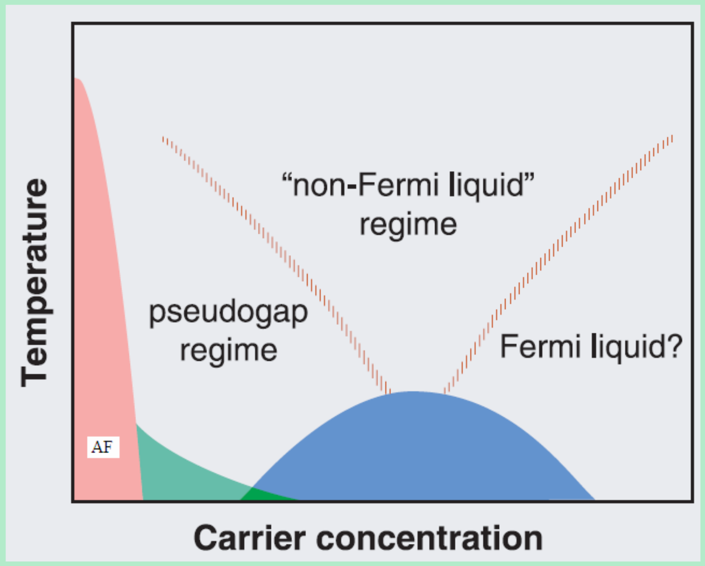
An introduction to High Temperature Superconductors



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Overview

- Recap
- Cuprate Electronic Structure – Models
- Cuprate Phase Diagram
  - *AF Mott Insulator*
  - *Superconducting Regime*
    - Under-doped
    - Optimally doped
    - Over-doped
- Resonating Valence Bond (RVB) picture – A simple explanation of Pseudogap

Recap: Free Fermi Gas

$$H = \sum_{i=1}^{n} \frac{p_i^2}{2m}$$

- Describes a collection of particles with momenta $\mathbf{p_i}$ and energy, E_i
- Since there is translational invariance, **p** is a good quantum number, electrons occupy **p** states following Pauli – Total Energy(E_F) Contour – Fermi-surface (FS)– Ground State.
- **Excitations :** Remove an electron from $k < k_F$, thus creating a hole there and placing it arbitrarily close to FS – Particle-hole excitation – *Gapless*
- **Specific Heat :** Only a fraction of electrons α T can get thermally activated. Thus U α $T.k_BT \rightarrow$ $\mathbf{C_v = \gamma T\ (\gamma\ \alpha\ g_0)}$
- **Magnetic Susceptibility :** constant α g_0 *(Pauli Paramagnet)*
- **Infinite Electrical Conductivity –** In presence of scatterers – Drude Formula

Recap : Landau Quasi-particle Idea

- A "particle" is an entity which has a well-defined energy for a given momentum.
- What if we add Interactions between electrons?
- **Landau's Idea** –one-to-one correspondence between states of non-interacting system to states of interacting system – No level crossing – Momentum still a good quantum number – An electron in a state is given a new dress by co-workers – **"Quasi-particle" or "collective excitation"**
- Example - Screening – An electron gets screened from other by those near it – For others, it is still a particle but has wore a new dress – "Quasi-particle"
- Interactions remove particles from certain eigen-states of a non-interacting Hamiltonian and put it into some other state – thus gives a life-time to the state.
- Thus, a quasi-particle is a "particle" with a finite life-time.

Recap : Superconductivity

- Superconductivity –resistivity of certain elements/compounds goes to zero on cooling through a critical temperature, T_c.
- Superconductors do not allow any magnetic field to penetrate through – Meissner effect
- High T_c Superconductivity
  - T_c was stuck at 23K till 1986, when Bednorz and Mueller discovered SC in certain transition metal oxide at 30K.
  - Very next year, Wu et al. discovered SC in YBCO above boiling point of Nitrogen – Study made easy
  - Not only technological importance – but show novel physics which challenged all existing notions of condensed matter

Types of Superconductors

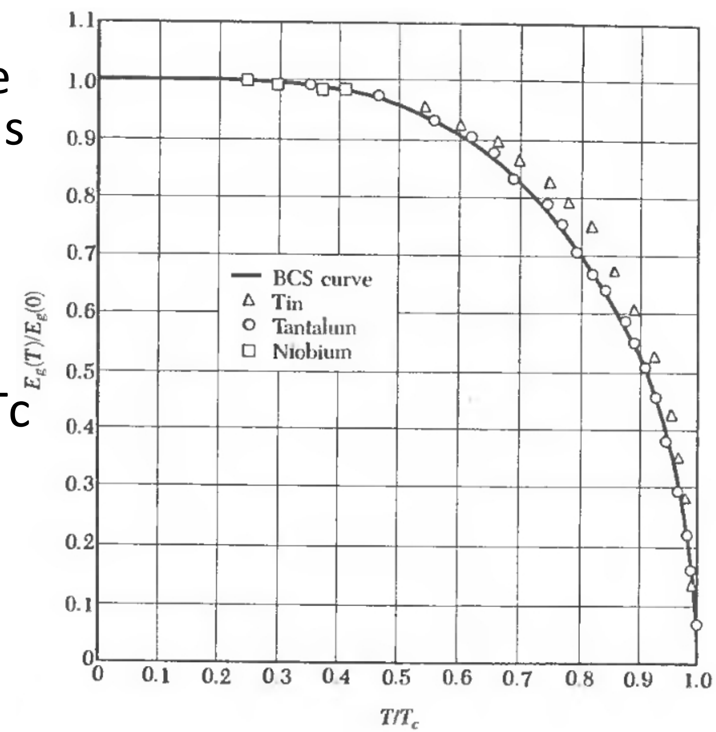
- ***Type I SC*** – As H is increased, M becomes zero at a critical field H_c.
- ***Type II SC*** – Two critical H_c – H_{c1} & H_{c2}. As H goes past H_{c1}, magnetic field lines penetrates in bundles (vortex). There can be surface currents on both sides of vortex. As H goes past H_{c2}, vortices come closer and kill SC – High Tc SC falls into this category.
- ***Important Length Scales***
  - *Coherence Length, ξ* – measure of the distance within which the SC electron concentration cannot change drastically in a spatially varying field.
  - *Penetration Depth*, λ – Magnetic field inside SC falls off exponentially over this length scale
- For SC and magnetic fields to coexist – $\lambda > \xi$
- Define Landau-Ginzburg constant, $\kappa = \lambda / \xi$, $\kappa_c = 0.707$
- $\kappa < \kappa_c$, field will not penetrate far enough to affect electrons within coherence length – Type I superconductivity
- $\kappa > \kappa_c$, superconductivity confined to small coherence length s.t. it can coexist with nearby magnetic field which has penetrated the material – Type II Superconductivity

Recap : Superconductivity

- Below Tc, entropy of SC state slightly lower than that of normal state –
  - *SC state more ordered than normal state*
  - *Only small fraction of electrons involved in SC – "super" electrons*
- Low T C_v exponential – *Excitations are gapped*
- Theories (Chronological Order)
  - *London Phenomenological Theory*
    - ✓ Postulate – Superconducting current is proportional to vector potential
    - ✓ Explains Meissner effect
  - *G-L Theory*
    - ✓ Extension of London theory
    - ✓ Phenomenological Order parameter, ns – explains critical behavior
    - ✓ Naturally incorporates type II superconductivity
  - *BCS Theory*

BCS Theory (1957)

- T_c depends on isotope mass of A cation – Phonons at play !
- ***BCS Theory*** based on phonon mediated electron-electron attraction has been extremely successful
- Cooper – Any attractive interaction between electrons outside Fermi surface will produce a bound state – Cooper pair
- There is a pairing wave-function which has an amplitude and a phase. The wave function has zero total angular momentum and thus, s-wave symmetry.
- In super-conducting state, the phase of all the pairs gets fixed and electrons move as a coherent cloud – zero resistance
- Gap arises as finite energy is required to break electron pairs.
- Gap goes smoothly to zero as T $\longrightarrow$ Tc – Second Order transition



Standard Results Summary

Property	Fermi Liquid	BCS Superconductors
Excitations	Gapless	Gapped
Specific Heat	$\sim T$	$\sim Exp(-\Delta/K_B T)$
Electrical Conductivity	$\sim T^2$	∞
Magnetism	Pauli Paramagnet	Diamagnet
	(non-zero Constant)	

Recap : Spectral Function

- For non-interacting case,

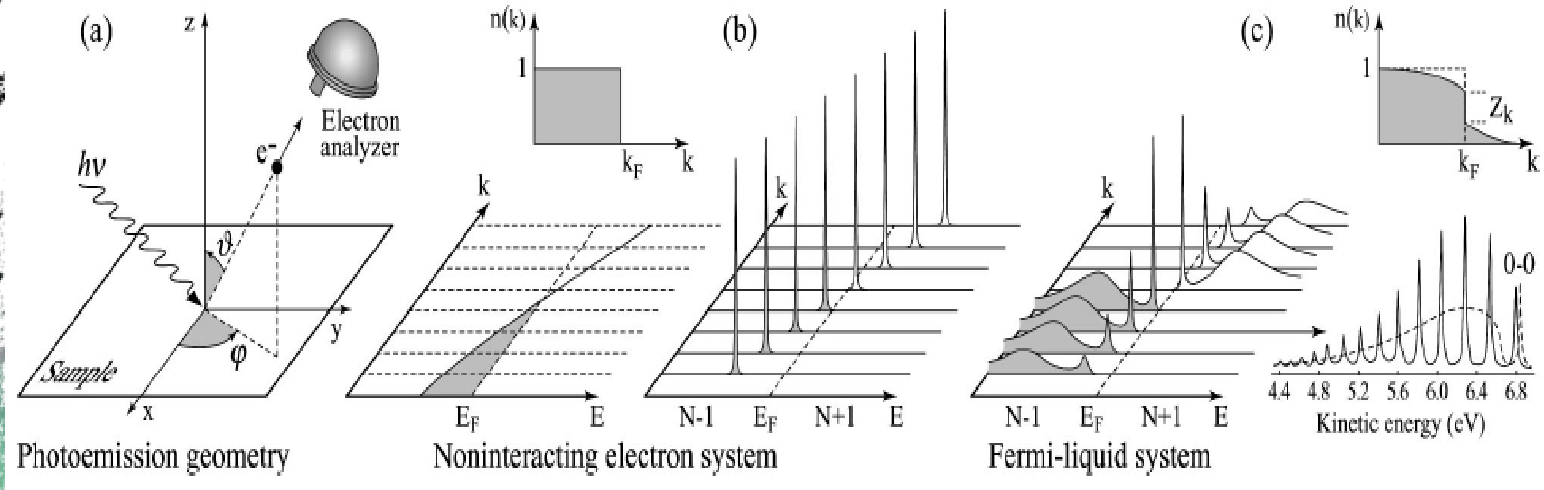
  Probability that state α has energy ω - Spectral function

- whenever Greens function has pole on negative imaginary axis or Spectral function has a Lorentzian part, We have a state which has life-time, $1/\Gamma$ and there are Quasi-particles excitations. These are particles which have well-defined energy dispersion and a finite lifetime (so that they can be observed).

- Many body Spectral Function, A(**k,** ω) measures the probability that an excitation (particle or hole) added to the **k**-state has energy ω – generalization of non-interacting DOS

- Spectral function for
  - *Free Fermi Gas – Delta function peaked at* $\xi_{\boldsymbol{k}}$
  - *BCS Superconductor* **–** *Two Delta functions peaked at +,-* E_k *– One for particle addition and other for hole addition (pair breaking)*

Angle Resolved Photoemission Spectroscopy (ARPES)

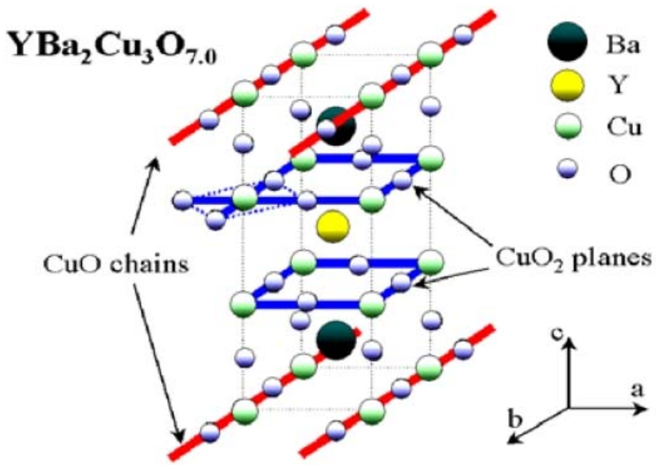


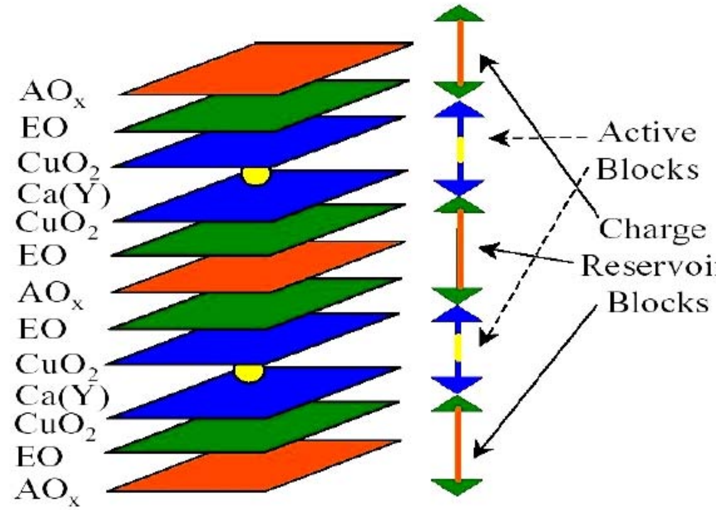
- Technique to measure $A^{-}(\mathbf{k},\omega)$
- A monochromatic radiation is incident on properly aligned single crystal sample – Emission of Photoelectrons – collected by Electron Analyzer – E_{kin} & **p** observed.
- Energy-momentum conservation :

$$E_{kin} = \hbar\nu - \phi - |E_B|$$
$$p_{||} = \hbar k_{||} = \sqrt{2mE_{kin}}\sin\vartheta$$

- Photon momentum & k_{perp} neglected – photon energies kept small to obtain good resolution - 2D Geometry
- Intensity is plotted as a f^n of E_B for fixed **k**

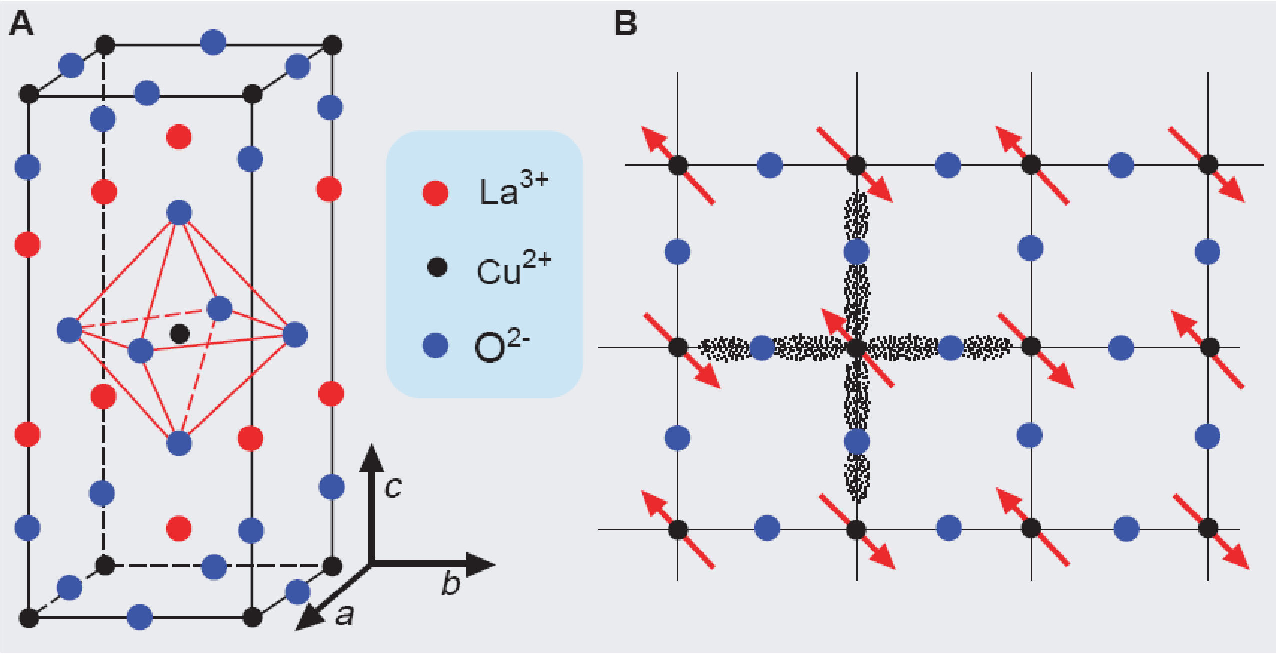
Cuprates: Material





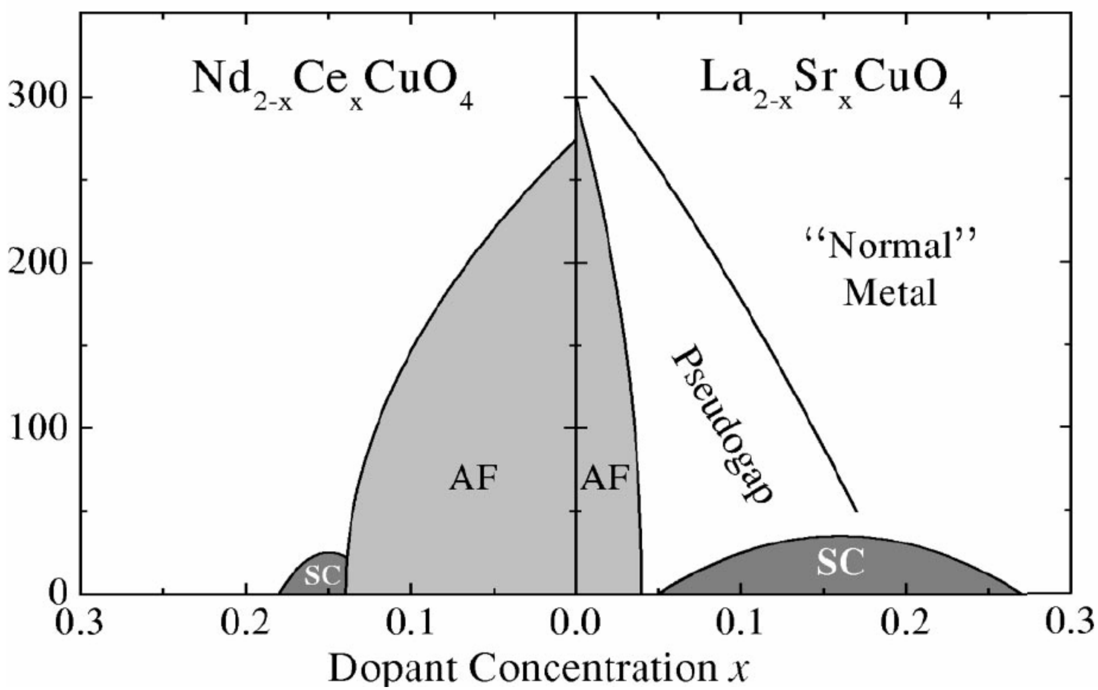
- Two sub-units – Active Blocks & Charge Reservoir Blocks
- *"Active Block"* – $(CuO_2/Ca/)_{n-1}CuO_2$ – Mobile Carriers Workspace
- *"Charge Reservoir Block"* - $EO/(AO_x)_mEO$
  - Storage for dopants
  - Provide Doping Charge
  - A = (Bi, Pb, Tl, Hg, Au, Cu, Ca, B, Al, Ga)
  - E=Alkaline Earth Metal (Sr, Ba)
- General Formula – $A_mE_2Ca_{n-1}Cu_nO_{2n+2+mx}$ – Terminology: A-m2(n-1)n
- Examples – $Bi_2Sr_2Ca_2Cu_3O_{10}$ – Bi-2223, $Y_1Ba_2Cu_3O_7$ – Y-1223

0210 compounds



- E_2Cu0_4 - La_2Cu0_4, Nd_2Cu0_4
- Key Structural Unit – CuO_2 planes with weak inter-planar coupling
- Hole Doping: Replace x fraction of La^{3+} with Sr^{2+} - Result: x holes per Cu
- Cu^{2+} - d^9 – Spin ½ on a planar square lattice
- Spins arrange in AF fashion to gain KE through Super-exchange.
- Electron Doping: Replace x fraction of Nd^{3+} with Ce^{4+} - Result: x e^- per Cu

Cuprates Phase Diagram

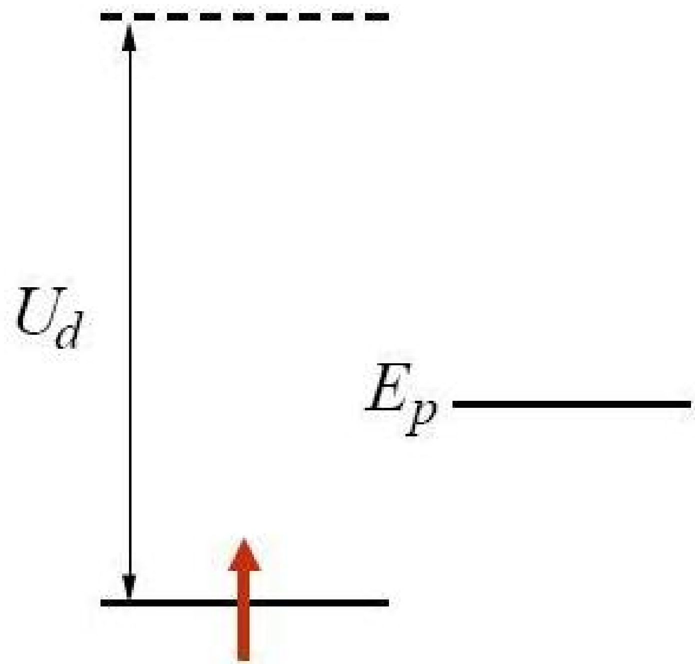


- Shows very rich phase diagram as a function of Doping
- AF Mott Insulator for small doping
- On further doping – SC
- Doping at which maximal T_C occurs – optimal doping.
- Lower dopings – Under-doping and Higher dopings- Over-doping
- Transition to "Strange" or "Normal" metal for $T > T_C$
- Exotic Pseudogap phase between AF and SC phases.

Electronic Structure

- Cu^{2+} is in d^9 configuration – octahedron environment of O^{2-}
- Jahn-Teller distortion of octahedron due to shift of apical oxygen splits the e_g orbitals – highest occupied orbital is $d_{x^2-y^2}$
- Thus Important degrees of freedom - $d_{x^2-y^2}$, p_x, p_y orbitals and a spin ½ at each site – 2d physics.
- Thus, a natural description – so called 3 band model
- Cu orbital is singly occupied, while oxygen orbitals are doubly occupied – finite hopping integral between Cu and oxygen orbitals

Energy Scales in 3 band Model



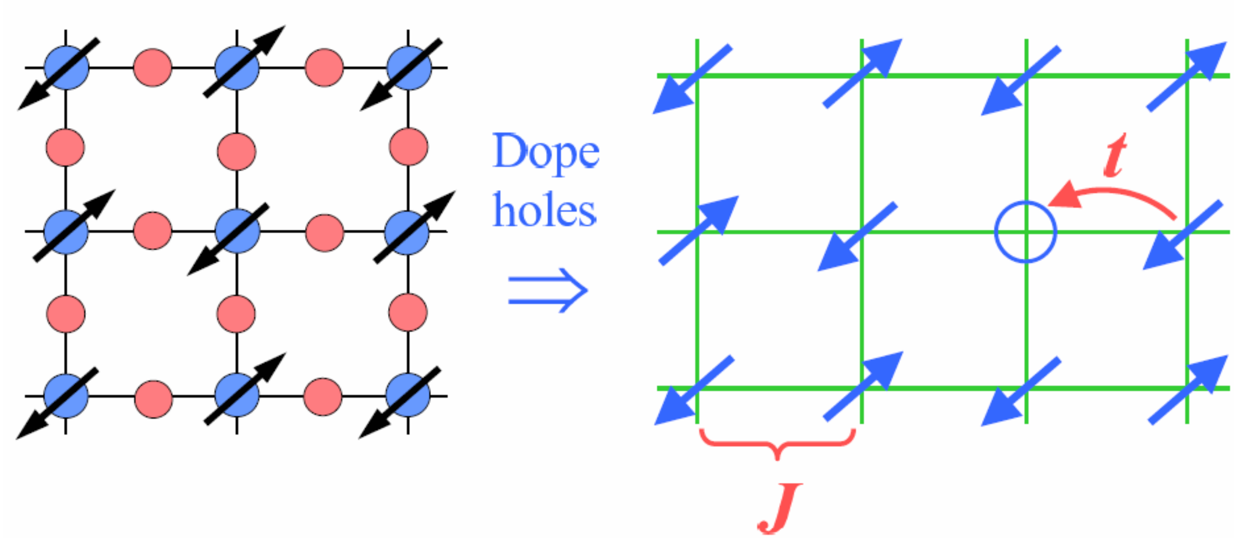
- Consider hole picture, Cu orbital occupied by a single hole with S = ½ and no hole on Oxygen p-orbital
- Cost for double occupancy – U_d (Much Larger than any other scale)
- Energy difference between p- and d- orbitals – E_p
- Hopping between p- and d-orbitals – t_{pd}
- If $t_{pd} << E_p$, the hole will form a local moment on Cu – Charge Transfer Insulator. Experimentally, Gap = 2.0 eV.
- Also, U_d is very high – All Cu sites has exactly one hole – Mott Insulator. Spins are localized in space.

3 band Model to t-J model

- Effective hopping between two Cu sites via oxygen sites $t = \frac{t_{pd}^2}{E_p}$
- Super-exchange mechanism gives rise to anti-ferromagnetic exchange between Cu spins $J = \frac{t^2}{E_p}$
- *J* is found to be 0.13 eV – Largest exchange interaction known
- Thus, we have anti-ferromagnetic Mott Insulator at zero doping.
- This gives rise to the celebrated t-J model –

$$H = P(-\sum_{<ij>,\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + J \sum_{<ij>} \vec{S}_i \cdot \vec{S}_j) P$$

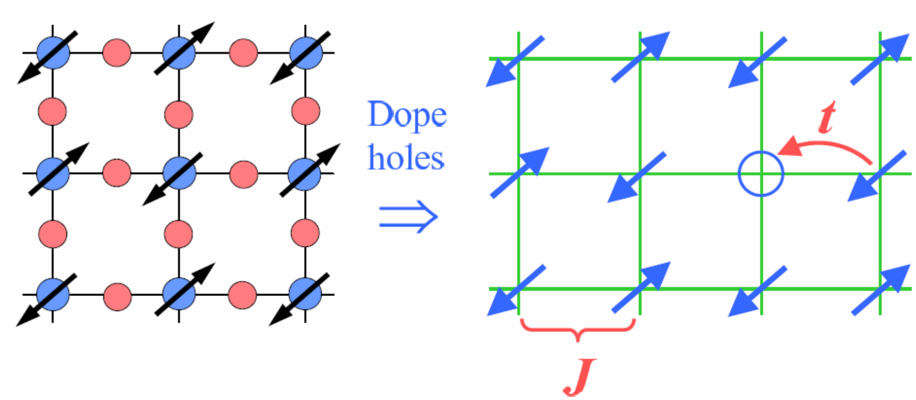
- P projects Hamiltonian on sub-space of no site double occupancy



t-J model

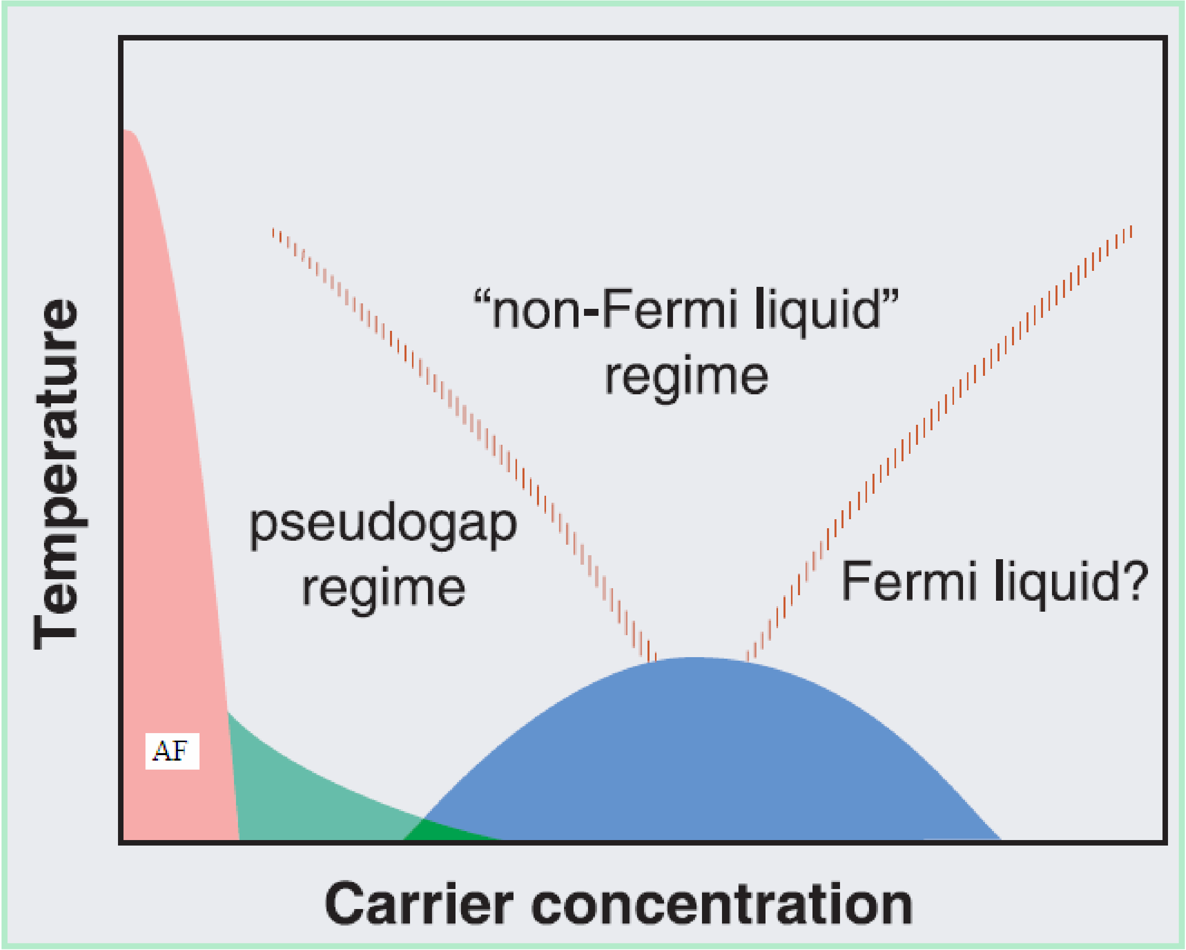
- When a hole is introduced into the system, it resides on Oxygen site due to large on-site Coulomb energy
- Doped hole resonates on 4 oxygen sites surrounding Cu – Spin of doped hole forms singlet with spin on Cu site – **Zhang-Rice singlet**
- In case of hole doping, Z-R singlet is the hopping entity.
- When an electron is doped into the system, it is equivalent to removal of a hole from Cu site. This hole vacancy can hop with t_{eff}
- Thus, in case of electron doping, doped electron is the hopping entity
- AF exists for much larger doping in electron doped compounds than hole doped compounds – Low SC transition temperature - No Pseudogap regime
- Viewpoint – Strongly correlated t-J model on a planar square lattice contains physics of High temperature superconductivity. It is equivalent to that of doping of a Mott Insulator.

Effect of Hole Doping



- A Doped hole likes to hop to lower its K.E.
- After 1 hop, it find itself in a ferromagnetic background
- Costs energy – Holes very effective in destroying AF
- Competition between t and J gives the phase diagram
- For xt >> J, K.E. should win – Fermi Liquid is expected as found.
- For xt ≤ J, Interesting physics – Low doping AF, SC for larger doping

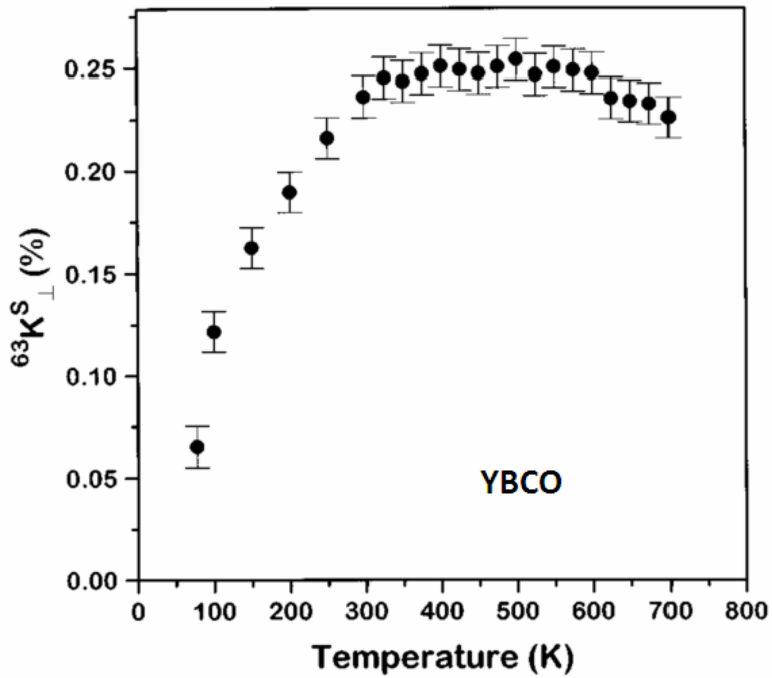
Superconducting regime

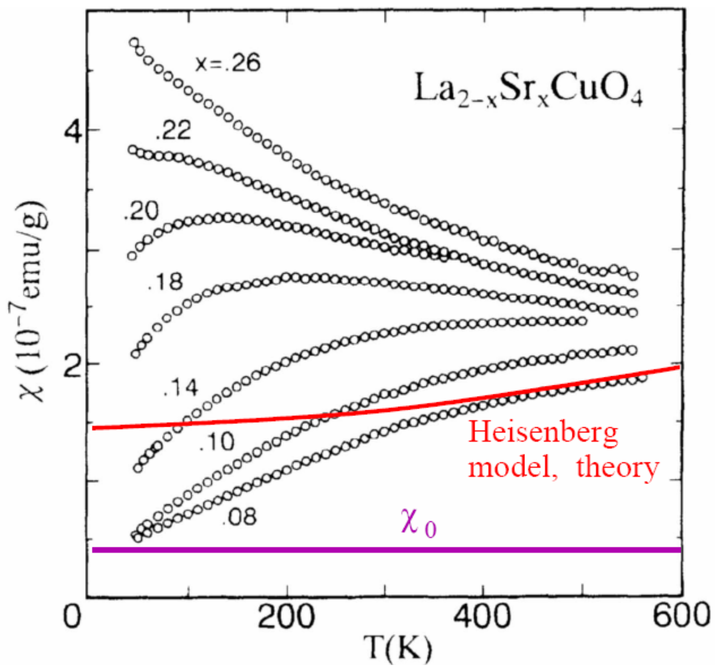


Superconducting state

- Doping range – $0.05 < x < 0.25$
- Underdoped - T_c increases with x
- Optimally doped – T_c largest
- Overdoped – T_c falling with x
- Well defined quasi-particles in the SC state
- Under-doped Normal State – Pseudogap, Optimally doped Normal State – “Strange Metal”, Overdoped Normal State – Fermi Liquid

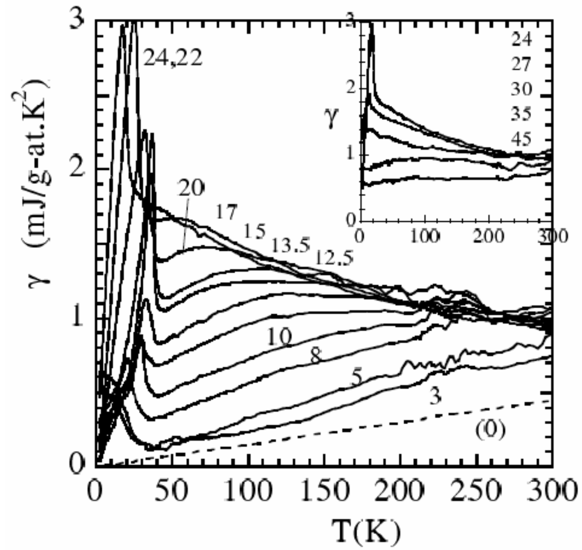
Pseudo Gap State: Knight Shift





- Knight Shift, K in NMR frequency – due to Conduction electrons – determines Susceptibility – should be constant for metals
- In under-doped YBCO, K is constant for high T - starts to come down well above $(Tc)^{max}$ – Quite Universal (See LSCO)
- Susceptibility falls well below that predicted by Heisenberg theory at zero doping – this reduction cannot be understood as fluctuations towards the anti-ferromagnet.
- This points to Singlet Formation and remarkably above critical temperature – Under-doped Normal state – Quite Abnormal !

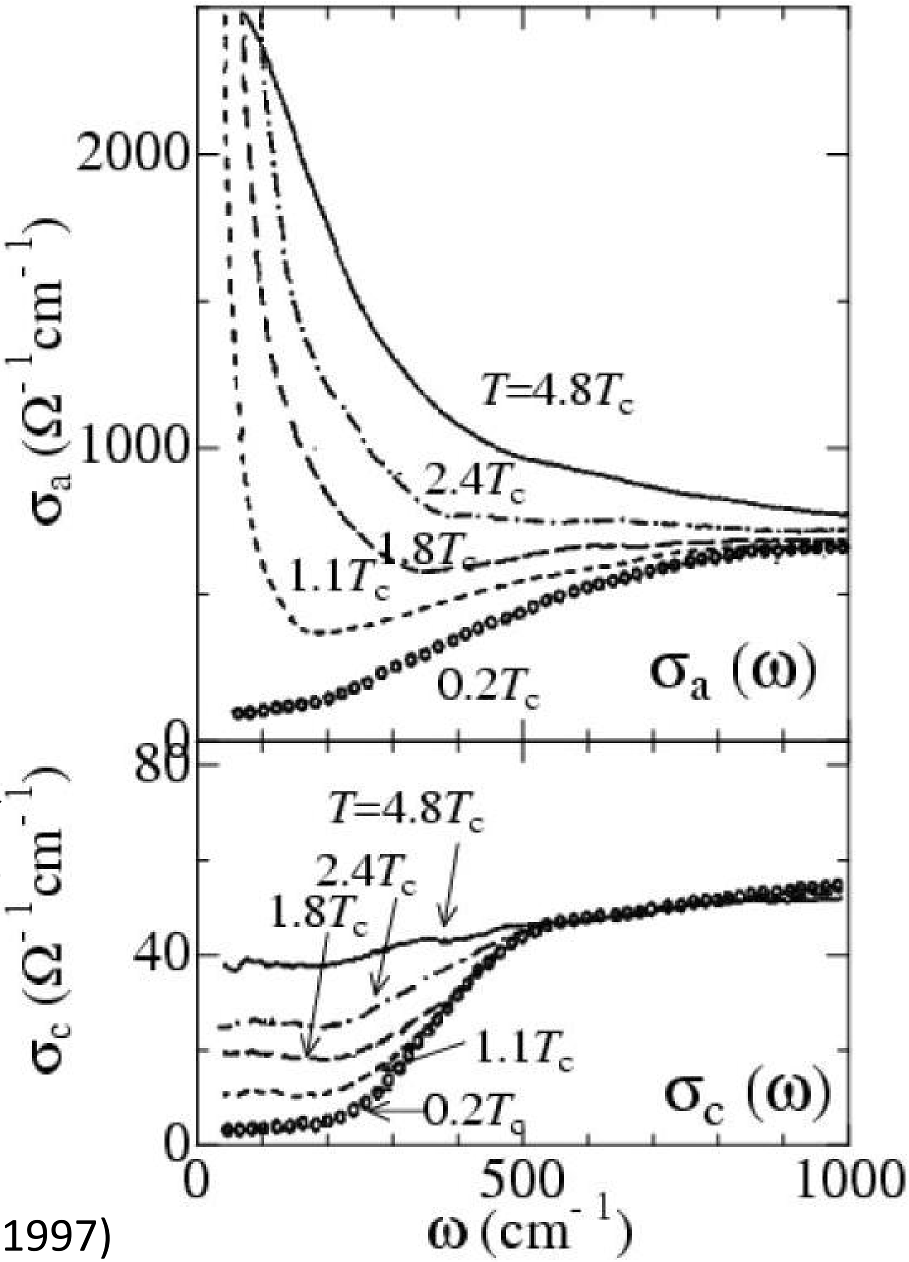
Pseudo Gap: Specific Heat



- γ – Linear T Coefficient of Specific Heat
- Shows marked decrease below room T which is above T_c (Compare inset pictures for optimal and over-doped regimes)
- This also suggests that spins are forming singlets and thus, spin entropy is gradually getting lost resulting in remarkable specific heat reduction
- Specific heat Jump at T_c - greatly reduced with decreasing doping

Pseudo Gap - Transport

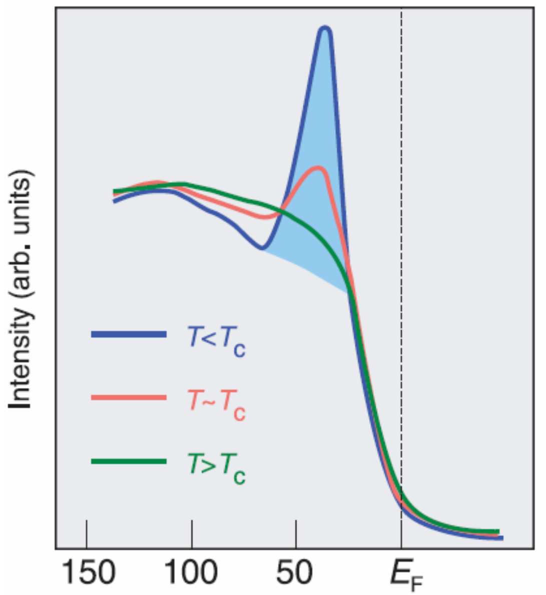
- At low ω, σ_{ab} shows Drude-like behavior – Width increases while Area decreases as temperature increases
- No sign of pseudogap – gap appearance in metals (CDW/SDW) – redistribution of area from Drude part to higher frequencies
- Area α doping, *x*. In SC state – delta function peak, ns/m α *x* – only doped holes contribute
- σ_c suggest gap for transport



YBCO (Uchida 1997)

Pseudo Gap – ARPES

- Along (0,π) direction, a gap exists (suppression of intensity at low energies) even above T_c though no QP excitations
- On lowering temperature through T_c, SC QP peak appears at the gap edge.
- Sharp QP excitations along (π, π) direction above and below T_c

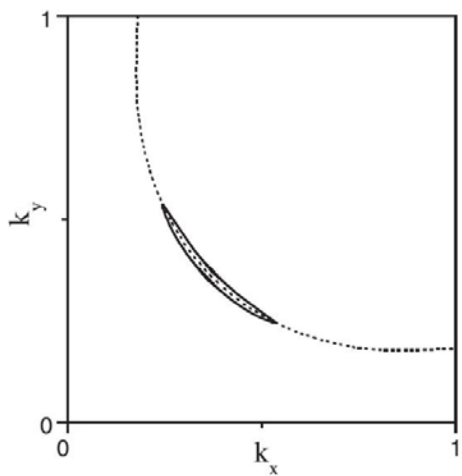


Pseudo Gap: Fermi Arc

- Fermi Surface (FS) obtained by finding k-points corresponding to minimum excitation energy.
- Below T_c, along FS, Gap shows d-wave symmetry - d-wave superconductor

$$\Delta(\vec{k}) = \Delta(\cos(kx) - \cos(ky))$$

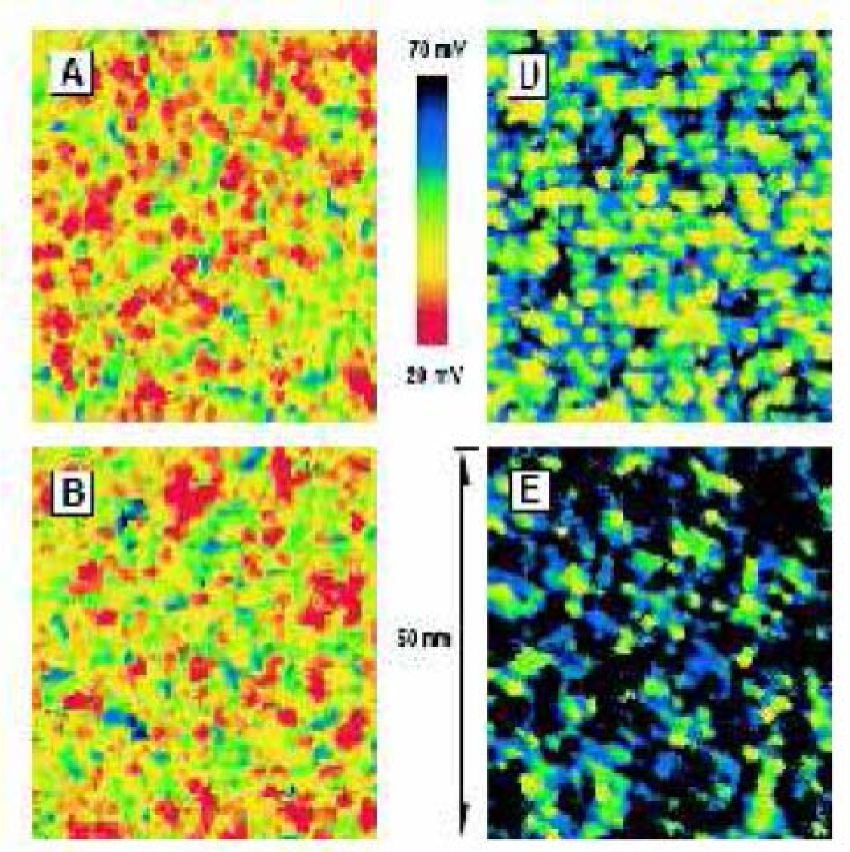
- Gap Vanishes along line joining (0,0) and (π, π) – Nodal QP
- Gap maximum at (0,π) - Anti-nodal QP
- For T>Tc: Gapless region expands to cover finite region near Nodal point – A Fermi surface or Fermi Arcs ? !!



Norman & Pepin 2003

Low Temperature STM

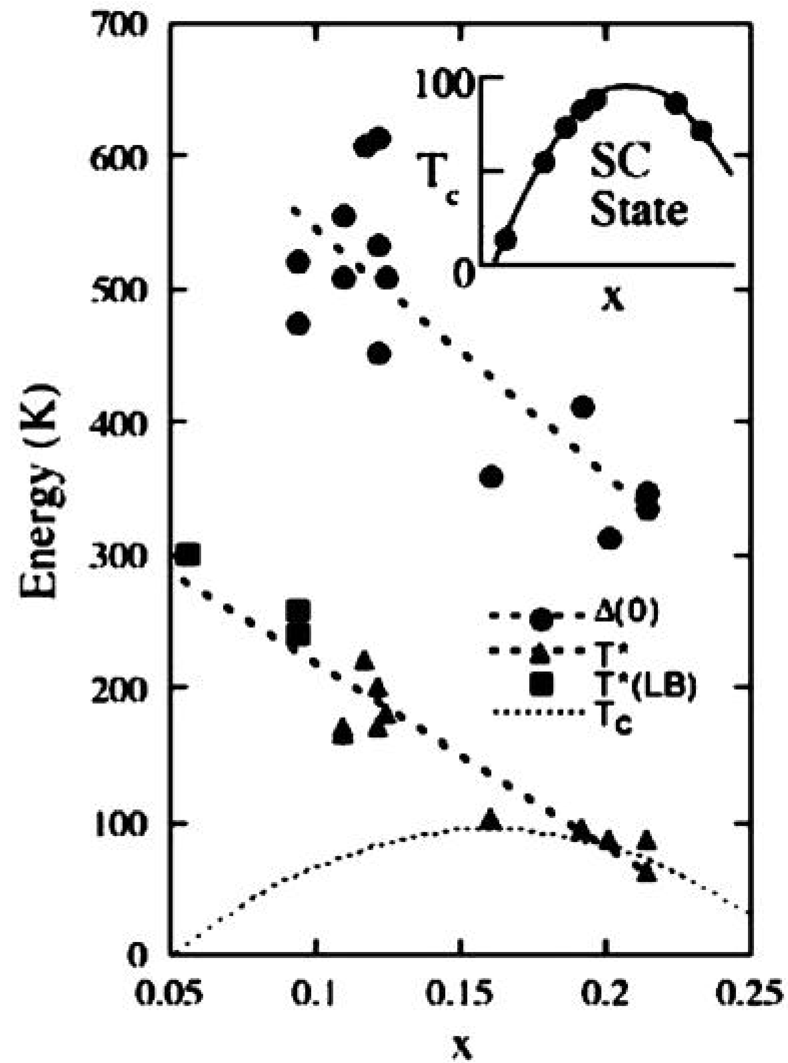
- STM gives real space information about local DOS which shows light on SC gap.
- Spatial inhomogeneity (length scales - 5-10 nm) – becomes more and more significant on underdoping
- Low lying DOS is homogeneous – can be associated with low lying QP near nodes
- Thus, spectra in the anti-nodal region is highly inhomogeneous in space while QP near nodal region are homogeneous and coherent



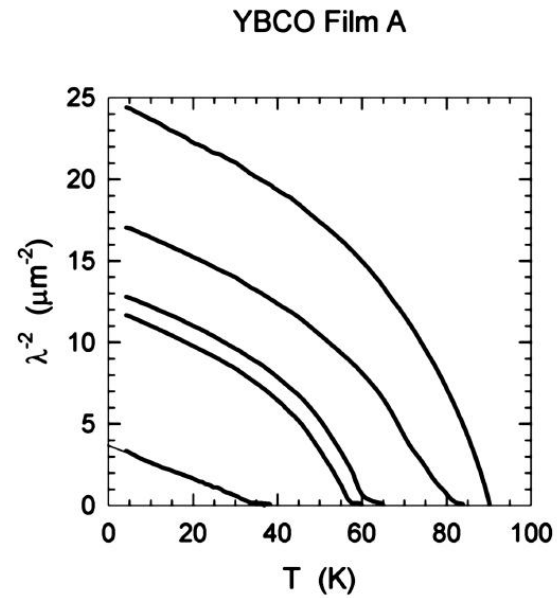
Bi-2212 (McElroy 2004)

Non-BCS Superconductivity

- Gap increases with decreasing doping while T_c decreases
- No QP excitations above T_c
- Different behavior from conventional SC where there are sharp QP in normal state and sharp peak pulls back from Fermi energy, thus opening SC gap.
- T* - temperature at which pseudogap first appears.



Super-fluid density

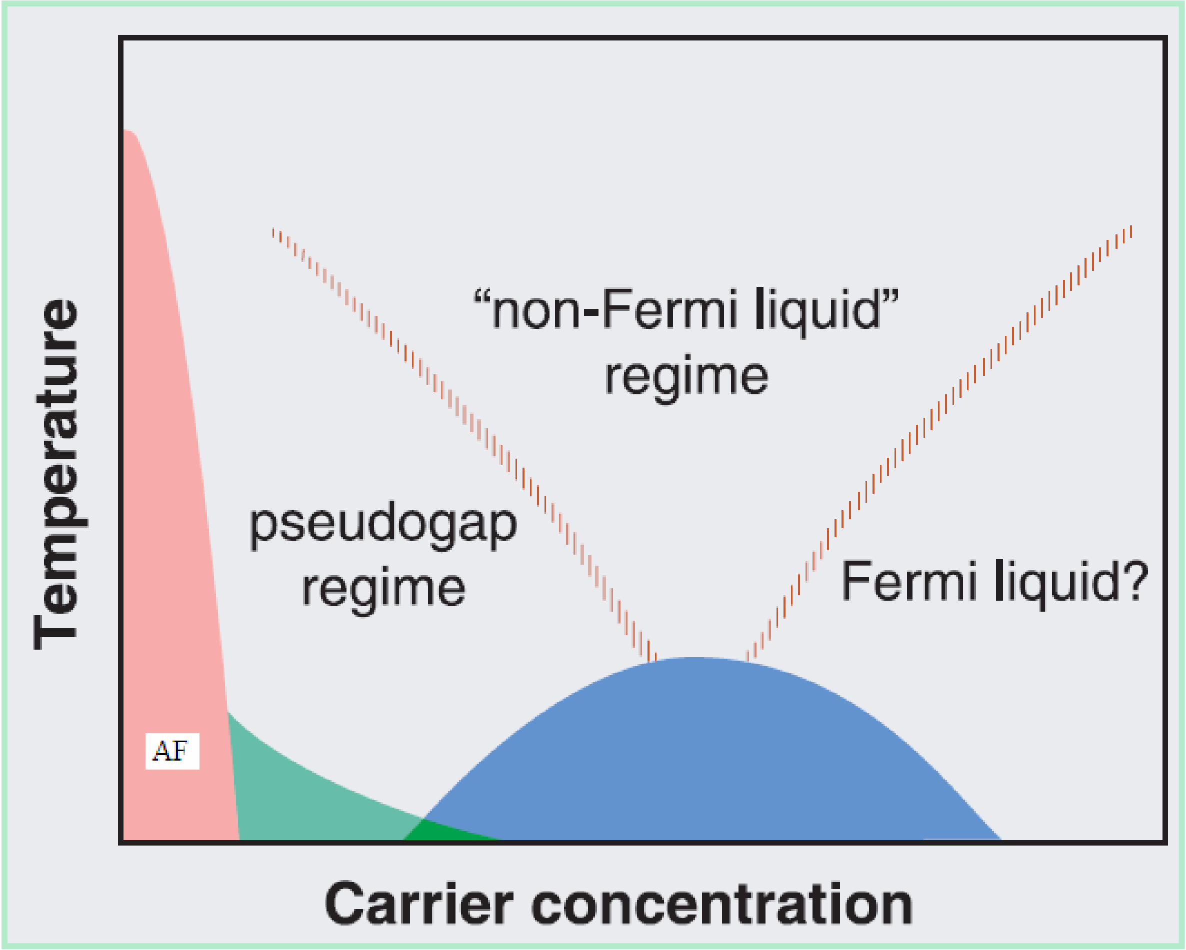


Boyce et al. 2000

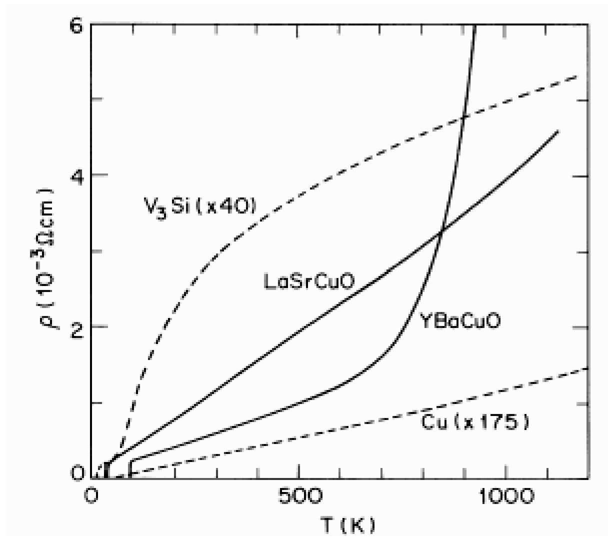
- BCS theory of a d-wave superconductor gives linear T dependence of super-fluid density – $\frac{n_s(T)}{m} = \frac{n_s(0)}{m} - \alpha T$

- BCS works well at low T – though
  - BCS gives n_s/m of order unity – here it is proportional to *x*
  - Mean field theories give α to be proportional to x – experimentally independent of doping – Open problem !!!
- Also, On under-doped side – $T_c = C\, n_s$ – Uemura Relation (C is independent of material)

Non-Fermi liquid regime

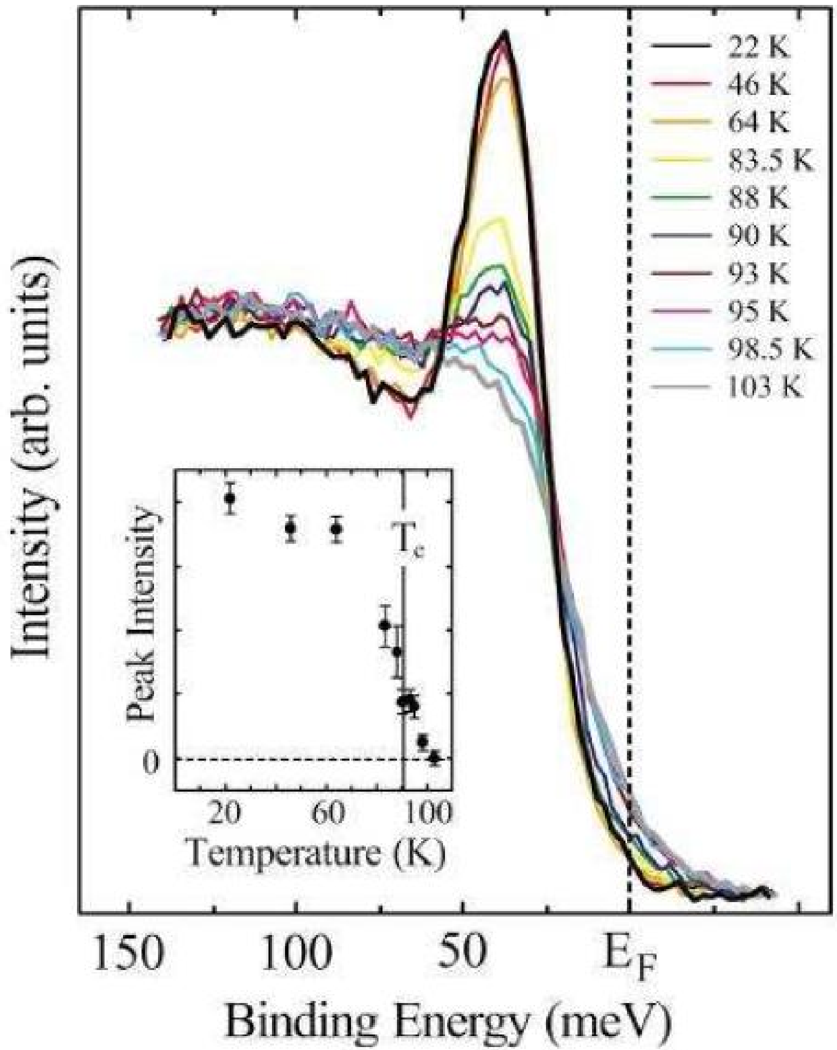


“Strange Metal”: Resistivity



- A metal resistivity should show T^2 behavior for low T .
- On increasing the temperature, other effects like phonon effects, scattering effects takes place which changes resistivity further.
- In this state, resistivity starts from zero and then go linear to temperatures as high as 600 K !!!

"Strange" Metal : ARPES



- In "Strange metals", SC gap vanishes
- No QP excitations – what sort of metal is this ? !!

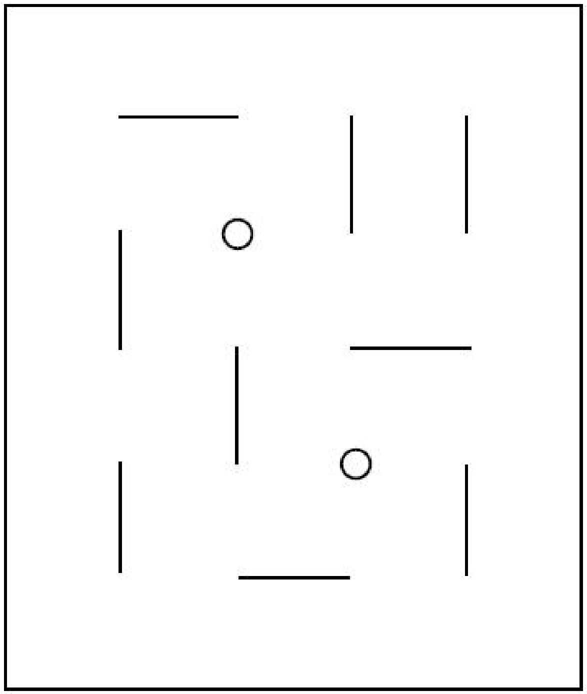
"Strange Metal"

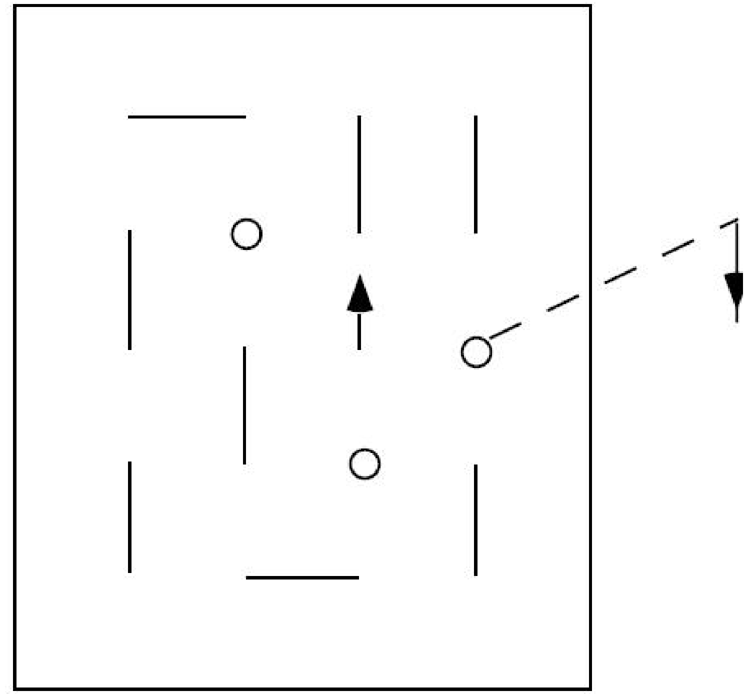
- Hall Coefficient is linear in T !
- Connected Fermi surface consistent with conventional band theory – How can one have FS for a metal when there are no QP ? – Controversial !
- For very large dopings – Fermi Metal

Summary : SC regime

- Sharp QP features below Tc
- In pseudo-gap regime, sharp QP features along nodal direction above Tc
- In normal state, no sharp QP like features
- Low temperature – BCS like
- Widemann-Franz Law is violated

Resonating valence bond (RVB)





- Hole mobility frustrates Neel Order – What is the best way to make both K.E. and Magnetic exchange energy happy ?
- Anderson tells Spins – Don't be chosy – Close your eyes – Hold hands of any mate you can find nearby when moved by holes
- Thus, a RVB state – superposition of singlets – holes move in the background of this liquid of spin singlets

RVB vs Neel

- In 1-d, $E_{neel} = -\frac{1}{4} J$, $E_{RVB} = -\frac{3}{8} J$: RVB is preferred ground state
- In 2-d, $E_{neel} = -\frac{1}{2} J$, $E_{RVB} = -\frac{3}{8} J$: RVB pose serious competition
- In 3-d, $E_{neel} = -\frac{1}{4} J$, $E_{RVB} = -\frac{3}{8} J$: Neel is preferred ground state
- Neel state has long range AF order – RVB has short range or power law decay of AF
- Since Neel state breaks the global spin rotation symmetry – gapless modes – *Magnons.* Finite energy required to break singlets – Excitations in RVB are gapped – *Spinons, Holons*.
- Magnons have spin-1 – Neel state has gapped S=0 excitations as well.
- Spinons have spin ½ and no charge – Holons have charge e but no spin.

Explanation of Pseudo Gap

- Singlet formation – decrease of uniform susceptibility – reduction of specific heat γ
- Holes responsible for in-plane transport – Area under Drude peak depends on doping only
- c-axis conductivity requires transportation of an electron across planes – This requires excitations which are gapped – we see a gap in $\sigma_c(\omega)$
- The pull-back of the leading edge in photoemission reflets energy cost to break a singlet