Examples of Lifshitz topological transition in interacting fermionic systems

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Outline

• Introduction to Lifshitz transition
• Dipolar fermions
• NaxCoO2 : motivation to consider fluctuations
• Interacting fermions in 2D: second order perturbation theory
• Interacting fermions in 2D: region of paramagnons
• Conclusions
What is a Lifshitz transition? Lifshitz JETP (1960)

- Topological transition of the Fermi surface/ no symmetry breaking
- possibilities: neck or pocket formation/collapsing

If $x$ is a controlling parameter (distance from the QCP):

E.g. in 3d: $\delta\Omega_{\text{sing}} \propto |x|^{5/2}$ for both types
Some recent examples/proposals

• Lifshitz transition in NaxCoO2: Okamoto et al. PRB RC (2010)
• Zeeman-driven Lifshitz transition in YbRh2Si2 : Hackl, Vojta PRL (2011)
• Lifshitz Transition in the Two Dimensional Hubbard Model; Kuang-Shing Chen, Zi Yang Meng et al. PRB (2012)
Dipolar fermions: Experimental setup

- Take advantage of dipolar interactions of the fermions at a finite magnetic field

\[ V(\vec{R}) = d^2 \frac{[1 - 3\cos^2 \theta]}{|\vec{R}|^3} \]

- Max attractive: \( \theta = 0 \)
- Max repulsive: \( \theta = \pi/2 \)
- Null: \( \theta = \arccos(1/\sqrt{3}) \)

\( d \): dipole moment
\( \theta \): angle between the vector that gives the relative position of the two dipoles and the external magnetic field

J. Quintanilla, S. Carr and JB
PRA RC(2009)
Dipolar Interaction

- Fourier transform of interaction for four values (0.2, 0.5, 1, 2) of the anisotropy parameter

\[ \alpha \equiv \frac{\alpha_\parallel}{\alpha_\perp} \]

to justify the use of nearest neighbor interaction for \( \alpha > 2 \):

\[ V(k) = V_0 \cos(k_\perp a_\perp) \]
Model

- Hamiltonian reads:

\[
H = -\sum_{i,l} \left( t_\parallel c_{i,l}^+ c_{i+1,l} + t_\perp c_{i,l}^+ c_{i,l+1} + h.c. \right) + V \sum_{i,l} c_{i,l}^+ c_{i,l+1} c_{i,l+1} c_{i,l}
\]

- Parameters: \( \mu / t_\parallel \quad t_\perp / t_\parallel \quad V / t_\parallel \)

- Effect of interaction: \( \varepsilon_k^* = -2t_\parallel \cos(k_\parallel) - 2t_\perp \cos(k_\perp) - \mu \)

- Meta-nematic phase transition:

\[
t_\perp^* = t_\perp + \frac{V}{\Omega} \sum_k \cos(k_\perp) n(\vec{k})
\]
Meta-nematic phase transition

Fermi surface becomes warped as perpendicular hopping is increased:

Increasing $t_\perp$  

Fermi-Surface becomes closed: topological change
Why “meta-nematic”?

- Meta-magnetic example: Analogy to Sr$_3$Ru$_2$O$_7$

  - First order transition for $V>0$
  - At $V=0$ no longer first order but continuous Lifshitz transition at
    $t_\perp = t_\parallel + \mu/2$
  - Quasi-1D $\rightarrow$ 2D transition: opposite to the notion of confinement
  - Density of states effect
More on meta-nematic

- By comparing energies we find the true position and size of jump.
- The jump has a BCS-like form:

\[ \Delta t^*_\perp = 2 \exp\left(-1/bV_c\right) \]

- S. Carr, J. Quintanilla and JB, PRB (2010)
Landau Theory

• Renormalized transverse hopping \(\rightarrow\) “effective order parameter”.
• Similarity to the well known binding energy of a Cooper pair in the presence of arbitrarily weak attractive interaction!
• Effect of interactions \(\rightarrow\) the continuous Lifshitz transition becomes first order.
Landau Theory

• Defining:

\[ x = \frac{(t_\perp^* - t_\perp^{OPT})}{t_\parallel} \]
\[ x_0 = \frac{(t_\perp - t_\perp^{OPT})}{t_\parallel} \]
\[ t_\perp^{OPT} = t_\parallel - \mu / 2 \]

• Using the logarithmic divergence of the DOS at van Hove energies at the points \((0, \pm \pi)\)

• Requiring the correct physics in absence of \(V\), we obtain the expansion:

\[
E \propto x^2 \left[ \ln |x| - \frac{1}{2} \right] - 2x(x - x_0 - aV) \ln |x| - Vbx^2 \ln^2 |x| \\
\Delta t_\perp^* = 2 \exp(-1/bV_c)
\]
• Collating the results of metanematic transition:
Finite temperature

- At finite $T$ reduced effect of van Hove singularities
- Critical end point on metamagnetic transition is regular:

$$\Delta t^*_\perp \propto (T_c - T)^{1/2}$$

S. Carr et al PRB (2010)
Finite-T phase diagram

• Density Wave dominates the phase diagram but there is still areas where the meta-nematic transition can be seen (even with an exponentially small $T_c$)
NaxCoO$_2$: motivation for fluctuations

- Quasi-2D metal
- Alternately stacked CoO$_2$ and Nax layers (conducting/reservoir)
- In most cases Na is randomly distributed $\rightarrow$ little influence on conducting layers
- Until now: Na-rich phase ($x \sim 0.7$) $\rightarrow$ Curie-Weiss metal
  Na-poor phase ($x \sim 0.3$) $\rightarrow$ Pauli paramagnetic metal
- $t_2g$ band from 3d Co orbitals responsible for most electronic properties $\rightarrow$ splits into $a_{1g}$ and 2 degenerate $e'_g$

D. Yoshizumi et al. (2007)
M.L. Foo et al. (2004)
G. Lang et al. (2008)
M. Yokoi et al. (2005)
OKAMOTO, NISHIO, HIROI (2010) Lifshitz transition?

**FIG. 2:** (color online) Temperature dependence of the magnetic susceptibility $\chi$ measured on cooling at a magnetic field of 1 T for a series of polycrystalline samples of Na$_x$CoO$_2$ for $0.61 \leq x \leq 0.63$. The dotted curve represents data for $x = 0.61$ after subtraction of Curie-like contribution from 0.2% impurity spins. The inset shows the $x$ dependence of the temperature derivative of $\chi$ at various temperatures, where curves are shifted upward by 2, 4, and $6 \times 10^{-6}$ cm$^3$ K$^{-1}$ mol$^{-1}$ for 50, 100 and 200 K data, respectively.
Specific heat and thermoelectric power
explanation by Okamoto et al.: non-rigid band/ resisting occupation!

But the Lifshitz transition occurs in the regime of strong magnetic fluctuations: need to understand deeper the coupling to magnetic fluctuations
Interacting fermions in 2D

- Consider interacting fermions in 2D with short-range interaction $U$ and with dispersion relation:

\[ \varepsilon(k) = \varepsilon_0(k) + \text{Re} \, \Sigma(k; k_{F2} = 0) \]

and we use the normalization for $k_{F1} = 1$, $\mu = \varepsilon(k = 0) \equiv 0$, $m_2 = 1$

First: to get a feeling use second order perturbation theory (SOPT) neglecting the scattering between the two Fermi surfaces.
- **Self-energy** \( \Sigma(k_F, \Omega = 0) = U^2 \int \frac{d^2q d\omega}{(2\pi)^3} G(k_F + \vec{q}, i\omega) \chi_0(-\vec{q}, -i\omega) \)

- \( \chi_0 = \chi_{01} + \chi_{02} \) susceptibility of free electrons (Lindhard function)

- **Units of energy:** \( \frac{k_{F1}^2}{m_2} \) (at \( \mu = 0 \)), momentum: \( k_{F1} \) (at \( \mu = 0 \))

- **Question:** effect of the formation of the pocket?

  \[ \Sigma(k_{F2}, i\omega = 0) \approx \frac{U^2}{8\pi^2} k_{F2}^2 \log \frac{\Lambda}{k_{F2}} \]

  \( \Sigma(k_{F1}, i\omega = 0) \): negligible dependence on pocket size

- **Luttinger theorem is respected:** \( n = \frac{1}{2\pi} (k_{F1}^2 - k_{F2}^2) \)
• To locate the chemical potential we need to consider:

\[ \varepsilon(k_{F2}) + \delta \Sigma(k_{F2}, \omega = 0) = \varepsilon(k_{F1}) + \delta \Sigma(k_{F1}, \omega = 0; k_{F2} \neq 0) \]

or:

\[ \frac{k_{F2}^2}{2} \left( \frac{U^2}{4\pi^2} \log \frac{\Lambda}{k_{F2}} - 1 \right) = \nu_{F1}(k_{F1} - 1) = \mu \]

Non-divergent terms containing \( k_{F2}^2 \) are effectively included in \( \Lambda \).

The actual chemical potential (corrected with the Hartree term) is:

\[ \mu_{\text{phys}} = \mu - U \frac{k_{F2}^2}{4\pi} \]

From the form of the transcendental equation: there is a region with 3 solutions for \( k_{F2} \).
\[
\mu_{\text{max}} = \frac{U^2}{16\pi^2} \Lambda^2 \exp\left(-\frac{8\pi^2}{U^2} - 1\right) \leftrightarrow k_{F2} = \Lambda \exp\left(-\frac{4\pi^2}{U^2} - \frac{1}{2}\right)
\]

Which solution wins?
Integrate the grand-canonical potential:

\[
d\Omega = -n \, d\mu_{\text{phys}}
\]
• Exponentially small jump in pocket size for small U
• Fermi-liquid picture valid (quasiparticle weight $Z$ independent of $k_F^2$ and damping $\propto \omega \log \omega$ (known non-analytic term)
• Exponentially small jump in density

Regime of paramagnons

By increasing U and using rings + ladders:

$$V(\vec{q},i\omega) = \frac{\chi_0(\vec{q},i\omega)}{1-U^2\chi_0^2(\vec{q},i\omega)} + \frac{U\chi_0^2(\vec{q},i\omega)}{1-U\chi_0(\vec{q},i\omega)}$$

Moriya (1973), Doniach and Engelsberg Phys Rev Lett (1968)
\[ \Sigma(\vec{k}, i\Omega) = U^2 \int \frac{d\omega \, d^2q}{(2\pi)^3} G(\vec{k} + \vec{q}, i\Omega + i\omega) V(\vec{q}, i\omega) \]

- For small momentum transfer vertex corrections approximately cancel with corrections of weight Z (Hertz and Edwards 1973)
- Then, self-energy reads:

\[ \Sigma(k_{F2}, \Omega = 0) \approx \frac{U_{\text{eff}}^2}{8\pi^2} \left[ k_{F2}^2 \left( \log \frac{\Lambda}{k_{F2}} + c_1 \right) + \frac{c_2}{\nu_{F1}} k_{F2}^2 + c_3 \right] \]

- and the Stoner criterion:

\[ U_{\text{St}} = \frac{2\pi}{1 + 1/\nu_{F1}} \]
Following same line of thought with SOPT: three possible solution of balance equation → one wins and the formation of pocket is 1st order.
• Some consequences:

• Jump in the specific heat before FM

• By increasing U and reaching Stoner then magnetism drives the Lifshitz 1st order.
Conclusions

• Lifshitz transitions although very sensitive seem to have been realized in physical systems.
• Other systems have been also reported lately (heavy fermions, pnictides etc.)
• Dipolar fermions in anisotropic optical lattices show clear meta-nematic transition (discontinuous).
• Main reason: effect of Van Hove singularities.
• NaxCoO2 shows a discontinuous Lifshitz transition accompanied by enhanced magnetic fluctuations.
• More systematic way to understand effects of fluctuations and FS reconstruction.
• Paramagnetic fluctuations + special dispersion relation may lead to a discontinuous appearance of a new pocket.