Nematic Order on the Surface of three-dimensional Topological Insulator\cite{1}

Hennadii Yerzhakov\textsuperscript{1}

Rex Lundgren\textsuperscript{2}, Joseph Maciejko\textsuperscript{1,3}

\textsuperscript{1} University of Alberta
\textsuperscript{2} Joint Quantum Institute, NIST/ The University of Maryland, College Park
\textsuperscript{3} Canadian Institute for Advanced Research

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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.

Model

OKF[4], spinless
\[ \hat{Q}_{ab}(r) = -\frac{1}{k_F^2} \psi^\dagger(r)(\partial_a \partial_b + \partial_b \partial_a - \delta_{ab} \partial \cdot \partial) \psi(r) \]

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

Here \( k_A = \Lambda \) for the undoped case representing momentum cut-off; \( k_A = k \) for the doped case.

The model Hamiltonian is
\[ \hat{H} = \hat{H}_0 + \hat{H}_{\text{int}} \]

\[ H_0 = \int \frac{d^2 k}{(2\pi)^2} \psi^\dagger_k (h(k) - \mu) \psi_k. \]

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

\[ h(k) = v_F \hat{z} \cdot (\sigma \times \hat{k}) = v_F \begin{pmatrix} 0 & i k e^{-i\theta_k} \\ -i k e^{i\theta_k} & 0 \end{pmatrix} \]

Mean Field Theory

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

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

Here without loss of generality we set

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

Quasi-particle energy

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

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

$$\bar{Q} = 0$$, circular

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

After summation over frequency

$$\mathcal{E}(\bar{Q}) = \frac{2}{f_2} \bar{Q}^2 - \frac{1}{2} \sum_s \int \frac{d^2k}{(2\pi)^2} |s \epsilon_\mathbf{k}(\bar{Q}) - \mu|, \ s = \pm 1$$
Mean Field Theory for undoped limit (zero chemical potential)

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

\[ \Delta = 2\bar{Q}/v_F \Lambda \quad \lambda = \frac{2f_2 \Lambda}{3\pi^2 v_F} \]

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

- Free energy reduces \( \mathcal{E}(\bar{Q}) = \frac{2}{f_2} \bar{Q}^2 - \int_{|k|<\Lambda} \frac{d^2 k}{(2\pi)^2} \epsilon_k(\bar{Q}) \)

\[ \alpha = -0.61 \]

\[ \lambda_c \approx 1.31 \]

\[ T=0 \]

\[ v_F(k) = v_F \left[ 1 + \alpha \left( \frac{k}{\Lambda} \right)^2 + \ldots \right] \]

\[ \Delta_c \]

\[ \frac{T}{v_F \Lambda} \]

\[ \lambda \]

Isotropic Phase

Nematic Phase

Metastable

TCP

\[ T^* \]

\[ T^{**} \]
Mean Field for doped limit

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

\[
\int_{|k-k_F|<\Lambda} \frac{d^2k}{(2\pi)^2} \equiv \int_{k_F-\Lambda}^{k_F+\Lambda} \frac{dk \cdot k}{2\pi} \int_0^{2\pi} \frac{d\theta_k}{2\pi}.
\]

- To leading order in $\Lambda/k_F$ 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 \( H_{MF} = \sum_k \psi_k^\dagger \mathcal{H}_k \psi_k \) where \( \mathcal{H}_k = v_F \hat{z} \cdot (\sigma \times k) - \mu + \bar{Q}_{ab}(\sigma_a \hat{k}_b + \sigma_b \hat{k}_a - \delta_{ab} \sigma \cdot \hat{k}) \)

The eigen-state with positive helicity is \( |\psi_+(k)\rangle = \frac{1}{\sqrt{2}} \left( \begin{array}{c} \frac{i e^{i \theta_k} f(\theta_k, \Delta_F)}{e^{2i \theta_k} - \Delta_F} \\ 1 \end{array} \right) \)

\[ f(\theta_k, \Delta_F) \equiv \sqrt{1 + \Delta_F^2 - 2 \Delta_F \cos 2\theta_k} \]

\[ s_k^x = \frac{(1 + \Delta_F) \sin \theta_k}{f(\theta_k, \Delta_F)}, \quad s_k^y = -\frac{(1 - \Delta_F) \cos \theta_k}{f(\theta_k, \Delta_F)} \]
Anisotropy of spin susceptibility

Spin susceptibility was calculated to the first order in $\Delta$ in the presence of a Zeeman term

$$\delta \mathcal{H}_k^Z = -\frac{1}{2} g \mu_B B \cdot \sigma$$

by using Kubo formula.

- For undoped limit

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

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

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

- For doped limit at zero temperature in the vicinity of QCP
Collective modes in the doped limit

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

\[
\hat{Q} = \psi^\dagger \Delta_1 \psi \tau_z + \psi^\dagger \Delta_2 \psi \tau_x,
\]

with

\[
\Delta_1 = -i(\sigma_x \hat{\partial}_x - \sigma_y \hat{\partial}_y),
\]

\[
\Delta_2 = -i(\sigma_x \hat{\partial}_y + \sigma_y \hat{\partial}_x).
\]

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

\[
S_{\text{eff}}[\mathbf{n}] = \frac{1}{2} \sum_{i q_n, \mathbf{q}} \mathbf{n}(\mathbf{q}, i q_n)^T \chi^{-1}(\mathbf{q}, i q_n) \mathbf{n}(-\mathbf{q}, -i q_n)
\]

\[
\chi^{-1}_{ij}(\mathbf{q}, i q_n) = \delta_{ij}(r + \kappa q^2) + M_{ij}(\mathbf{q}, i q_n)
\]

\[
M(\mathbf{q}, i q_n) = i s \mathcal{N}(\mu) \int_0^{2\pi} \frac{d\phi}{2\pi} \frac{1}{i s - \cos(\phi - \theta_{\mathbf{q}})}
\]

\[
\times \begin{pmatrix}
\sin^2 2\phi & -\sin 2\phi \cos 2\phi \\
-\sin 2\phi \cos 2\phi & \cos^2 2\phi
\end{pmatrix},
\]

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

At criticality

\[
\omega_1(q) \approx \sqrt{\frac{\kappa}{2 \mathcal{N}(\mu)}} v_F q^2,
\]

\[
\omega_2(q) \approx -\frac{i v_F \kappa}{\mathcal{N}(\mu)} q^3
\]

\[z=3\]
Collective modes in the doped limit

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

\[ \delta \langle s_i(q, \omega) \rangle \propto \Pi_{i,j}^R(q, \omega) \delta n_j(q, \omega) \]

\[ \Pi_{i,j}^R(r, t) = -i \theta(t) \left\langle \left[ (\psi^\dagger \sigma_i \psi)(r, t), (\psi^\dagger \Delta_j \psi)(0, 0) \right] \right\rangle \]

It is shown that \( \Pi_{i,j}^R \) 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

\[ \Sigma(k, ik_n) = \frac{T}{V} \sum_{q, iq_n} \sum_{ij} \Delta_i(\hat{k}) G_0(k - q, ik_n - iq_n) \Delta_j(\hat{k}) \chi_{ij}(q, iq_n) \]

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

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

\[ \Sigma_0(k, ik_n) = -i \omega_0^{1/3} |k_n|^{2/3} \text{sgn} k_n. \]

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

\[ \Sigma(k, ik_n) = (1 - \sigma_y \cos 3\theta_k - \sigma_x \sin 3\theta_k) |\cos 2\theta_k|^{-2} \Sigma_0(k, ik_n) \]

\[ Z_k = \frac{1}{1 - \text{Re}[\Sigma^*(k, \omega)]'} \bigg|_{\omega = \Omega_k} \]

- 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.