Lecture III: Strong Correlation: Mott Transition

▷ References:

N. F. Mott, *Metal-Insulator Transitions*, Taylor-Francis 1990

P. W. Anderson, *Concepts in Solids*, Harwood Publishing

P. W. Anderson, *Local moments and localized states*, Rev. Mod. Phys. **50**, 191 (1978)

▷ Band theory of metals:

Completely filled and empty bands give insulating behaviour while partially filled bands conduct $\rightsquigarrow$ metals

H. Bethe, *Theory of the diffraction of electrons in crystals*, Ann. Phys. **87**, 5 (1928).

A. Sommerfeld, *An electronic theory of the metals based on Fermi's statistics. I. General consideration, conductivity and surface emission phenomena*, Z. Phys. **47**, 1 (1928).

F. Bloch, *The electron theory of ferromagnetism and electrical conductivity*, Z. Phys. **57**, 545 (1929).

Band picture consolidated with realisation that small band-gap materials could be made metallic by thermal excitation of carriers or chemical doping $\rightsquigarrow$ *semi-conductots*

A. H. Wilson, Proc. R. Soc. London, Ser. **A133**, 458 (1931); Proc. R. Soc. London, Ser. **A134**, 277 (1931).

R. H. Fowler, Proc. R. Soc. London, Ser. **A140**, 505 (1933); Proc. R. Soc. London, Ser. **A141**, 56 (1933).

However, early on, it was found that some compounds (e.g. Ni0) do not respect this classification:

J. H. de Boer and E. J. W. Verway, Proc. Phys. Soc. London, Sec. **A49**, 59 (1937).

Some materials which should involve a half-filled band (i.e. "one electron per site") behave as insulators

Following suggestion by Peierls,

R. Peierls, Proc. Phys. Soc. London, Ser. **A49**, 72 (1937).

> *"it is quite possible that the electrostatic interaction between the electrons prevents them from moving at all. At low temperatures the majority of the electrons are in their proper places in the ions. The minority which have happened to cross the potential barrier find therefore all the other atoms occupied, and in order to get through the lattice have to spend a long time in ions already occupied by other electrons. This needs a considerable addition of energy and so is extremely improbable at low temperatures."*

it was argued by Mott that strong electron correlations drive system insulating

N. F. Mott, Proc. Phys. Soc. London, Ser. **A62**, 416 (1949).

Qualitatively, behaviour can be understood from a "simple" model of strongly correlated electrons:

▷ <u>The Mott-Hubbard Model</u>

Consider lattice "tight-binding" Hamiltonian:

$$\hat{H}_0 = -t\sum_{\langle ij\rangle} c^\dagger_{i\sigma}c_{j\sigma} + \text{h.c.} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} n_{\mathbf{k}\sigma}$$

e.g. simple 2d cubic lattice $\epsilon_{\mathbf{k}} = -2t(\cos k_x a + \cos k_y a)$

together with local "on-site" interaction:

$$\hat{H}_I = U\sum_i n_{i\uparrow}n_{i\downarrow}$$

generally (and here) $U > 0 \quad \longleftrightarrow \quad$ Coulomb repulsion

Control parameters: U/t, temperature, electron density, (and dimensionality)

▷ Expected properties of the half-filled system (viz. $n = n_\uparrow + n_\downarrow = 1$):

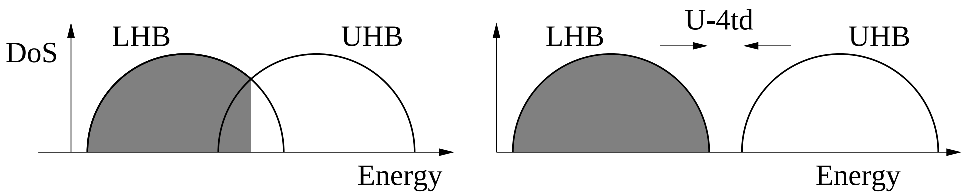
(i) $U/t \ll 1$ expect Fermi-liquid behaviour *(caveat: perfect "nesting" symmetry can induce weak transition to insulating spin or charge density wave — see below; also depends on dimensionality)*

(ii) $U/t \gg 1$ expect electrons to localise (one per atomic orbital). Since charge excitation involves site double occupancy (energy cost U), there is a charge gap $\rightsquigarrow$ <u>Mott insulator</u>.

▷ How does insulating phase (ii) develop from metallic phase (i)? — the <u>Mott transition</u>

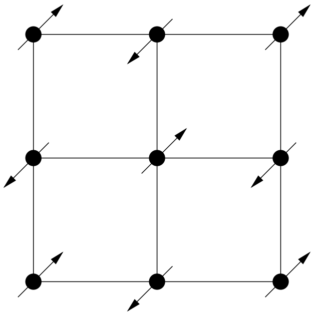
▷ Three principle and complementary ideas expounded in the literature

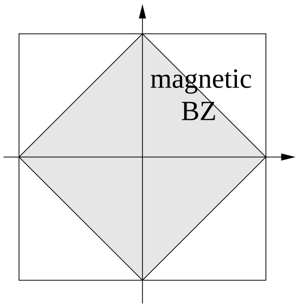
(a) Mott-Hubbard: rooted in a modified band picture



and not directly linked to any kind of magnetism...

(b) Slater: nesting symmetry $\rightsquigarrow$ development of (antiferro)magnetic order; splits the band and creates insulating phase (J. C. Slater, *Magnetic Effects and the Hartree-Fock Equation*, Phys. Rev. **82**, 538 (1951).)



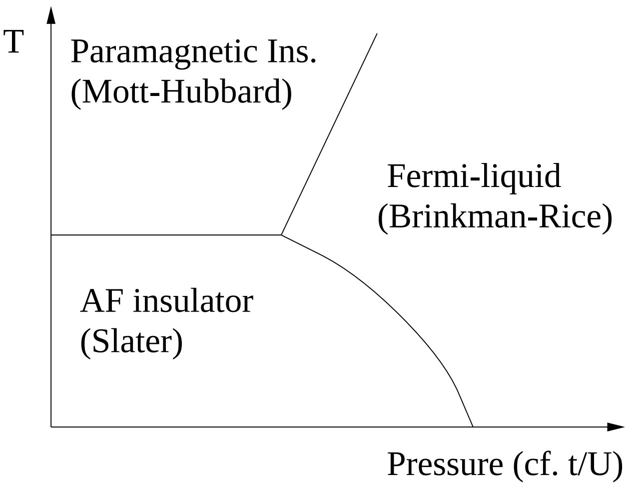


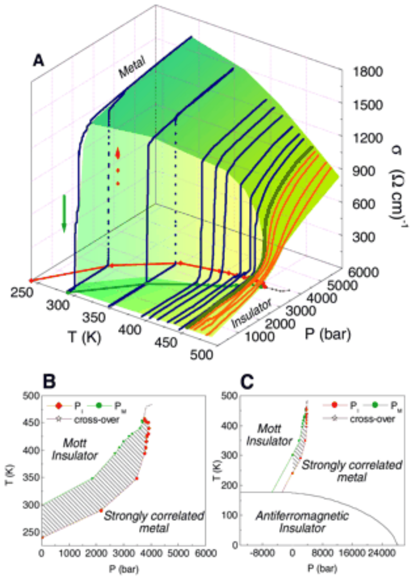
(c) Brinkman and Rice: seamless connection to Fermi-liquid theory through divergence of effective mass (W. F. Brinkman and T. M. Rice, *Application of Gutzwiller's Variational Method to the Metal-Insulator Transition*, Phys. Rev. B **2**, 4302 (1970).)

$$\frac{m^*}{m} \sim \frac{1}{U_{\text{crit}} - U}$$

▷ Which picture is correct? To some extent, all "phases" realized in experiment:

e.g. V_2O_3





At present, reliable theory largely unavailable

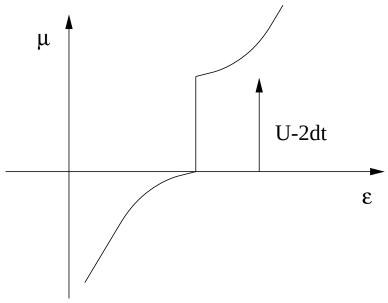
it remains one of the great outstanding problems of condensed mattter!

Some(?) intuition provided by "exact" solution in limit of infinite dimension (but poor description of magnetism)...

...and exact solution in one-dimension

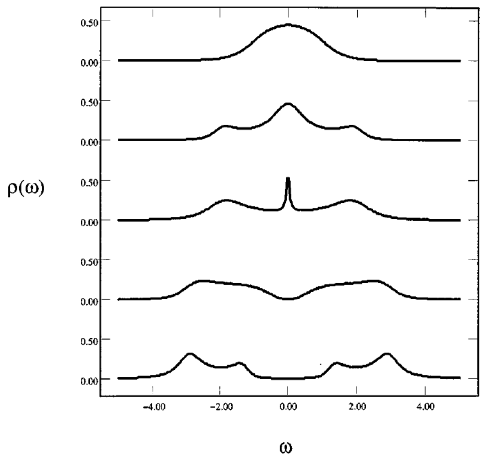
▷ Phase diagram away from half-filling?

Naively, one expects a jump in the chemical potential as one crosses the transition:



...with transition to metal when $U < 4dt$

However, bands change with density *(it is not a "rigid band system")*. In thermodynamic limit, the jump (if it exists) may not correspond directly to the Hubbard gap (e.g. as seen in the $d = \infty$ system, mid-gap states could emerge)



In 1d: obtain a Luttinger liquid for $n \neq 1$ (see later lectures)

In 2d: it has been suggested (notably by Anderson) that the doped Mott insulator may, indeed, not be a Fermi-liquid at all!

▷ Nature of Mott insulating state ($n = 1, U/t \gg 1$)?

Suppose one electron per site ⇝ massive 2^N spin degeneracy — lifted at second order of perturbation theory...

In limit $U/t \gg 1$, can treat

$$\hat{H}_0 = -t \sum_{\langle ij \rangle} c^\dagger_{i\sigma} c_{j\sigma} + \text{h.c.}$$

as perturbation on local Hubbard interaction $\hat{H}_I = U \sum_i n_{i\uparrow} n_{i\downarrow}$:

$$\Delta E = -\langle \psi_0 | \hat{H}_0 \frac{1}{\epsilon_0 - \hat{H}_I} \hat{H}_0 | \psi_0 \rangle$$

What intuition is provided by "two-site" problem?:

same spin: $\quad \uparrow_1 \quad \uparrow_2 \quad \longrightarrow \quad$ frozen (Pauli exclusion)

opposite spin: $\quad \uparrow_1 \quad \downarrow_2 \quad \xrightarrow{\hat{H}_0} \quad \overbrace{0_1 \qquad \uparrow\downarrow_2}^{\frac{1}{\epsilon_0 - \hat{H}_I}} \quad \xrightarrow{\hat{H}_0} \quad \begin{cases} \uparrow_1 & \downarrow_2 \\ -\downarrow_1 & \uparrow_2 \end{cases}$

note sign change due to exchange

...in operator form, using the identity,

$$\hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 = -\frac{1}{2} c^\dagger_{1\alpha} c^\dagger_{2\beta} c_{1\beta} c_{2\alpha} - \frac{1}{4} \hat{n}_1 \hat{n}_2$$

obtain (exercise)

$$\hat{H} = J \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 - \frac{J}{4}, \qquad J = \frac{4t^2}{U} > 0$$

i.e. an antiferromagnetic exchange interaction of spins

eigenstates:

$$\begin{array}{lll} S = 1 & \text{triplet} & \begin{cases} |\uparrow\uparrow\rangle & S_z = 1 \\ \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) & S_z = 0 \\ |\downarrow\downarrow\rangle & S_z = -1 \end{cases} \\ S = 0 & \text{singlet} & \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \qquad S_z = 0 \end{array}$$

ground state is a singlet with energy $E = -\frac{3J}{4}$

▷ *Note that, unlike a ferromagnetic interaction (viz. $J < 0$), the classical ground state ($|\uparrow\downarrow\rangle$ or $|\downarrow\uparrow\rangle$) is not, by itself, an eigenstate — consequence of non-trivial zero-point energy*

▷ Generalised to many-site system, effective Hamiltonian of insulating phase given (up to irrelevant constant) by the quantum spin 1/2 antiferromagnetic Heisenberg Hamiltonian

$$\hat{H} = J \sum_{\langle ij \rangle} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j$$

▷ Nature of ground state?

For a time, it was thought that zero-point fluctuations might destroy AF ordered phase even at $T = 0$!

In fact, ground state usually ordered but depends sensitively on lattice geometry, and dimensionality (see next lecture)

Doping away from half-filling? Lattice $t - J$ Hamiltonian

$\hat{P}_s$ — projection onto singly occupied sub-space

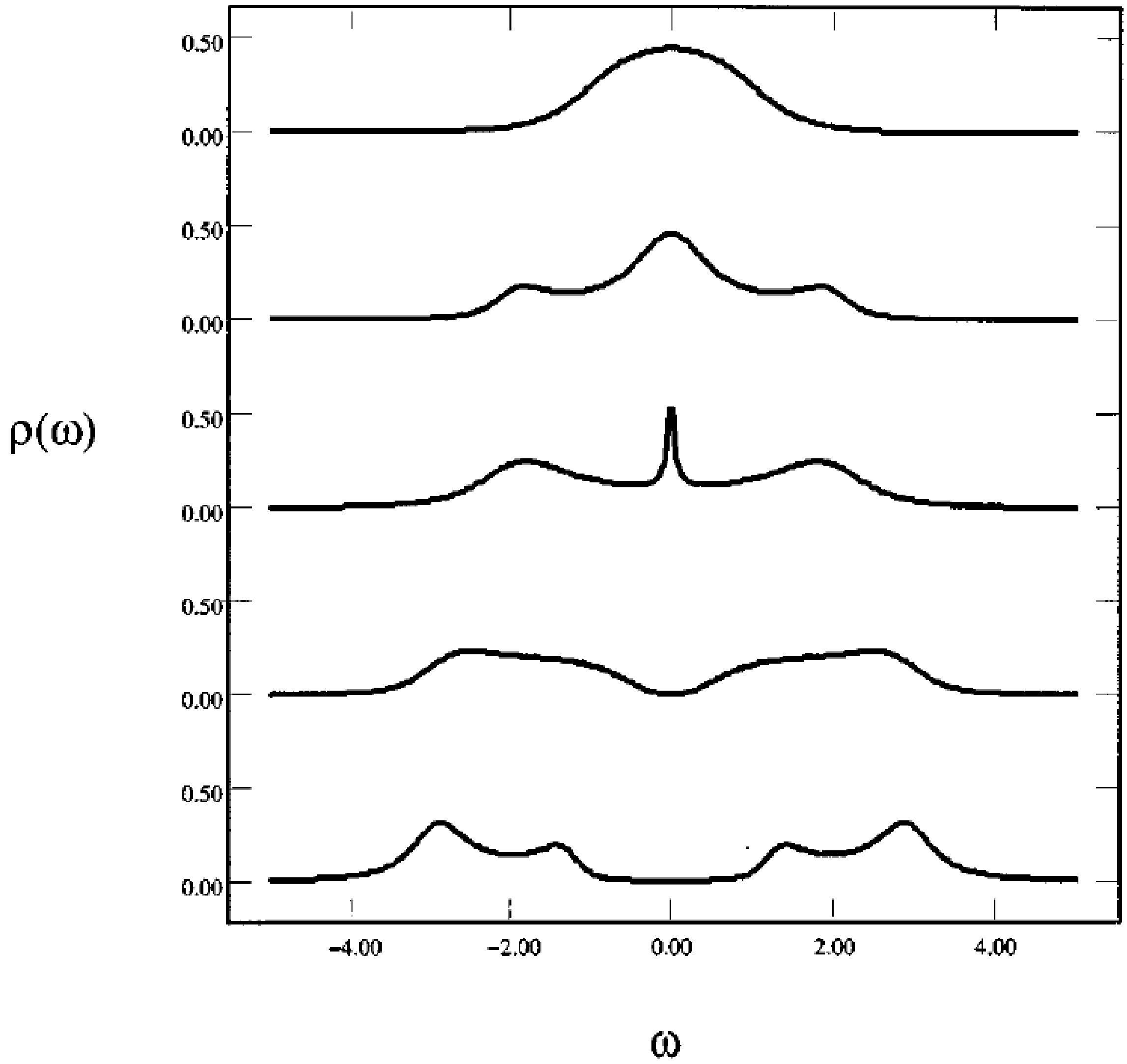
$$\hat{H} = -t \sum_{\langle ij \rangle} \hat{P}_s c^\dagger_{i\sigma} c_{j\sigma} \hat{P}_s + J \sum_{\langle ij \rangle} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j$$

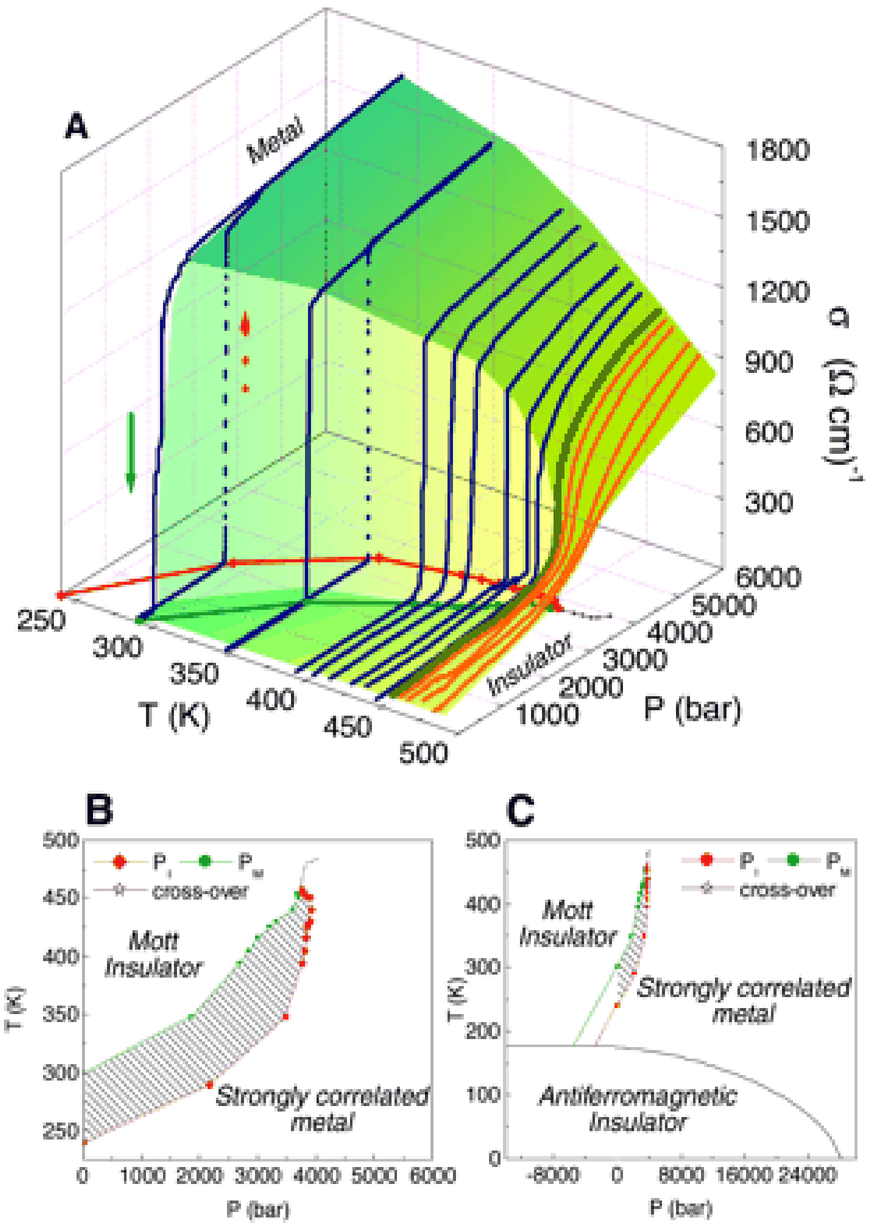
phase diagram? (lesson from cuprates?)

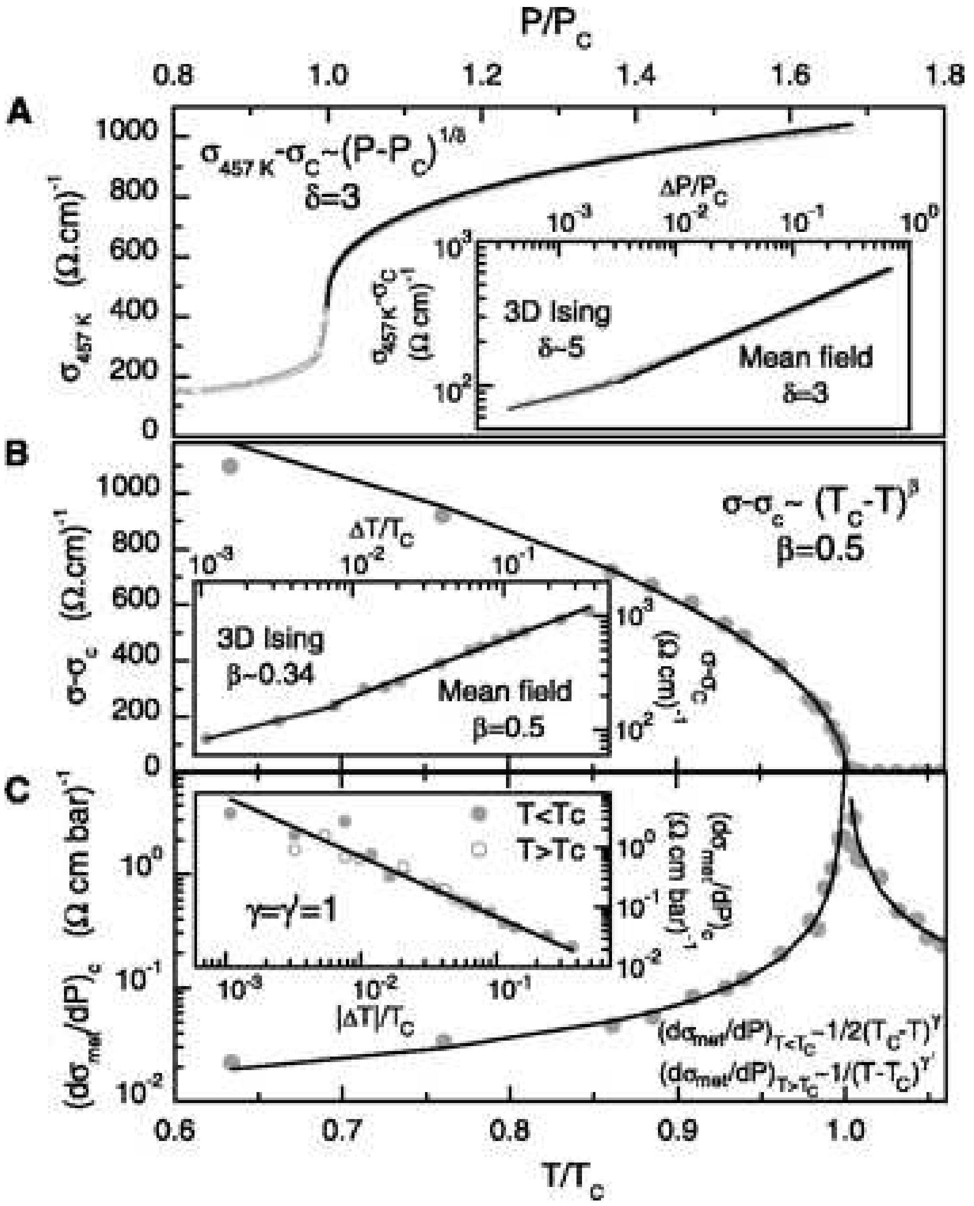
▷ Summary: In the half-filled system, strong electron interaction leads to

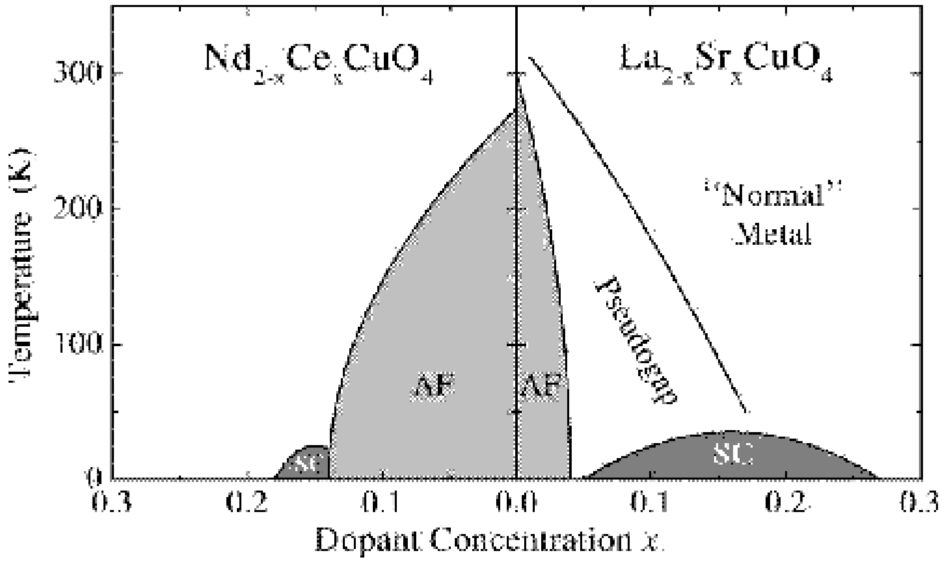
- Mott transition to insulating phase;
- formation of local magnetic moments;
- with a quantum AF ground state *(cf. tendency of Hund's rule in atoms which favours ferromagnetic correlations — exercise: why the difference?)*

According to classification in lecture 1., development of magnetic state, which involves breaking of continuous spin symmetry, should be accompanied by appearance of low-energy collective excitations — spin waves. Goal of next lecture is to explore nature of spin wave excitations in the magnetic state


ρ(ω)
0.50
0.00
0.50
0.00
0.50
0.00
0.50
0.00
0.50
0.00
-4.00
-2.00
0.00
2.00
4.00
ω


A
Metal
Insulator
1800
1500
1200
900
600
300
σ (Ω cm)$^{-1}$
250
300
350
400
450
500
T (K)
1000
2000
3000
4000
5000
6000
P (bar)
B
Mott Insulator
Strongly correlated metal
cross-over
T (K)
P (bar)
C
Mott Insulator
Strongly correlated metal
Antiferromagnetic Insulator
cross-over
T (K)
P (bar)


P/P_C
A
$\sigma_{457\,K}-\sigma_C \sim (P-P_C)^{1/\delta}$
δ=3
ΔP/P_C
3D Ising
δ~5
Mean field
δ=3
B
$\sigma-\sigma_c \sim (T_C-T)^\beta$
β=0.5
ΔT/T_C
3D Ising
β~0.34
Mean field
β=0.5
C
T<Tc
T>Tc
γ=γ′=1
|ΔT|/T_C
$(d\sigma_{met}/dP)_{T<T_C} \sim 1/2(T_C-T)^\gamma$
$(d\sigma_{met}/dP)_{T>T_C} \sim 1/(T-T_C)^{\gamma'}$
T/T_C



$Nd_{2-x}Ce_xCuO_4$
$La_{2-x}Sr_xCuO_4$
"Normal" Metal
Pseudogap
AF
AF
SC
SC
Temperature (K)
300
200
100
0
0.3
0.2
0.1
0.0
0.1
0.2
0.3
Dopant Concentration x