Examples of Lifshitz topological transition in interacting fermionic systems

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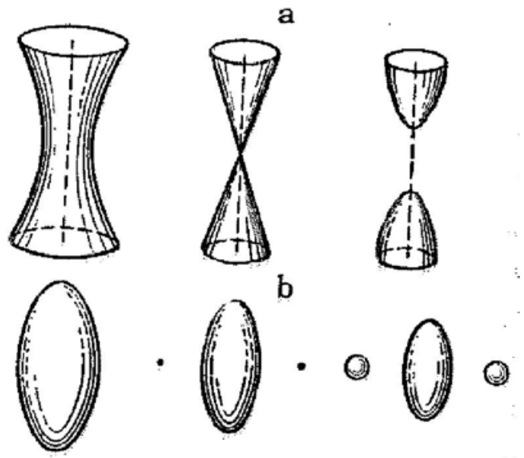
Outline

- 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 controling parameter (distance from the QCP):

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

Some recent examples/proposals

- Electron-doped iron arsenic superconductors: Liu et al. Nature (2010)
- 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

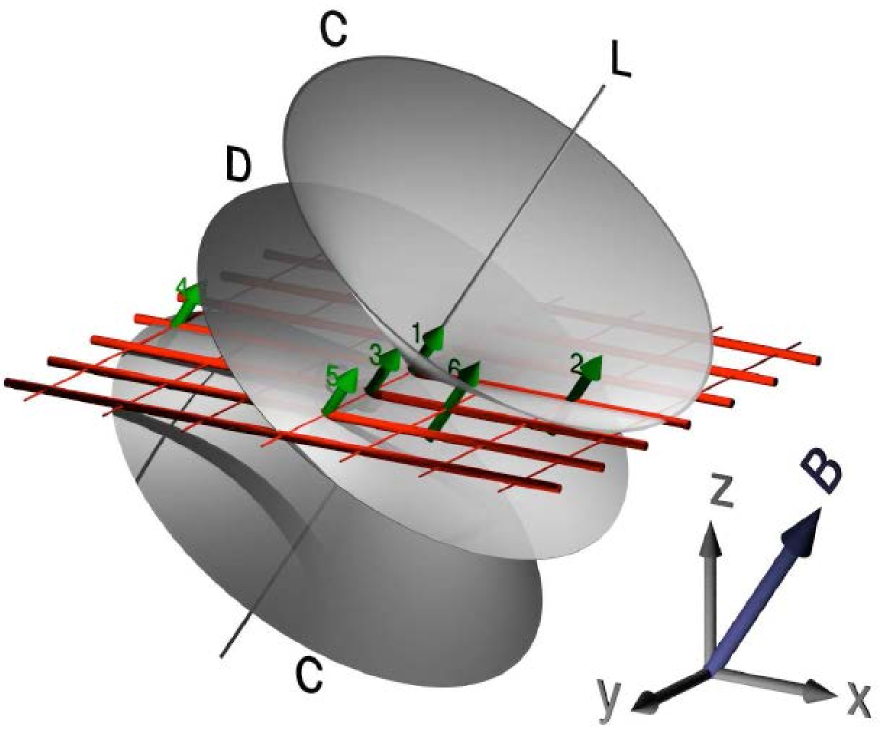
- Take advantage of dipolar interactions of the fermions at a finite magnetic field

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

d: dipole moment

θ: 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)



- Max attractive: θ=0
- Max repulsive: θ=π/2
- Null: θ=arccos(1/$\sqrt{3}$)

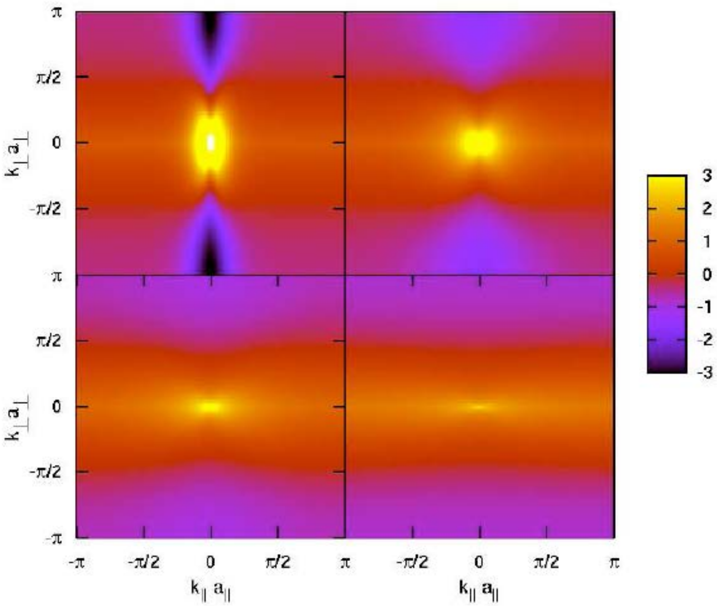
Dipolar Interaction

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

$$\alpha \equiv \frac{a_{||}}{a_{\perp}}$$

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

$$V(k) = V_0 \cos(k_{\perp} a_{\perp})$$



Model

- Hamiltonian reads:

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

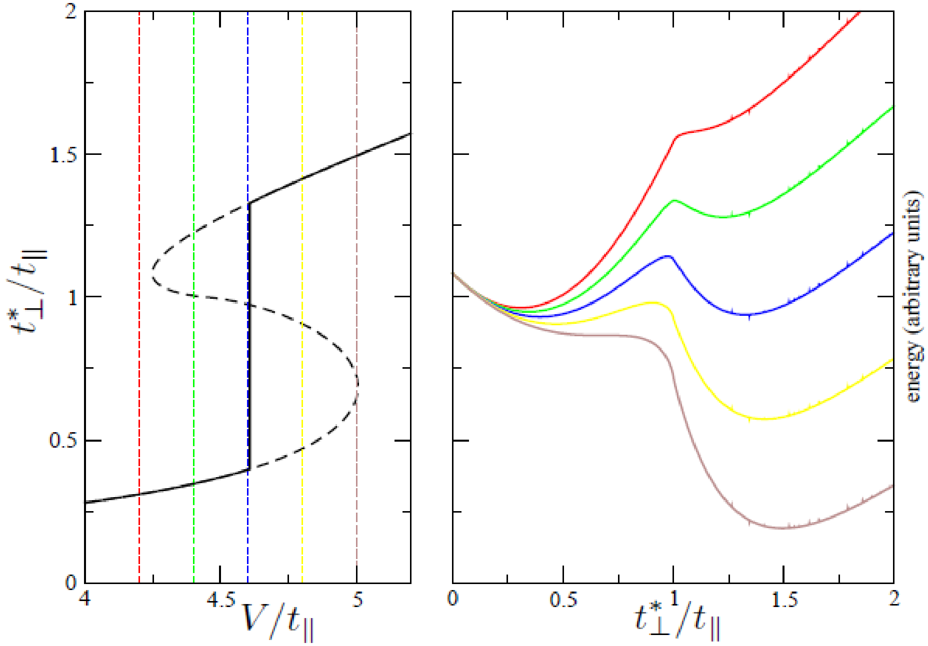
- Parameters: $\mu / t_{\|}$ $\quad t_{\perp} / t_{\|}$ $\quad V / t_{\|}$

- Effect of interaction: $\varepsilon^{*}_{k} = -2t_{\|}\cos(k_{\|}) - 2t^{*}_{\perp}\cos(k_{\perp}) - \mu$

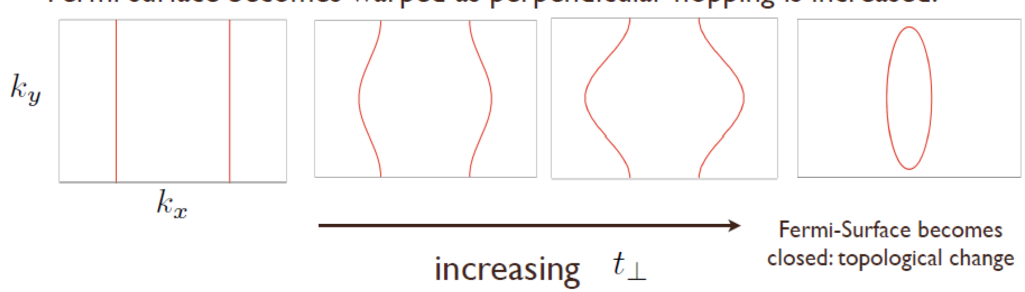
- Meta-nematic phase transition:

$$t^{*}_{\perp} = t_{\perp} + \frac{V}{\Omega}\sum_{\vec{k}} \cos(k_{\perp})\, n(\vec{k})$$

Meta-nematic phase transition

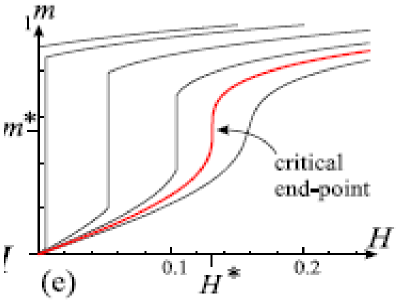


Fermi surface becomes warped as perpendicular hopping is increased:



Why "meta-nematic"?

- Meta-magnetic example: Analogy to $Sr_3Ru_2O_7$



- First order transition for V>0
- At V=0 no longer first order but continuous Lifshitz transition at

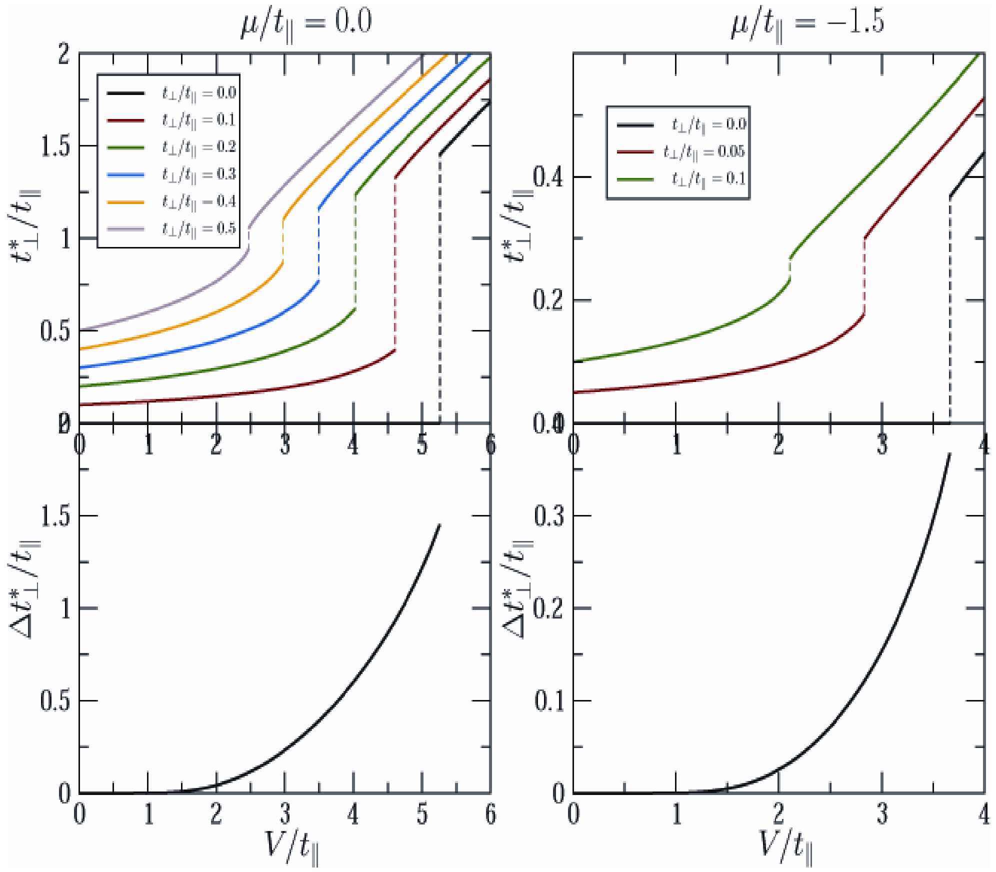
$$t_\perp = t_\parallel + \mu / 2$$

- Quasi-1D → 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:

$$\Delta t_{\perp}^{*} = 2\exp(-1/bV_c)$$



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

Landau Theory

- Renormalized transverse hopping → "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 → the continuous Lifshitz transition becomes first order.

Landau Theory

- Defining:

$$x = (t_\perp^* - t_\perp^{QPT})/t_\parallel$$

$$x_0 = (t_\perp - t_\perp^{QPT})/t_\parallel$$

$$t_\perp^{QPT} = t_\parallel - \mu/2$$

- Using the logarithmic divergence of the DOS at van Hove energies at the points

$$(0, \pm\pi)$$

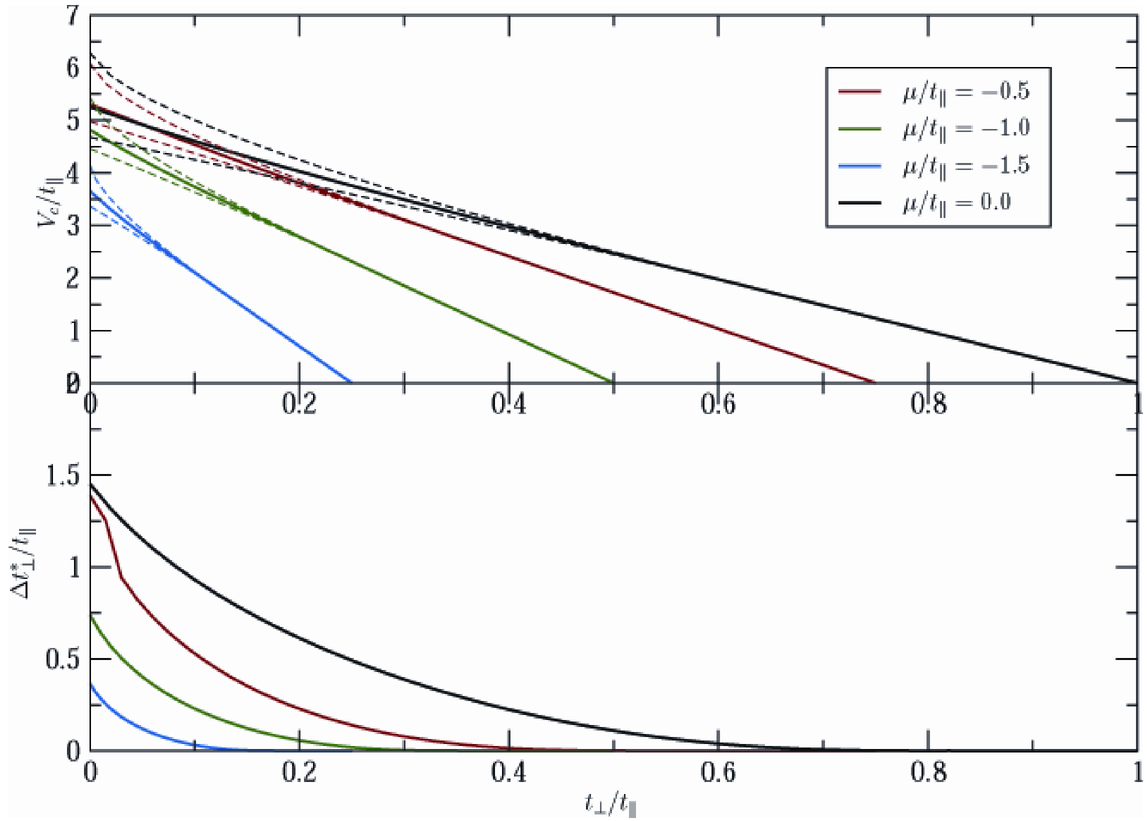
- Requiring the correct physics in absence of V, we obtain the expansion:

$$E \propto x^2[\ln|x| - \frac{1}{2}] - 2x(x - x_0 - aV)\ln|x| - Vbx^2\ln^2|x|$$

$$\Delta t_\perp^* = 2\exp(-1/bV_c)$$

Partial Phase Diagram

- Collating the results of meta-nematic transition:

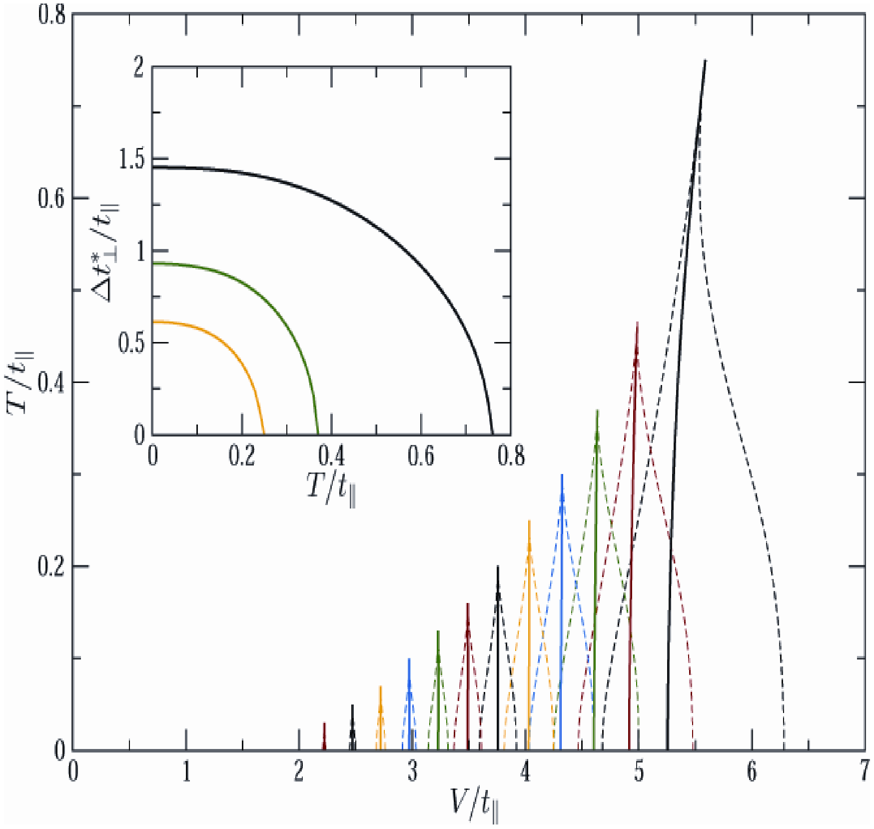


Finite temperature

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

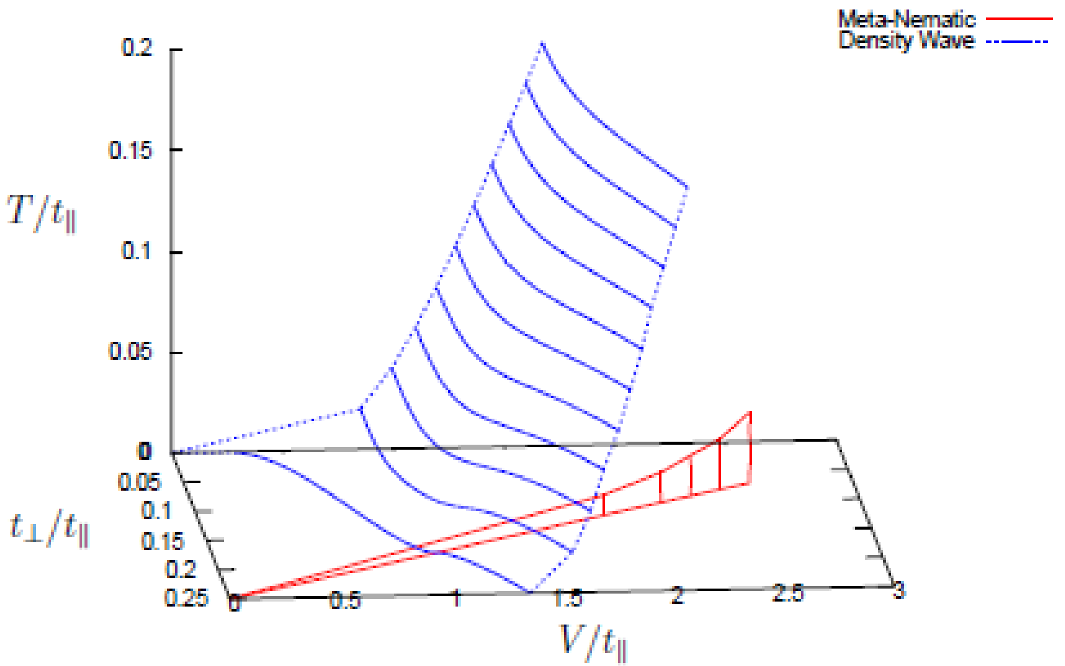
$$\Delta t_{\perp}^{*} \propto (T_c - T)^{1/2}$$

S.Carr et al PRB (2010)



Finite-T phase diagram

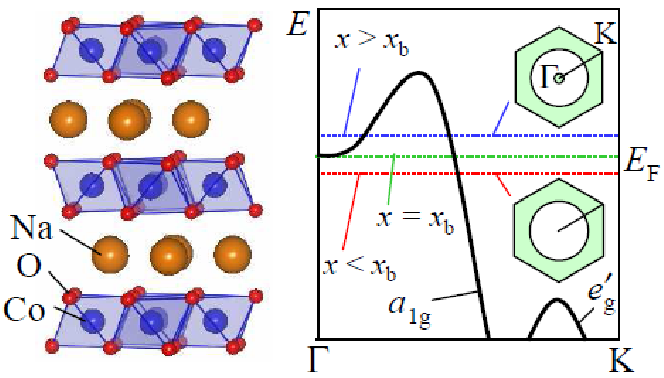
- Density Wave dominates the phase diagram but there is still areas where the meta-nematic transition can be seen (even with an exponentially small Tc)



Phase diagram at $\mu = -1.5t_{\parallel}$.

Na_xCoO_2: motivation for fluctuations

- Quasi-2D metal
- Alternately stacked CoO_2 and Na_x layers
  (conducting/reservoir)
- In most cases Na is randomly distributed → little influence on conducting layers
- Until now: Na-rich phase (x ~ 0.7) → Curie-Weiss metal
  Na-poor phase (x ~ 0.3) → Pauli paramagnetic metal
- t_{2g} band from 3d Co orbitals responsible for most electronic properties → 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?

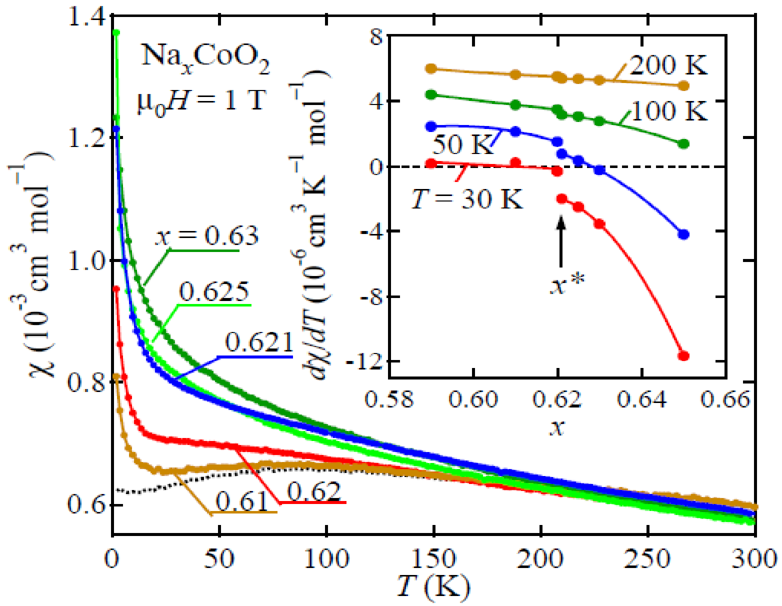
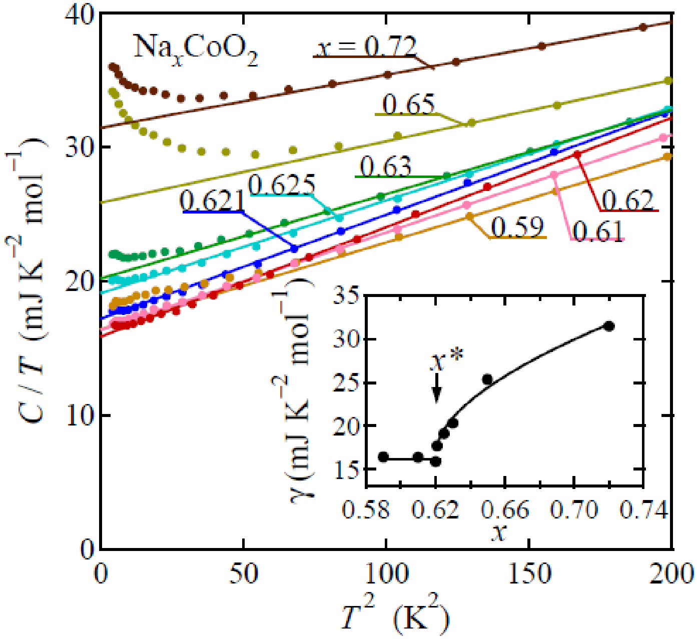
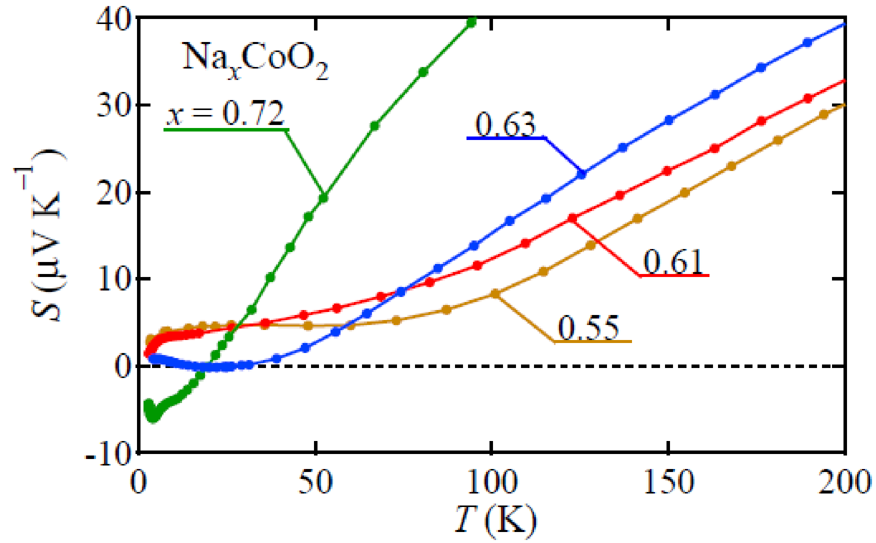


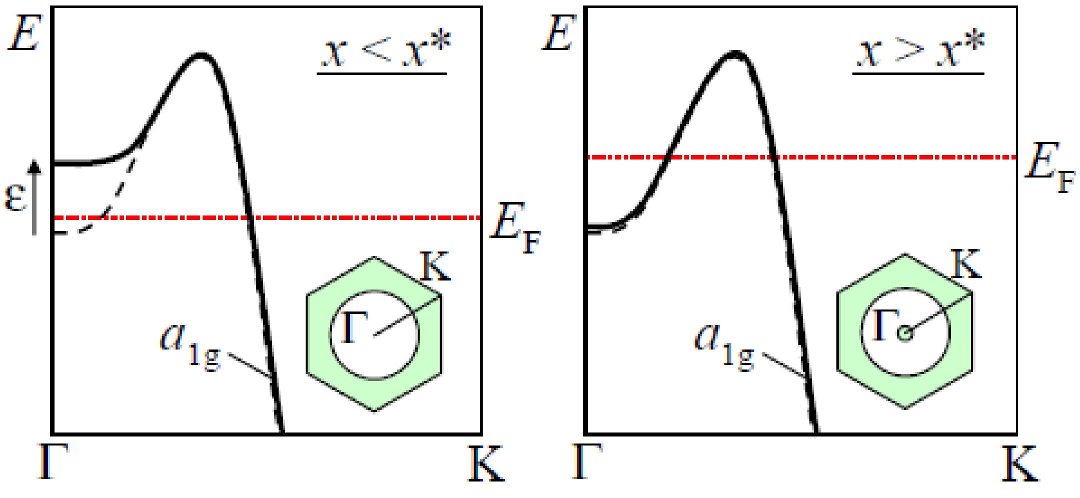
FIG. 2: (color online) Temperature dependence of the magnetic susceptibility χ measured on cooling at a magnetic field of 1 T for a series of polycrystalline samples of Na_xCoO_2 for $0.61 \leq x \leq 0.63$. The dotted curve represents data for $x = 0.61$ after subtraction of Curie-like contribution from 0.2% impurity spins. The inset shows the x dependence of the temperature derivative of χ 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





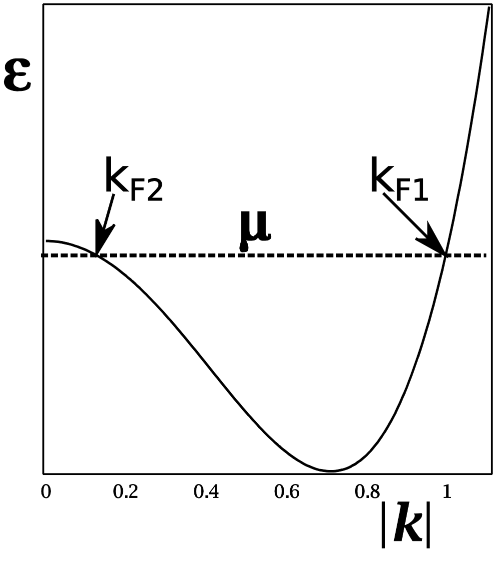
explanation by Okamoto et al.:
non-rigid band/ resisting occupation!



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:



where $\varepsilon(k) = \varepsilon_0(k) + \mathrm{Re}\,\Sigma(k; k_{F2} = 0)$

and we use the normalization

for $k_{F1} = 1$ $\mu = \varepsilon(k = 0) \equiv 0$ $\mathrm{m}_2 = 1$

First: to get a feeling use second order perturbation theory (SOPT) neglecting the scattering between the two Fermi surfaces.

- Self-energy $\Sigma(k_F,\Omega=0)=U^2\int\frac{d^2q d\omega}{(2\pi)^3}G(\vec{k}_F+\vec{q},i\omega)\chi_0(-\vec{q},-i\omega)$
- $\chi_0=\chi_{01}+\chi_{02}$ 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?

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

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

- 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:

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

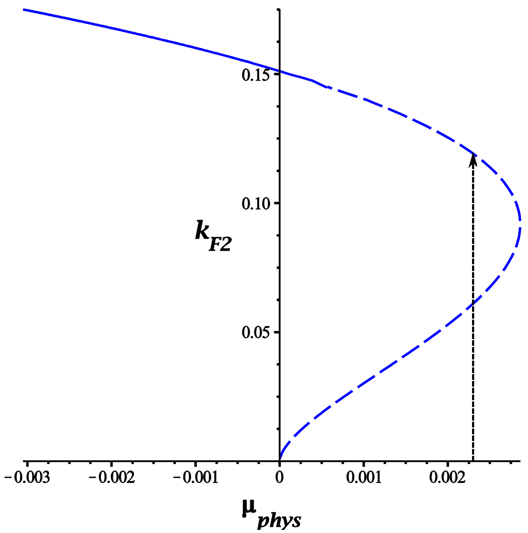
Non-divergent terms containing k_{F2}^2 are effectively included in Λ.

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

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

From the form of the transcendental equation: there is a region with 3 solutions for k_{F2}

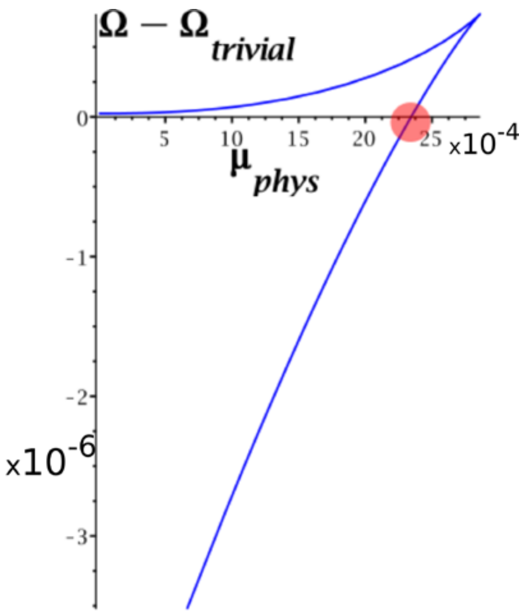
$$\mu_{\max} = \frac{U^2}{16\pi^2}\Lambda^2 \exp(-\frac{8\pi^2}{U^2} - 1) \quad \leftrightarrow \quad k_{F2} = \Lambda \exp(-\frac{4\pi^2}{U^2} - \frac{1}{2})$$



Which solution wins?

Integrate the grand-canonical potential:

$$d\Omega = -n \, d\mu_{phys}$$



- Exponentially small jump in pocket size for small U
- Fermi-liquid picture valid (quasiparticle weight Z independent of k_{F2} 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:

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

W. F. Brinkman and S. Engelsberg Phys. Rev. 169, 417 (1968)
M. T. Beal-Monod, S- K. Ma, D. R. Fredkin Phys. Rev. Lett. 20, 929 (1968)
P. W. Anderson and W. F. Brinkman Phys. Rev. Lett. 30, 1108 (1973)
Moriya (1973) , Doniach and Engelsberg Phys Rev Lett (1968)

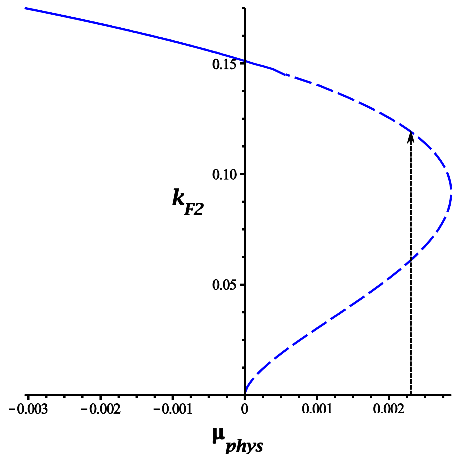
$$\Sigma(\vec{k}, i\Omega) = U^2 \int \frac{d\omega\, d^2 q}{(2\pi)^3} G(\vec{k}+\vec{q}, i\Omega + i\omega) V(\vec{q}, i\omega)$$

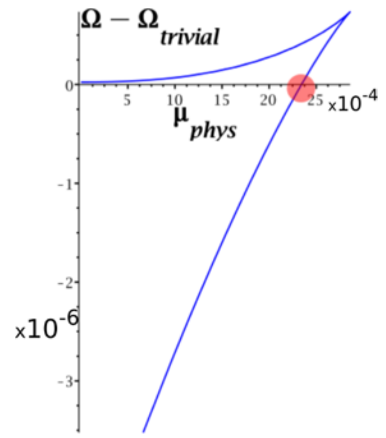
- For small momentum transfer vertex corrections approximately cancel with corrections of weight Z (Hertz and Edwards 1973)
- Then, self-energy reads:

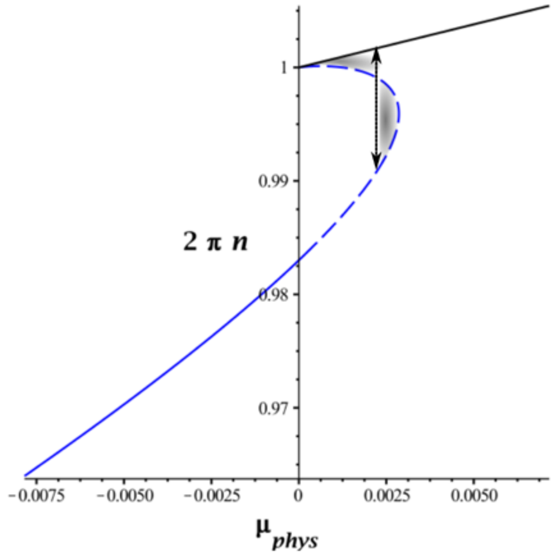
$$\Sigma(k_{F2}, \Omega = 0) \approx \frac{U_{eff}^2}{8\pi^2} \left[k_{F2}^2 \left(\log \frac{\Lambda}{k_{F2}} + c_1 \right) + \frac{c_2}{\upsilon_{F1}} k_{F2}^2 + c_3 \right]$$

- and the Stoner criterion: $U_{St} = \dfrac{2\pi}{1 + 1/\upsilon_{F1}}$

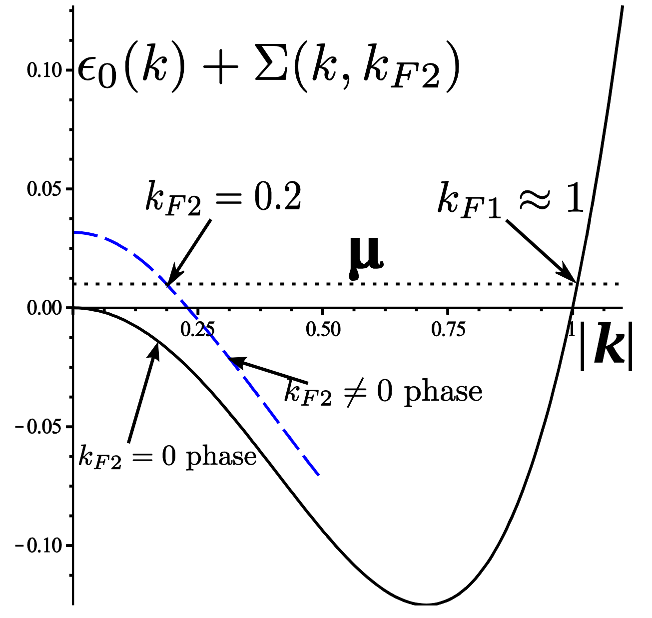
Following same line of thought with SOPT: three possible solution of balance equation ➔ one wins and the formation of pocket is 1st order.







- 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.