## MECHANISM

## requires going beyond BCS theory to include inelastic scattering

In conventional superconductors we use Eliashberg theory to include the electron-

A serious limitation of BCS theory is that it is not good for relating the T<sub>c</sub> value to microscopic parameters characterizing the normal state complexities of a metal.  $T_c = 1.13 h \omega_D e^{-1/N(0)V}$ 

Just qualitative model Not quantitative in its conceptualization Fermi sea

Need to go beyond this!

Interaction beyond band structure are introduced through a self energy

Think of electron as propagating in a medium consisting of all other electrons and phonon i.e. lattice vibrations AND in cuprates spin fluctuations [magnetism is around the corner]

Electron acquires a lifetime [imaginary part of self energy] and Electron spectral density



### Self energy $\Sigma(\mathbf{k},\omega)$ gives renormalizations

#### Electron Spectral Function A(k, w)

 $A(k,\omega)$  is measured in Angle-Resolved Photoemission Spectroscopy (ARPES)

$$A(\mathbf{k},\omega) = \frac{1}{\pi} \frac{|\Sigma_2|}{(\omega - \varepsilon_{\mathbf{k}} - \Sigma_1)^2 + \Sigma_2^2}$$



To describe the electron -phonon interaction as it enters Eliashberg theory, in principle we need:

1] phonons -frequencies and polarization vectors

2] electronic band structure and wavefunctions

3] coupling between electron and an ion displaced from equilibrium

 $\alpha(\omega)$ 

**α(ω)** 

This is a lot of detailed information; but it can all be econdensed into a single function:  $F(\omega)$ 

$$\alpha^{2}(\omega)F(\omega) \equiv \alpha^{2}F(\omega)$$

Analogous to the phonon frequency distribution  $F(\omega)$  or the electronic density of states  $N(\varepsilon)$ .

<u>**Phonons:</u>** dispersion  $\omega(k)$ , frequency distribution F( $\omega$ )</u>

Lattice vibrations or phonons are measured by inelastic neutron scattering



#### Neutron groups

definite momentum transfer to phonon analyzed as a function of energy transfer to phonon



(1.40, 1.40, 1.40)

(1425, 1425, 1425)

200

100

200r

100

Fig. 4.10. A set of 'constant q' scans in Pb taken at various points along the diagonal in the Brillouin zone. Reproduced from Ref. [89]

B. Brockhouse et al., Phys. Rev. 128, 1099 (1962).

For the high Tc oxides spin polarized inelastic neutron scattering [monitor spin flip] can be used to get the magnetic excitations spin waves or spin fluctuations[damping] See a very famous 41mev resonance In YBCO, different energies in other materials

#### Famous 41 mev spin one resonance



Bourges et. al. see later for reference

**Phonon frequency distribution** 

$$F(\boldsymbol{\omega}) = \frac{1}{N} \sum_{\mathbf{k}j} \delta(\boldsymbol{\omega} - \boldsymbol{\omega}_j(\mathbf{k}))$$

N is number of points in FBZ; j is phonon branch index

Note that frequency distribution is a single function while dispersion curves are <u>many</u> frames, one for each direction in FBZ, yet for the lattice specific heat knowing  $F(\omega)$  is enough!! – much, much simpler

For simple metal, one atom per unit cell  $F(\omega)$  is normalized to 3



Stedman et al., Phys. Rev. 162, 549 (1967).

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[ζζο]

[ιζο]

## If you image these through the electrons use

### weighted distribution with electronphonon weighting

$$\mathbf{v}^{2}(\boldsymbol{\omega})F(\boldsymbol{\omega}) \equiv \alpha^{2}F(\boldsymbol{\omega})$$

Analogous to the phonon frequency distribution  $F(\omega)$  or the electronic density of states  $N(\varepsilon)$ .

#### Furthermore,



Renormalization due to electron-phonon interaction can change dispersion curve (ie. energy-momentum relationship  $\varepsilon_k$ ).

**Electron Self-Energy** 

$$\Sigma(k,\omega) = \langle \overset{\mathbf{I}}{\longrightarrow} \rangle$$



Medium changes electron energy dispersion curve and gives a finite lifetime to be in a particular k state, ie,  $\epsilon = E + i\Gamma$ 

$$\Sigma(\omega) = \int_{0}^{\infty} d\Omega \alpha^{2} F(\Omega) \ln \left| \frac{\Omega - \omega}{\Omega + \omega} \right| - i\pi \int_{0}^{|\omega|} d\Omega \alpha^{2} F(\Omega)$$

#### Example of how $\alpha^2 F(\omega)$ determines properties

 $\lambda$  the electron-phonon mass renormalization

Electron pulls ions off equilibrium positions



Heavier by  $[1+\lambda]$ i.e. m\*=m $[1+\lambda]$  Electron moves with polarization cloud of lattice charge



Electron spectral density for noninteracting case

$$A(\mathbf{k},\omega) = \delta(\omega - \varepsilon_{\mathbf{k}})$$

Want to include lifetimes, change to Lorentzian with width  $\Gamma,$  also change energy to  $\mathsf{E}_{\mathsf{k}}$ 

$$A(\mathbf{k}, \omega) = \frac{1}{\pi} \frac{\Gamma}{(\omega - E_{\mathbf{k}})^{2} + \Gamma^{2}}$$
  
Broadening  
New dispersion  
$$E_{\mathbf{k}} = \varepsilon_{\mathbf{k}} + \operatorname{Re}[\Sigma(E_{\mathbf{k}})]$$



Scattering rate due to phonon is zero till energy 'wp' at which point it increases out of zero



Scattering rate is zero till excitation energy of electron is large enough to create a phonon at which point it rises out of zero.

Rise reflects the available phonon frequency distribution



### The mode in Y123 Ortho-II

Quasiparticle scattering rate due to absorption of a real thermally created phonon

Thermally excited Phonon w is absorbed by electron. Empty states are always available for such scattering

No threshold for such scattering with real phonons

### Ortho II, alternating full and empty Cu-O chain



Can invert I-V characteristics to get electron-phonon spectral density through Eliashberg equations



#### **Electron-phonon spectral density in Pb**

Tunneling: McMillan and Rowell, Phys. Rev. Lett. 14, 108 (1965).

#### Calculations:

Tomlinson and Carbotte, Phys. Rev. B 13, 4738 (1976). This function contains all of the complicated information on electron and phonon dynamics and the coupling between them that enters superconductivity.

## Remarkable condensation of required information!



# Inversion of optical data

## How to get information on mechanism from optics

Can get distribution of bosons that scatter electrons from an analyses of scattering rates

What is recovered is a weighted boson distribution i.e. weighted by appropriate electron -boson coupling In conventional superconductors, tunneling has been method of choice to get information on gap and phonons

Optics has been hard, good metals reflectance near 1

In poor metals such as oxides, optics has been great!

**INVERSION** 

$$\alpha^{2} F(\mathbf{v}) \sim W(\omega) = \frac{1}{2\pi} \frac{\omega_{p}^{2}}{4\pi} \frac{d^{2}}{dv^{2}} \left\{ \mathbf{v} \operatorname{Re} \frac{1}{\sigma(\mathbf{v})} \right\}$$

Calculation of conductivity from Pb
Electron-phonon spectral density and differentiation to get it back

Normal state only

Solid curve is input and others are output at two temperatures  $\begin{array}{c} 1.5 \\ (3) \\$ 

In theory!



#### **Electron-phonon spectral density from optics**

Old data for Pb good agreement with tunneling



#### It works beautifully!

B. Farnworth and T. Timusk, Phys. Rev. B 10, 2799 (1974); ibid 14, 5119 (1976).

#### Hwang et. al. [Timusk-group] Nature,427,714 [2004]

Optical scattering rate in Bi2212 across the doping range

from underdoped to





# What should we see if its spin fluctuation exchange ?

Expect to see a picture of local spin susceptibility i e BZ average

In cuprates see a broad background and sometimes a prominent spin one resonance in magnetic susceptibility at specific momentum [pi.pi] great specific see

#### Famous 41 mev spin one resonance



Ph. Bourges, Y. Sidis, H.F. Fong, B. Keimer, L.P. Regnault, J. Bossy, A.S. Ivanov, D.L. Lilius, and I.A. Aksay, in High Temperature Superconductivity, eds. S.E. Barnes, *et al.*, CP483 (American Institute of Physics, Amsterdam, 1999), p. 207.

#### The neutron resonance mode



Hayden et. Al. PRL 76,1344 [1996] Stock et.al. PRB 71,024522 [2005] Bourges et.al. PRB 53,876 [1996] and other Bourges references

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#### Temperature and doping dependence ...

#### Temperature

Y123



Dai et al., Science 284, 1344 (1999)

#### Temperature and doping dependence ....

**Temperature** 

Y123



Dai et al., Science 284, 1344 (1999)

#### Doping





He et al., PRL 86, 1610 (2001)

Two energy scales in spin susceptibility of La1.64Sr0.16CuO4



B Vignolle et al Nature Phys 3,163 [2007]

Averaged over the B Z

## What does optics see?

Phonons Spin fluctuations Both? [most likely case]?

Listen carefully and tell me what you think

### Inversion in LSCO

Get two peak structure at low T And evolution to single peak at room temp

Good agreement with neutrons

Looks real good !



Hwang et. al. Phys. Rev. Lett., 100, 137005 [2008]

#### Temperature and Doping evolution of Electron-Boson Spectral Function

Sharp peak goes away with increasing temperature and doping



#### Hwang et al ,PRB 75, 144506 [2007]



#### Redistribution of spectral weight with temperature in OP doped Bi2212



#### J. Hwang et. al. Phys. Rev. Lett. 102 , 027003 [2009] Hg Ba2 Cu O4+, Tc=90K



## Optical scattering rate

Same temperature evolution as Bi2212 Resonance energy moves up and amplitude is reduced with increasing temperature



Spectral density extends to high energy and evolves with temperature

#### Summary of optical resonance energy vs Tc



## Angular resolved photo emission



Electron spectral density



ARPES measures this function at negative energy only

Self energy  $\Sigma(\mathbf{k},\omega)$  gives renormalizations

Renormalized dispersion in Pb: Electron-phonon interaction

$$E_{\mathbf{k}} = \varepsilon_{\mathbf{k}} + \operatorname{Re}[\Sigma(E_{\mathbf{k}})]$$

## Schachinger et al PRB 67, 214508 [2003]



## The Kink in ARPES



Bogdanov, Lanzara et. al. Phys. Rev. Lett. 85,2581 [2000]

## The Kink in ARPES



Bogdanov, Lanzara et. al. Phys. Rev. Lett. 85,2581 [2000]



Johnson et. al. PRL 87,177007 [2001]

#### **Bi-2212** near the nodal region



Quasiparticle self energy



#### Schachinger - Carbotte , inversion [PRB 77,094524 [2008] of nodal direction ARPES data in Bi2212 by X. J. Zhou-gro



## Spectrum extends to high energy and evolves with temperature

W. Zhang et. al. [X. J. Zhou-group] PRL 100,107002 [2008] :Bi2212

#### Features at 70,115,150 meV interpreted by authors as not phonons



Momentum resolution 0.004 A-1 Tc=91K, energy resolution 0.56 meV

#### On the other hand

L. Zhao et. al. [X. J. Zhou-group] APS Portland 2010



heavily over-doped [BI PB] 2SR 2CU O6+ , Coupling to multiple phon modes at 70 meV, lamda=





#### **Tunneling Spectroscopy**



## Tunneling measures the electron density of states N[ $\omega$ ] DoS

## For superconducting-normal junction it is $N[\omega]$ that enters

## For superconductor-superconductor junctions it's a convolution of the two DoS

### peak-dip-hump in Tunneling

#### Bi-2212 (SIS junction)



Tunneling  $\leftrightarrow$  INS



Zasadzinski et al. Phys. Rev. Lett. 87, 067005 (2001)

## Four different techniques give very similar results for the energy of boson peak

ARPES gives about6Tunneling gives about5Optics gives about8/1.43= about5.5Neutron gives about5.4

All in units of the critical temperature

Good agreement about resonance but its origin remains controversial

Extent to high energy of spectral density and its evolution with temperature indicate spin fluctuations

Probably both are involved What do you think?

## We have come a long way! wonderful journey of discoveries

## BUT it is not over yet

END

#### Lanzara et. al. Nature ,421, 510 [2001]



Signatures of underlying Electron Boson spectrum seen in

Neutron scattering **INS** 

Angular resolved photo emission ARPES

Tunneling SIS junctions

Optics IR-spectroscopy

#### Coherence in underdoped state and beyond



Y. S. Lee et. al. [Basov-group] PRB 72,054529 [2005]

#### Padilla et. al. [Basov-group] PRB 72,060511 [2005]



#### Stock et.al. PRB 71,024522 [2005]



Local spin susceptibility from spin polarized neutron scattering

Bourges PRB 53,876 [1996]





#### Hayden et.al. < PRL 76,1344 [1996]



Local spin susceptibility from polarized spin neutron scattering

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