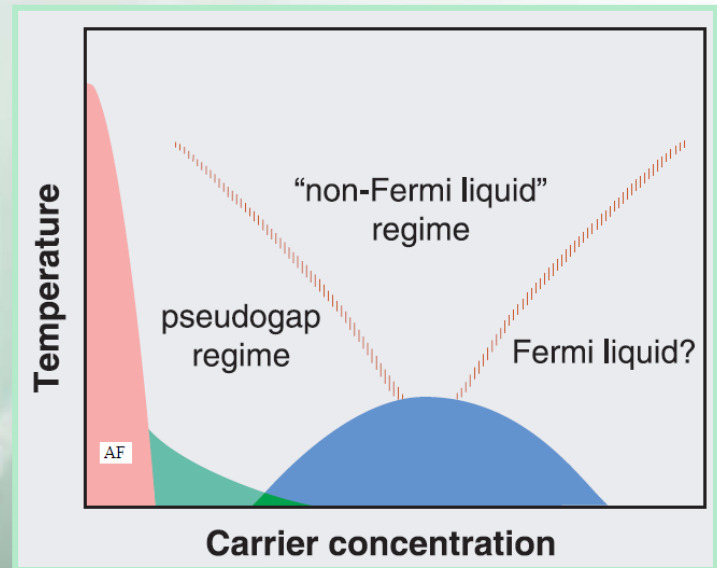
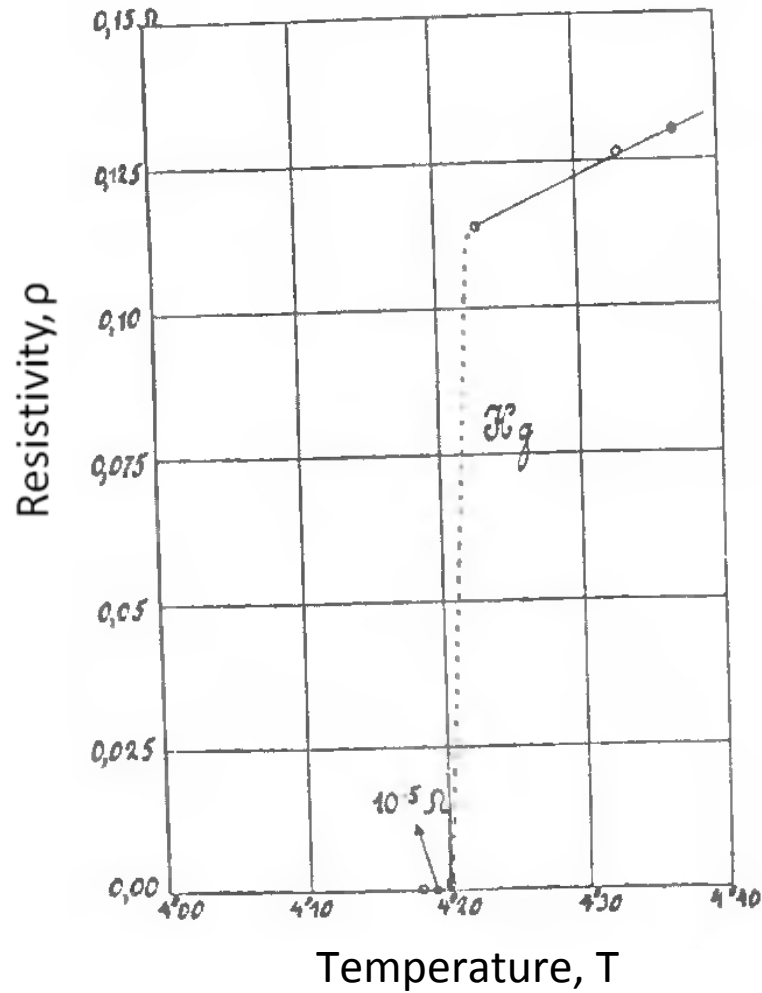


An introduction to High Temperature Superconductors



Sandeep Pathak
Materials Research Center,
IISc Bangalore

Kamerlingh Onnes - 1911



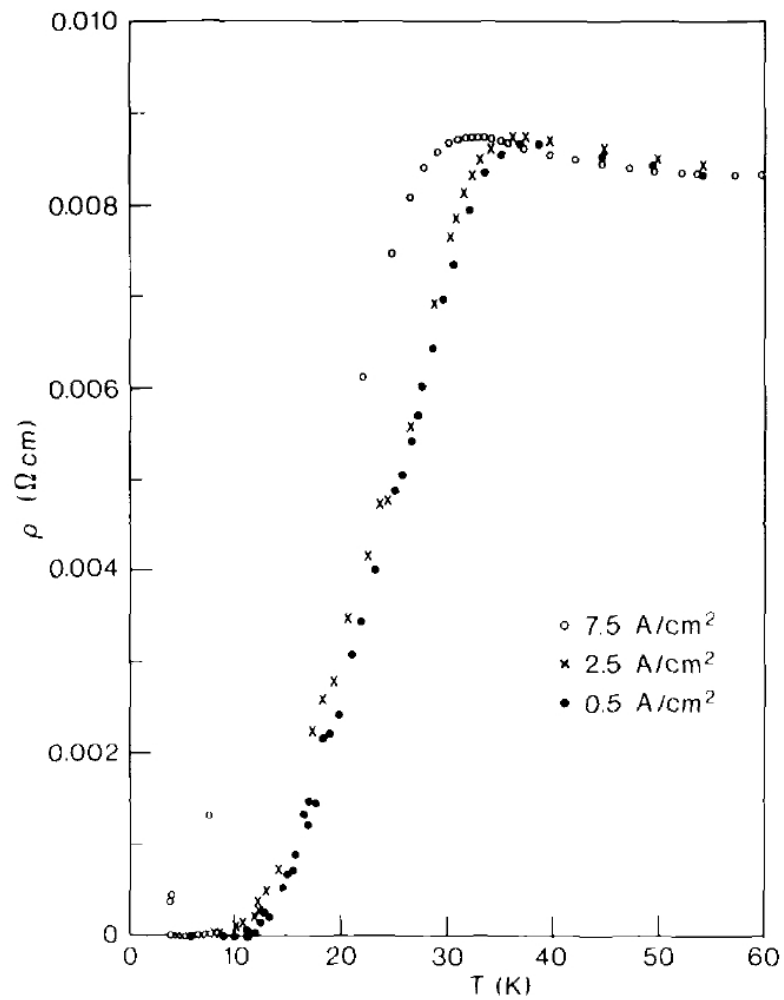
Not a rare phenomenon !!!

H ?	S	s-d								s-p						He	
Li 20 50 GPa	Be 0.026	<div style="border: 1px solid black; padding: 5px; text-align: center;"> Elements T_c[K] applied pressure </div>								B 11 250 GPa	C 4 B doped	N	O 0.6 120 GPa	F	Ne		
Na	Mg									Al 1.19	Si 8.5 12 GPa	P 6 17 GPa	S 17 160 GPa	Cl	Ar		
K	Ca 15 150 GPa	Sc 0.3 21 GPa	Ti 0.4	V 5.3	Cr	Mn	Fe 2 21 GPa	Co	Ni	Cu	Zn 0.9	Ga 1.1	Ge 5.4 11.50 GPa	As 2.7 24 GPa	Se 7 13 GPa	Br 1.4 150 GPa	Kr
Rb	Sr 4 50 GPa	Y 2.8 15 GPa	Zr 0.6	Nb 9.2	Mo 0.92	Tc 7.8	Ru 0.5	Rh .0003	Pd	Ag	Cd 0.55	In 3.4	Sn 3.72	Sb 3.5 8.5 GPa	Te 7.4 35 GPa	I 1.2 25 GPa	Xe
Cs 1.5 5 GPa	Ba 5 15 GPa	La 5.9	Hf 0.13	Ta 4.4	W 0.01	Re 1.7	Os 0.65	Ir 0.14	Pt	Au	Hg 4.15	Tl 2.39	Pb 7.2	Bi 8.5 9 GPa	Po	At	Rn
Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt									

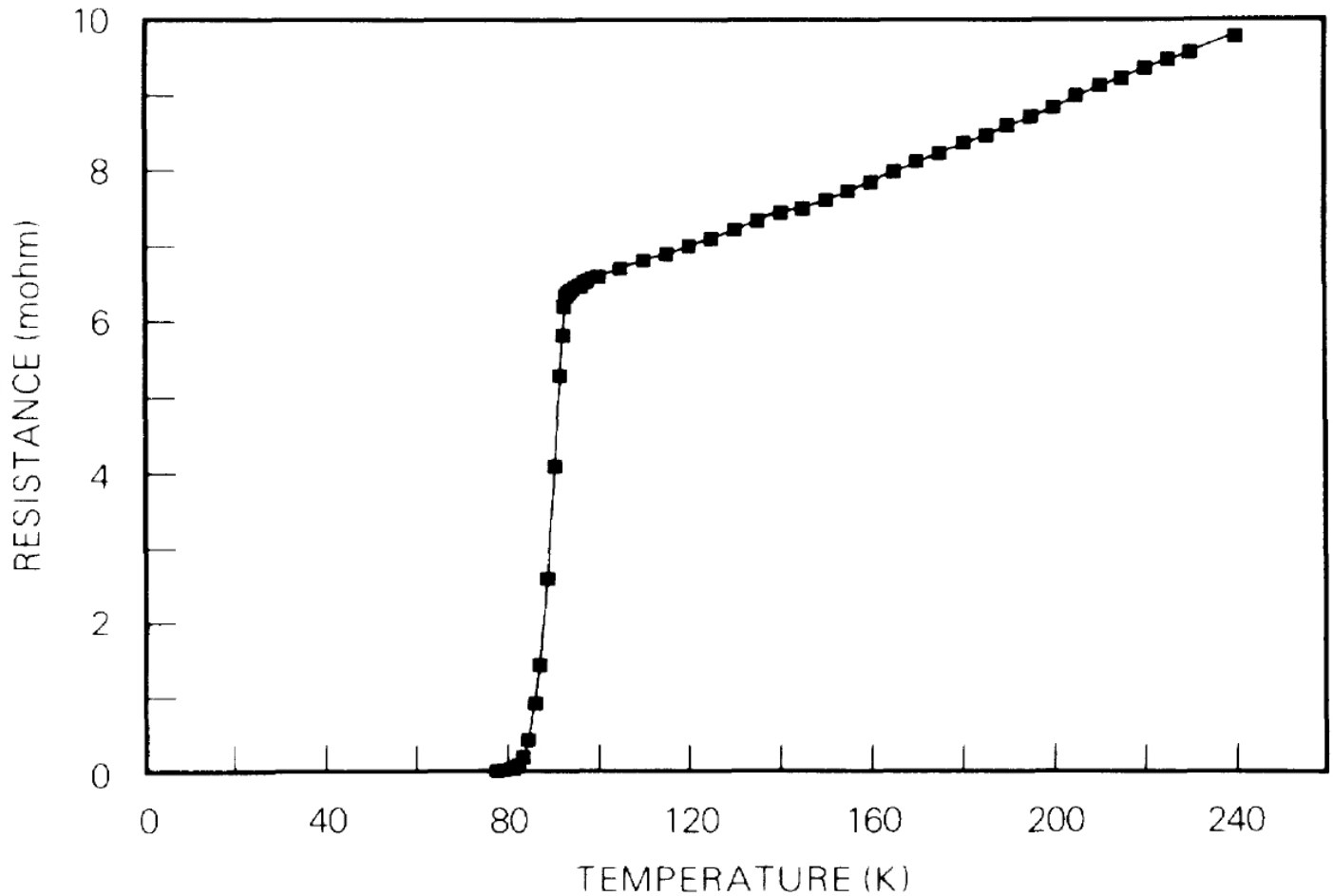
s-f	Ce 1.7 5 GPa	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu 1.1 18 GPa
	Th 1.4	Pa 1.4	U 0.2	Np 0.075	Pu	Am 0.8	Cm	Bk	Cf	Es	Fm	Md	No	Lr



Bednorz & Muller - 1986



Superconductivity above Liquid Nitrogen temperature !!!

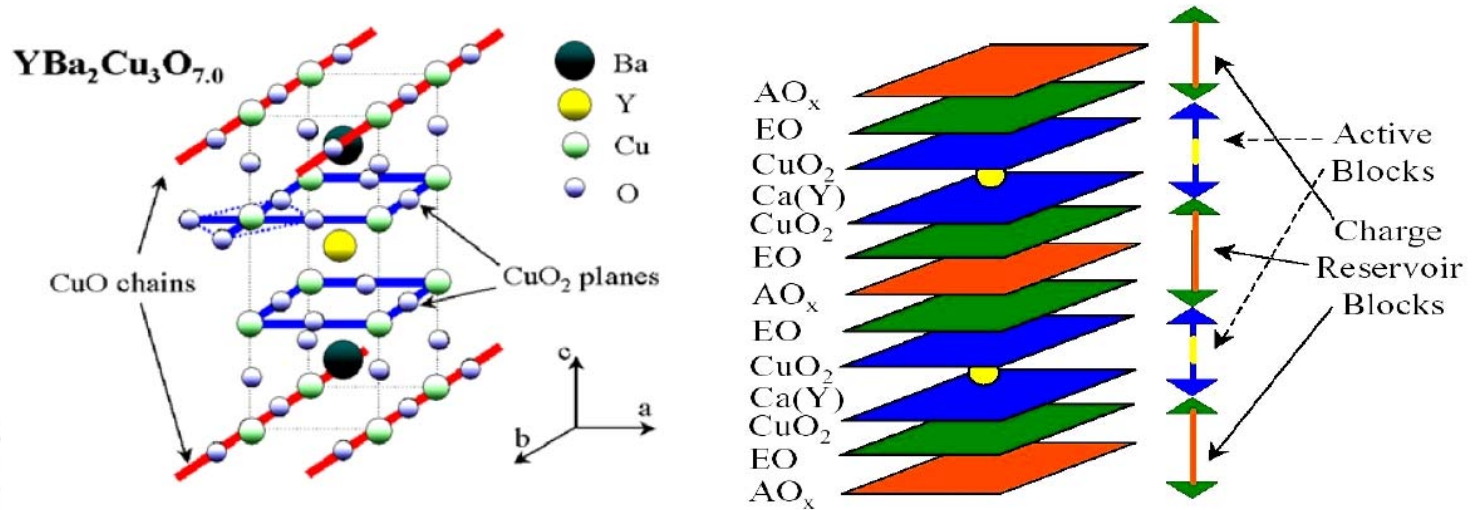


Wu et al (1987)

Plan of the talk

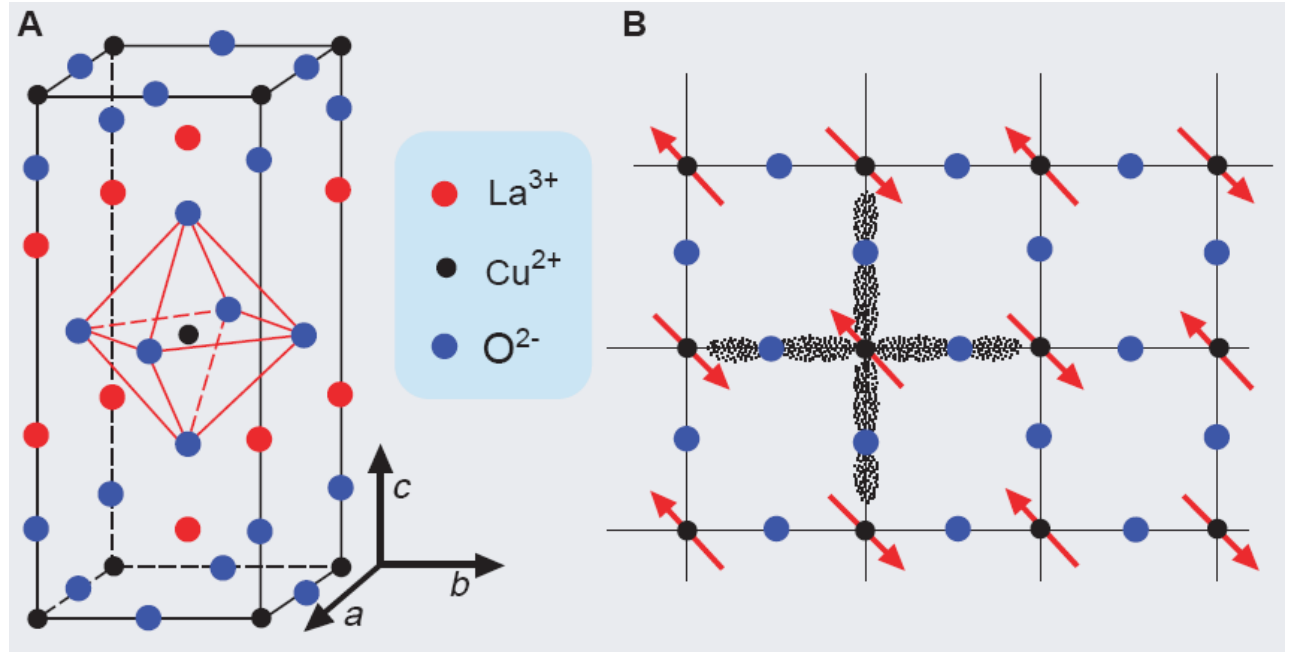
- High T_c Buzz - Cuprate Material
- Recap
 - Fermi Liquid Theory – Quasi-particle (QP) Idea
 - Superconductivity – Cooper Calculation – BCS Results
 - Concretizing QP Idea – Greens Function – Spectral Function – ARPES
- High T_c phases
 - AF Mott Insulator
 - Pseudo-gap regime
 - Super-conducting state
 - “Normal” metal regime
- Theoretical Models

Cuprates: Material



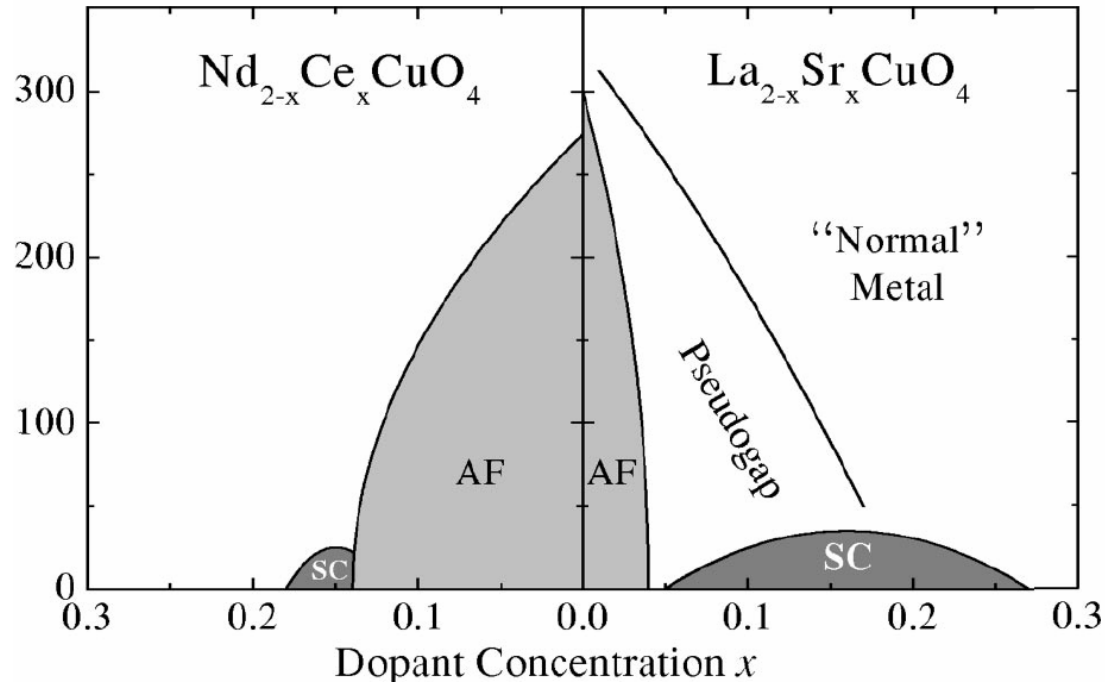
- Two sub-units – Active Blocks & Charge Reservoir Blocks
- “Active Block” – (CuO₂/Ca/)_{n-1} CuO₂ – Mobile Carriers Workspace
- “Charge Reservoir Block” - EO/(AO_x)_m EO
 - Storage for dopants
 - Provide Doping Charge
 - A = (Bi, Pb, Tl, Hg, Au, Cu, Ca, B, Al, Ga)
 - E=Alkaline Earth Metal (Sr, Ba)
- General Formula – A_mE₂Ca_{n-1}Cu_nO_{2n+2+mx} – Terminology: A-m2(n-1)n
- Examples – Bi₂Sr₂Ca₂Cu₃O₁₀ – Bi-2223, Y₁Ba₂Cu₃O₇ – Y-1223

0210 compounds



- E_2CuO_4 - La_2CuO_4 , Nd_2CuO_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 $\frac{1}{2}$ 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.

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, \mathbf{p} is a good quantum number, electrons occupy \mathbf{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 $\propto T$ can get thermally activated. Thus $U \propto T \cdot k_B T \rightarrow C_v = \gamma T$ ($\gamma \propto g_0$)
- **Magnetic Susceptibility** : constant $\propto g_0$ (*Pauli Paramagnet*)
- **Infinite Electrical Conductivity** – In presence of scatterers – Drude Formula

Landau Quasi-particle Idea

- What if we add Interactions between electrons?
- 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”
- Landau’s Idea – There is 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”**
- All the non-interacting physics remains the same in spite of high Coulomb energy per particle – mass get renormalized
- **Interactions → Fermi-Gas to Fermi-Liquid**

Superconductivity

- As metals are cooled below certain temperature, the electrical resistance goes to zero and this phase is called a superconductor (SC).
- Differences from perfect conductor
 - A superconductor does not allow Magnetic field (H) to penetrate through it. Persistent surface currents are set in such a way that H is cancelled – ***Meissner effect (1933) – Perfect Diamagnetism*** – Magnetization, $M = -H$, while in metals, flux can not change on cooling through transition
 - Perfect Conductor - No persistent currents



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.

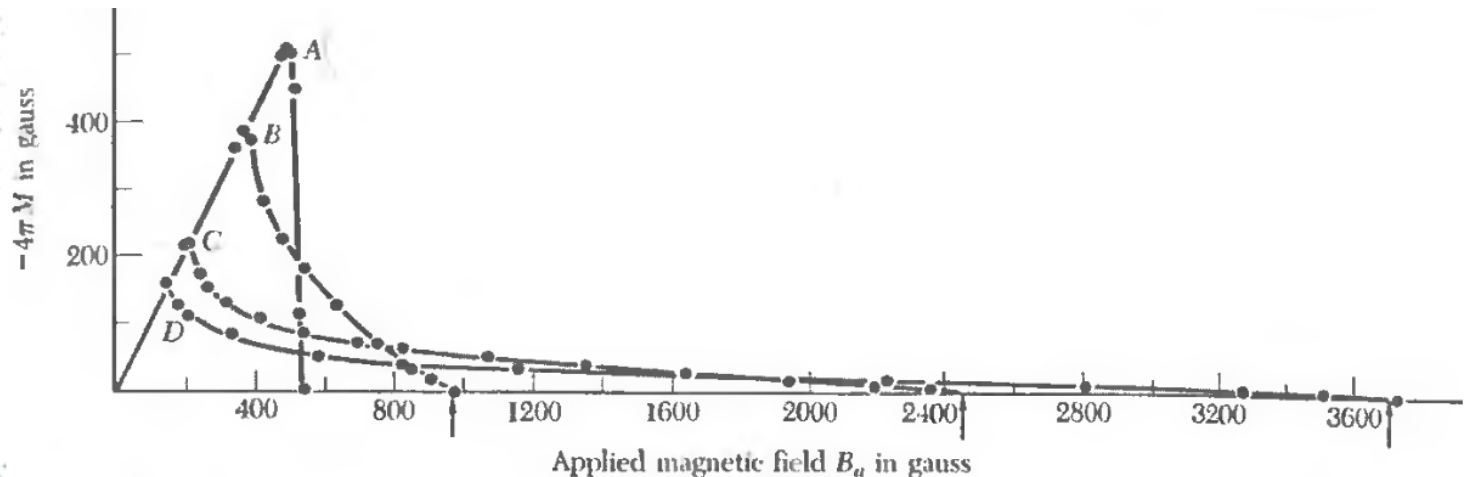
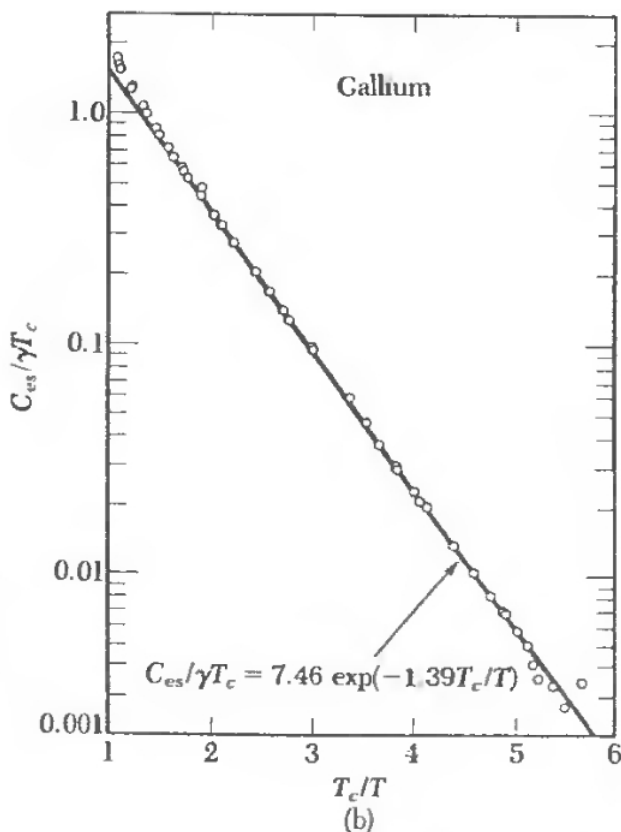
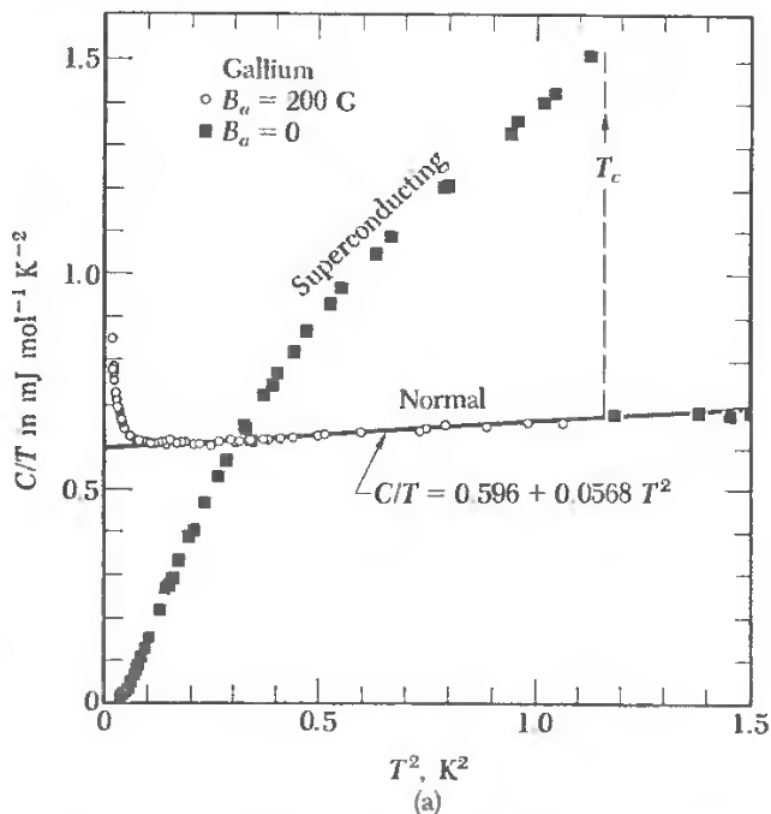


Figure 5a Superconducting magnetization curves of annealed polycrystalline lead and lead-indium alloys at 4.2 K. (A) lead; (B) lead-2.08 wt. percent indium; (C) lead-8.23 wt. percent indium; (D) lead-20.4 wt. percent indium. (After Livingston.)

Specific Heat

- Below T_c , SC state has lower entropy than normal state – more ordered. Small Difference – *Small fraction of conduction electrons participate in the transition*. Two fluid picture – “normal” and “super”
- Low T C_v exponential – *Excitations are gapped*



London phenomenological theory (1935)

- Postulate – Superconducting current is proportional to vector potential

$$\vec{j}_s(\vec{r}) = -\frac{1}{\mu_0 \lambda^2} \vec{A}$$

$$\lambda = \left(\frac{m c}{\mu_0 q^2 n_s} \right)^{\frac{1}{2}}$$

- Explains Meissner effect

$$\nabla \times \vec{j}_s = -\frac{1}{\mu_0 \lambda^2} \vec{B}$$

$$\Rightarrow \nabla \times \vec{j}_s = -\frac{1}{\mu_0 \lambda^2} \vec{B}$$

$$\Rightarrow \nabla \times \vec{B} = \mu_0 \vec{j}_s : \text{Maxwell's equation}$$

$$\Rightarrow \nabla \times \nabla \times \vec{B} = \mu_0 \nabla \times \vec{j}_s = -\frac{1}{\lambda^2} \vec{B}$$

$$\Rightarrow \nabla^2 \vec{B} = \frac{1}{\lambda^2} \vec{B}$$

- Constant Magnetic field cannot reside inside a superconductor
- Since, λ diverges as transition temperature is reached, n_s was presumed to go continuously to zero at T_c – Second Order phase transition
- Standard Reference for Second Order Transitions : Landau!

G-L description of SC state (1950)

- G-L introduced a phenomenological order parameter, $\Psi(\mathbf{r})$ s.t. $\Psi^*(\mathbf{r}) \Psi(\mathbf{r}) = n_s$ – super-fluid density ($n_s \rightarrow 0$ as $T \rightarrow T_c^+$)
- In the vicinity of SC-Metal transition, Free energy density of SC state, F_s can be expanded in terms of $\Psi(\mathbf{r})$

$$F_s = F_N + a(T) |\psi|^2 + \frac{1}{2} b(T) |\psi|^4 + \frac{1}{2m} |(-i\hbar\nabla - qA/c)\psi|^2 + \frac{B^2}{2\mu_0}$$

- Uniform space solution is given by

$$|\psi_0|^2 = -\frac{a(T)}{b(T)} = n_s$$

or

$$\psi = 0$$

- This implies $a(T)$ should be less than 0 for $T < T_c$ and vice-versa.

$$a(T) = a_1(T - T_c), a_1 > 0$$

- It is easy to see that

$$H_c(T) \sim (T - T_c)$$

G-L Theory: London equation

- By minimizing w.r.t. \mathbf{A} and requiring that $\Psi \approx \Psi_0$

$$j_s(\vec{r}) = -(iq\hbar/2m)(\psi^* \nabla \psi - \psi \nabla \psi^*) - (q^2/mc)\psi^* \psi \vec{A}$$

$$j_s(\vec{r}) = -(q^2/mc)\psi^* \psi \vec{A} : \text{London equation}$$

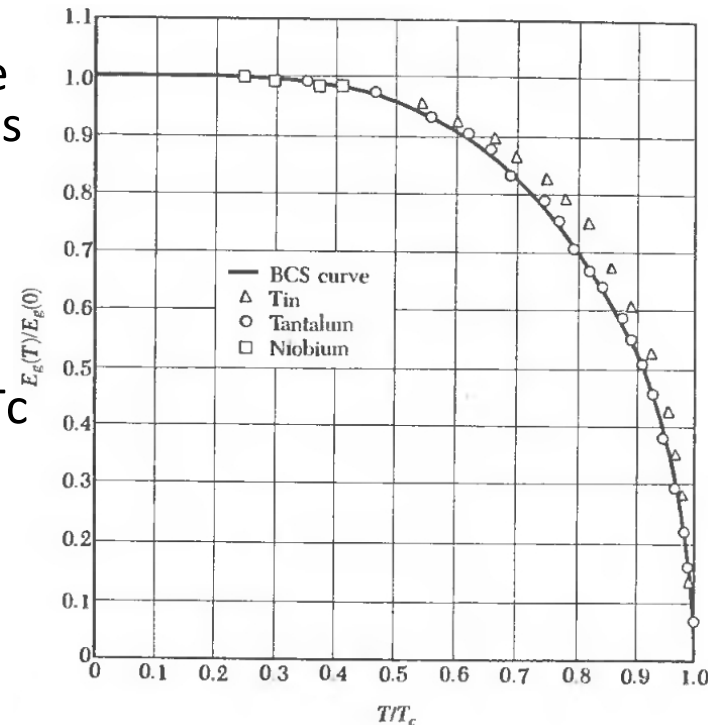
- Length Scale describing super-fluid stiffness

$$\xi^2 = \frac{\hbar^2}{2ma}$$

- Larger the magnitude of ξ , harder for $|\psi|$ to fluctuate – measure of the distance within which the SC electron concentration cannot change drastically in a spatially varying field.
- Criterion for Type I or Type II Superconductors
- Type I behavior supported when $\xi > \lambda$ and Type II for $\xi < \lambda$
- Define Landau-Ginzburg constant, $\kappa = \lambda / \xi$
- For usual SC, κ does not exceed 3 usually, but, for High Tc Cuprates, $\kappa = 100$!!!

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 an 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 $T \rightarrow T_c$ – Second Order transition



Standard Results Summary

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

Greens Function

- Suppose we have a Hamiltonian $H = H_0 + V$
- We ask the question, given state $|\Psi_0\rangle$ at time $t=0$, what is time evolution of the state? $\left(i\frac{\partial}{\partial t} - H_0\right)|\psi\rangle = V(t)|\psi\rangle$

- Define Greens function to be solution of

$$\left(i\frac{\partial}{\partial t} - H_0\right)G(t-t') = \delta(t-t')$$

- In terms of Greens Function,

$$|\psi(t)\rangle = |\psi_0\rangle + \int_0^t dt' G(t-t')V(t')|\psi(t')\rangle$$

$$|\psi(t)\rangle_0 = U(t)|\psi_0\rangle, U(t) = e^{-iH_0 t}$$

- Consider $V=0$ (non-interacting) case,

$$H_0 = \sum_{\alpha} \varepsilon_{\alpha} |\alpha\rangle\langle\alpha|$$

$$U(t) = \sum_{\alpha} e^{-i\varepsilon_{\alpha} t} |\alpha\rangle\langle\alpha| \Rightarrow U(\omega) = \sum_{\alpha} \delta(\omega - \varepsilon_{\alpha}) |\alpha\rangle\langle\alpha|$$

$$U_{\alpha\alpha}(\omega) = \delta(\omega - \varepsilon_{\alpha})$$

Thus, $\text{tr}U(\omega) = \text{DOS}$

$U_{\alpha\alpha}(\omega)$ - Probability that state α has energy ω - Spectral function

Properties of Greens Function

- Greens function is *causal* → Kramer's Kronig relations – Real and Imaginary parts of the Green's function are not independent.
- Spectral function completely determines Greens function

$$\left(i \frac{\partial}{\partial t} - H_0 \right) G(t) = \delta(t)$$

$$\Rightarrow (\omega I - H_0) G(\omega) = I \Rightarrow G(\omega) = (\omega I - H_0)^{-1}$$

$$\Rightarrow G(\omega) = \sum_{\alpha} \frac{|\alpha\rangle\langle\alpha|}{\omega - \varepsilon_{\alpha}}$$

$$G_{\alpha\alpha}(\omega^+) = P \left(\frac{1}{\omega - \varepsilon_{\alpha}} \right) - i\pi\delta(\omega - \varepsilon_{\alpha})$$

$$\text{Thus, } \boxed{-\frac{1}{\pi} \text{Im}(G_{\alpha\alpha}(\omega^+)) = \text{Spectral function, } A_{\alpha}(\omega)}$$

$$\text{and, } \boxed{-\frac{1}{\pi} \text{Im}(\text{tr}G(\omega^+)) = \text{DOS}}$$

- Take Fourier transform – $G_{\alpha\alpha}(t) = -i\theta(t)e^{-i\varepsilon_{\alpha}t}$

$$G(\omega) = \int d\omega' \frac{\sum_{\alpha} \delta(\omega' - \varepsilon_{\alpha}) |\alpha\rangle\langle\alpha|}{\omega - \omega'}$$

$$\boxed{G(\omega) = \int d\omega' \frac{\rho(\omega')}{\omega - \omega'}}$$

Importance of Spectral Function

- If Greens function has pole at $\omega = \Omega - \Gamma$, i.e.

$$G_{\alpha\alpha}(\omega) = \frac{Z_{\alpha}}{\omega - (\Omega - i\Gamma)}$$

$$\text{Then, } G_{\alpha\alpha}(\omega) = \frac{Z_{\alpha}(\omega - \Omega)}{((\omega - \Omega)^2 + \Gamma^2)} - i \frac{Z_{\alpha}\Gamma}{((\omega - \Omega)^2 + \Gamma^2)}$$

$$-\frac{1}{\pi} \text{Im}(G_{\alpha\alpha}(\omega^+)) = \frac{Z_{\alpha}\Gamma / \pi}{((\omega - \Omega)^2 + \Gamma^2)} = A_{\alpha}(\omega)$$

- Then, $G_{\alpha\alpha}(t) = -i\theta(t)e^{-i\Omega t - \Gamma t}$
- This means that 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, $A(\mathbf{k}, \omega)$

- Define $A^+(\vec{k}, t-t') = \langle N | c_{\vec{k}}(t) c_{\vec{k}}^\dagger(t') | N \rangle$
 $A^-(\vec{k}, t-t') = \langle N | c_{\vec{k}}^\dagger(t') c_{\vec{k}}(t) | N \rangle$ $A(\vec{k}, \omega) = A^+(\vec{k}, \omega) + A^-(\vec{k}, \omega)$
- If a particle (A^+) or hole (A^-) is added to a N-particle system at time, t' , does it still look like a particle or hole at time, t ?
- Since particle is to be added at an energy, $\omega > \mu$ and hole at energy, $\omega < \mu$
 $A^+(\vec{k}, \omega) = \theta(\omega - \mu) A(\vec{k}, \omega)$
 $A^-(\vec{k}, \omega) = \theta(\mu - \omega) A(\vec{k}, \omega) = n_F^-(\omega) A(\vec{k}, \omega)$
- After simple algebra, it turns out that
 $A^+(\vec{k}, \omega) = \sum_n |\langle n, N+1 | c_{\vec{k}}^\dagger | N \rangle|^2 \delta(\omega - (\omega_n + \mu))$
 $A^-(\vec{k}, \omega) = \sum_n |\langle n, N-1 | c_{\vec{k}} | N \rangle|^2 \delta(\omega - (-\omega_n + \mu))$
- Delta function counts if the n^{th} excited state has energy ω measured from chemical potential and if it does, what is the weight of the added excitation in that state. *Thus, $A(\mathbf{k}, \omega)$ measures the probability that an excitation (particle or hole) added to the \mathbf{k} -state has energy ω – generalization of non-interacting DOS*

$A(\vec{k}, \omega)$ – Properties & Sum Rules

- General Structure –
$$A(\vec{k}, \omega) = \frac{1}{\pi} \frac{Z_{\vec{k}} \left(\frac{1}{\Gamma_{\vec{k}}} \right)}{(\omega - E_{\vec{k}})^2 + \left(\frac{1}{\Gamma_{\vec{k}}} \right)^2} + A^{inc}(\vec{k}, \omega)$$

- Sum Rules

$$\int_{-\infty}^{\infty} d\omega A(\vec{k}, \omega) = 1$$

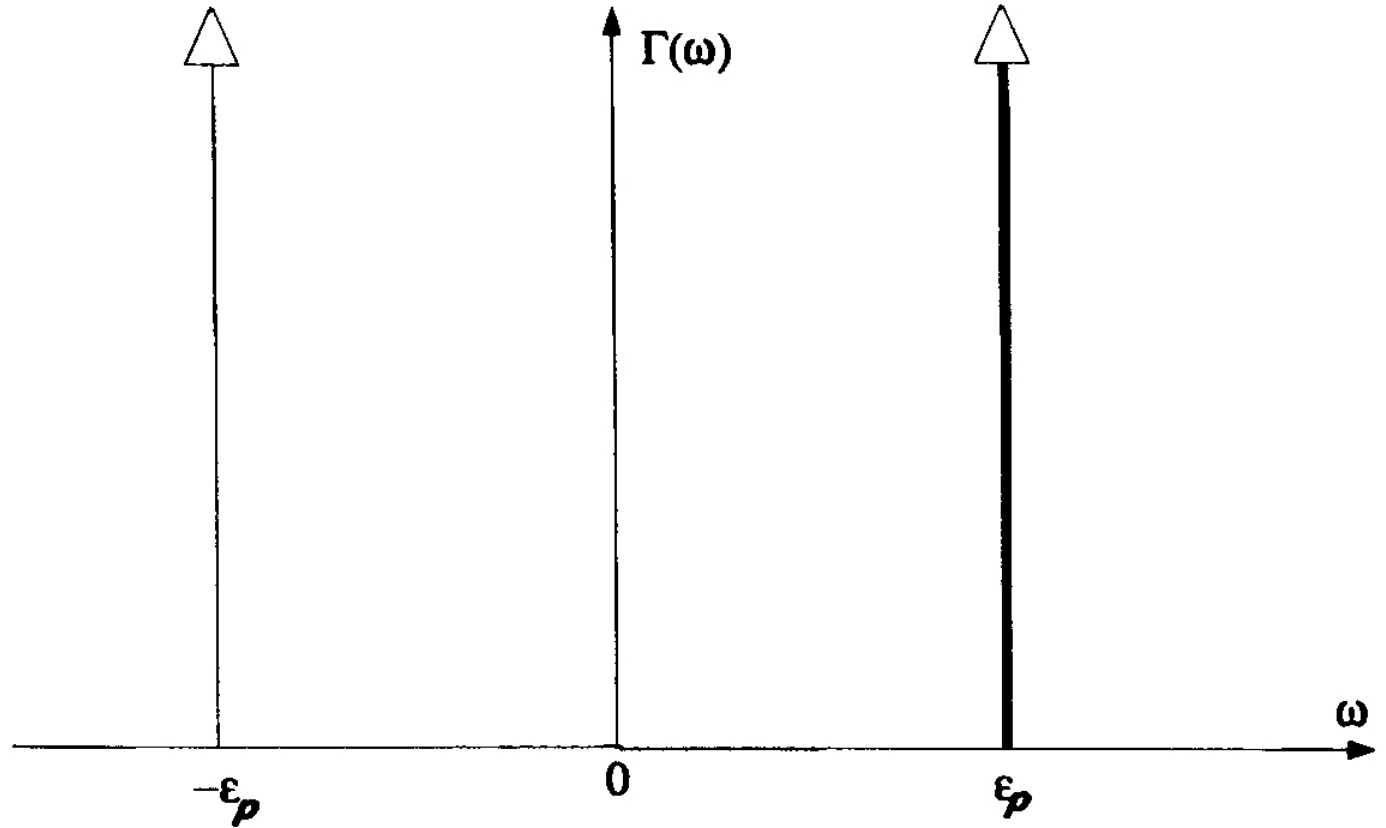
$$\int_{-\infty}^{\infty} d\omega A^+(\vec{k}, \omega) = \langle c_{\vec{k}} c_{\vec{k}}^{\dagger} \rangle$$

$$\int_{-\infty}^{\infty} d\omega A^-(\vec{k}, \omega) = \langle n_{\vec{k}} \rangle$$

- Spectral function for

- *Fermi System – Delta function peaked at ξ_k*
- *BCS Superconductor – Two Delta functions peaked at $\pm E_k$ – One for particle addition and other for hole addition (pair breaking)*

$A(\mathbf{k}, \omega)$ for superconductors



Spectral density of the retarded Green's function in the superconductor.

- Note that QP are infinitely lived even inspite of interactions.

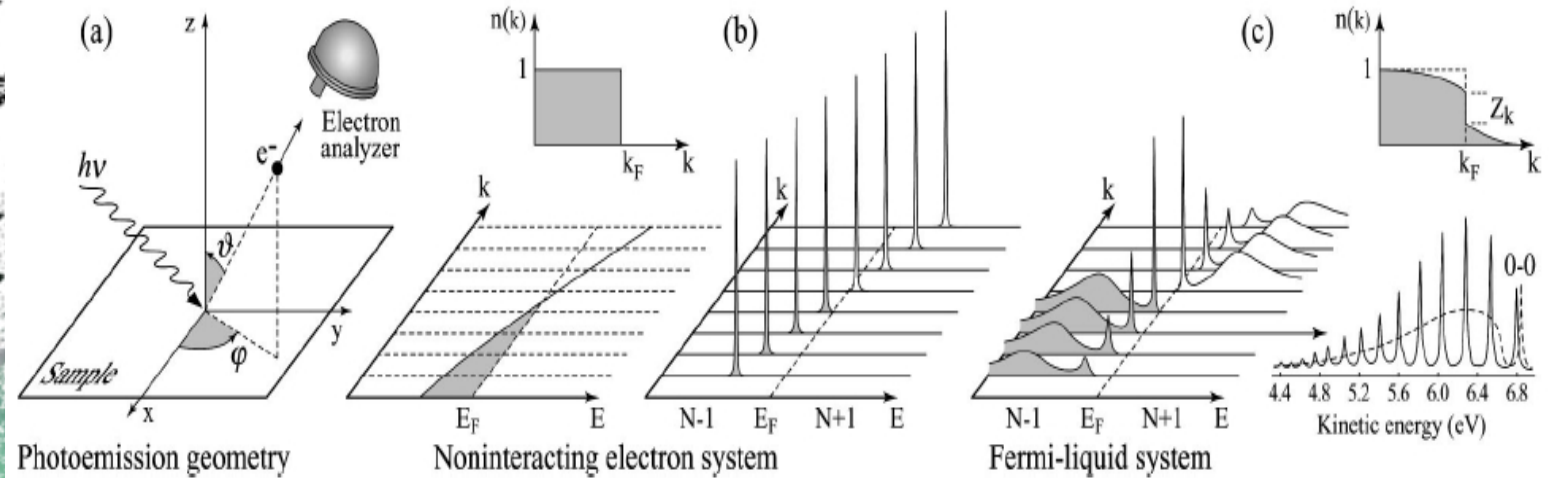
Many Body Greens Function

- Taking analogy from non-interacting case, define

$$G(\vec{k}, \omega) = \int d\omega' \frac{A(\vec{k}, \omega')}{\omega - \omega'}$$

$$\Rightarrow G(\vec{k}, t) = -i\theta(t) \langle G | \{c_{\vec{k}}(t), c_{\vec{k}}^\dagger(t')\} | G \rangle$$

Angle Resolved Photoemission Spectroscopy (ARPES)

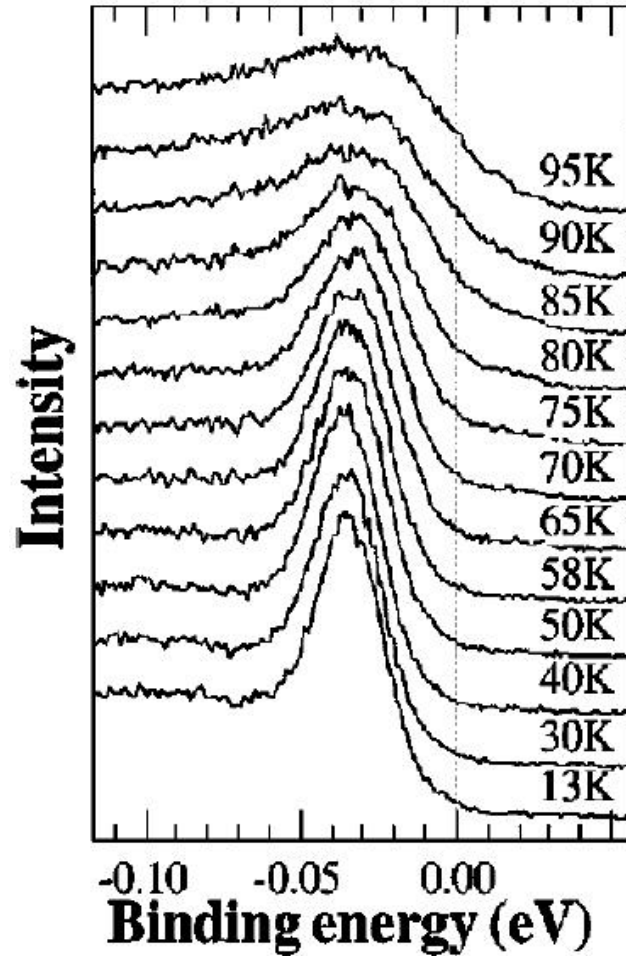


- Technique to measure $A^-(\mathbf{k}, \omega)$
- A monochromatic radiation is incident on properly aligned single crystal sample – Emission of Photoelectrons – collected by Electron Analyzer – E_{kin} & \mathbf{p} observed.
- Energy-momentum conservation :

$$E_{kin} = \hbar \nu - \phi - |E_B|$$

$$p_{||} = \hbar k_{||} = \sqrt{2mE_{kin}} \sin \mathcal{G}$$
- 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 \mathbf{k}

ARPES: SC – Normal Transition



- Bi₂Sr₂CaCu₂O_{8+δ} ($T_c = 87$ K) Randeria et al, 1995

Surprises awaiting to appear !

- Undoped Cuprate – Mott Insulator – Expected to be metal by band theory
- Non-BCS d-wave superconductor below T_c
- Non-Fermi Liquid metal for $T > T_c$
- For very high doping, fermi metal

