7. Frustration in metals

So far: insulators with local-moment degrees of freedom (= spins)

charge fluctuations unimportant

Now: conducting states with electron degrees of freedom, Fermi surfaces etc + magnetism. Electrons interact via Coulomb int.!

7.1. Fermi liquids and non-Fermi liquids

Electrons in conventional metals behave as Fermi Liquids (FL).

Fermi Liquid: (Landau)

- metallic state which can be adiabatically connected to Fermi gas of non-interacting electrons.
- elementary excitations are weakly interacting (!) electrons and holes, with quantum numbers $S = \frac{1}{2}$, $Q = \pm e$, but possibly renormalized mass.

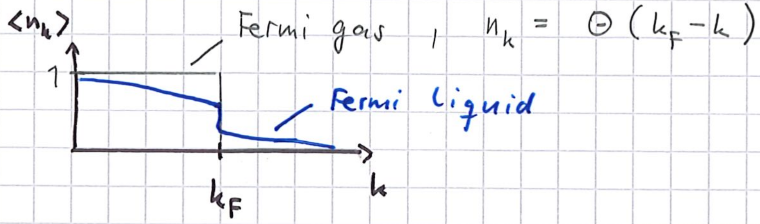
More precisely, ground state and low-lying excited states of FL are in one-to-one correspondence to that of a Fermi gas.

Observable consequences: FL has

- specific heat $C = \gamma \cdot T$ at low T, $\gamma \sim$ const
- resistivity $\rho = \rho_0 + A T^2$ at low T, ρ_0 from defects
- Fermi surface $\hat{=}$ $(d-1)$-dimensional manifold in momentum space where $\langle n_{k\sigma} \rangle = \langle c^\dagger_{k\sigma} c_{k\sigma} \rangle$ jumps discontinuously at $T=0$.

Low-energy excitations of FL can be understood as quasiparticles (QP) (with $S = 1/2$ and $|Q| = e$), i.e. electrons or holes dressed by interaction effects.

Momentum distribution (at $T=0$)



Jump height in $\langle n_k \rangle$ defines <u>quasiparticle weight</u> Z_k, $0 \le Z_k \le 1$.

Single-particle spectral function $A(k,\omega) = -\frac{1}{\pi} \operatorname{Im} G_c(k,\omega)$,
$G_c(k,\tau) = -T_\tau \langle c_k(\tau)\, c_k^\dagger(0) \rangle$, displays quasiparticle peak at $\omega = \mu$ along Fermi surface, with weight Z_k ($Z_k = 1$ in Fermi gas)

Recall: $\int d\omega \; A(k,\omega) = 1$, $A(k,\omega) \geq 0 \quad \forall\, k,\omega$.

Electron-electron interaction leads to finite lifetime of quasiparticles $<$ away from Fermi surface / at finite temperatures.

Inverse lifetime $\hat{=}$ <u>scattering rate Γ</u> $\hat{=}$ broadening of δ peak in $A(k,\omega)$

Fermi liquid has <u>$\Gamma \propto \max(T^2, (\omega-\mu)^2)$</u> at small T and $|\omega-\mu|$.

<u>Luttinger theorem</u>

Momentum-space volume enclosed by Fermi surface equals that in non-interacting limit (!), i.e. all electrons contribute to Fermi volume:

$$V_{FL} = (n_{tot} \underbrace{\bmod 2}_{\text{accounts for filled bands}})$$

assuming spin-degenerate bands. (Fermi surface defined at $T=0$ only!)

Remarks

FL behavior of interacting electrons is hypothesis, can be proven for generic lattice models in $d \geq 3$ for weak interactions. Often, also strongly interacting electron systems behave as FL (often with $Z_k \ll 1$).

In $d = 1$, FL behavior is not realized even for weak interactions; instead, 1d interacting electrons behave as Luttinger liquids (bosonic density excitations, power laws in many observables, $Z_k = 0$).

In $d = 2$, situation is not fully clear, but many research point towards FL behavior at weak interactions.

Luttinger theorem can be proven non-perturbatively, provided that FL hypothesis concerning excitations holds. (Oshikawa 2000)

FL concept can be generalized to semimetals (like graphene); key is one-to-one correspondence of low-lying many-body states to non-interacting limit.

FL behavior is in principle expected if $\omega, T \ll \underbrace{\varepsilon_F}_{10^3 \ldots 10^4 K}$. In solids, phonons provide additional scales: $\Theta_{\text{Debye}} \simeq 100 \ldots 1000\,K$, $\Delta\rho_{\text{Phonons}} \propto T^5$. In practice $\rho(T) - \rho_0 \propto T^2$ is only observed at low T (e.g. $T < 100$ K or lower).

Non-Fermi Liquids

Metallic states whose behavior fall outside the FL paradigm are usually called non-Fermi Liquids (nFL). Often, one observes $\rho(T) - \rho_0 \propto T^x$ with $x \neq 2$.

nFL behavior can have various sources:

a) no well-defined fermionic QP (example: Luttinger Liquid)

b) fermionic QP exist, but their scattering is anomalous (e.g. $\Gamma \propto T$ instead of T^2) (can occur near quantum phase transitions)

c) FL-like QP exist, but Fermi volume violates Luttinger's theorem (example: fractionalized Fermi Liquid, see later)

d) strong disorder may generate effective nFL behavior

⋮

Note: Systems may display FL behavior, but only at very low T (e.g. < 1 K), and intermediate-T regime may look nFL-like.

7.2. Conventional order vs. liquid states

Metals can display symmetry-breaking (= ordered) phases like insulators, i.e., may break lattice translation and/or spin rotation symmetry.

Depending on the band filling, ordered states may become (band) insulators: If ordered state enlarges the unit cell by factor M, a band insulator may emerge from band filling $\langle n \rangle$ per spin if $M \cdot \langle n \rangle$ is an integer. ATTN: Generically, the onset of symmetry breaking leaves metallicity intact (bands will be backfolded due to larger unit cell), but insulator may emerge for stronger order.

Example:

paramagnetic metal | AF metal | AF insulator → control parameter

This can be obtained in a mean-field theory for electrons in the presence of magnetism:

$$H_{MF} = - \sum_{\langle ij \rangle \sigma} t_{ij} c^{+}_{i\sigma} c_{j\sigma} + g \sum_i \vec{m}_i \cdot c^{+}_{i\sigma} \vec{\sigma}_{\sigma\sigma'} c_{i\sigma'}$$

where $\vec{m}_i$ represents spontaneous magnetization of ordered state (which in principle needs to be determined self-consistently, but can be assumed to have a particular form).

A magnetic metal often behaves like a Fermi Liquid (suitably generalized: quasiparticle properties may become spin-dependent etc.)

For non-symmetry-breaking states, there are important conceptual differences between insulators and metals:

- For local-moment insulators, a non-symmetry-breaking state at $T=0$ with half-odd-integer spin per unit cell must be fractionalized and topological ($\curvearrowright$ spin liquid, Lieb-Schultz-Mattis-Hastings theorem)

- For a metal, a non-symmetry-breaking state may simply be a Fermi liquids (!).

Metals can display other (non-trivial) symmetric states.
Example: Fractionalized Fermi liquid (FL^*)

FL^* is most easily obtained in two-band (or two-orbital) system, where one band („c") is a conventional (weakly interacting) metal, while the other („f") is strongly correlated, half-filled, and forms a fractionalized spin liquid. Both bands are assumed to be weakly coupled; such a coupling does not qualitatively alter the system's properties.

FL^* does not break symmetries and features both conventional metallic quasiparticles and fractionalization in the spin sector. It violates Luttinger's theorem, as only the c electrons contribute to Fermi volume:

$$V_{FL^*} = (n_c \bmod 2) \neq (n_{tot} \bmod 2)$$

$$n_{tot} = n_f + n_c = 1 + n_c$$

Conceptually, it is not easy to define a „metallic spin liquid":

- Most definitions of topology fail in the presence of a Fermi surface.

- Local-moment formation in a metal cannot be defined sharply.

- Fractionalization (e.g. into spinons) cannot be easily distinguished from the response of a metallic particle-hole continuum.

One (the only ?) sharp distinction is by Fermi volume: If a symmetric state displays a Fermi surface of charge-e spin-$\frac{1}{2}$ quasiparticle, but violates Luttinger's theorem, it cannot be a Fermi liquid. The Luttinger violation implies that not all electrons contribute to the Fermi volume, hence the state may be a „metallic spin liquid". (FL^* deserves to be called this way.)

7.3. Routes to frustrated metals

What are the (microscopic) settings where one can expect to find a frustrated metal?

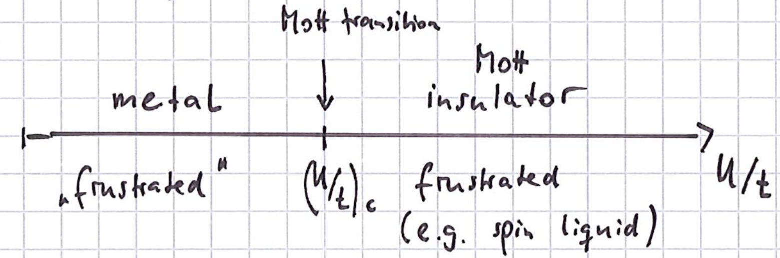
(a) Hubsard models on geometrically frustrated lattices

(e.g. kagome, pyrochlore)

$$H = -\sum_{\langle ij \rangle} t_{ij} \, c^{+}_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

Focus on $\langle n \rangle = 1$. $U/t \to \infty$ ↷ frustrated Heisenberg model

Generic phase diagram at $T=0$:



It is natural to expect that signatures of frustration are also visible in metallic phase, at least close to Mott transition.

Which signatures can be expected?

- reduced kinetic energy (see below)
- strong short-range magnetic correlations (but no magnetic order)
- potential instabilities to other phases (e.g. superconducting near Mott transition)
- ... ?

(This field is little studied, as numerical simulations are hard: quantum Monte Carlo sign problem)

Frustration and reduced kinetic energy:

On a bipartite lattice with nearest-neighbor hopping t, the (hopping) band width is $2t \cdot z$, where z is the coordination number. (square lattice ↝ bandwidth $8t$)

The minimum and maximum of the dispersion are realized for plane waves where neighboring sites have phase shift 0 and π, respectively. This corresponds to the maximum kinetic energy (bandwidth) (for fixed t)

On frustrated lattices, a plane wave which has π phase shift between neighboring sites does not exist, hence the bandwidth is smaller than $2tz$. (The non-existence of this single-particle state is obviously equivalent to the non-existence of a simple Néel antiferromagnetic state, ↑↓↑↓↑↓.)

↝ Geometric frustration in single-particle hopping implies narrow bands $\hat{=}$ heavy / slow particles.

In extreme cases, the bandwidth may be zero (!).

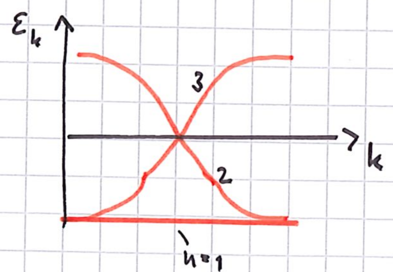
Example: Kagome lattice

$$H = -t \sum_{\langle ij \rangle} \left(c_i^+ c_j + h.c. \right) = \sum_{n=1}^{3} \varepsilon_{k,n} \, c_{k,n}^+ c_{k,n}$$

Unit cell of 3 sites ↝ 3 bands

One of the 3 bands is perfectly flat!

↝ Hopping Hamiltonian has eigenstates which are localized in real space!

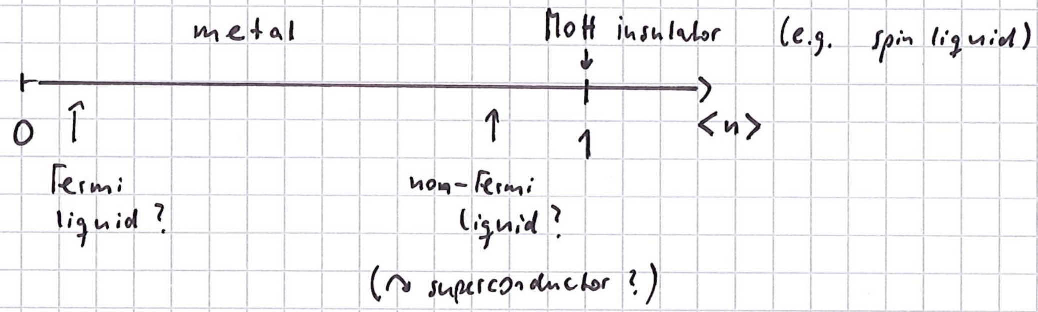


6) Doped frustrated Mott insulators

Work at $U/t \gg 1$, but at $\langle n \rangle \neq 1$, i.e. start from half-filled Mott insulator on frustrated lattice and then vary electron concentration.

$\langle n \rangle \leq 1$:
$$H_{\text{eff}} = -\sum_{\langle ij \rangle} t_{ij} \left(\tilde{c}^{+}_{i\sigma} c_{j\sigma} + \text{h.c.} \right) + \sum_{\langle ij \rangle} J_{ij} \left(\vec{S}_i \cdot \vec{S}_j - \frac{n_i n_j}{4} \right)$$

„t-J model", $\tilde{c}^{+}_{i\sigma} = c^{+}_{i\sigma} (1 - n_{i,-\sigma})$ forbids double occupancy



For $\langle n \rangle \neq 1$, the system can be expected to be metallic. For $\langle n \rangle \ll 1$, interaction effects are likely weak ↝ expect Fermi-liquid behavior.

The behavior near half-filling is little understood even for non-frustrated lattices. Various non-FL states have been proposed. Numerics remains inconclusive.

ATTN: On the square lattice, the doped Mott insulator problem is believed to represent the physics of cuprate high-temperature superconductors. (Nobel prize 1987)

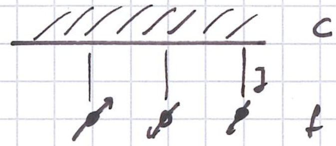
(c) RKKY frustration and Kondo lattices

Consider two bands
- weakly correlated conduction electrons, $\langle n_c \rangle \neq 1$
- strongly correlated f electrons, $\langle n_f \rangle = 1$

$$\underline{H} = \underline{-\sum_{\langle ij\rangle\sigma} t_{ij} \left(c_{i\sigma}^{+} c_{j\sigma} + h.c. \right) + \underset{J>0}{J} \sum_i \underset{\text{spin moment of f electron}}{\vec{S}_i} \cdot \underbrace{\tfrac{1}{2} c_{i\sigma}^{+} \overset{\text{Pauli}}{\vec{\sigma}_{\sigma\sigma'}} c_{i\sigma'}}_{\text{spin moment of c electron}}}$$

„Kondo lattice model"

A direct interaction of the local moments $\left(I_{ij} \vec{S}_i \cdot \vec{S}_j \right)$ has been neglected (is small for f electrons). But local moments interact via conduction electrons:



For small J, the effective interaction is

$$\underline{I_{ij}^{\text{eff}}} \propto \underline{J^2 \chi_c \left(\vec{r}_i - \vec{r}_j \right)}$$

where $\chi_c(\vec{r})$ is the spin susceptibility of c electrons. I_{ij}^{eff} has been derived in second-order perturbation theory in J; it is called <u>RKKY interaction</u> (Ruderman, Kittel, Kasuya, Yosida). In a three-dimensional metal, $\chi_c(\vec{r})$ decay as $1/r^3$

$\rightarrow$ RKKY interaction is long-ranged. Moreover, its sign oscillates with wavelength k_F^{-1} ($k_F \hat{=}$ Fermi momentum)

Due to these oscillations, RKKY interaction is partially frustrated even on bipartite (unfrustrated) lattices!

In Kondo lattices, the dynamics of the local moments is governed by two competing effects:

- RKKY interaction (prefers ordered magnet or spin liquid of f moments)
- Kondo screening: larger J promotes singlet formation between c and f electrons ↷ f moments screened (↷ FL with heavy quasiparticles)

Energy scales: $I_{RKKY} \propto J^2 \rho_0$ ρ_0: c-electron density of states

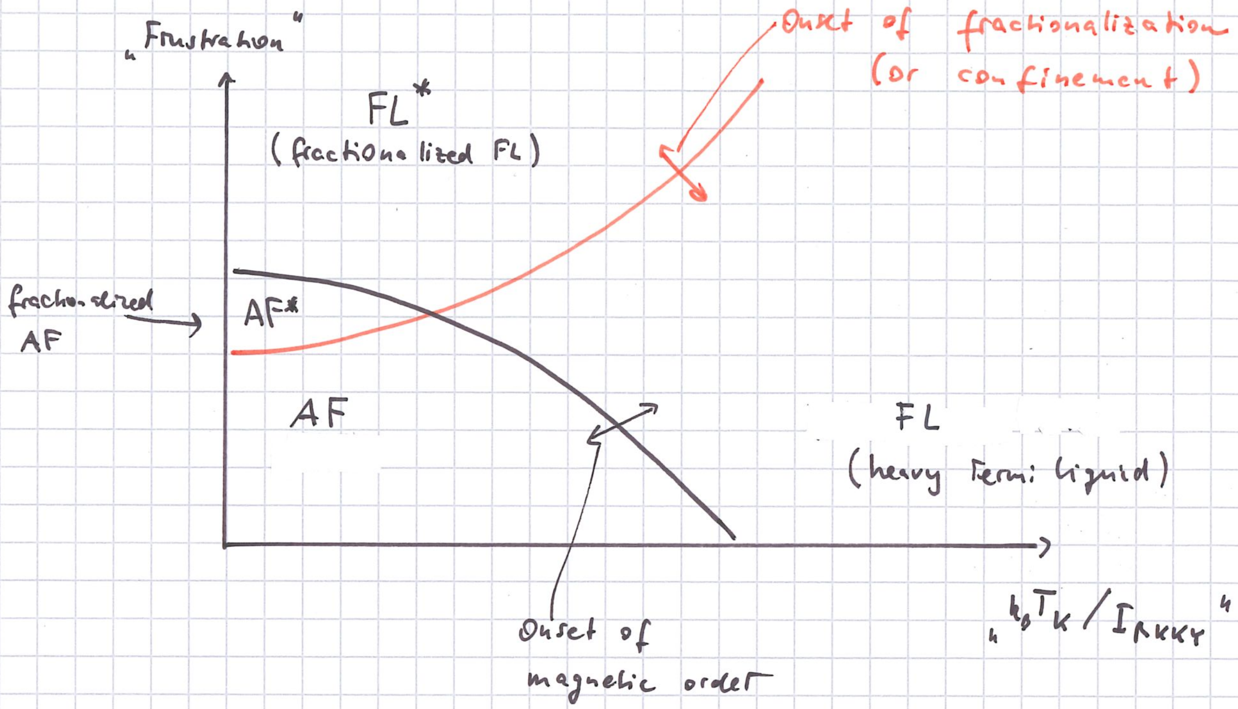
Kondo temperature: $k_B T_K \propto \exp\left(-\frac{1}{J \rho_0}\right)$

↷ Kondo screening wins at large J, RKKY wins at small J.

If RKKY wins but is strongly frustrated, the f moments may settle into a spin liquid. The resulting metal is a fractionalized Fermi liquid (FL*), see Sec 7.2.

7.4. Global phase diagrams (of Kondo lattices)

Kondo lattice, $T=0$, $\langle n_c \rangle \neq 1$ $\curvearrowright$ all phases metallic



Generically, two different types of transitions can occur:

- Onset of magnetic order $\hat{=}$ symmetry-breaking transition

- Onset of fractionalization / confinement $\hat{=}$ no symmetry breaking, but breakdown / onset of Kondo screening $\hat{=}$ jump in Fermi volume (recall: FL* violates Luttinger theorem)