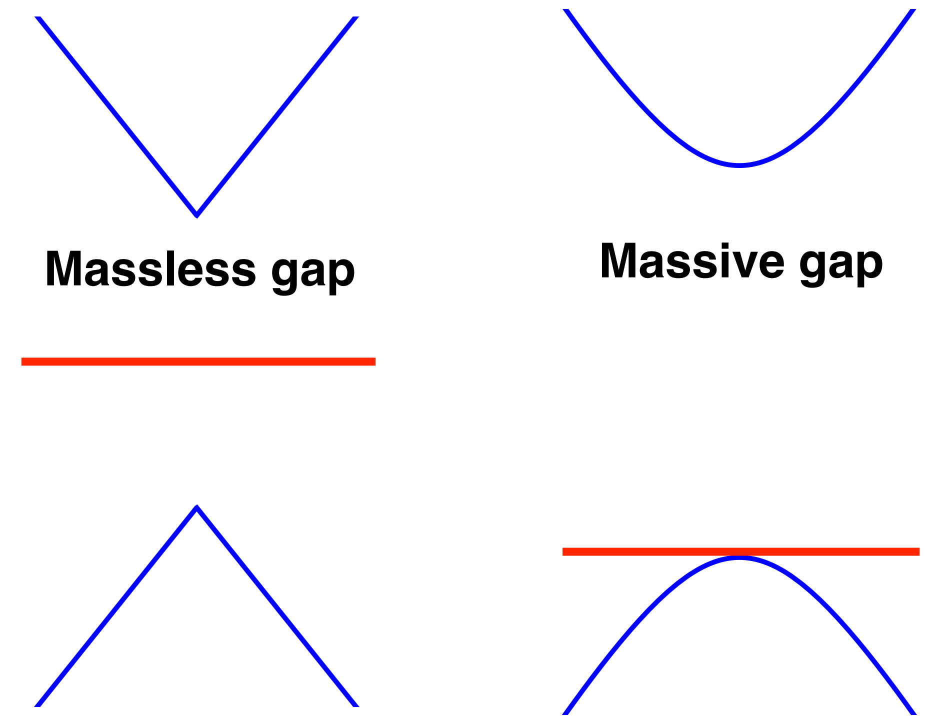
$$\boxed{\varepsilon_n = \hbar v\sqrt{2n}\frac{|1+\alpha_n k_\circ \ell_B|}{\ell_B}}$$

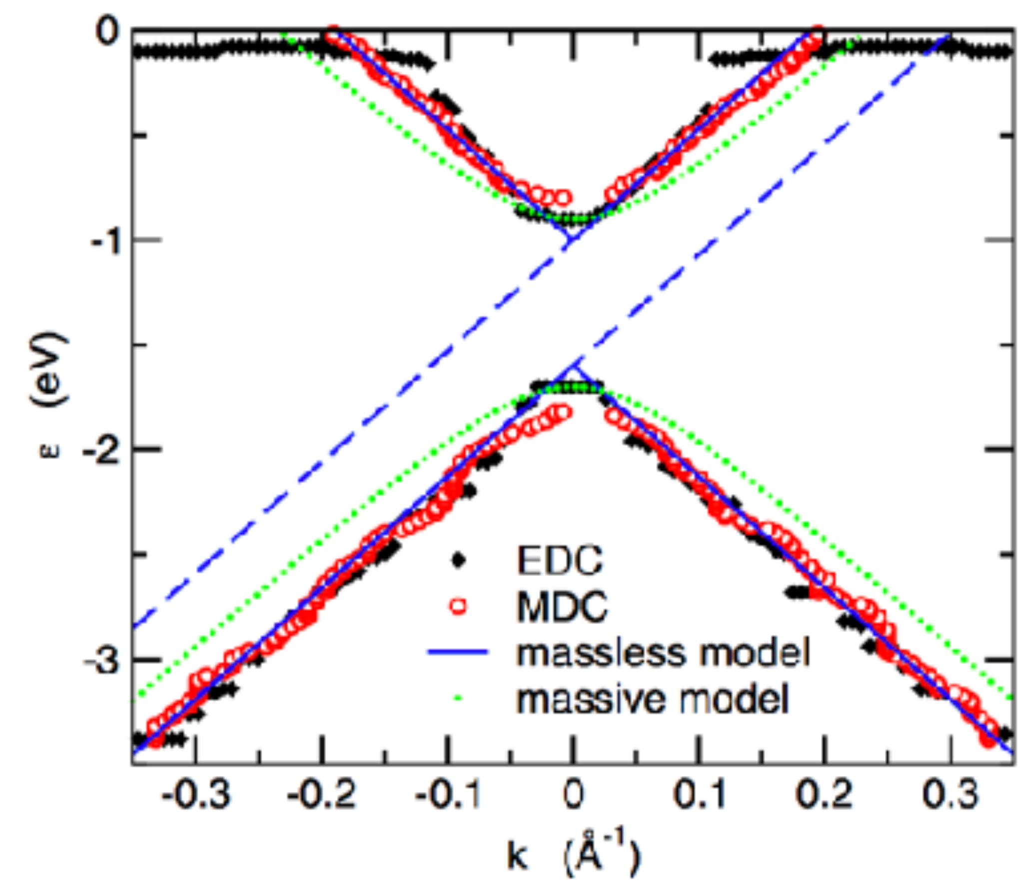
$$n = 0, 1, 2, \ldots$$

$$\ell_B = \sqrt{\hbar/eB}$$

$$\alpha_n = (2n-1)^{-1/2} + (2n+1)^{-1/2}$$

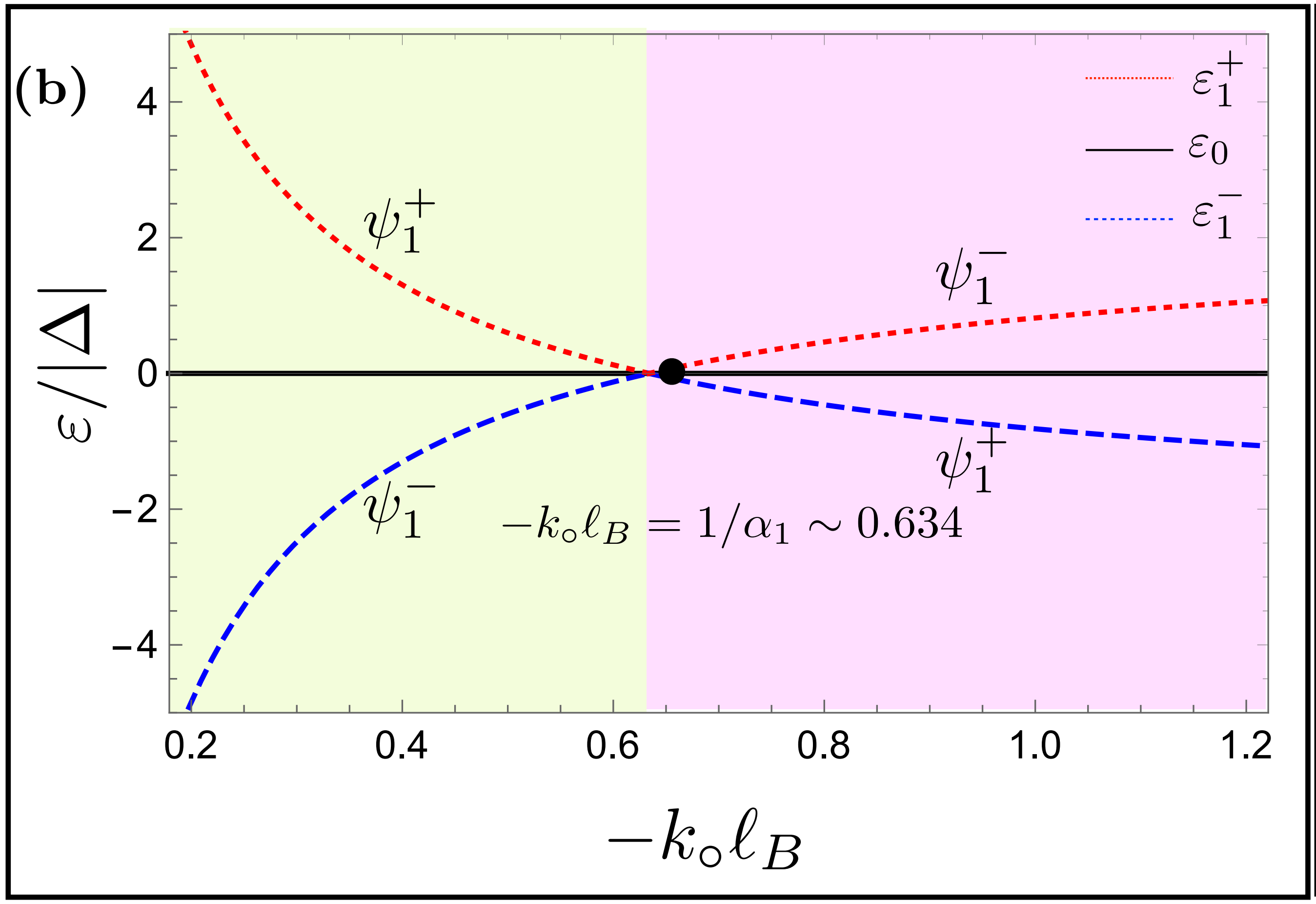
$$\boxed{|\psi_n^\pm\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}\pm\text{sign}\,(1+\alpha_n k_\circ \ell_B)\,|n-1\rangle \\ |n\rangle\end{pmatrix}}$$

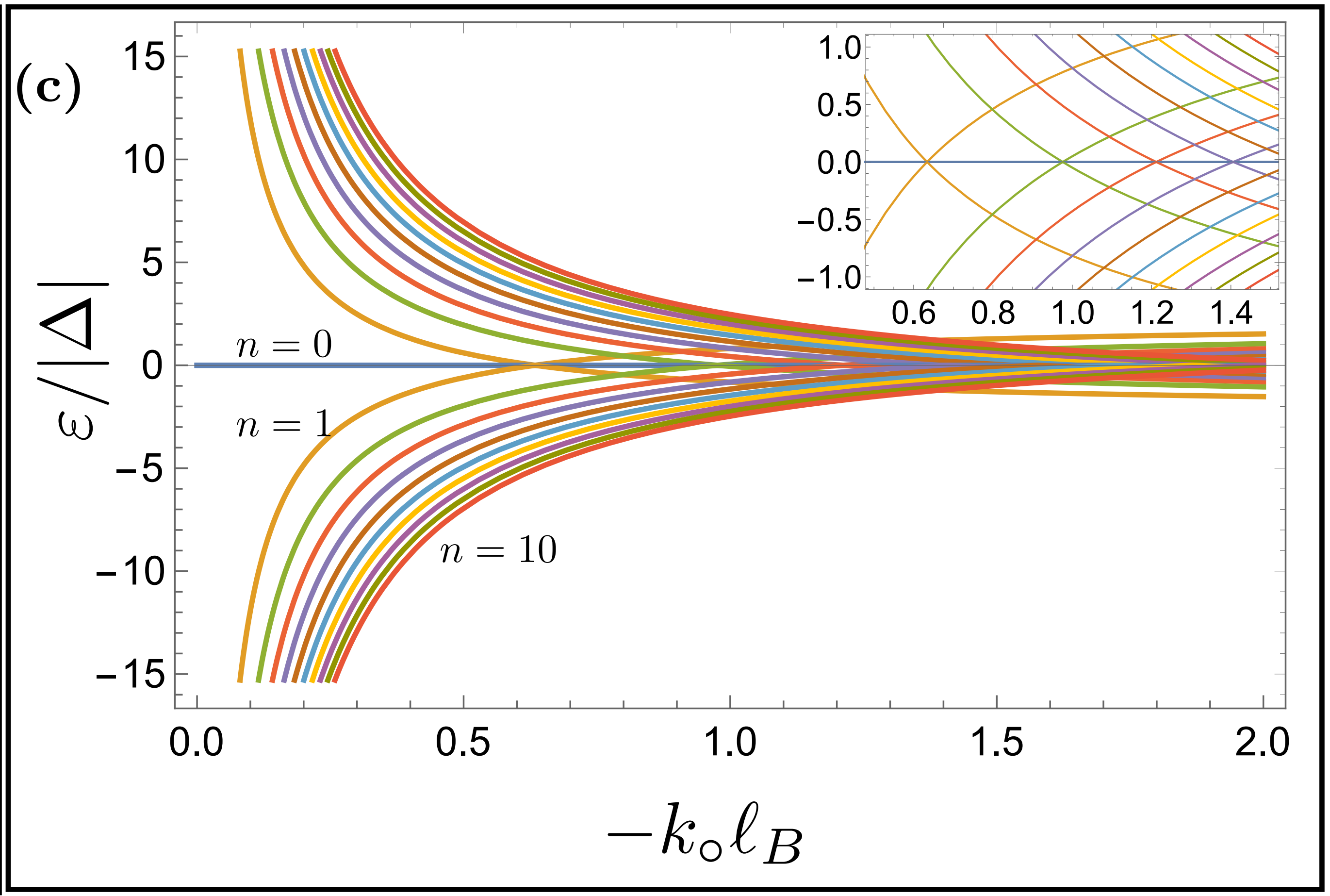




E. Cappelluti et al, AdP, 526, 387(2014).

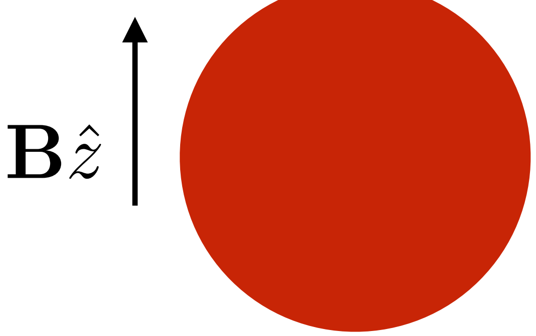
Landau level inversion in nodal circle phase





Landau level: 3D case

Nodal sphere



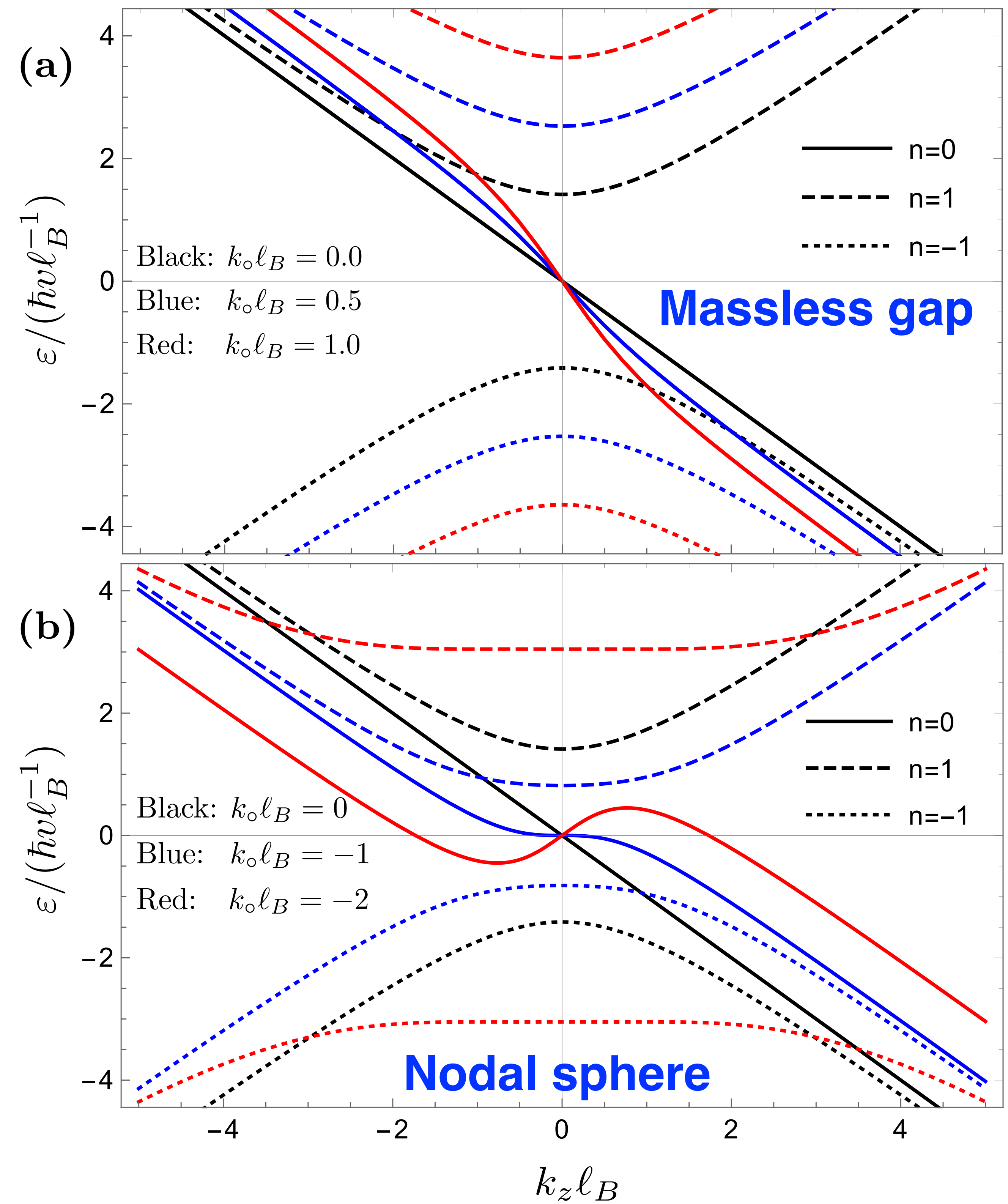
$$\boxed{\tilde{\varepsilon}_n^{\pm}(k_z) = \pm\sqrt{\varepsilon_n^2 + [m(n,k_z)]^2}}$$

$$\boxed{\tilde{\varepsilon}_0(k_z) = -m(n,k_z)}$$

$$\boxed{m(n,k_z) = \hbar v k_z \left(1 + \frac{k_\circ \ell_B}{\sqrt{2n+1+(k_z\ell_B)^2}}\right)}$$

Critical value

$$k_\circ \ell_B = -\sqrt{2n+1}$$



Summary

- **Massless gap opening and Nodal circle/sphere with a infinite-range interaction**
- **Infinite-interaction induced by momentum-conserving scattering of electron from a Boson mode**
- **Sheet singularity of Berry curvature in nodal sphere metal**
- **Landau levels: zero energy level, level inversion**

Thank you!