Nematic Order on the Surface of three-dimensional Topological Insulator[1]

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[1] RL, HY, JM arXiv:1702.07364 (2017)

Outline

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Nematic Instability and Motivation

- RL and JM in [2] developed Landau Theory for Helical Fermi Liquids which suggest possibility of isotropic–nematic transition in 3D TIs.
- Electron-electron interaction may lead to spontaneous breaking of rotational symmetry [3], in particular to nematic order.
- Nematic OP is traceless symmetric rank two tensor. As TrQ^3 in 2D is zero, it is expected that isotropic-nematic transition is continuous.
- No theoretical description for nematic order on the surface of 3D TIs.

[2] RL and JM, Phys. Rev. Lett. 115, 066401 (2015)
[3] I.Ya. Pomeranchuk, Zh. Eksp. Toer. Fiz. 35, 524 (1958) [Sov. Phys. JETP 8, 361 (1959)]

Model

OKF[4], spinless

$$\hat{Q}_{ab}(\boldsymbol{r}) = -\frac{1}{k_F^2}\psi^\dagger(\boldsymbol{r})(\partial_a\partial_b + \partial_b\partial_a - \delta_{ab}\boldsymbol{\partial}\cdot\boldsymbol{\partial})\psi(\boldsymbol{r})$$

Helical

$$\hat{Q}_{ab}(\boldsymbol{r}) = -\frac{i}{k_A}\psi^\dagger(\boldsymbol{r})(\sigma_a\partial_b + \sigma_b\partial_a - \delta_{ab}\boldsymbol{\sigma}\cdot\boldsymbol{\partial})\psi(\boldsymbol{r})$$

Here $k_A = \Lambda$ for the undoped case representing momentum cut-off;

$k_A = k$ for the doped case.

- The model Hamiltonian is $\hat{H} = \hat{H}_0 + \hat{H}_{int}$

$$H_0 = \int \frac{d^2k}{(2\pi)^2}\psi_{\boldsymbol{k}}^\dagger(h(\boldsymbol{k}) - \mu)\psi_{\boldsymbol{k}},$$

$$H_{\text{int}} = -\frac{f_2}{4}\int d^2r\,\text{Tr}\left(\hat{Q}(\boldsymbol{r})^2\right)$$

$$h(\boldsymbol{k}) = v_F\hat{\boldsymbol{z}}\cdot(\boldsymbol{\sigma}\times\boldsymbol{k}) = v_F\begin{pmatrix} 0 & ike^{-i\theta_{\boldsymbol{k}}} \\ -ike^{i\theta_{\boldsymbol{k}}} & 0 \end{pmatrix}$$

[4] V. Oganesyan, S.A. Kivelson, and E. Fradkin, Phys.Rev. B 64, 195109 (2001)

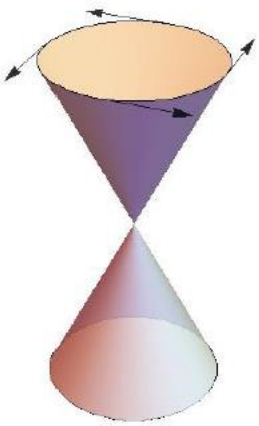
Mean Field Theory

•Integrating out fermionic field we obtain the following form for the Free energy

$$\mathcal{F}(\bar{Q}) = \frac{2}{f_2}\bar{Q}^2 - \frac{T}{V}\sum_{ik_n}\sum_{\boldsymbol{k}} \ln\left[(k_n - i\mu)^2 + \epsilon_{\boldsymbol{k}}(\bar{Q})^2\right]$$

Here without loss of generality we set

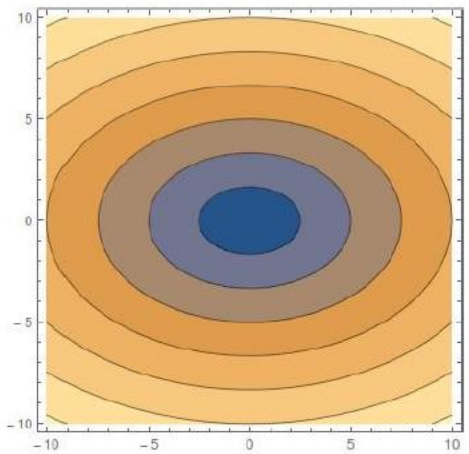
$$\bar{\boldsymbol{Q}} = \begin{pmatrix} 0 & \bar{Q} \\ \bar{Q} & 0 \end{pmatrix}$$



Quasi-particle energy

$$\epsilon_{\boldsymbol{k}}(\bar{Q}) = \sqrt{(\epsilon^0_{\boldsymbol{k}})^2 - 4\bar{Q}\epsilon^0_{\boldsymbol{k}}\frac{k}{k_A}\cos 2\theta_{\boldsymbol{k}} + 4\bar{Q}^2\left(\frac{k}{k_A}\right)^2}$$

$$\epsilon^0_{\boldsymbol{k}} = v_F k$$



$\bar{Q} = 0$, circular

$\bar{Q} \neq 0$, elliptical

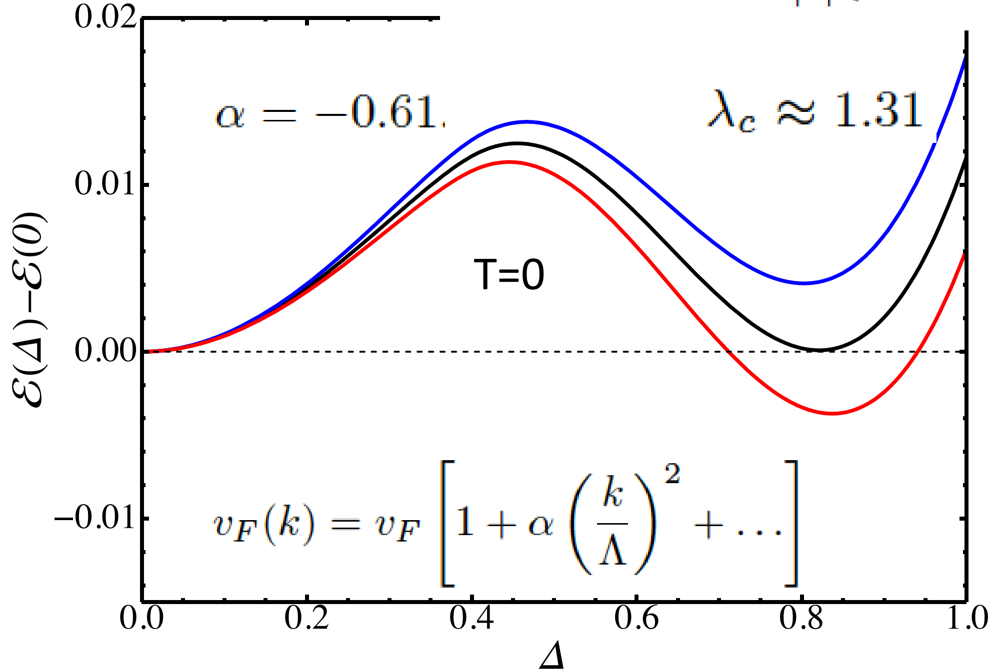
After summation over frequency

$$\mathcal{E}(\bar{Q}) = \frac{2}{f_2}\bar{Q}^2 - \frac{1}{2}\sum_{s}\int \frac{d^2k}{(2\pi)^2}|s\epsilon_{\boldsymbol{k}}(\bar{Q}) - \mu| \ , \ s = \pm 1$$

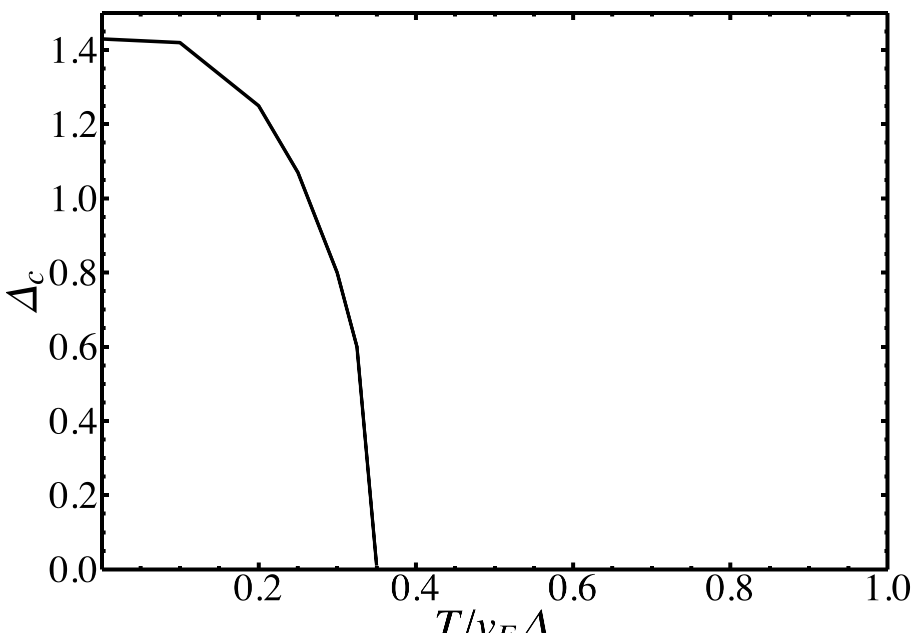
Mean Field Theory for undoped limit (zero chemical potential)

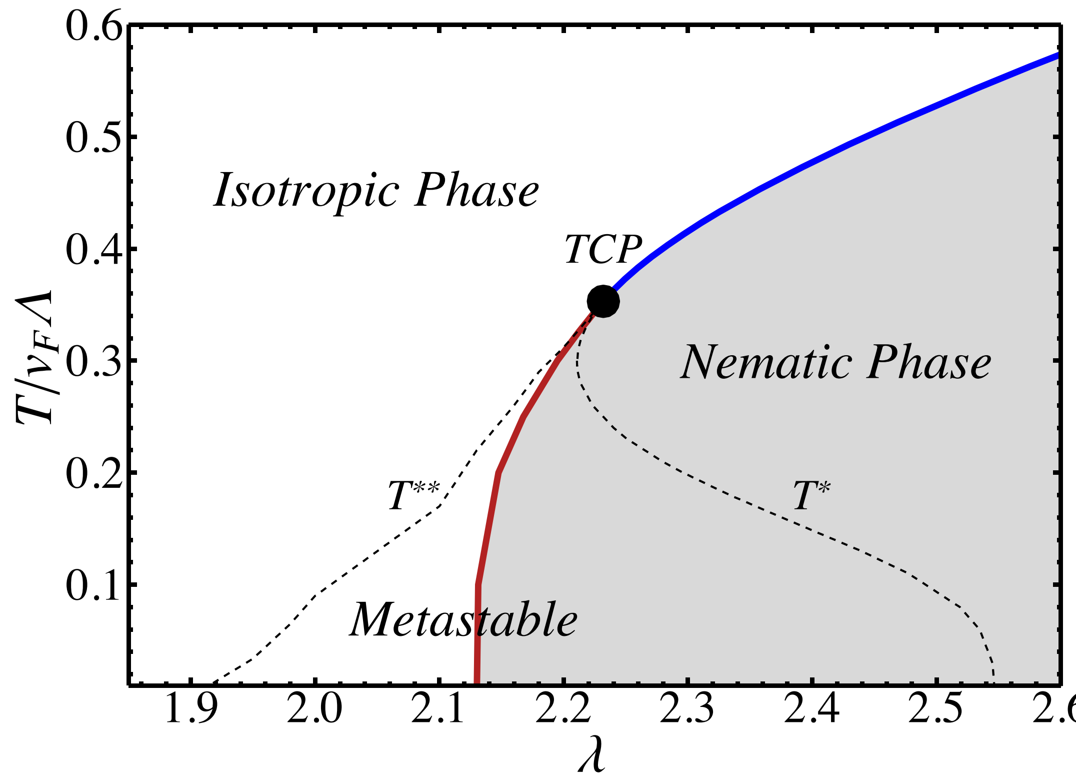
- Free energy reduces $\mathcal{E}(\bar{Q}) = \frac{2}{f_2}\bar{Q}^2 - \int_{|\boldsymbol{k}|<\Lambda} \frac{d^2k}{(2\pi)^2}\epsilon_{\boldsymbol{k}}(\bar{Q}) \rightarrow \mathcal{E}(\Delta) = \frac{v_F\Lambda^3}{3\pi^2}\left[\frac{\Delta^2}{\lambda} - |\Delta - 1| E\left(-\frac{4\Delta}{(\Delta-1)^2}\right)\right]$

$$\Delta = 2\bar{Q}/v_F\Lambda \qquad \lambda = 2f_2\Lambda/3\pi^2 v_F$$



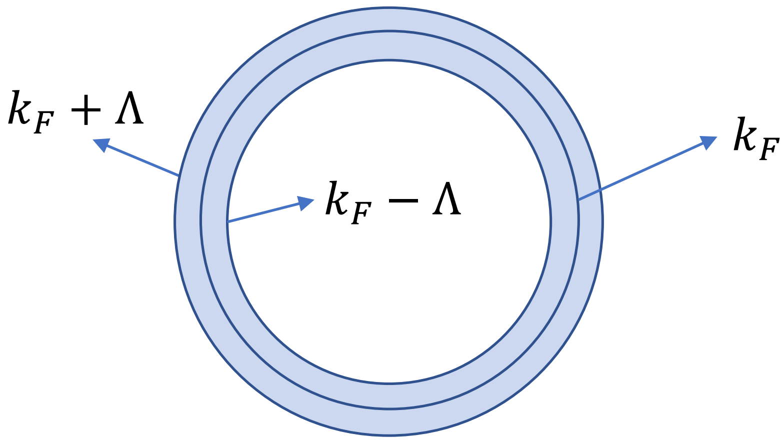
$$\mathcal{F}(\bar{Q}) = \frac{2}{f_2}\bar{Q}^2 - T\sum_s \int_{|\boldsymbol{k}|<\Lambda} \frac{d^2k}{(2\pi)^2} \ln\left(1 + e^{-s\epsilon_{\boldsymbol{k}}(\bar{Q})/T}\right)$$





Mean Field for doped limit

• In the doped limi $\mu \gg v_F\Lambda$, where Λ is a cut-off momentum around the Fermi surface



$$\int_{|k-k_F|<\Lambda} \frac{d^2k}{(2\pi)^2} \equiv \int_{k_F-\Lambda}^{k_F+\Lambda} \frac{dk\,k}{2\pi} \int_0^{2\pi} \frac{d\theta_{\boldsymbol{k}}}{2\pi};$$

• To leading order in Λ/k_F we obtain for energy

$$\mathcal{E}(\bar{Q}) - \mathcal{E}(0) = \left(\frac{2}{f_2} - \mathcal{N}(\mu)\right)\bar{Q}^2 + \frac{\mathcal{N}(\mu)}{4\mu^2}\bar{Q}^4 + \mathcal{O}(\bar{Q}^6)$$

, where $\mathcal{N}(\mu) = \mu/(2\pi v_F^2)$ is non-interacting density of states at the Fermi surface.

• Thus we found continuous phase transition even at zero temperature. This result is in full compliance with the results of RL, JM article [2].

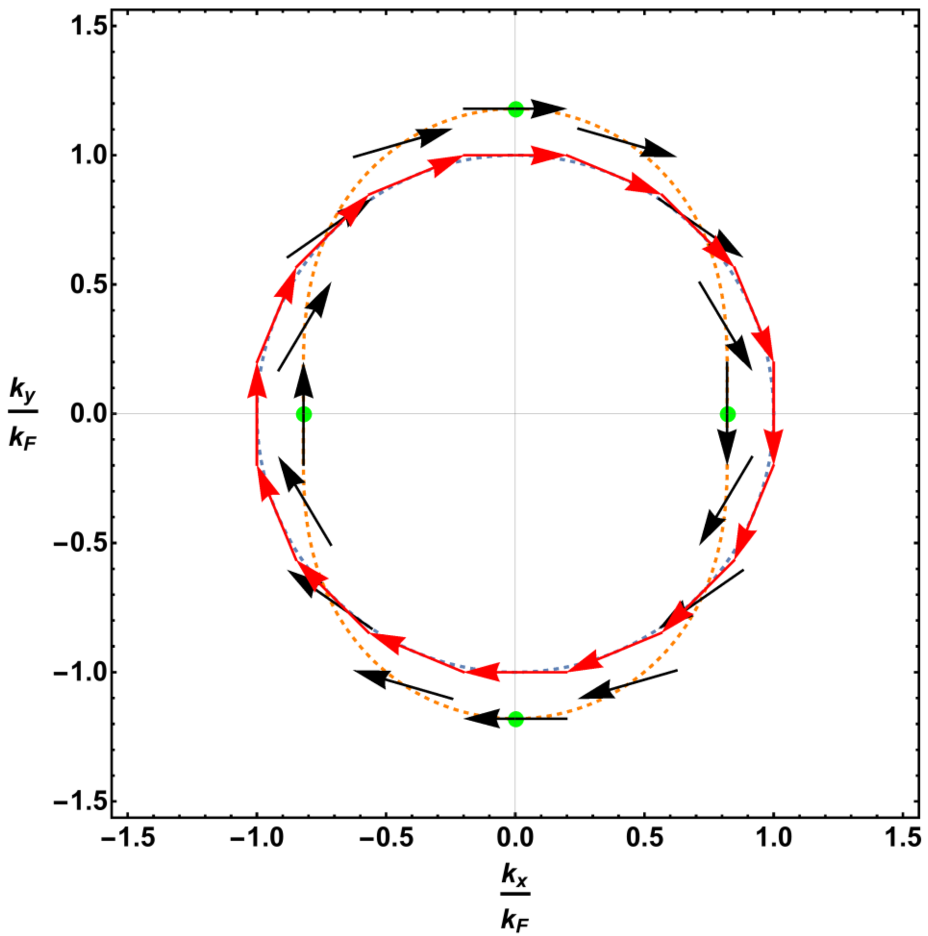
Doped limit. Breakdown of spin-momentum locking

- In mean-field $H_{\mathrm{MF}} = \sum_{\boldsymbol{k}} \psi^{\dagger}_{\boldsymbol{k}} \mathcal{H}_{\boldsymbol{k}} \psi_{\boldsymbol{k}}$ where $\mathcal{H}_{\boldsymbol{k}} = v_F \hat{\boldsymbol{z}} \cdot (\boldsymbol{\sigma} \times \boldsymbol{k}) - \mu + \bar{Q}_{ab}(\sigma_a \hat{k}_b + \sigma_b \hat{k}_a - \delta_{ab} \boldsymbol{\sigma} \cdot \hat{\boldsymbol{k}})$

$\hat{k}_a = k_a / k.$

- The eigen-state with positive helicity is $|\psi_+(\boldsymbol{k})\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} i e^{i\theta_{\boldsymbol{k}}} \frac{f(\theta_{\boldsymbol{k}}, \Delta_F)}{e^{2i\theta_{\boldsymbol{k}}} - \Delta_F} \\ 1 \end{pmatrix}$

$f(\theta_{\boldsymbol{k}}, \Delta_F) \equiv \sqrt{1 + \Delta_F^2 - 2\Delta_F \cos 2\theta_{\boldsymbol{k}}}$



$$s^x_{\boldsymbol{k}} = \frac{(1 + \Delta_F) \sin \theta_{\boldsymbol{k}}}{f(\theta_{\boldsymbol{k}}, \Delta_F)}, \qquad s^y_{\boldsymbol{k}} = -\frac{(1 - \Delta_F) \cos \theta_{\boldsymbol{k}}}{f(\theta_{\boldsymbol{k}}, \Delta_F)}.$$

Anisotropy of spin susceptibility

Spin susceptibility was calculated to the first order in Δ in the presence of a Zeeman term $\delta\mathcal{H}_{\boldsymbol{k}}^{Z} = -\frac{1}{2}g\mu_B \boldsymbol{B}\cdot\boldsymbol{\sigma}$ by using Kubo formula

.

- for undoped limit → $\chi_{xx}(T) - \chi_{yy}(T) = \frac{g^2\mu_B^2\Lambda}{8\pi v_F} F\left(\frac{T}{v_F\Lambda}\right)\Delta(T)$

$$\chi_{xx} - \chi_{yy} = \frac{1}{4}g^2\mu_B^2\mathcal{N}(\mu)\frac{\Lambda}{k_F}\Delta_F$$

- for doped limit at zero temperature in the vicinity of QCP

In contrast, for regular nematic Fermi liquid spin susceptibility is isotropic.

Collective modes in the doped limit

Following OKF, it is convenient to represent order parameter in terms of Pauli matrices

$$\hat{Q} = \psi^\dagger \Delta_1 \psi \tau_z + \psi^\dagger \Delta_2 \psi \tau_x$$

$$\begin{cases} \Delta_1 = -i(\sigma_x \hat{\partial}_x - \sigma_y \hat{\partial}_y) \\ \Delta_2 = -i(\sigma_x \hat{\partial}_y + \sigma_y \hat{\partial}_x) \end{cases}$$

Performing Hubbard-Stratonovich transformation and expanding the action to second order in bosonic field $\boldsymbol{n} = (n_1, n_2)$ the effective action

$$S_{\text{eff}}[\boldsymbol{n}] = \frac{1}{2} \sum_{iq_n, \boldsymbol{q}} \boldsymbol{n}(\boldsymbol{q}, iq_n)^T \chi^{-1}(\boldsymbol{q}, iq_n) \boldsymbol{n}(-\boldsymbol{q}, -iq_n)$$

$$\chi^{-1}_{ij}(\boldsymbol{q}, iq_n) = \delta_{ij}(r + \kappa q^2) + M_{ij}(\boldsymbol{q}, iq_n)$$

$$M(\boldsymbol{q}, iq_n) = is\mathcal{N}(\mu) \int_0^{2\pi} \frac{d\phi}{2\pi} \frac{1}{is - \cos(\phi - \theta_{\boldsymbol{q}})} \times \begin{pmatrix} \sin^2 2\phi & -\sin 2\phi \cos 2\phi \\ -\sin 2\phi \cos 2\phi & \cos^2 2\phi \end{pmatrix},$$

with essentially the same bosonic propagator as in the spinless case [OKF].

At criticality

overdamped

$$\omega_1(q) \approx \sqrt{\frac{\kappa}{2\mathcal{N}(\mu)}} v_F q^2, \qquad \omega_2(q) \approx -\frac{i v_F \kappa}{\mathcal{N}(\mu)} q^3$$

undamped

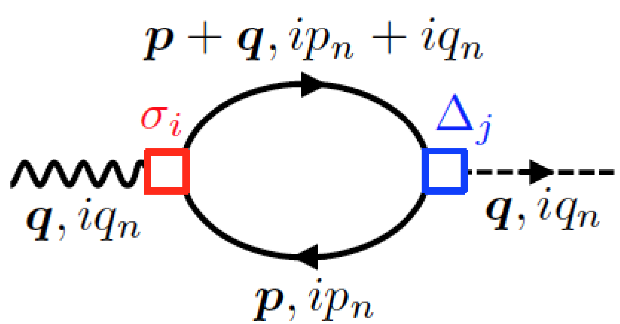
z=3

Collective modes in the doped limit

Nematic fluctuations may induce spin fluctuations in a helical FL. Using Kubo formula

$$\delta\langle s_i(\boldsymbol{q},\omega)\rangle \propto \Pi^R_{ij}(\boldsymbol{q},\omega)\delta n_j(\boldsymbol{q},\omega)$$

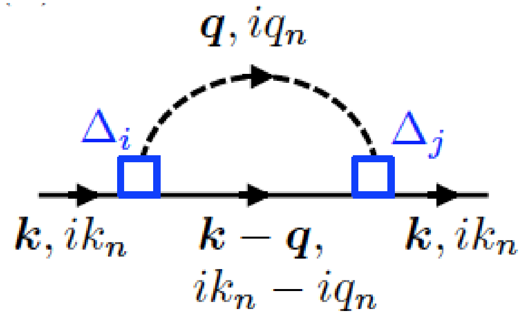
$$\Pi^R_{ij}(\boldsymbol{r},t) = -i\theta(t)\left\langle\left[(\psi^\dagger\sigma_i\psi)_{(\boldsymbol{r},t)},(\psi^\dagger\Delta_j\psi)_{(\boldsymbol{0},0)}\right]\right\rangle$$



It is shown that Π^R_{ij} is not equal zero in isotropic phase, the same is expected for nematic phase.

Electron Self-Energy

- At one-loop order fermionic self-energy is



$$\Sigma(\boldsymbol{k}, ik_n) = \frac{T}{V}\sum_{\boldsymbol{q}, iq_n}\sum_{ij}\Delta_i(\hat{\boldsymbol{k}})\mathcal{G}_0(\boldsymbol{k}-\boldsymbol{q}, ik_n - iq_n)\Delta_j(\hat{\boldsymbol{k}})\chi_{ij}(\boldsymbol{q}, iq_n)$$

- At the critical point $r = 0$ for $|k - k_F| \ll k_F$ and $|k_n| \ll \mu$,

$$\Sigma(\boldsymbol{k}, ik_n) = \left(1 + \hat{\boldsymbol{z}}\cdot(\boldsymbol{\sigma}\times\hat{\boldsymbol{k}})\right)\Sigma_0(\boldsymbol{k}, ik_n),$$

$$\Sigma_0(\boldsymbol{k}, ik_n) = -i\omega_0^{1/3}|k_n|^{2/3}\,\mathrm{sgn}\,k_n$$

$$\omega_0 \sim \mathcal{N}(\mu)^{-1}(v_F\kappa)^{-2}$$

- In the nematic phase using several approximations the self-energy is estimated to

$$\Sigma(\boldsymbol{k}, ik_n) = (1 - \sigma_y\cos 3\theta_{\boldsymbol{k}} - \sigma_x\sin 3\theta_{\boldsymbol{k}})\,|\cos 2\theta_{\boldsymbol{k}}|^{-2}\,\Sigma_0(\boldsymbol{k}, ik_n)$$

- $Z_{\mathbf{k}} = \dfrac{1}{1 - \mathrm{Re}[\Sigma^\star(\mathbf{k},\omega)]'\Big|_{\omega=\Omega_{\mathbf{k}}}}$ - thus we observe non-Fermi liquid behaviour at QCP and in the Nematic phase

Conclusions

- Owing to strong spin-orbit coupling, nematic order parameter in helical Fermi liquid involves both momentum and spin, unlike the case of the spin-degenerate Fermi liquid.
- For undoped limit, we surprisingly found first-order phase transition which evolves into continuous one at a finite temperature tricritical point.
- For doped limit, phase transition is continuous even at zero temperature.
- The consequences of developing nematic order are partial breakdown of spin-momentum locking, spin susceptibility anisotropy (both limits).
- Nematic fluctuations may induce spin fluctuations.
- Non-Fermi liquid behaviour at QCP and in the nematic phase.