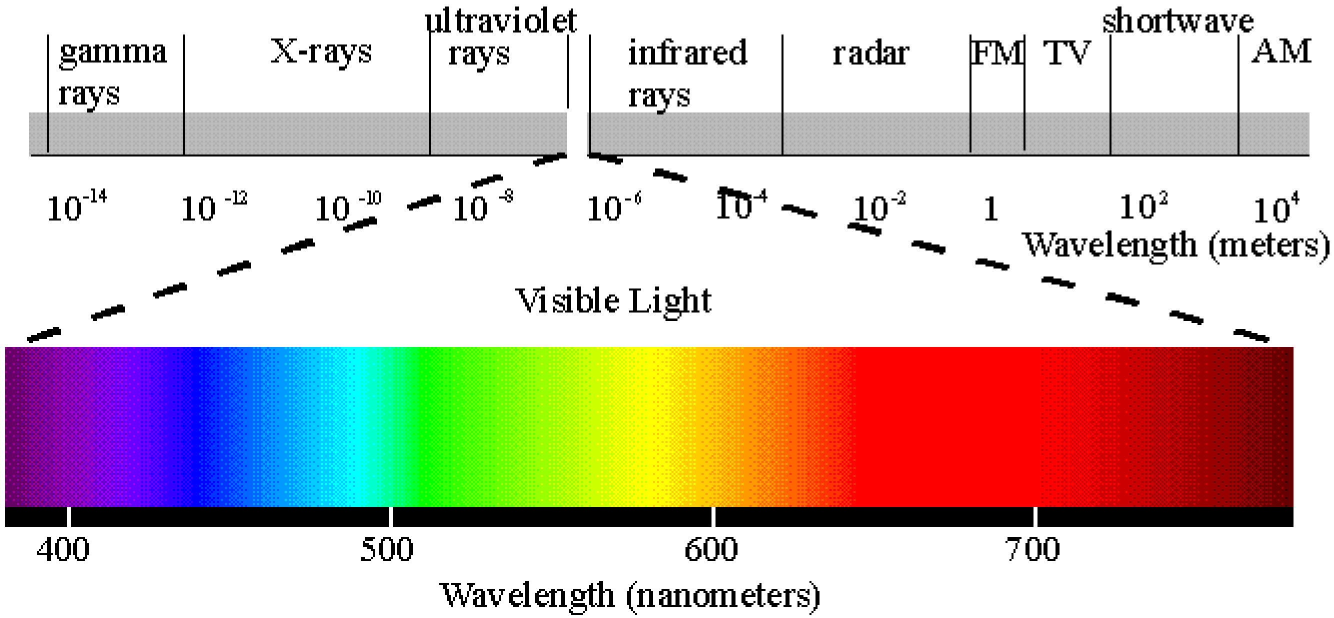
-

- Kramers-Kronig

- $MgTi_2O_4$ $CuIr_2S_4$ Peierls

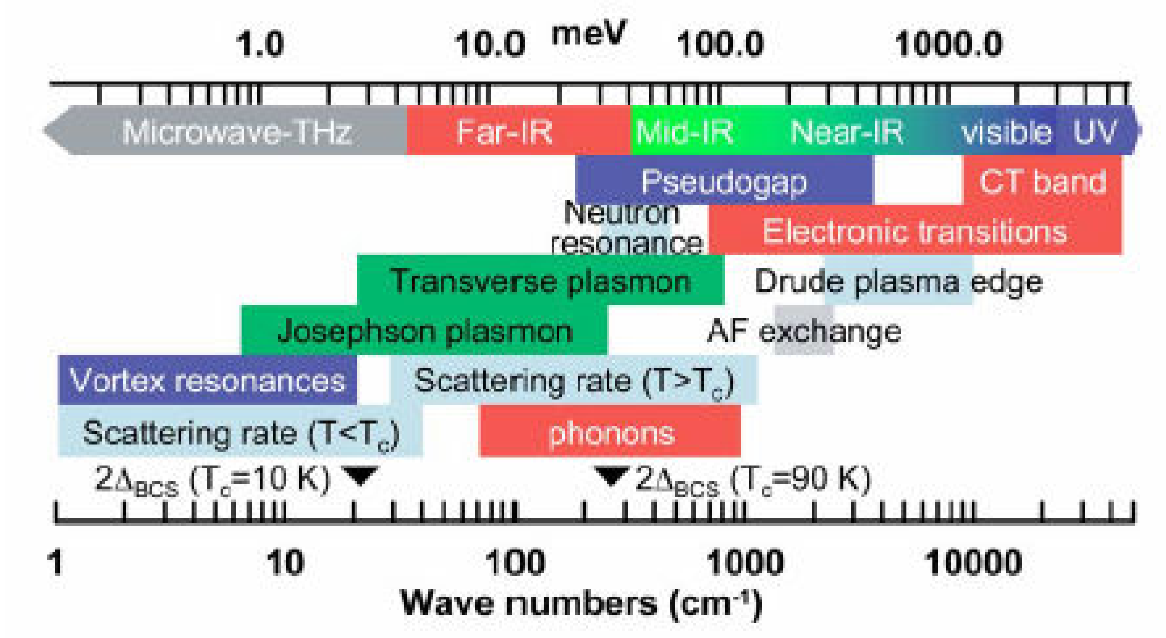
- Cu_xTiSe_2

Light



gamma rays
X-rays
ultraviolet rays
infrared rays
radar
FM
TV
shortwave
AM
10^{-14}
10^{-12}
10^{-10}
10^{-8}
10^{-6}
10^{-4}
10^{-2}
1
10^{2}
10^{4}
Wavelength (meters)
Visible Light
400
500
600
700
Wavelength (nanometers)

D. N. Basov, T. Timusk, Rev Mod Phys 2005



1 eV = 8065 cm-1 = 11400 K

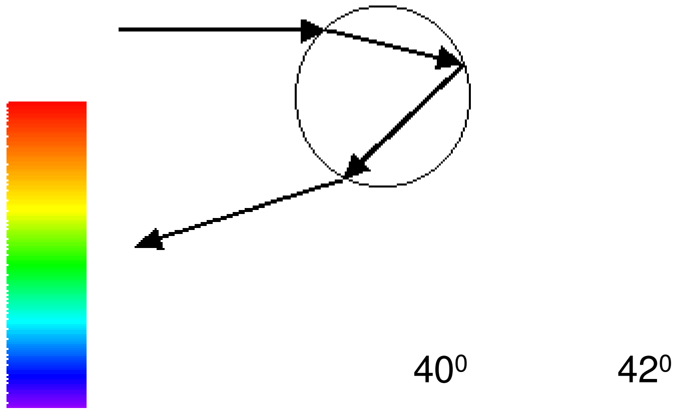
1.24 eV=10000 cm-1

ν 10000/λ

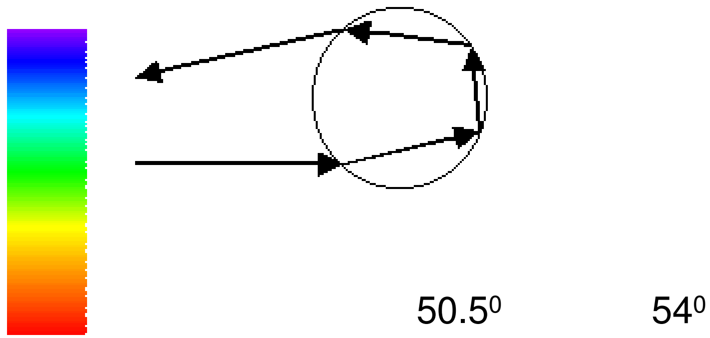
(ν: cm-1) (λ: μm)

Rainbow

Primary Bow

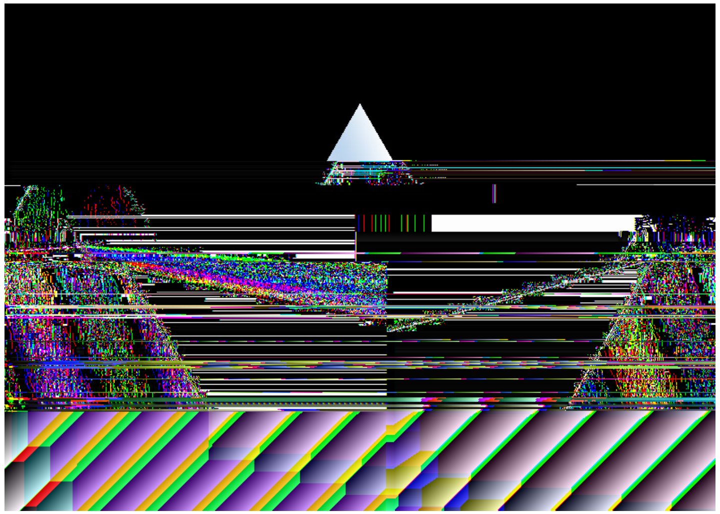


Secondary Bow (reflected twice)



1666 Newton

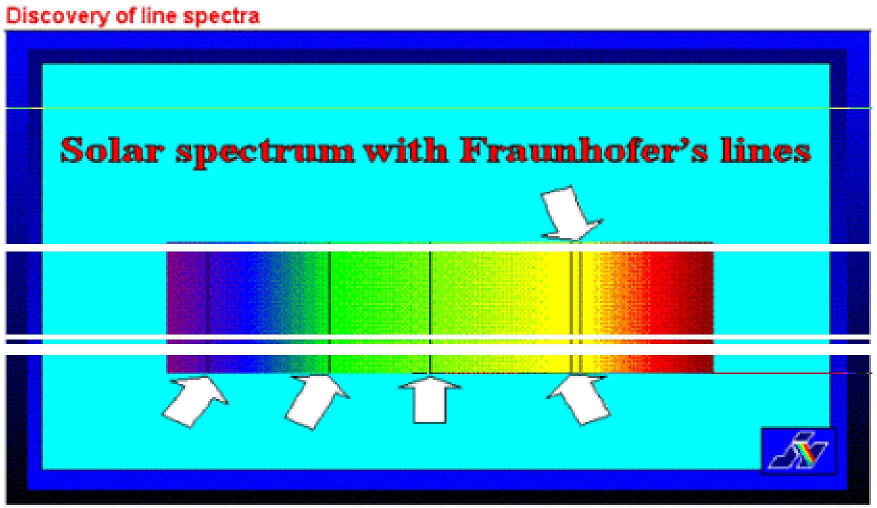
Newton spectrum



Newton' s analysis of light was the beginning of the science of spectroscopy.

W Herschel (1800)

J.W. Ritter (1801)

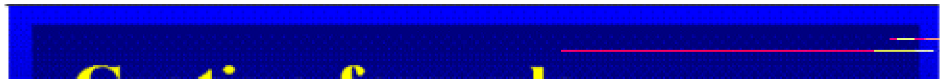


Joseph Fraunhofer(1787-1826)

1814 Fraunhofer lines.

T. Young
Fraunhofer

Fraunhofer

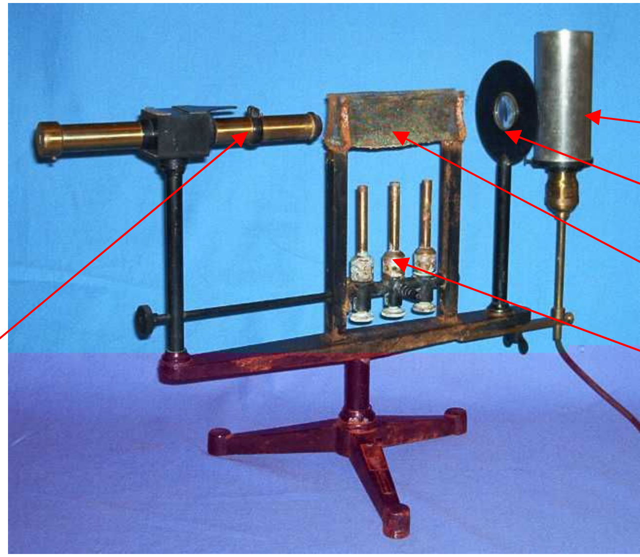


Fraunhofer

Fraunhofer 33 Kirchhoff

1848
Foucault

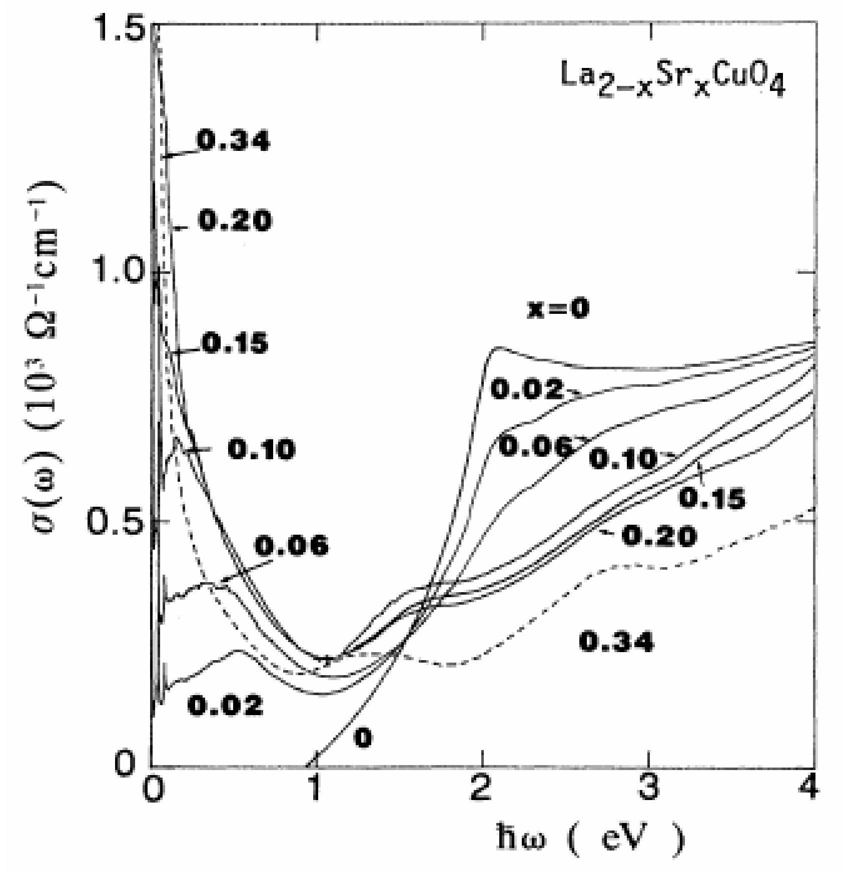
Na

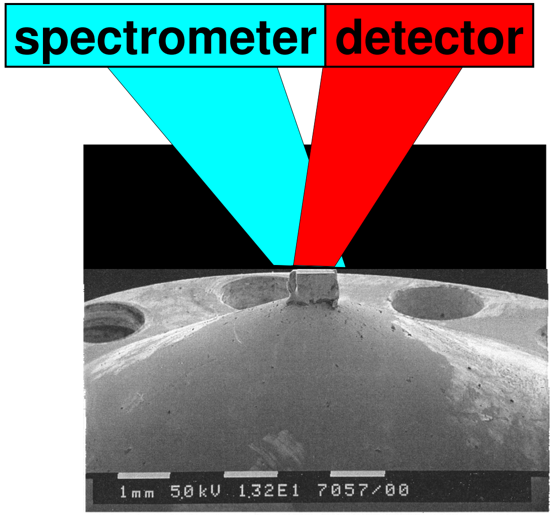


NaCl

During the latter half of the nineteenthofathinfa 5 2 9 9 (§ (f] T J e 4 9

Optical conductivity





- $R(\omega)$
- $\varepsilon(\omega)$, $\sigma(\omega)$

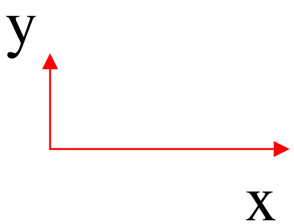
  $R(\omega)$ Kramers-Kronig
-

Optical properties of solids

1. Optical constants
2. Kramers-Kronig transformation
3. Interband transition
4. Intraband transition
   - Drude model
   - Non-Drude spectra of strongly correlated electrons
   - Optical spectra of a superconductor

1. Optical constants

Consider an electromagnetic wave in a medium



$$E_y = E_0 e^{i(qx-\omega t)} = E_0 e^{i\omega(x/v-t)} = E_0 e^{i\omega(\frac{nx}{c}-t)}$$

where $v \equiv \omega/q = c/n(\omega)$, $n(\omega)$: refractive index

If there exists absorption,

$$E_y = E_0 e^{-\frac{\omega K x}{c}} e^{i\omega(\frac{nx}{c}-t)}$$

K: attenuation factor

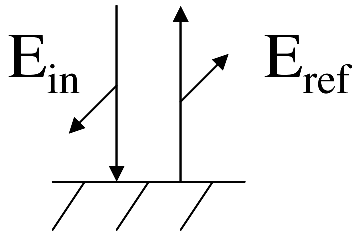
Intensity

$$\mathrm{I} \propto E_y^2 = E_0^2 e^{-\frac{2\omega K x}{c}}$$

Introducing a complex refractive index: $N(\omega) \equiv n(\omega) + iK(\omega)$

$$E_y = E_0 e^{i\omega(\frac{N(\omega)x}{c}-t)}$$

Reflectivity



$$\frac{E_{ref}}{E_{in}} \equiv r = r(\omega)e^{i\theta(\omega)}$$

$$= \frac{n+iK-1}{n+iK+1} = \sqrt{\frac{(n-1)^2+K^2}{(n+1)^2+K^2}}e^{i\theta(\omega)}$$

$$R = |E_{ref}/E_{in}|^2 = |r(\omega)|^2 = \frac{(n-1)^2+K^2}{(n+1)^2+K^2}$$

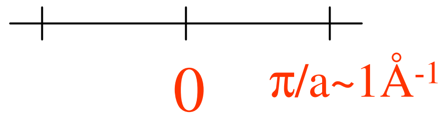
$$tg\,\theta = \frac{2K}{n^2+K^2-1}$$

$$n = \frac{1-R}{1+R-2R^{1/2}\cos\theta}$$

$$k = \frac{-2R^{1/2}\sin\theta}{1+R-2R^{1/2}\cos\theta}$$

If n, K are known, we can get R, θ; vice versa.

Dielectric function



$$D(q,\omega) \equiv \varepsilon(q,\omega)E(q,\omega)$$

$$photon, q \rightarrow 0, \varepsilon = \varepsilon(\omega, q \rightarrow 0) = \varepsilon(\omega)$$

Infrared
$q=2\pi/\lambda \sim 10^{-4}$ Å^{-1}

$$\because \sqrt{\varepsilon(\omega)} = N(\omega)$$

$$\Rightarrow \varepsilon(\omega) \equiv \varepsilon_1(\omega) + i\varepsilon_2(\omega) = (n(\omega) + iK(\omega))^2$$

$$\begin{cases} \varepsilon_1(\omega) = n^2(\omega) - K^2(\omega) \\ \varepsilon_2(\omega) = 2n(\omega)\cdot K(\omega) \end{cases}$$

conductivity

$$\sigma = \sigma_1(\omega) + \sigma_2(\omega)$$

By electrodynamics, $\varepsilon(\omega) = 1 + \dfrac{4\pi i \sigma(\omega)}{\omega}$

In a solid, considering the contribution from ions or from high energy electronic excitations

$$\varepsilon(\omega) = \varepsilon_\infty + \frac{4\pi i \sigma(\omega)}{\omega}$$

Now, we have several pairs of optical constants:

$$\begin{cases} n(\omega),\ K(\omega) \\ R(\omega),\ \theta\,(\omega) \\ \varepsilon_1(\omega),\ \varepsilon_2(\omega) \\ \sigma_1(\omega),\ \sigma_2(\omega) \end{cases}$$

But only $R(\omega)$ can be measured experimentally.

Kramers-Kronig

Kramers-Kronig transformation:

$$P(\omega) = \chi(\omega)E(\omega)$$

χ(ω)

FT

$$P(t) = \int_{-\infty}^{\infty} dt'\,\chi(t-t')E(t')$$

$$E_r(\omega) = r(\omega)E_i(\omega)$$

$$E_r(t) = \int_{-\infty}^{\infty} dt'\,r(t-t')E_i(t')$$

$$\chi(\omega) = \alpha(\omega)F(\omega)$$

$$\chi(t) = \int_{-\infty}^{\infty} dt'\,\alpha(t-t')F(t')$$

ω

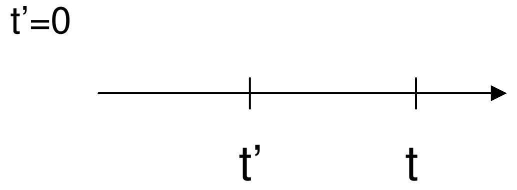
t

α(t-t')

Causality:

t<t', α(t-t')=0,

$$\alpha(\omega) = \int_{-\infty}^{\infty} \alpha(t) e^{i\omega t} dt = \int_{0}^{\infty} \alpha(t) e^{i\omega t} dt$$

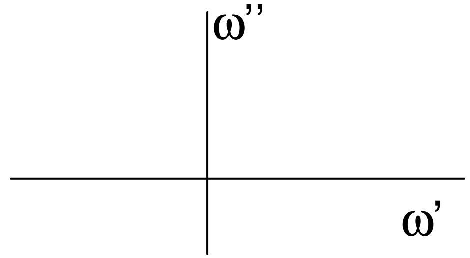


α(ω) ω

$$\omega \rightarrow \omega = \omega' + i\omega''$$

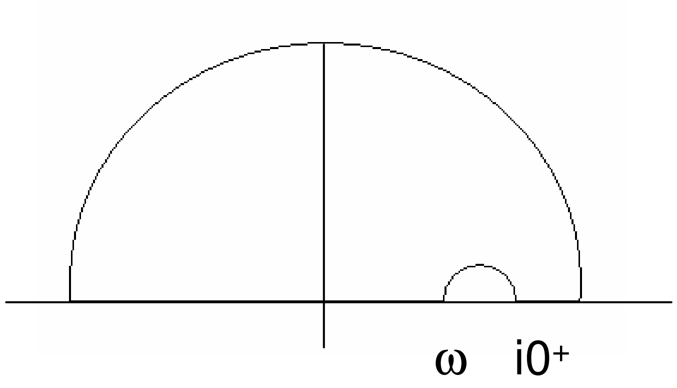
$$\alpha(\omega) = \int_{0}^{\infty} \alpha(t) e^{i(\omega' + i\omega'')t} dt = \int_{0}^{\infty} \alpha(t) e^{-\omega'' t} e^{i\omega t} dt$$

$\because t > 0, e^{-\omega'' t}$ α(ω) ω



Consider the integral

$$\oint \frac{\alpha(\omega')d\omega'}{\omega'-\omega+i0^+}$$



ω i0+

0

ω'→∞ α(ω') →0

0

$$\oint \frac{\alpha(\omega')d\omega'}{\omega'-\omega+i0^+} = \int_{-\infty}^{\infty} \frac{\alpha(\omega')d\omega'}{\omega'-\omega+i0^+} = 0$$

$$\because \frac{1}{x \mp i0^+} = \frac{P}{x} \pm i\pi\delta(x)$$

$$\Rightarrow \frac{1}{\pi i} P\int_{-\infty}^{\infty} \frac{\alpha(\omega')d\omega'}{\omega'-\omega} - \alpha(\omega) = 0$$

α(ω) α₁(ω)+iα₂(ω)

K-K

$$\alpha_1(\omega) = \frac{1}{\pi} P\int_{-\infty}^{+\infty} \frac{\alpha_2(\omega')\mathrm{d}\omega'}{\omega'-\omega}$$

$$\alpha_2(\omega) = \frac{-1}{\pi} P\int_{-\infty}^{+\infty} \frac{\alpha_1(\omega')\mathrm{d}\omega'}{\omega'-\omega}$$

$$\frac{1}{x \mp i0^{+}} = \frac{P}{x} \pm i\pi\delta(x)$$

$$\because \frac{1}{x - i\delta} = \frac{x + i\delta}{x^2 + \delta^2} = \frac{x}{x^2 + \delta^2} + i\frac{\delta}{x^2 + \delta^2}$$

δ→0+ $\frac{x}{x^2 + \delta^2} = \frac{1}{x}$ for x≠0 $\frac{P}{x}$

$$\frac{x}{x^2 + \delta^2} = 0$$

$P\int_{-\infty}^{\infty} \frac{f(x)}{x} dx$ x=0

δ→0+ $\frac{\quad}{\ ^2 \quad ^2}$ for x≠0

K-K

$$\because \alpha(\omega)=\int_0^{\infty}\alpha(t)e^{i\omega t}dt$$

$$\therefore \alpha_1(\omega)=\int_0^{\infty}\alpha(t)\cos(\omega t)dt \qquad \alpha_1(\omega)=\alpha_1(-\omega)$$

$$\alpha_2(\omega)=\int_0^{\infty}\alpha(t)\sin(\omega t)dt \qquad \alpha_2(\omega)=-\alpha_2(-\omega)$$

$$\alpha_2(\omega)=\frac{-1}{\pi}P\int_{-\infty}^{0}\frac{\alpha_1(\omega')\mathrm{d}\omega'}{\omega'-\omega}+\frac{-1}{\pi}P\int_0^{\infty}\frac{\alpha_1(\omega')\mathrm{d}\omega'}{\omega'-\omega}$$

ω'→-ω'

$$=\frac{1}{\pi}P\int_0^{\infty}\frac{\alpha_1(\omega')\mathrm{d}\omega'}{\omega'+\omega}+\frac{-1}{\pi}P\int_0^{\infty}\frac{\alpha_1(\omega')\mathrm{d}\omega'}{\omega'-\omega}$$

$$=\frac{-2\omega}{\pi}P\int_0^{\infty}\frac{\alpha_1(\omega')\mathrm{d}\omega'}{\omega'^2-\omega^2}$$

$$=\frac{-1}{\pi}P\int_0^{\infty}[d\ln\left|\frac{\omega'+\omega}{\omega'-\omega}\right|]\alpha_1(\omega')$$

$$\frac{1}{\frac{\omega'+\omega}{\omega'-\omega}}\frac{(\omega'-\omega)d\omega'-(\omega'+\omega)d\omega'}{(\omega'-\omega)^2}=\frac{-2\omega d\omega'}{\omega'^2-\omega^2}$$

$$=\frac{-1}{\pi}P\int_0^{\infty}\ln\left|\frac{\omega'+\omega}{\omega'-\omega}\right|]\frac{d\alpha_1(\omega')}{d\omega}$$

$$\alpha_1(\omega) = \frac{2}{\pi} P \int_0^{+\infty} \frac{\omega' \alpha_2(\omega') \mathrm{d}\omega'}{\omega'^2 - \omega^2}$$

:

$$r(\omega) = \sqrt{R(\omega)} e^{i\theta}$$

$$\Rightarrow \ln r(\omega) = (1/2) \ln R(\omega) + i\theta$$

$$\theta = \frac{\omega}{\pi} P \int_0^{\infty} \frac{\ln R(\omega')}{\omega^2 - \omega'^2} d\omega'$$

Low- ω extrapolation:

Insulator: R~ constant

Metal: Hagen-Rubens

Superconductor: two-fluids model

High-ω extrapolation:

R~ ω^{-p} (p~4)

$$D = E + 4\pi P$$

$$\Rightarrow 4\pi P = [\varepsilon(\omega) - 1] E$$

$$\varepsilon_1(\omega) - 1 = \frac{2}{\pi} P \int_0^{+\infty} \frac{\omega' \varepsilon_2(\omega') \mathrm{d}\omega'}{(\omega')^2 - \omega^2}$$

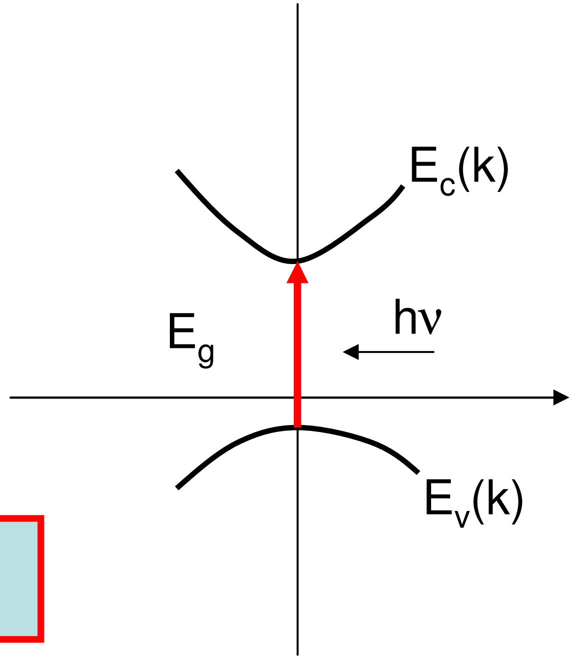
$$\varepsilon_2(\omega) = -\frac{2\omega}{\pi} P \int_0^{+\infty} \frac{[\varepsilon_1(\omega') - 1] \mathrm{d}\omega'}{(\omega')^2 - \omega^2}$$

k'=k.

$$|\,v,k>, E_v(k)$$

$$|\,c,k>, E_c(k)$$

$$\hbar\omega = E_c(k) - E_v(k) \equiv E_{cv}(k)$$

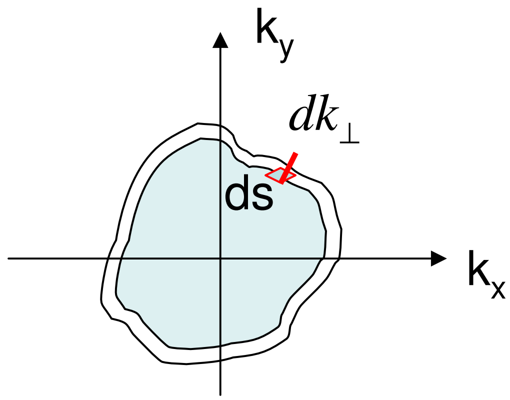


Kubo-Greenwood

van Hove

E—E+ΔE ΔZ

$$N(\varepsilon) = \lim \frac{\Delta Z}{\Delta E}$$



k E(k)=const E E +ΔE

ΔZ k V/(2π)^3,

ΔZ V/(2π)^3•(E—E+ΔE)

E—E+ΔE $dsdk_\perp$

$$\Delta Z = \frac{V}{(2\pi)^3}\int d\vec{k} = \frac{V}{(2\pi)^3}\int ds dk_\perp$$

ds $dk_\perp$

$$= (\frac{V}{(2\pi)^3}\int \frac{ds}{|\nabla_k E|})\Delta E$$

$$\because \Delta E = |\nabla_k E(k)| \cdot dk_\perp$$

$|\nabla_k E|$

$$N(E) = \lim \frac{\Delta Z}{\Delta E} = \frac{V}{(2\pi)^3}\int \frac{ds}{|\nabla_k E|}$$

E(k) N(E).

$$E = \frac{(\hbar\vec{k})^2}{2m^*}$$

$$\nabla_k E(k) = \left(\frac{\hbar^2 k_x}{m^*}, \frac{\hbar^2 k_y}{m^*}, \frac{\hbar^2 k_z}{m^*}\right)$$

$$|\nabla_k E(k)| = \frac{\hbar^2}{m^*}\sqrt{k_x^2 + k_y^2 + k_z^2} = \frac{\hbar^2 k}{m^*} = \frac{\hbar^2}{m^*}\left(\frac{2m^*}{\hbar^2}\right)^{1/2}\sqrt{E(k)}$$

$$N(E) = \frac{2V}{(2\pi)^3}\int_0^{\pi}\int_0^{2\pi}\frac{k^2 \sin\theta d\theta d\varphi}{\left(\frac{2\hbar^2}{m^*}\right)^{1/2} E^{1/2}} = \frac{V}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2} E^{1/2}$$

$\nabla_k E(k) = 0$ $\equiv$ van Hove singularity

Obviously, the density of states will be high if a band is flat.

$$N(E) = \frac{V}{(2\pi)^3} \int \frac{ds}{|\nabla_k E|}$$

$$\hbar\omega = E_c(k) - E_v(k) \equiv E_{cv}(k)$$

E $E_{cv}(k)$

Hamiltonian $H_0 = \frac{\vec{p}^2}{2m} + U(r)$

$$H = \frac{(\vec{p} - \frac{e}{c}\vec{A})^2}{2m} + U(r) = \frac{1}{2m}\vec{p}^2 + U(r) - \frac{e}{mc}\vec{A}\cdot\vec{p} = H_0 + H'$$

A^2

Coulomb $\nabla\cdot\mathbf{A}$ 0 $\because \vec{p}\cdot\vec{A} - \vec{A}\cdot\vec{p} = -i\hbar\nabla\cdot\vec{A}$

$$\vec{E}(t) = -\frac{1}{c}\frac{\partial\vec{A}(t)}{\partial t} \longrightarrow \boxed{\vec{E} = i\omega\vec{A}/c}$$

H' |v, k> → |c, k>

$$W_{v,\vec{k}\to c,\vec{k}} = \frac{2\pi}{\hbar}|<v,\vec{k}\,|\,H'\,|\,c,\vec{k}>|^2\ \delta(E_c(k) - E_v(k) - \hbar\omega)$$

$$\vec{A}(t) = A_0\vec{e}_s e^{-i\omega t}$$

↑

(∇_rxA(t) 0)

$$W_{v,\vec{k}\to c,\vec{k}} = \frac{2\pi}{\hbar} \left| \frac{e}{mc} A_0 \vec{e}_s \cdot < v,\vec{k} \,|\, \vec{p} \,|\, c,\vec{k} > \right|^2 \delta(E_{vc}(k) - \hbar\omega)$$

$$= \frac{2\pi e^2}{\hbar m^2 \omega^2} |\, \vec{p}(E_{vc}(k)) \,|^2 \; \delta(\hbar\omega - E_{vc}(k)) \,|\, E \,|^2$$

|v, k> → |c, k>

|v, k> → |c, k>

$$W_{v\to c} = \frac{2}{V}\sum_k W_{v,\vec{k}\to c,\vec{k}} = 2\int_{BZ} \frac{d^3k}{(2\pi)^3} \cdot \frac{2\pi e^2}{\hbar m^2 \omega^2} |\, \vec{p}(E_{vc}(k)) \,|^2 \; \delta(\hbar\omega - E_{vc}(k)) \,|\, E \,|^2$$

$$E_{vc}(k) = \hbar\omega$$

$$2\int_{BZ} \frac{d^3k}{(2\pi)^3} \delta(\hbar\omega - E_{vc}(k)) = J(\hbar\omega)$$

$$W_{v\to c} = \frac{2\pi e^2}{\hbar m^2 \omega^2} J(\hbar\omega) \,|\, \vec{p}_{vc}(\hbar\omega) \,|^2 |\, E \,|^2$$

$$\hbar\omega W_{v\to c} = \frac{2\pi e^2}{m^2\omega} J(\hbar\omega)\,|\,\vec{p}_{vc}(\hbar\omega)\,|^2\,|\,E\,|^2$$

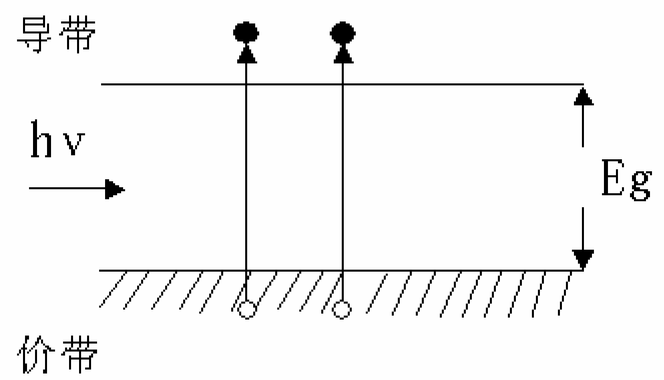
$\sigma_1|E|^2 \quad (1/4\pi)\omega\varepsilon_2(\omega)|E|^2$

$$\varepsilon_2(\omega) = \frac{8\pi^2 e^2}{m^2\omega^2} J(\hbar\omega)\,|\,\vec{p}_{vc}(\hbar\omega)\,|^2$$

$\varepsilon_2(\omega)$ Kramers-Kronig

A.

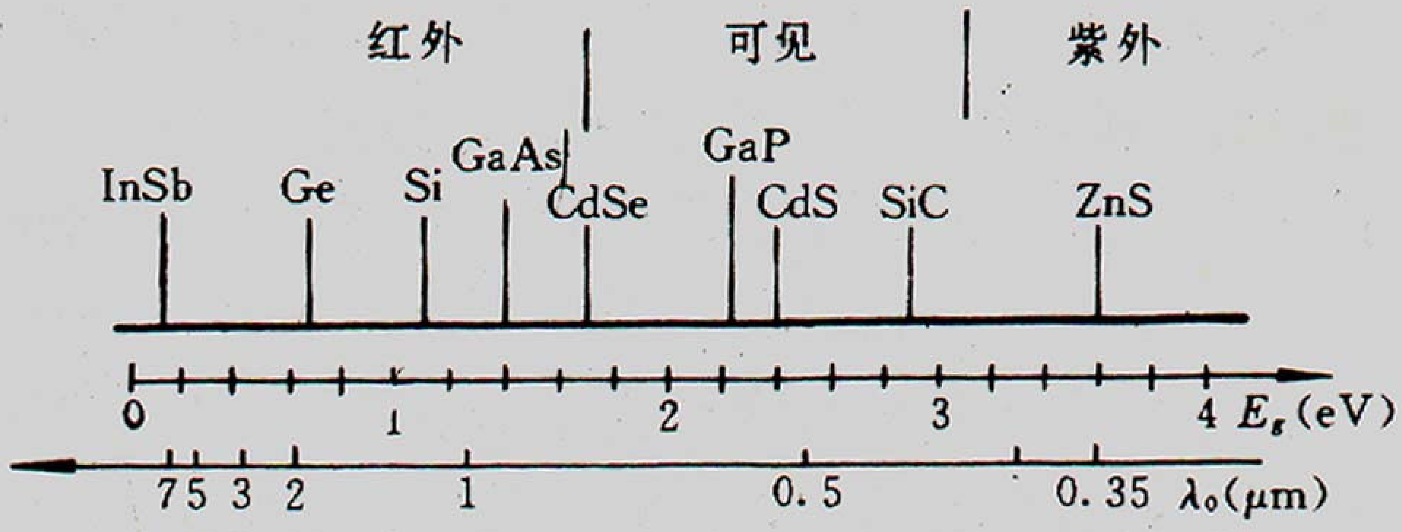
OK



—

GaAs: Eg= 1.5eV

Si: Eg= 1.12eV

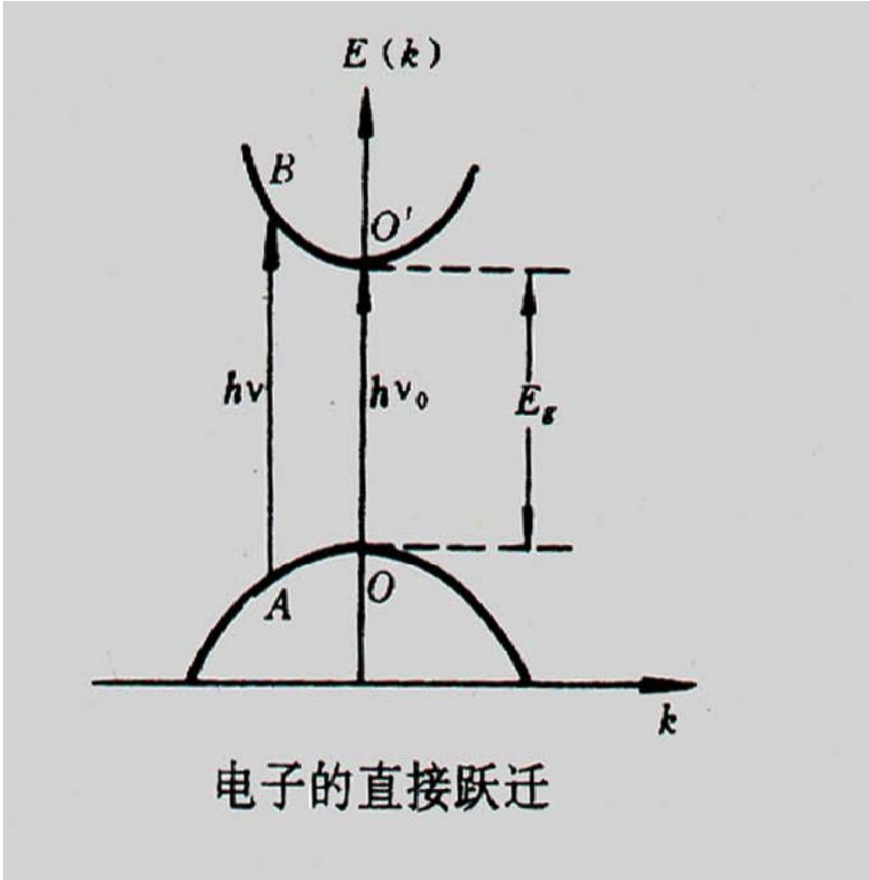


E_g 和 λ_0 的对应关系

B.

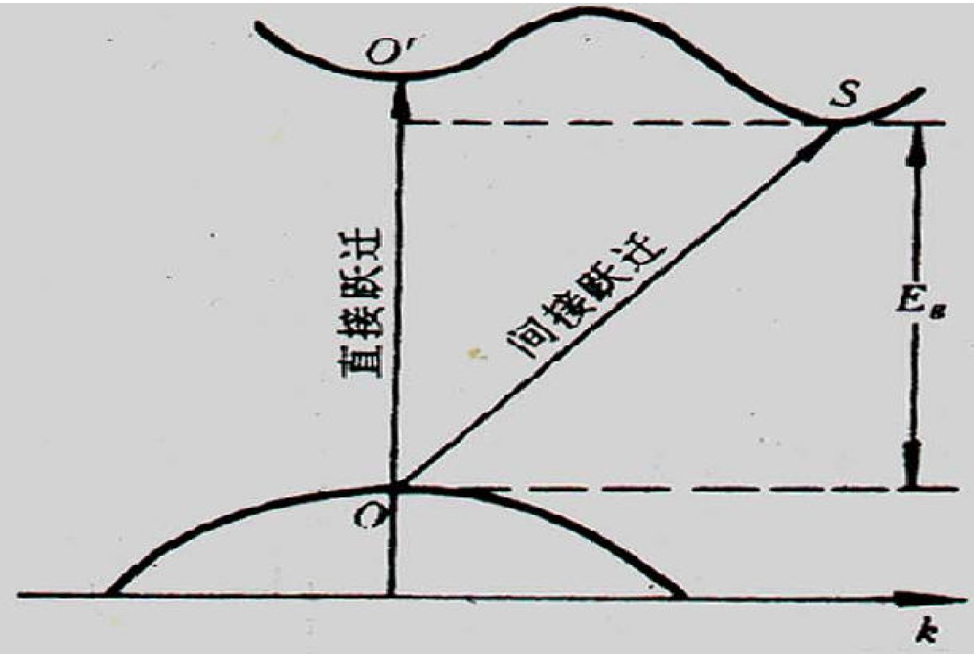
(k

GaAs



$$\alpha(h\nu)=\begin{cases}A(h\nu-E_g)^{\frac{1}{2}} & h\nu\geq E_g\\ 0 & h\nu<E_g\end{cases}$$

Si：间接带隙半导体



直接跃迁和间接跃迁

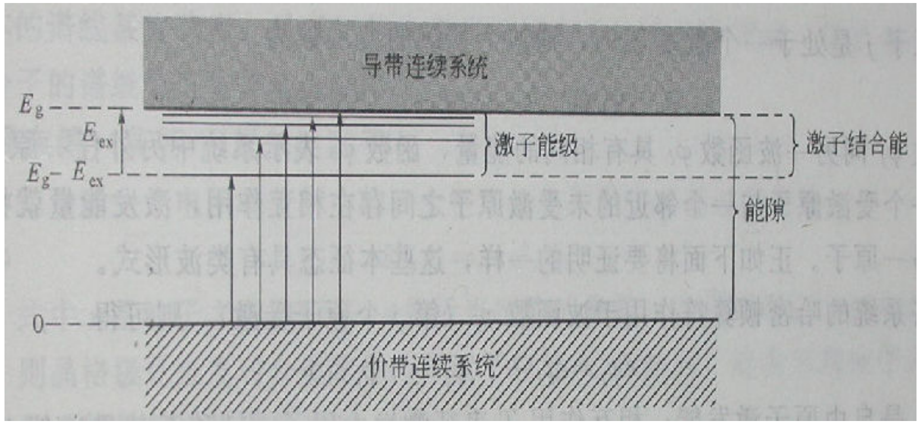
C.

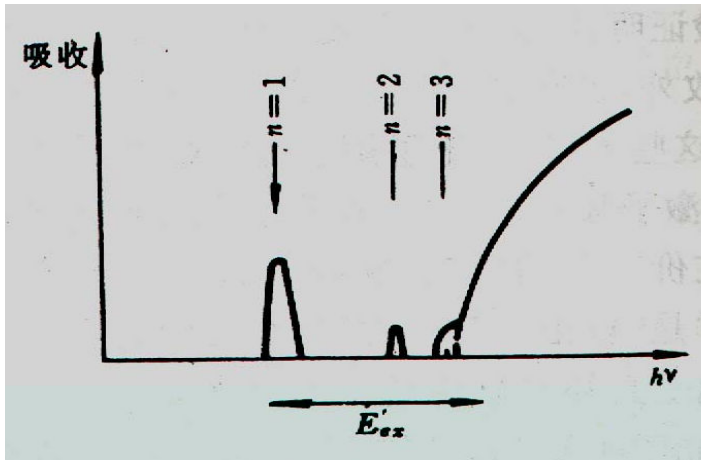
i).

E_g

, E_b

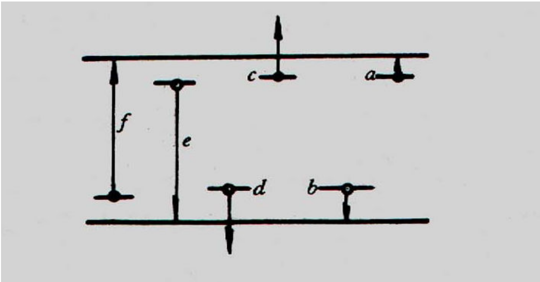
$$h\nu = E_g - E_b$$





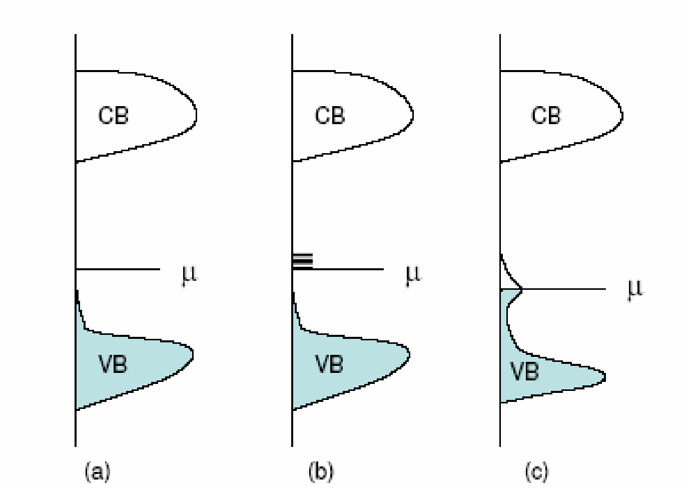
激子吸收光谱

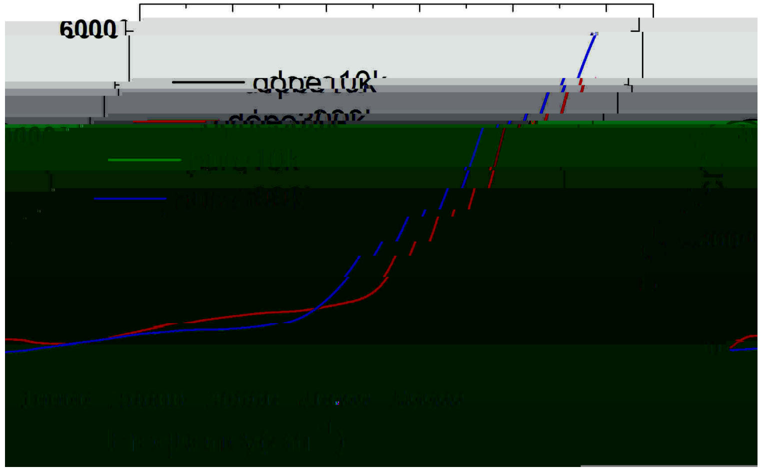
ii). 杂质吸收



杂质吸收中的电子跃迁

B-doped Diamond D Wu et al. PRB 06





iii). 声子吸收

Drude model

Drude

Drude

Boltzman

Kubo →0

$$\sigma(\omega) = \frac{\sigma_0}{1 - i\omega\tau}$$

$$\sigma_0 = \frac{ne^2\tau}{m^*} = \frac{\omega_p^2\tau}{4\pi}$$

$$\frac{d\vec{P}}{dt} + \frac{\vec{\mathrm{P}}}{\tau} = -e\vec{E}$$

$$\vec{\mathrm{p}}(t) = m^*\vec{\mathrm{v}}$$

$$\vec{E} = \vec{E}_0 e^{i(\vec{q}\cdot\vec{r}-\omega t)}$$
$$\vec{P} = \vec{P}_0 e^{i(\vec{q}\cdot\vec{r}-\omega t)}$$

$$\Rightarrow \quad -i\omega\vec{\mathrm{P}}(\omega) = -e\vec{E}(\omega) - \frac{1}{\tau}\vec{\mathrm{P}}(\omega) \quad \Rightarrow \quad \vec{\mathrm{P}}(\omega) = \frac{e}{i\omega - 1/\tau}\vec{E}(\omega)$$

$$\vec{J}(t) = -ne\,\vec{\mathrm{v}}(t) = -ne\,\vec{\mathrm{P}}(\omega)/m^*$$

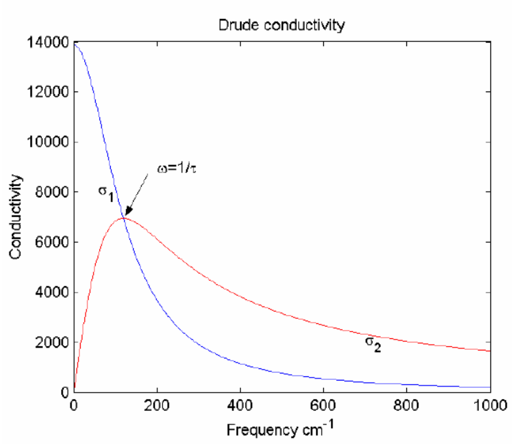
$$\vec{J}(\omega) = -\frac{ne}{m^*}\vec{\mathrm{P}}(\omega) = \frac{ne^2\tau/m^*}{1-i\omega\tau}\vec{E}(\omega)$$

$$\Rightarrow \quad \sigma(\omega) = \frac{\sigma_0}{1-i\omega\tau} = \frac{\omega_D^2}{4\pi}\frac{1}{1/\tau - i\omega}$$

$$\sigma_0 = \frac{ne^2\tau}{m^*} = \frac{\omega_p^2\tau}{4\pi}$$

$$\sigma_1(\omega) = \frac{\sigma_0}{1+\omega^2\tau^2} = \frac{\omega_p^2\tau}{4\pi}\frac{1}{1+\omega^2\tau^2}$$

$$\sigma_2(\omega) = \frac{\sigma_0\omega\tau}{1+\omega^2\tau^2} = \frac{\omega_p^2\tau}{4\pi}\frac{\omega\tau}{1+\omega^2\tau^2}$$



$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega) = 1 + \frac{4\pi i}{\omega}\sigma(\omega)$$

$$\varepsilon(\omega) = \varepsilon_\infty + \frac{4\pi i}{\omega}\sigma(\omega)$$

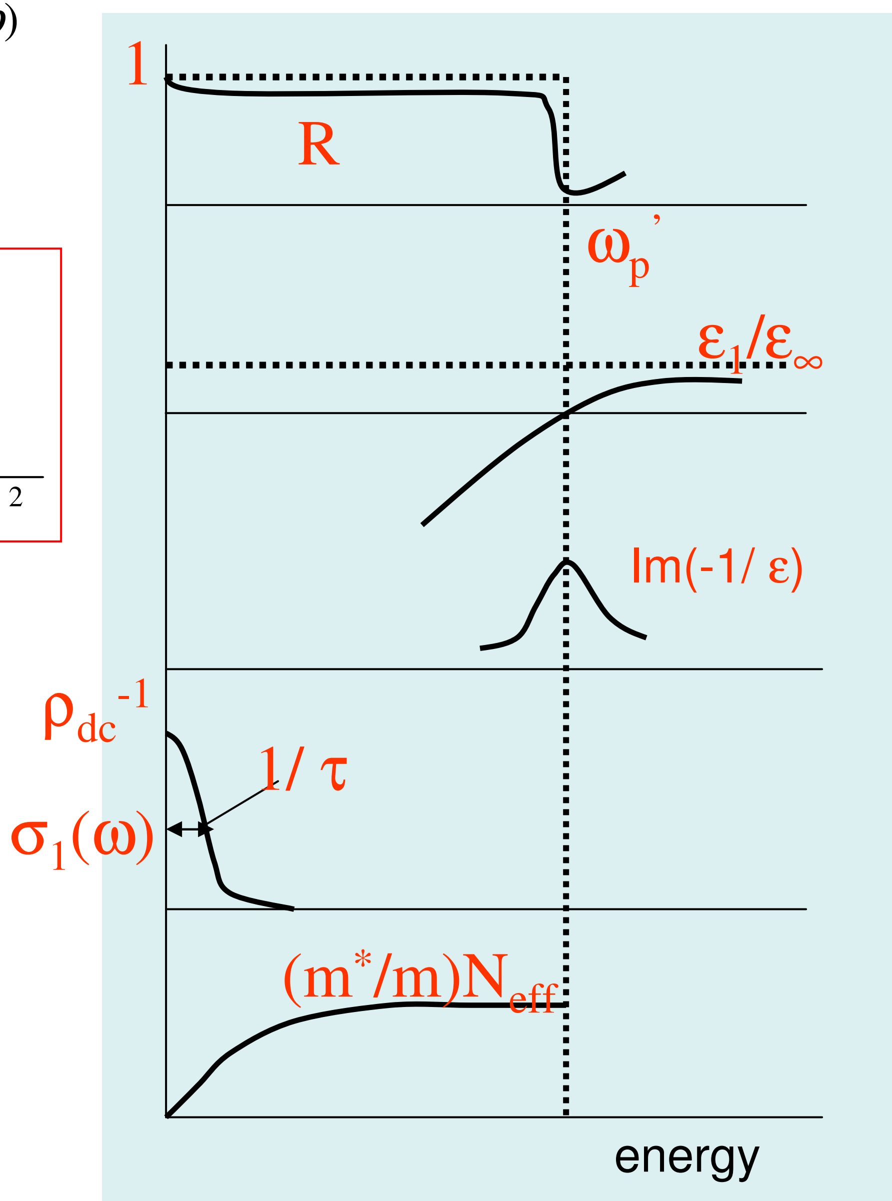
$$\Rightarrow \quad \varepsilon_1 = \varepsilon_\infty - \frac{\omega_p^2}{\omega^2 + 1/\tau^2}$$

$$\varepsilon_2 = \frac{4\pi\sigma_1}{\omega} = \frac{\omega_p^2 \tau}{\omega}\frac{1}{1+\omega^2\tau^2}$$

$$\mathrm{Im}\left[\frac{1}{-\varepsilon(\omega)}\right] = \frac{\omega_p'^2 \omega/\tau}{(\omega^2 - \omega_p'^2)^2 + \omega^2\tau^{-2}}$$

$$\omega_p' = \omega_p / \sqrt{\varepsilon_\infty}$$

$$\int_0^\infty \sigma_1(\omega)d\omega = \frac{\omega_p^2}{8}$$



1.Hagen-Rubens regime

At low-frequency limit $\omega\tau \ll 1$

$$\begin{cases} \sigma_1(\omega) = \dfrac{\sigma_0}{1+\omega^2\tau^2} = \dfrac{\omega_p^2\tau}{4\pi}\dfrac{1}{1+\omega^2\tau^2} \\ \sigma_2(\omega) = \dfrac{\sigma_0\omega\tau}{1+\omega^2\tau^2} = \dfrac{\omega_p^2\tau}{4\pi}\dfrac{\omega\tau}{1+\omega^2\tau^2} \end{cases} \Rightarrow$$

$$\sigma_1(\omega) \approx \sigma_0$$

$$\sigma_2(\omega) \approx \sigma_0\omega\tau = \frac{\omega_p^2\tau^2}{4\pi}\omega \ll \sigma_1$$

$$\begin{cases} \varepsilon_1 = \varepsilon_\infty - \dfrac{\omega_p^2}{\omega^2 + 1/\tau^2} \\ \varepsilon_2 = \dfrac{4\pi\sigma_1}{\omega} = \dfrac{\omega_p^2\tau}{\omega}\dfrac{1}{1+\omega^2\tau^2} \end{cases}$$

$$\varepsilon_1 = \varepsilon_\infty - \frac{\tau^2\omega_p^2}{1+\omega^2\tau^2} \approx \varepsilon_\infty - \tau^2\omega_p^2$$

$$\varepsilon_2 = \frac{\omega_p^2\tau}{\omega}\frac{1}{1+\omega^2\tau^2} \approx \frac{\omega_p^2\tau}{\omega} = \frac{4\pi\sigma_0}{\omega} \gg \varepsilon_1$$

$$\begin{cases} n = \dfrac{1}{\sqrt{2}}\sqrt{\sqrt{\varepsilon_1^2+\varepsilon_2^2}+\varepsilon_1} \\ k = \dfrac{1}{\sqrt{2}}\sqrt{\sqrt{\varepsilon_1^2+\varepsilon_2^2}-\varepsilon_1} \end{cases}$$

$$n = k = \frac{1}{\sqrt{2}}\sqrt{\varepsilon_2} = \sqrt{\frac{2\pi\sigma_0}{\omega}} \gg 1$$

$$R = \frac{(n-1)^2+k^2}{(n+1)^2+k^2} = \frac{n^2-2n+1+k^2}{n^2+2n+1+k^2} = \frac{1-2/n+1/n^2+k^2/n^2}{1+2/n+1/n^2+k^2/n^2} \approx \frac{2-2/n}{2+2/n} \approx 1-2/n = 1-\sqrt{\frac{2\omega}{\pi\sigma_0}}$$

2. Relaxation regime

$$1/\tau < \omega < \omega_p$$

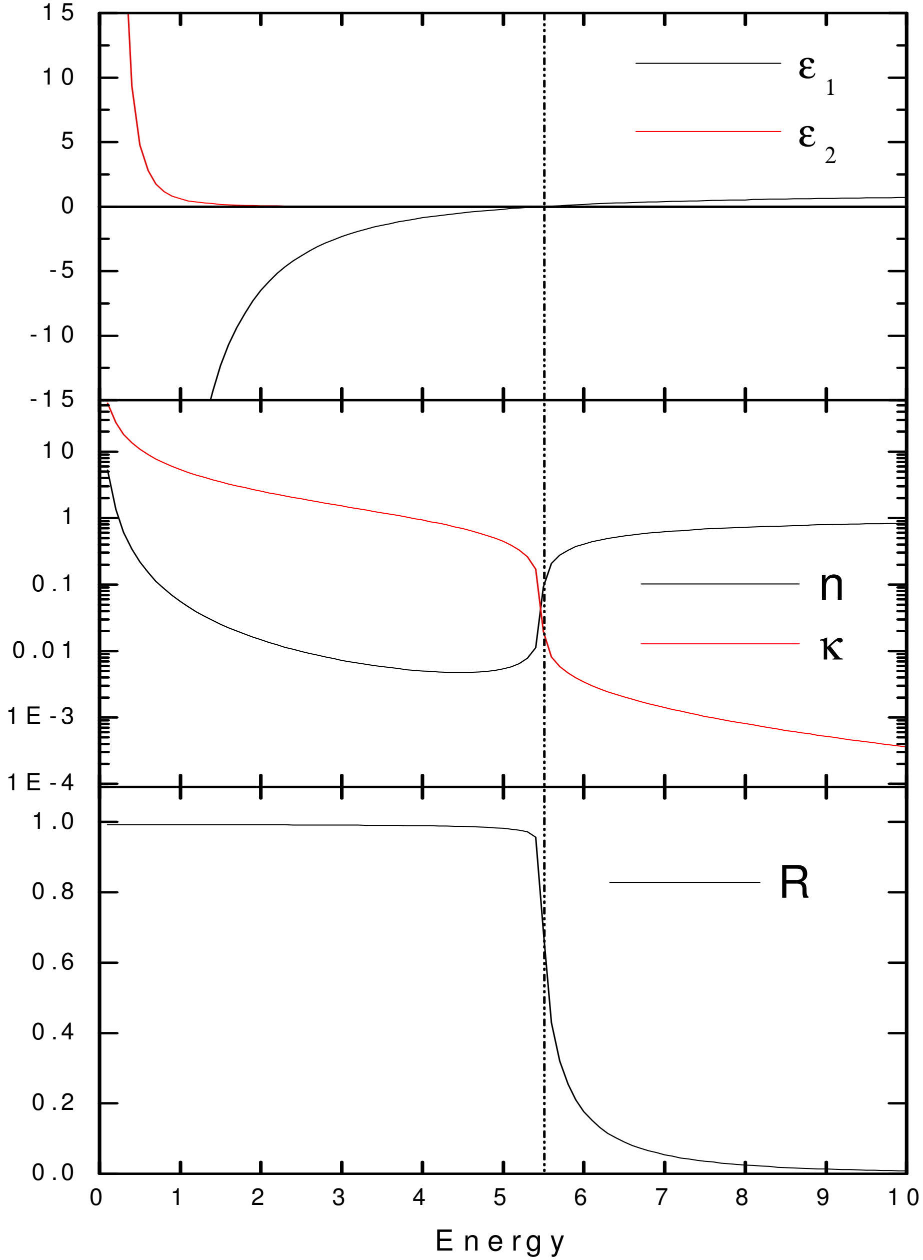
$$\begin{cases} 4\pi\sigma_1(\omega) = \dfrac{\omega_p^2\tau}{1+\omega^2\tau^2} \approx \dfrac{\omega_p^2}{\omega^2\tau} \\ 4\pi\sigma_2(\omega) = \dfrac{\omega\omega_p^2\tau^2}{1+\omega^2\tau^2} \approx \dfrac{\omega_p^2}{\omega} \end{cases} \qquad \begin{cases} \varepsilon_1 = \varepsilon_\infty - \dfrac{\omega_p^2}{\omega^2} \\ \varepsilon_2 = \dfrac{\omega_p^2}{\omega^3\tau} \end{cases} \qquad \begin{cases} n \approx \dfrac{\omega_p}{2\tau\omega} \\ k \approx \dfrac{\omega_p}{\omega} \end{cases}$$

⇒ $R \simeq 1 - \dfrac{2}{\omega_p\tau}$ a constant if τ is constant, otherwise $1-R \propto 1/\tau$

3. Ultraviolet transparency regime

$$\omega \gg \omega_p$$

$\varepsilon_1 \to \varepsilon_\infty$ (ε_1 crosses zero at $\omega = \omega_p/\sqrt{\varepsilon_\infty}$) $R \to 0$

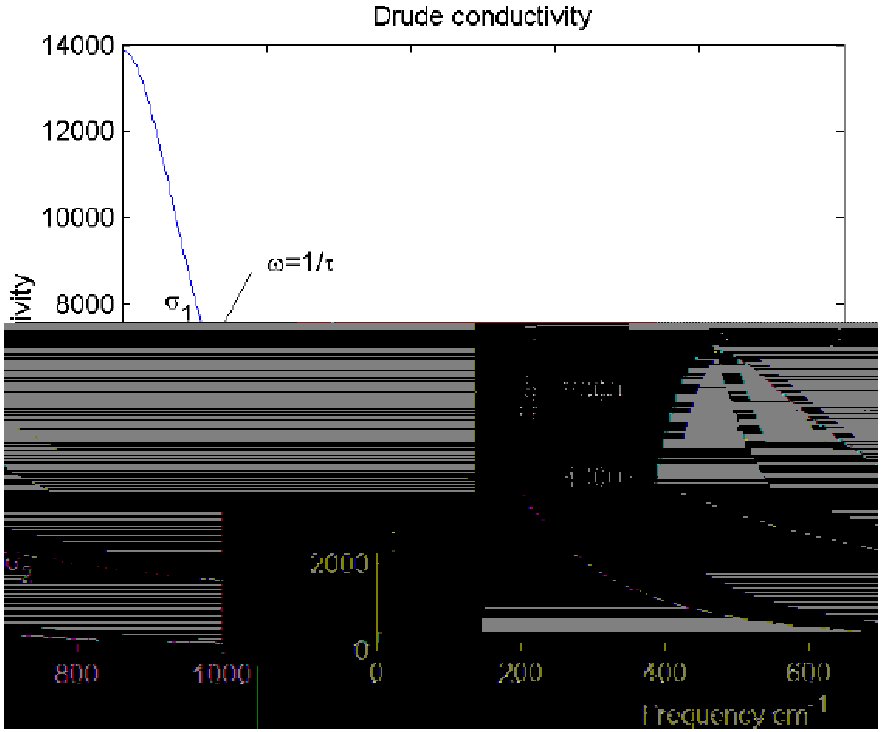


Plot of Drude Model spectra

$$\sigma(\omega) = \frac{\omega_D^2}{4\pi} \frac{1}{1/\tau \quad i\omega}$$

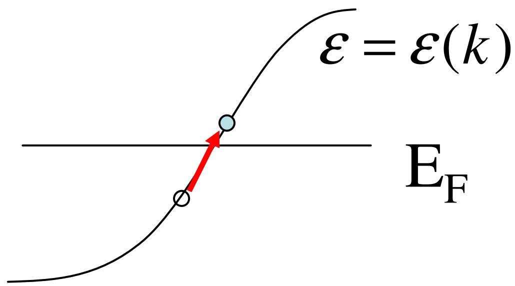
$$\Gamma = 0.02\mathrm{eV}$$

$$4\pi Ne^2 / m = \omega_p^2 = 30$$



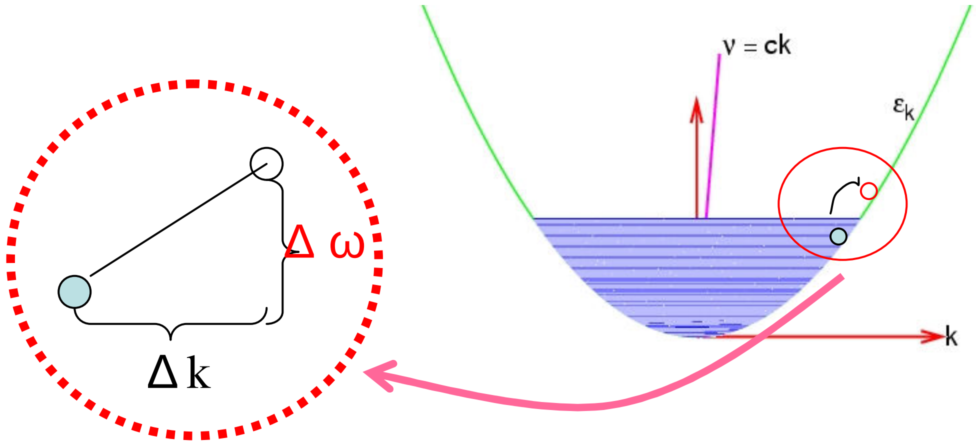
Intraband transition particle-hole

Boson mode

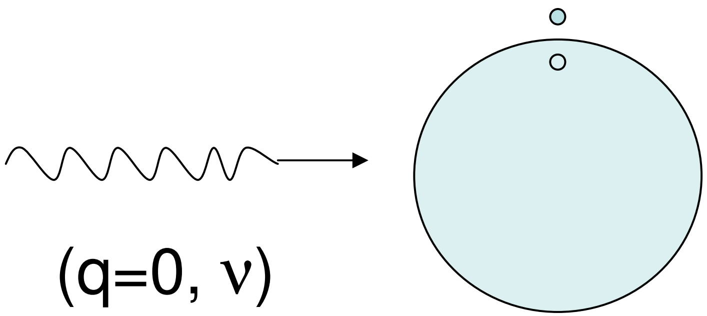


Absorption processes

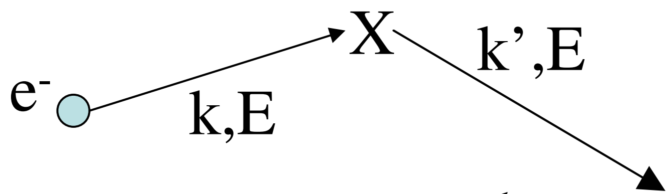
Infrared light <u>cannot</u> be absorbed by electron-hole pair creation



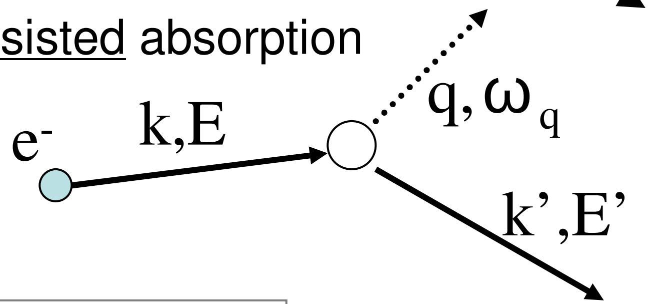
(The impurities or boson modes are needed to transfer the momemtum of particle-hole excitations. This is called impurities or boson-assisted absorptions.)



<u>(a) Impurity-assisted</u> absorption



<u>(b) boson-assisted</u> absorption



Holstein process, if phonons are involved.

Boltzmann

$$\frac{\partial f}{\partial t} + \vec{v}_k \bullet \nabla_r f + \dot{\vec{k}} \bullet \nabla_k f = \left(\frac{\partial f}{\partial t}\right)_{coll}$$

f=f(, , t)

k

$$\dot{\vec{k}} = \frac{\partial \vec{k}}{\partial t} = -\frac{e}{\hbar}\left(\vec{E} + \frac{1}{c}\vec{v}_k \times \vec{H}\right) = -\frac{e}{\hbar}\vec{E}$$

$$f = f_0 + f_1 \qquad f_0 = \frac{1}{1 + \exp[(\varepsilon_k - \varepsilon_F)/k_B T]}$$

$$\left(\frac{\partial f}{\partial t}\right)_{coll} = \frac{f - f_0}{\tau} = -\frac{f_1}{\tau}$$

$$\frac{\partial f}{\partial k} = \frac{\partial f}{\partial \varepsilon}\frac{\partial \varepsilon}{\partial k}, \qquad \vec{v}_k = \hbar^{-1}\nabla_k \varepsilon(\vec{k})$$

$$-\frac{\partial f^1}{\partial t} = \vec{v}_k \bullet \nabla_r f_1 - e\vec{E} \bullet \vec{v}_k \frac{\partial f^0}{\partial \varepsilon} + \frac{f^1}{\tau}$$

FT

$$J(q,\omega) = -\frac{2e^2}{(2\pi)^3}\int f^1 v_k dk = \frac{2e^2}{(2\pi)^3}\int dk \frac{\tau\vec{E}(\vec{q},\omega)\cdot\vec{v}_k(-\frac{\partial f^0}{\partial\varepsilon})}{1-i\omega\tau+iv_k\cdot q\tau} v_k$$

$$\hat{\sigma}(\vec{q},\omega) = \frac{2e^2}{(2\pi)^3} \iint \frac{\tau \vec{v}_k \vec{v}_k}{1 - i\omega\tau + i\vec{v}_k \cdot \vec{q}\tau} \left(-\frac{\partial f^0}{\partial \varepsilon}\right) \frac{dS}{\hbar v_k} d\varepsilon$$

$$= \frac{2e^2}{(2\pi)^3} \int_{\varepsilon=\varepsilon_F} \frac{\tau \vec{v}_k \vec{v}_k}{1 - i\omega\tau + i\vec{v}_k \cdot \vec{q}\tau} \frac{dS_F}{\hbar v_k}$$

q→0

$$\hat{\sigma}(q,\omega) = -\frac{e^2}{4\pi^3\hbar} \int \frac{\tau \vec{v}_k \vec{v}_k}{v_k} \frac{dS_F}{1 - i\omega\tau} = \sigma_{dc} \frac{1}{1 - i\omega\tau}$$

Kubo

Hamiltonian $$H_0 = \frac{1}{2m}\sum_{i=1}^{N}\vec{p}_i^{\,2} + \sum_{i=1}^{N} V_i(\vec{r}_i) + \frac{1}{2}\sum_{i,j=1}\frac{e^2}{|\vec{r}_i - \vec{r}_j|}$$

$$H = \frac{1}{2m}\sum_{i=1}^{N}[\vec{p}_i - \frac{e}{c}\vec{A}(\vec{r}_i)]^2 + \sum_{i=1}^{N} V_i(\vec{r}_i) + \frac{1}{2}\sum_{i,j=1}\frac{e^2}{|\vec{r}_i - \vec{r}_j|} = H_0 + H'$$

A^2

$$H' = -\frac{e}{2mc}\sum_{i=1}^{N}[\vec{p}_i\cdot\vec{A}(\vec{r}_i) + \vec{A}(\vec{r}_i)\cdot\vec{p}_i] = -\frac{e}{mc}\sum_{i=1}^{N}\vec{p}_i\cdot\vec{A}(\vec{r}_i)$$

Coulomb $\nabla\cdot\mathbf{A}$ 0

$$\vec{J}(\vec{r}) = \frac{e}{2m}\sum_{i=1}^{N}[\vec{p}_i\delta(\vec{r}-\vec{r}_i) + \delta(\vec{r}-\vec{r}_i)\vec{p}_i]$$

$$H' = -\frac{1}{c}\int d\vec{r}\,\vec{J}(\vec{r})\cdot\vec{A}(\vec{r},t)$$

$$H' = -\frac{1}{c}\vec{J}(\vec{q})\cdot\vec{A}(\vec{q})$$

H'　　　　　|s> → |s'>

$$W_{s\to s'} = \frac{2\pi}{\hbar^2} |< s | H' | s' >|^2 \ \delta[\omega - (\omega_{s'} - \omega_s)]$$

$$= \frac{2\pi}{\hbar^2 c^2} < s' | \vec{J}(\vec{q}) | s >< s | \vec{J}^*(\vec{q}) | s' >| \vec{A}(\vec{q}) |^2 \ \delta[\omega - (\omega_{s'} - \omega_s)]$$

$$W = \sum_{s,s'} W_{s\to s'} = \frac{2\pi}{\hbar^2 c^2} \sum_{s,s'} < s' | \vec{J}(\vec{q}) | s >< s | \vec{J}^*(\vec{q}) | s' > | \vec{A}(\vec{q}) |^2 \ \delta[\omega - (\omega_{s'} - \omega_s)]$$

$$\delta(\omega) = \frac{1}{2\pi} \int \exp(-i\omega t) dt$$

$$W = \frac{1}{\hbar^2 c^2} \sum_{s,s'} \int dt \exp(-i\omega t) < s' | \vec{J}(\vec{q}) | s >< s | \exp(-i\omega_{s'} t) \vec{J}^*(\vec{q}) \exp(-i\omega_s t) | s' > | \vec{A}(\vec{q}) |^2$$

Schrodinger　　　J(q)　J^*(q)

Heisenberg

$$\vec{J}(\vec{q},t) = e^{iH_0 t/\hbar} \vec{J}(\vec{q}) e^{-iH_0 t/\hbar}$$

$$\vec{J}^*(\vec{q},t) = e^{-iH_0 t/\hbar} \vec{J}^*(\vec{q}) e^{iH_0 t/\hbar}$$

$$\sum_{s'} | s' >< s' | = 1$$

$$P = \hbar\omega W = |\vec{A}(\vec{q})|^2 \frac{\omega}{\hbar c^2} \sum_s \int dt < s | \vec{J}(\vec{q},0) \vec{J}^*(\vec{q},t) | s > \exp(-i\omega t)$$

$\vec{E} = i\omega\vec{A}/c$

$$= |\vec{E}(\vec{q})|^2 \frac{1}{\hbar\omega} \sum_s \int dt < s | \vec{J}(\vec{q},0) \vec{J}^*(\vec{q},t) | s > \exp(-i\omega t)$$

$$\frac{1}{\quad} \qquad \left\langle \qquad\qquad ^{*} \qquad\qquad \right\rangle$$

i a constant correlation time τ for all states

$$\vec{J}(\vec{q},t)=\vec{J}(\vec{q},0)\exp(-t/\tau)$$

$$\vec{J}(\vec{r})=\frac{e}{2m}\sum_{i=1}^{N}[\vec{p}_i\delta(\vec{r}-\vec{r}_i)+\delta(\vec{r}-\vec{r}_i)\vec{p}_i]$$

$$\vec{J}(\vec{q})=\int\vec{J}(\vec{r})\exp(-i\vec{q}\cdot\vec{r})d\vec{r}=-\frac{e}{m}\sum_j\vec{p}_j$$

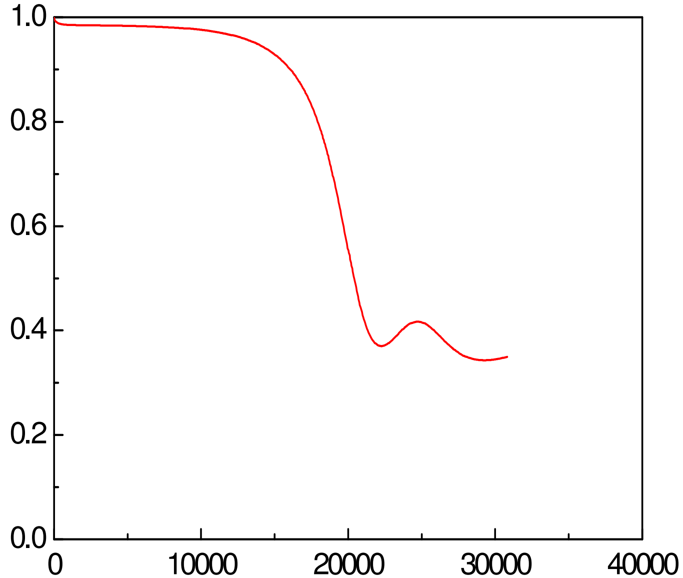
ii only zero wavevector is considered (local limit) $\exp(i\vec{q}\cdot\vec{r})\approx 1$

$$\Rightarrow\quad \sigma(\omega)=\frac{e^2}{m^2\hbar\omega}\int dt\exp\{\text{-i}\omega t-|t|\tau\}\sum_{s,s',j}|\langle s'|\quad|s\rangle|^2$$

$$2\sum_{s,s',j}\frac{|\langle s'|\quad|s\rangle|^2}{m\hbar\omega_{s's}}=f_{s's}$$

the osillator strength

$$\sigma(\omega)=\frac{e^2\tau}{m}\frac{f_{s's}}{1-i\omega\tau}\xrightarrow{f_{s's}=N}\sigma(\omega)=\frac{Ne^2\tau}{m}\frac{1}{1-i\omega\tau}$$



1.0
0.8
0.6
0.4
0.2
0.0
0
10000
20000
30000
40000

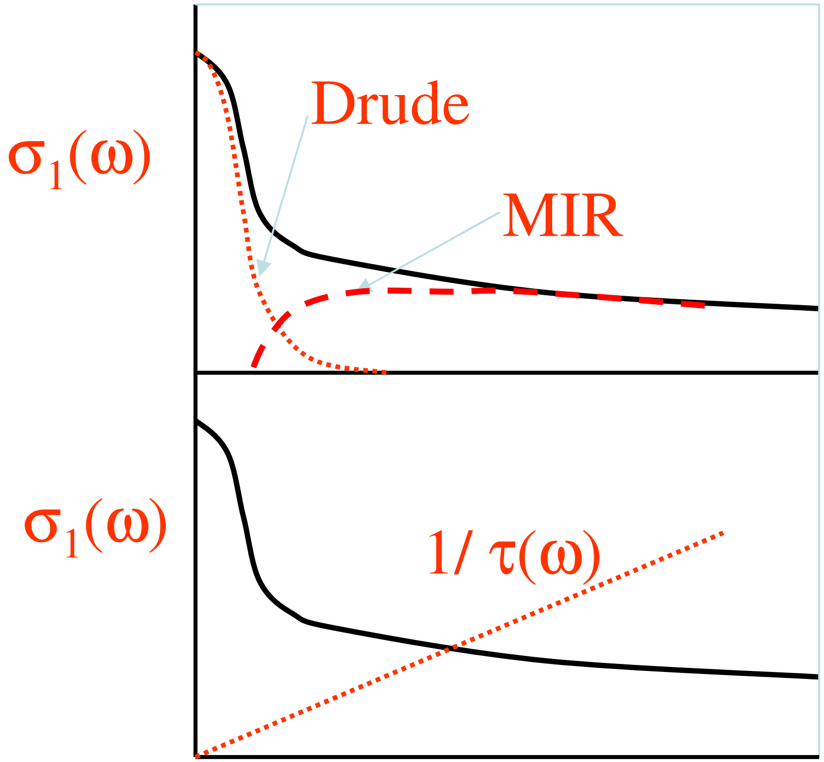
Non-Drude spectra of strongly correlated electrons

General feature: a sharp peak at ω=0

+ a long tail extending to high energies

For example: cuprates

Two possible interpretations



Drude Model $\sigma(\omega) = \frac{\omega_p^2}{4\pi}\frac{1}{1/\tau - i\omega}$

Extended Drude Model

Let $M(\omega,T) = 1/\tau(\omega,T) - i\omega\lambda(\omega,T)$

$1/\tau(\omega,T)$: Frequency dependent scattering rate

λ: Mass enhancement $m^* = m(1+\lambda)$

$$\sigma(\omega,T) = \frac{\omega_p^2}{4\pi}\frac{1}{M(\omega,T) - i\omega}$$

$$= \frac{\omega_p^2}{4\pi}\frac{1}{1/\tau(\omega,T) - i\omega[1+\lambda(\omega,T)]}$$

$$= \frac{1}{4\pi}\frac{\omega_p^{*2}}{1/\tau^*(\omega,T) - i\omega}$$

$1/\tau(\omega,T) = (\omega_p^2/4\pi)\mathrm{Re}(1\ \sigma(\omega))$

$1+\lambda(\omega) = (\omega_p^2/4\pi\omega)\mathrm{Im}(1\ \sigma(\omega))$

e.g. Marginal Fermi Liquid model:

$M(\omega,T)$ γ δ00 1+2 10 μ i 11 λ 22 12 λ 2 12 λ 11 0 0 1 0 0 χμ /1 1202 φ 0

$g^2N^2(0)\quad \frac{}{2}x \quad i \quad \ln\frac{x}{c}$

Drude

Extended Drude Model

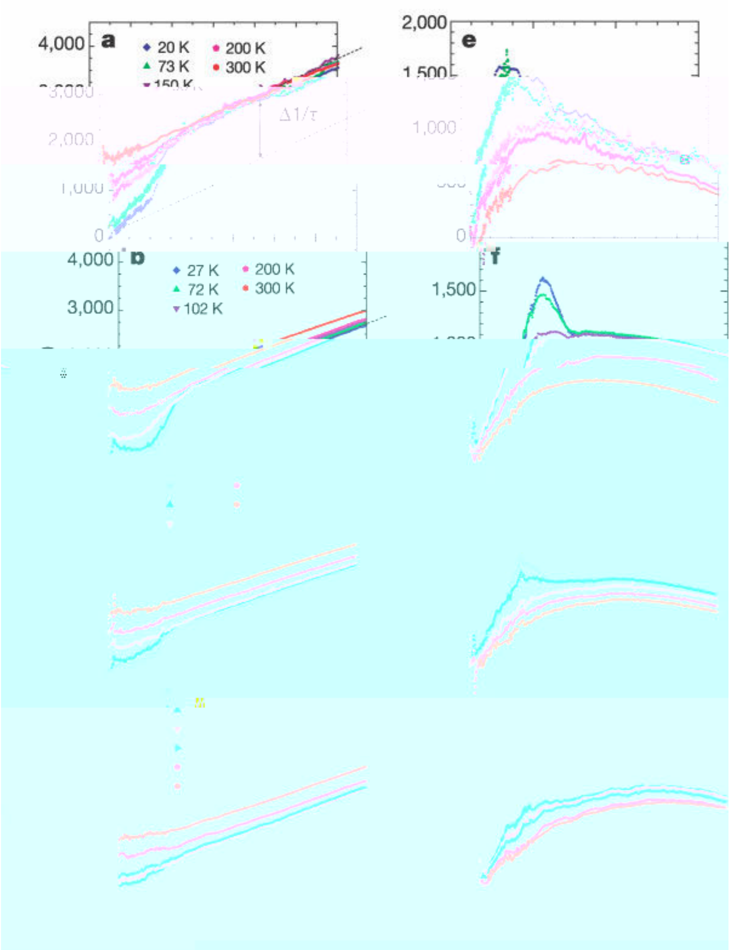
$$\sigma(\omega,T) = \frac{\omega_p^2}{4\pi}\frac{1}{(\gamma(\omega,T) - i\omega)}$$

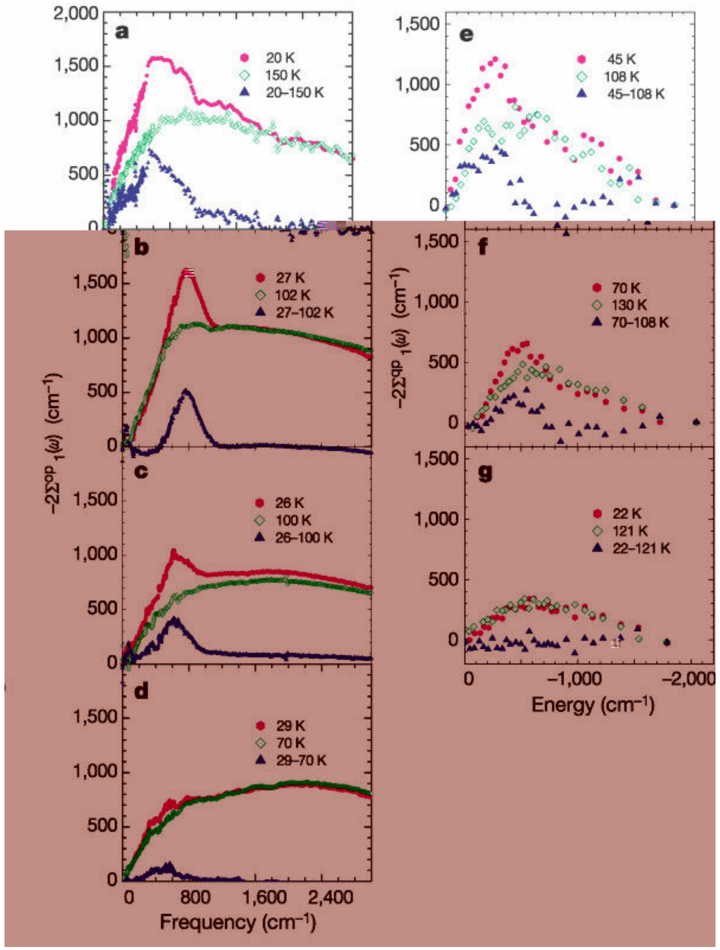
According to Little and Varma,

$$\gamma(\omega) = -2i\Sigma^{op}$$
$$= -2i[\Sigma_1(\omega) + i\Sigma_2(\omega)]$$

1/τ(ω)   m*/m

$$\gamma_1(\omega) = 1/\tau(\omega) = 2\Sigma_2$$
$$\gamma_2(\omega) = \omega(1 - m^*/m) = -2\Sigma_1$$



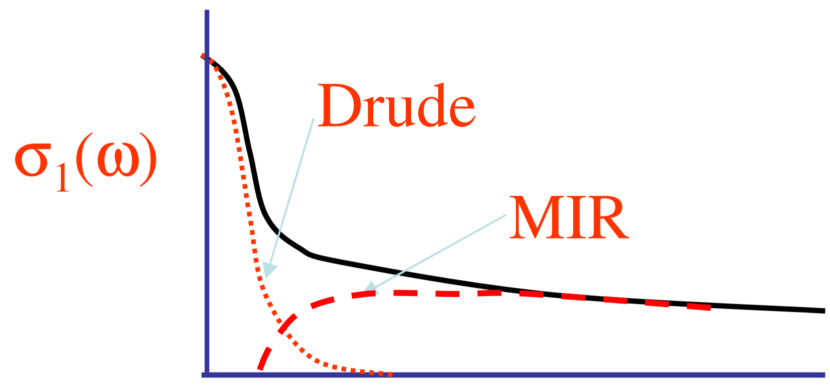


Hwang, Timusk, Gu,
Nature 427, 714 (2004)

(2) Two component picture

Drude component + mid-IR component

Drude component	mid-IR component
Sharp peak at ω=0	Long tail at high energies
Free carriers weakly coupled with boson excitations	Bound carriers strongly coupled with phonons, etc.



Optical spectra of a superconductor

T=0, London electrodynamics gives

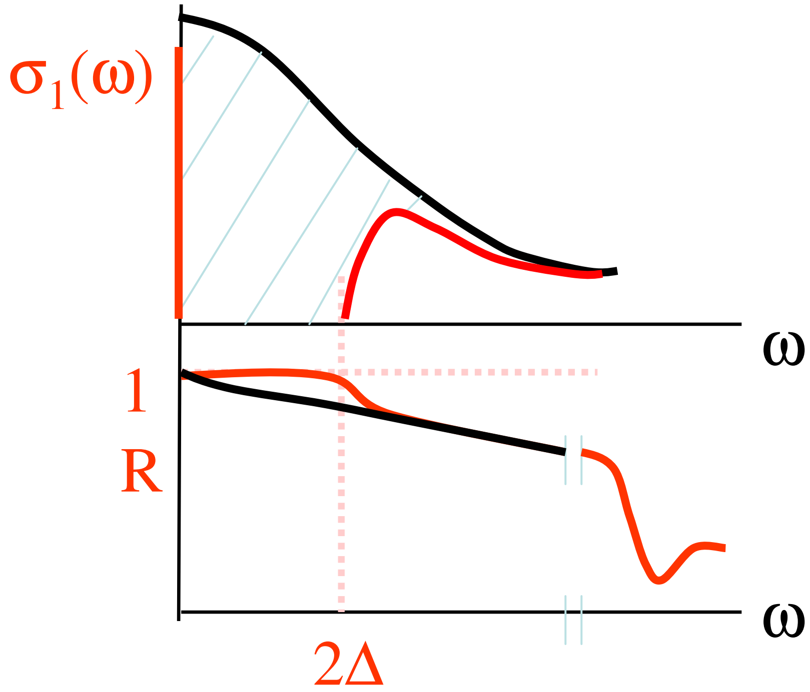
$$\sigma = \frac{1}{8}\omega_{ps}^2\delta(\omega) + i\omega_{ps}^2/4\pi\omega \;\Rightarrow\; \frac{1}{\lambda_L^2} = \frac{8}{c^2}\int_0^\infty (\sigma_1^n - \sigma_1^s)\,d\omega \quad \text{or} \quad \frac{1}{\lambda_L^2} = \frac{4\pi}{c^2}\omega\sigma_2(\omega)$$

dirty limit: $\xi > l \Leftrightarrow 2\Delta < \Gamma$

Absorption starts at Δ

clean limit: $\xi < l \Leftrightarrow 2\Delta > \Gamma$

Absorption starts at **$2\Delta+\Omega$.**



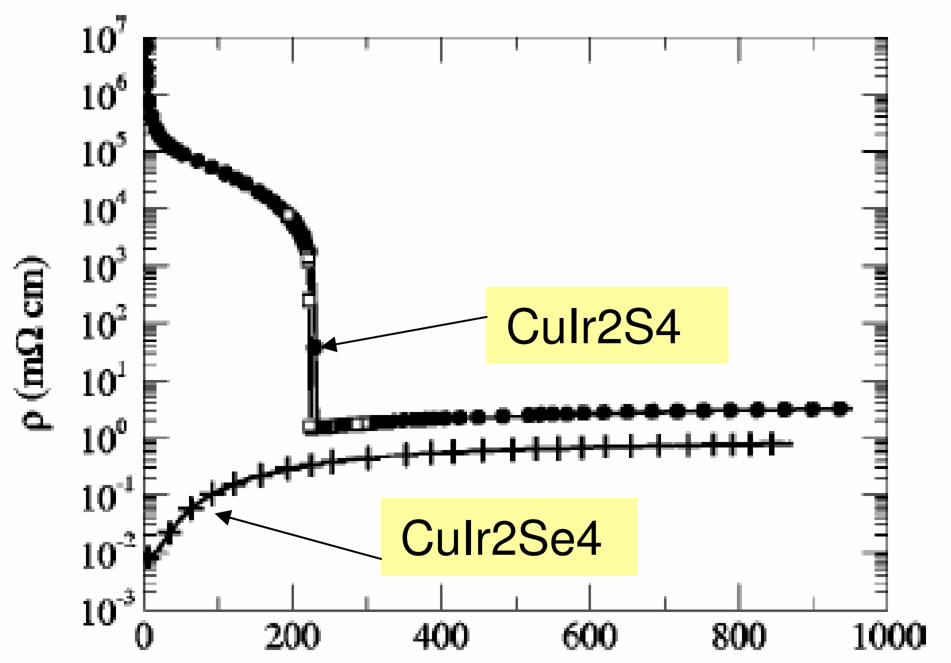
pippard coherence length $\xi = v_F/\pi\Delta$, $\Gamma = 1/\tau = v_F/l$

Optical study of CuIr2S4 and MgTi2O4: support for orbital-Peierls transitions

- Metal-insulator transitions in CuIr2S4 and MgTi2O4
- Orbital Peierls transition scenario by Khomskii
- Optical data---evidence for orbital Peierls transitions

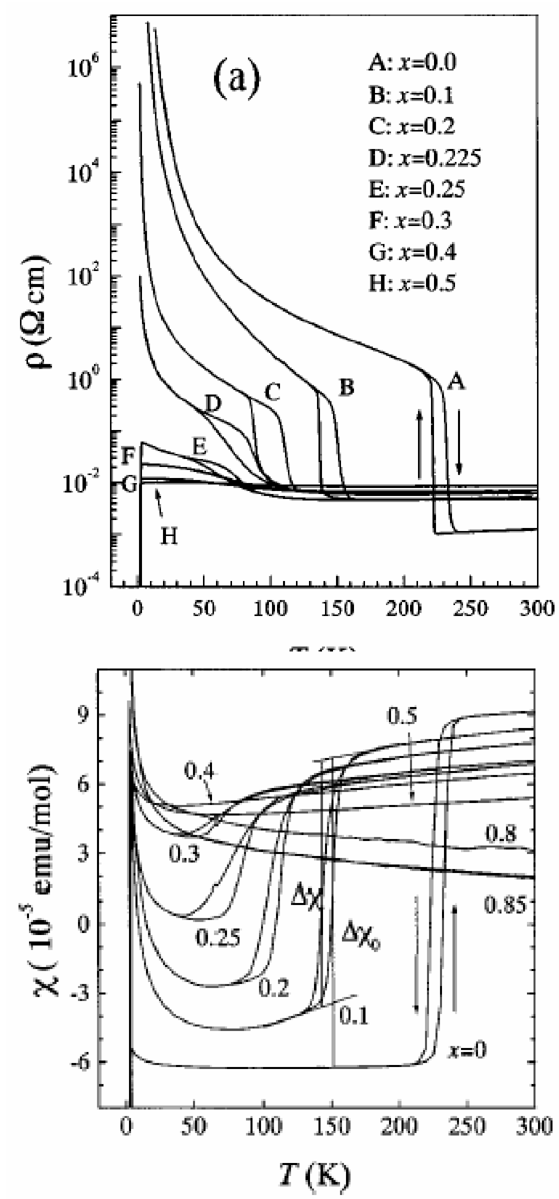
Peierls (Metal-insulator) transition may occur in some dimension-reduction systems

CuIr2S4



Metal-Insulator transition at ~230K

Discovered in 1994 by S. Nagata et al.

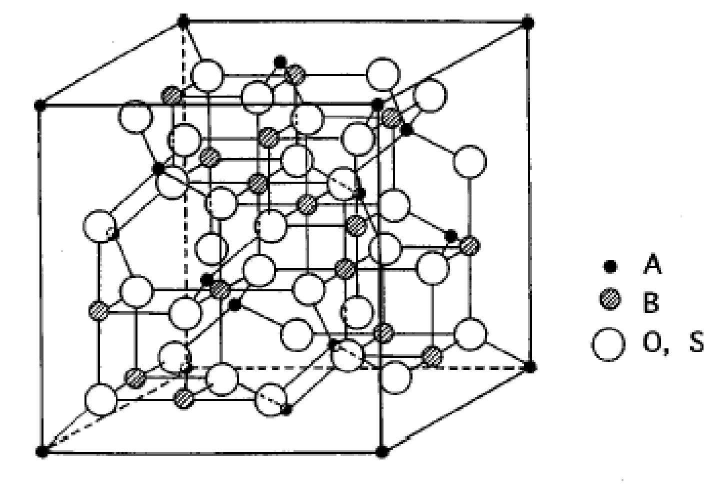


Zn substitution,

G. H. Cao, et al. PRB 64, 214514 (2001)

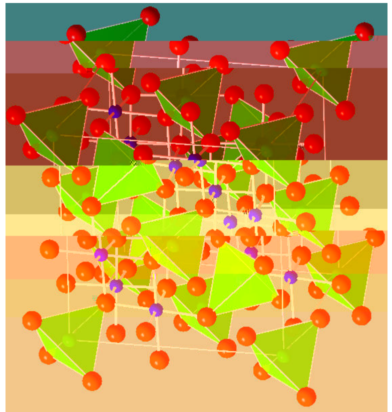
Structure feature

$A_{tet}[B_2]_{oct}S_4$

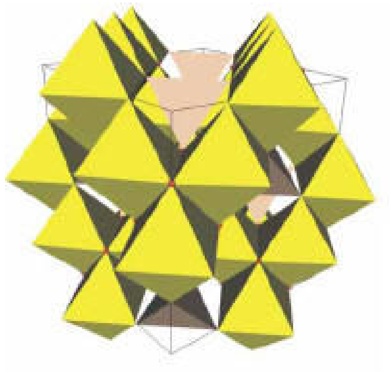


cubic

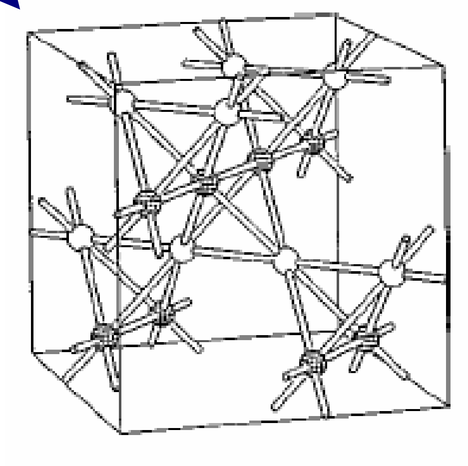
A site
tetrahedra



B site
octahedra



B-site only, pyrochlore lattice



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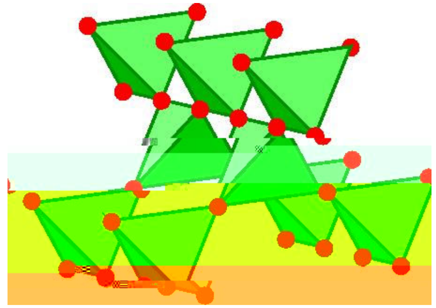


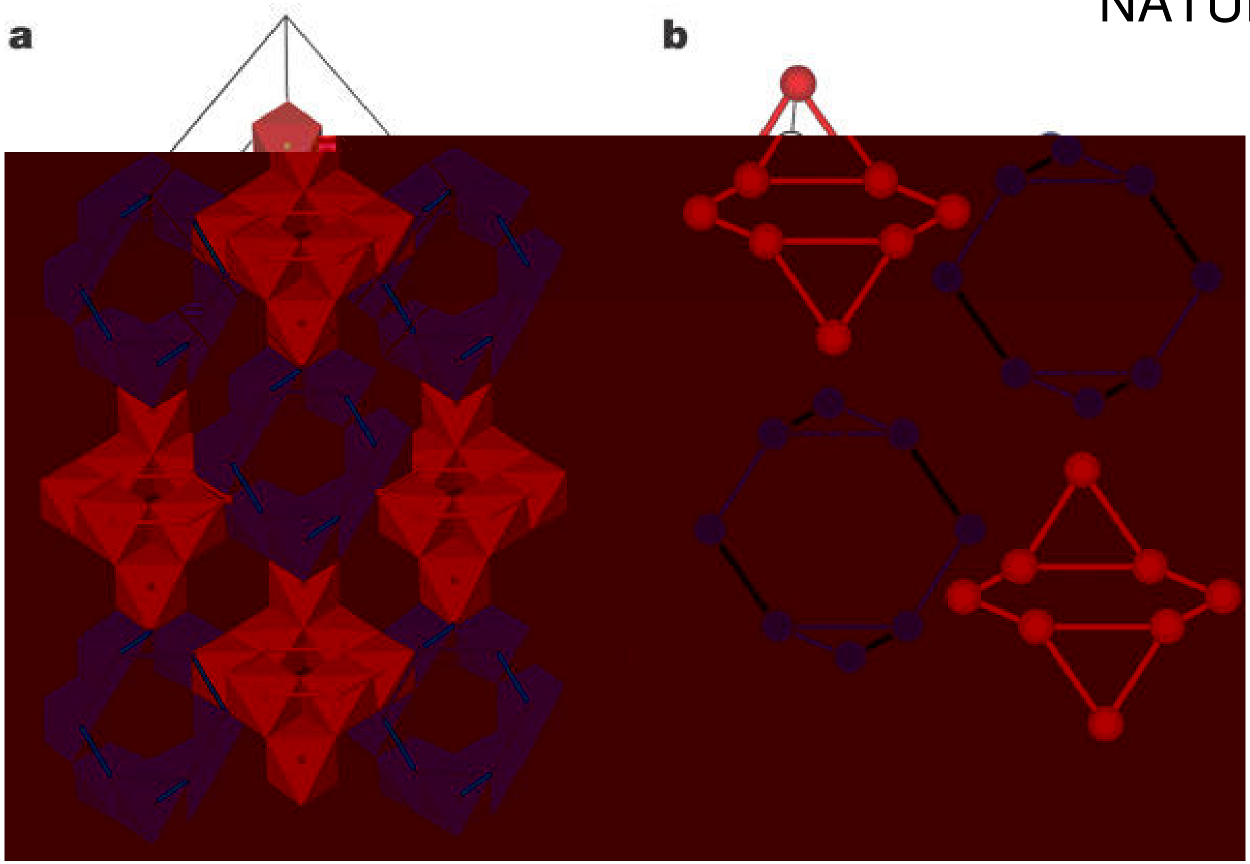
6 chains by three orbitals

A site cation has fully filled orbital (e.g. Cu^{1+}, Mg^{2+});

the physical properties are determined by the B site cations.

Formation of isomorphic Ir 3+ and Ir 4+ octamers and spin dimerization in CuIr2S4

P G Radaelli, et al., NATURE 416, 155 (2002)



Low-T structure

$Cu^{+I}Ir^{3+}Ir^{4+}S_4^{2-}$

Ir: $5d^7 6s^2$

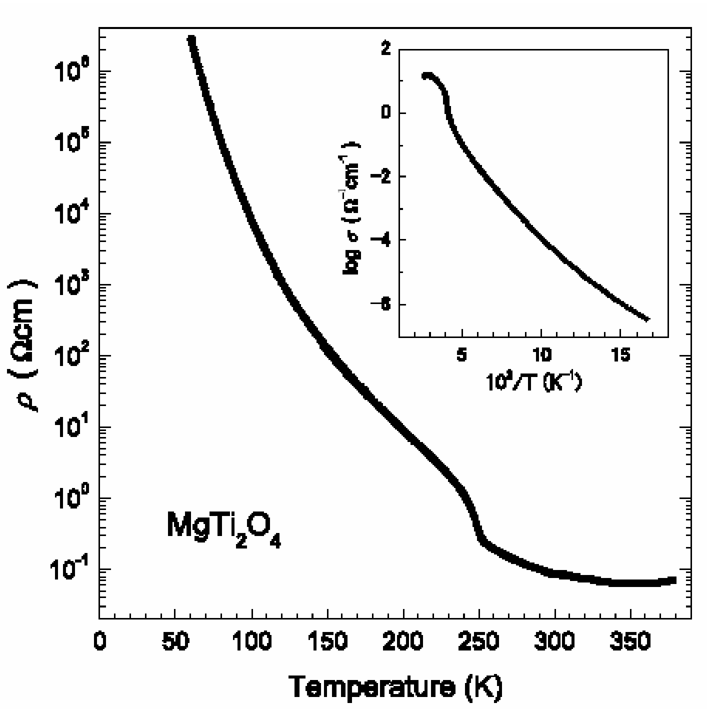
Ir3+ is nonmagnetic ($t_{2g}^6 e_g^0$, s=0)

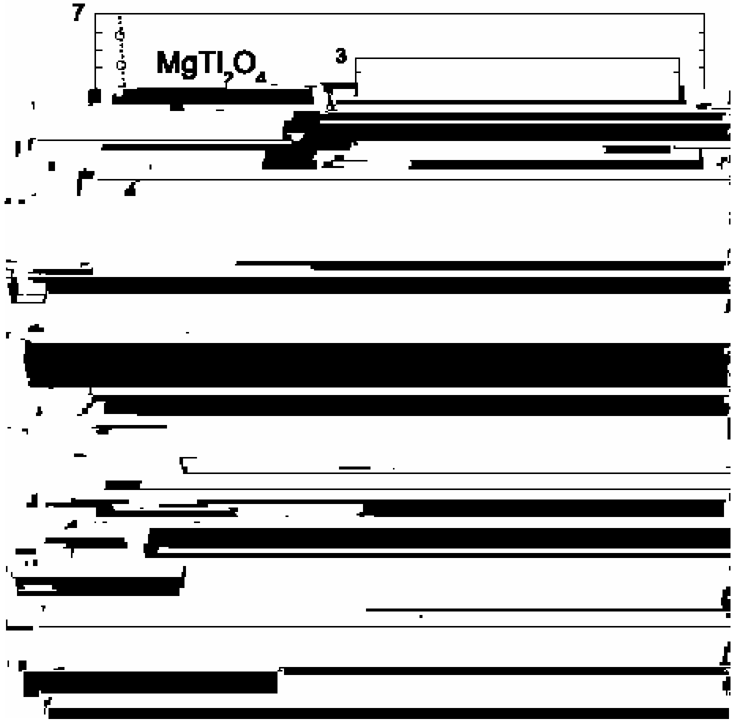
Ir4+ has a local moment ($t_{2g}^5 e_g^0$, s=1/2) (for low spin state)

Observation of Phase Transition from Metal to Spin-Singlet Insulator in $MgTi_2O_4$ with $S = 1/2$ Pyrochlore Lattice

Masahiko ISOBE and Yutaka UEDA*

JPSJ 2002



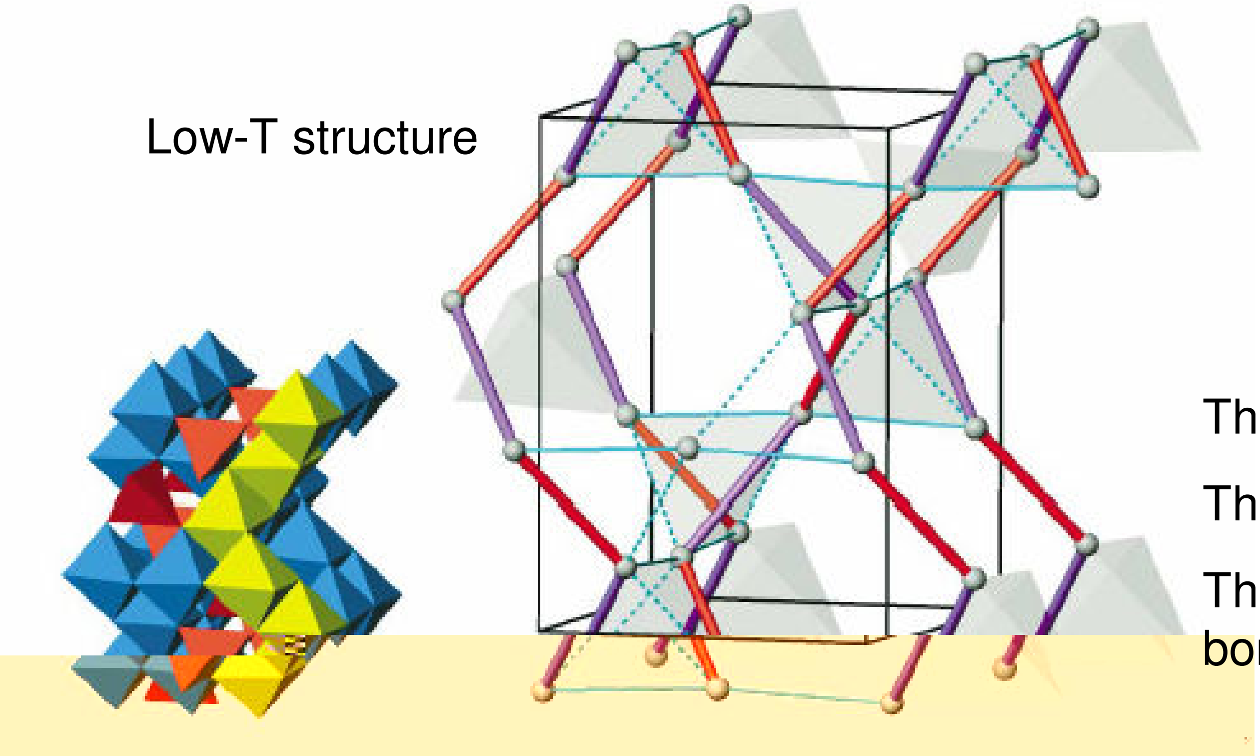


VOLUME 92, NUMBER 5 PHYSICAL REVIEW LETTERS week ending 6 FEBRUARY 2004

Spin Singlet Formation in $MgTi_2O_4$: Evidence of a Helical Dimerization Pattern

M. Schmidt,[1,2] W. Ratcliff II,[3] P. G. Radaelli,[1,4] K. Refson,[1] N. M. Harrison,[5,6] and S. W. Cheong[3]

Low-T structure



Ti: $3d^2 4s^2$

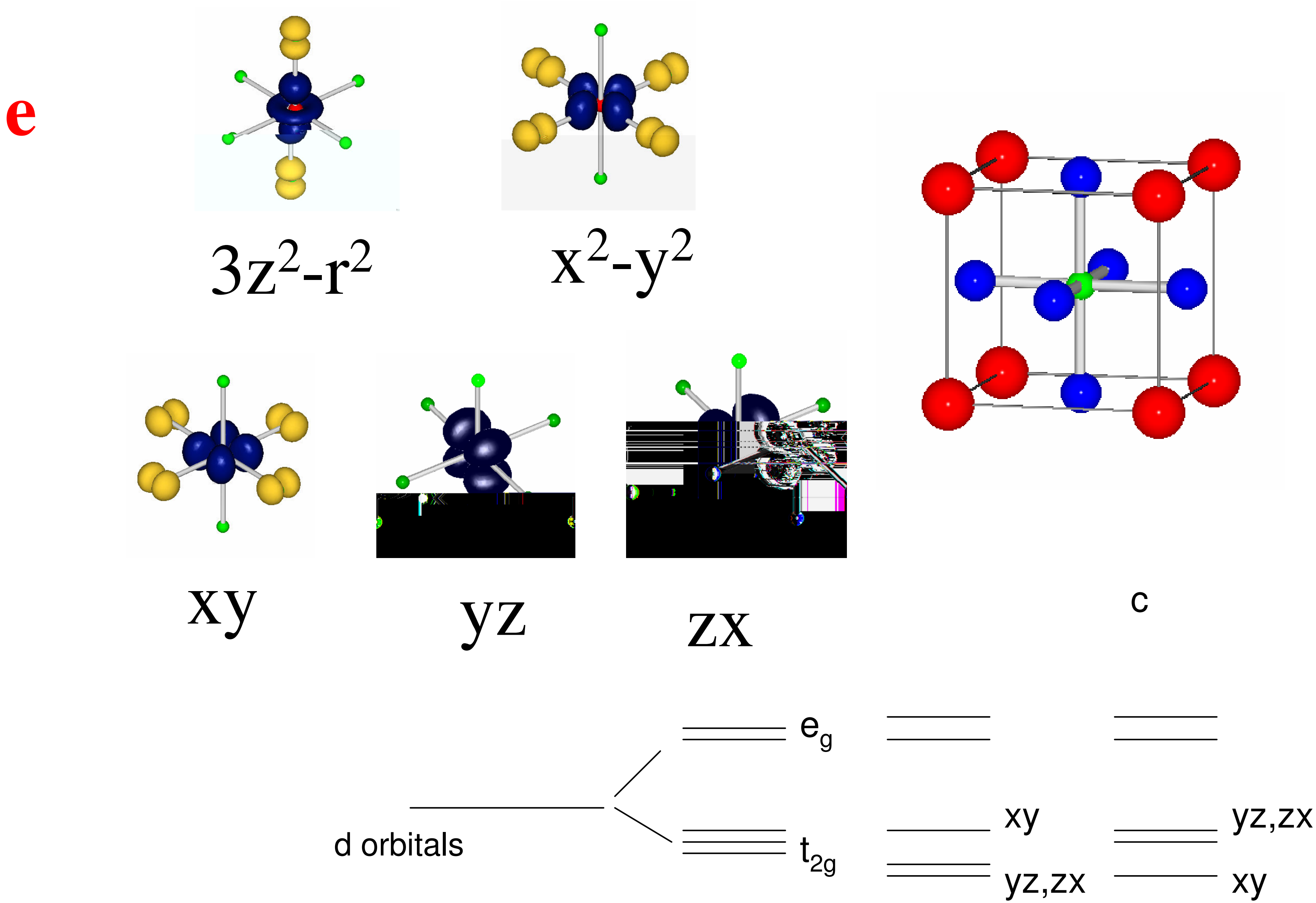
Ti^{3+}, $3d^1$, s=1/2

(dimerized)

The red: the shortest bond

The purple: the longest bond

The blue: the intermediate bond



e
3z2-r2
x2-y2
xy
yz
zx
c
eg
t2g
d orbitals
xy
yz,zx
yz,zx
xy

PHYSICAL REVIEW LETTERS

Below T_{MIT}

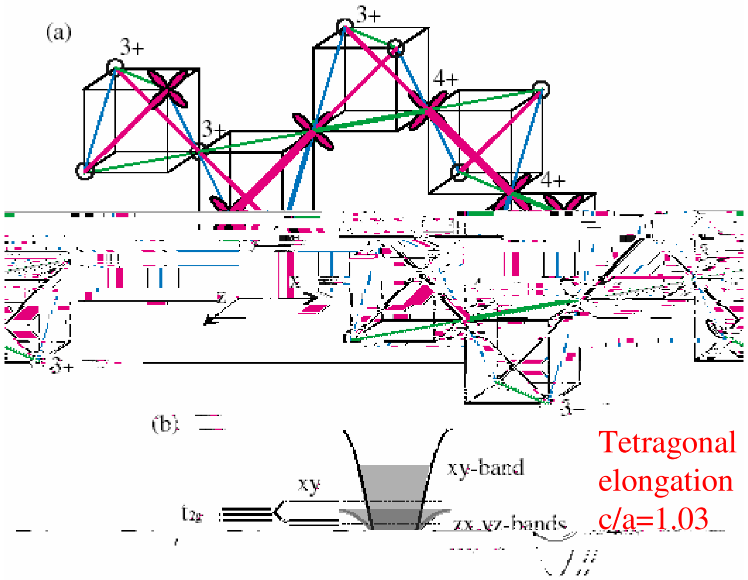
Orbitally Induced Peierls State in Spinels

D.I. Khomskii[1,2] and T. Mizokawa[3]

Ir^{3+}: $t_{2g}^{6}e_{g}^{0}$, s=0

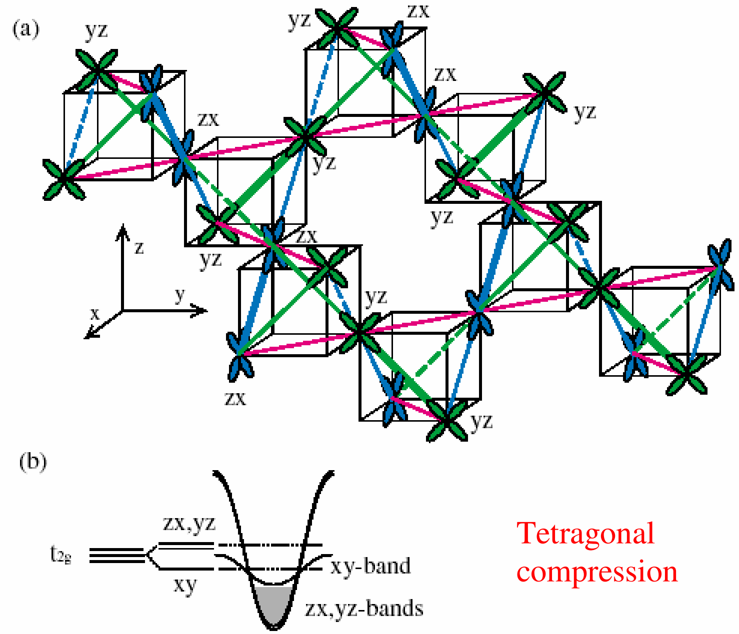
Ir^{4+}: $t_{2g}^{5}e_{g}^{0}$, s=1/2

Ti^{3+}: $3d^1$, s=1/2



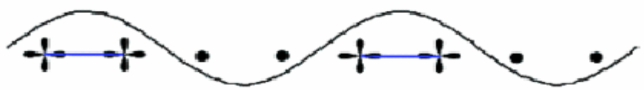
Tetragonal elongation c/a=1.03

ordering in $CuIr_2S_4$. FIG. 2 (color). (a) Charge and orbital ... singlet bonds are ... Octamer is shown by thick lines. ... (b) Schematic ... $CuIr_2S_4$.



Tetragonal compression

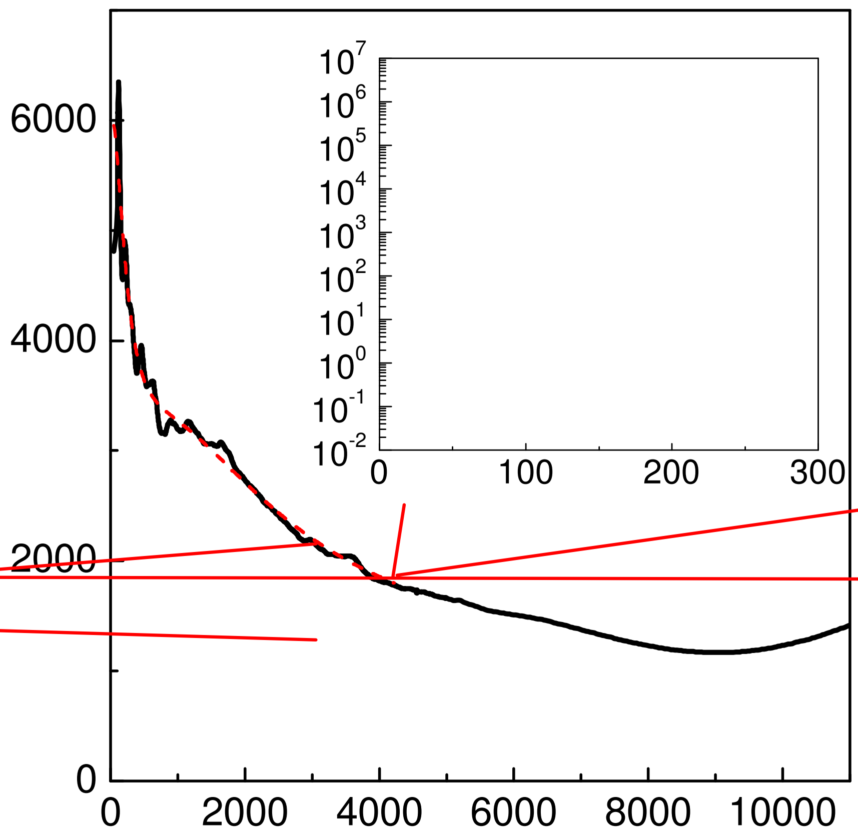
FIG. 3 (color). (a) Orbital ordering in $MgTi_2O_4$. ... singlet bonds are shown by double, intermediate single, and long dashed lines. yz orbitals are shown in green and zx orbitals blue. (b) Schematic electronic structure of $MgTi_2O_4$. ... different orientation of coordinate axes as compared with Figs. 1 and 2.



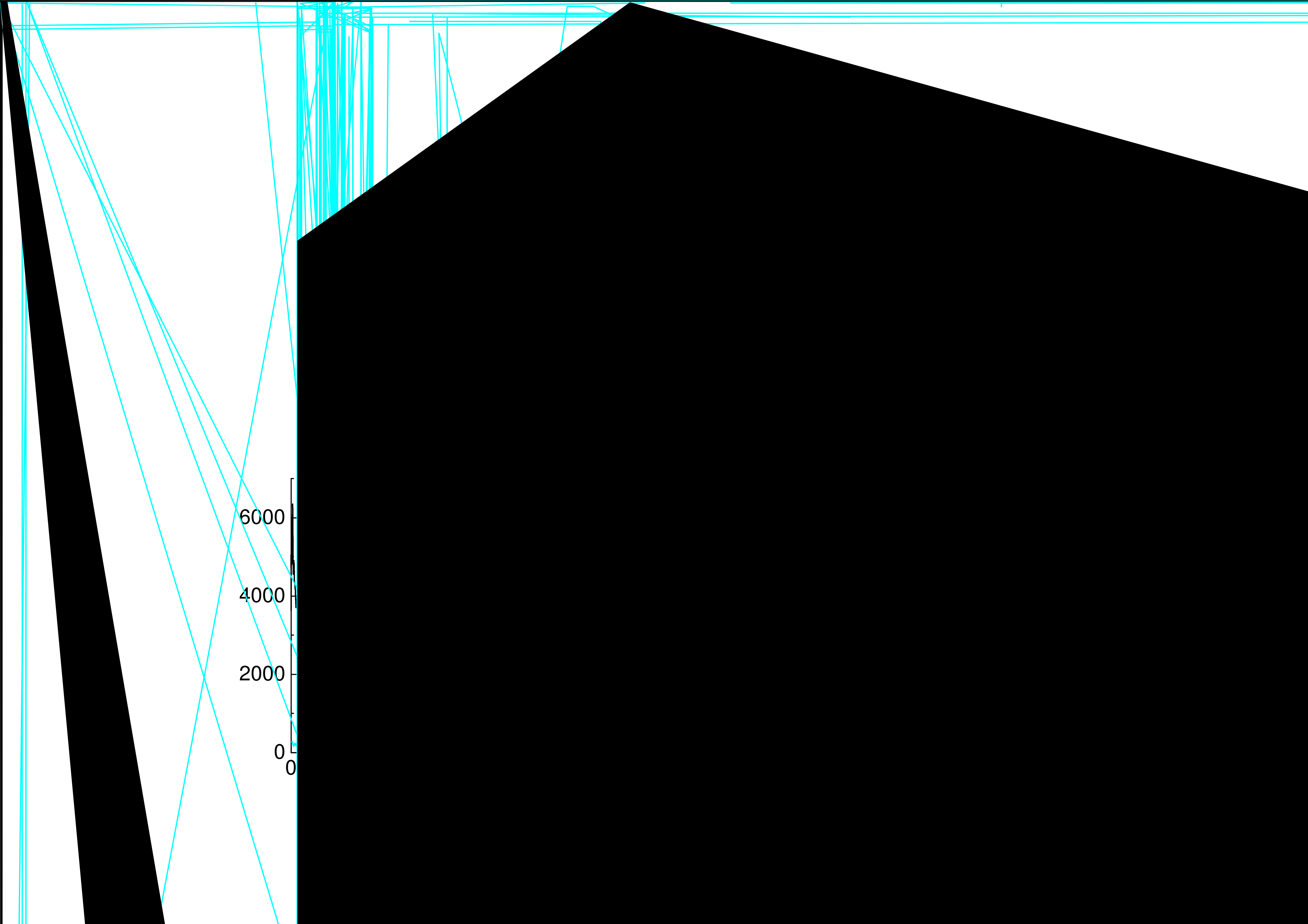
tetramerization

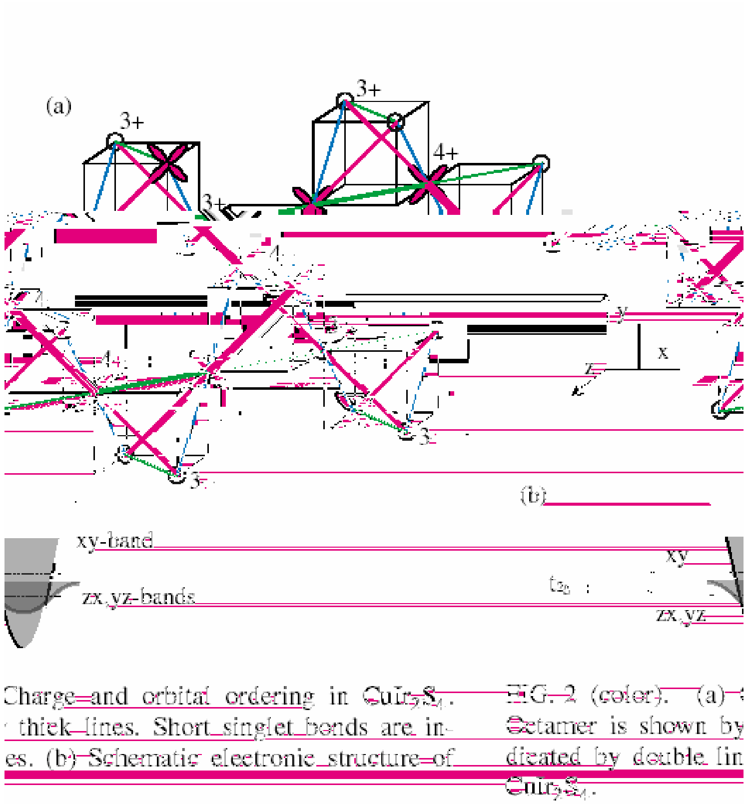
Electrons arranged in chains formed by respective orbitals!!

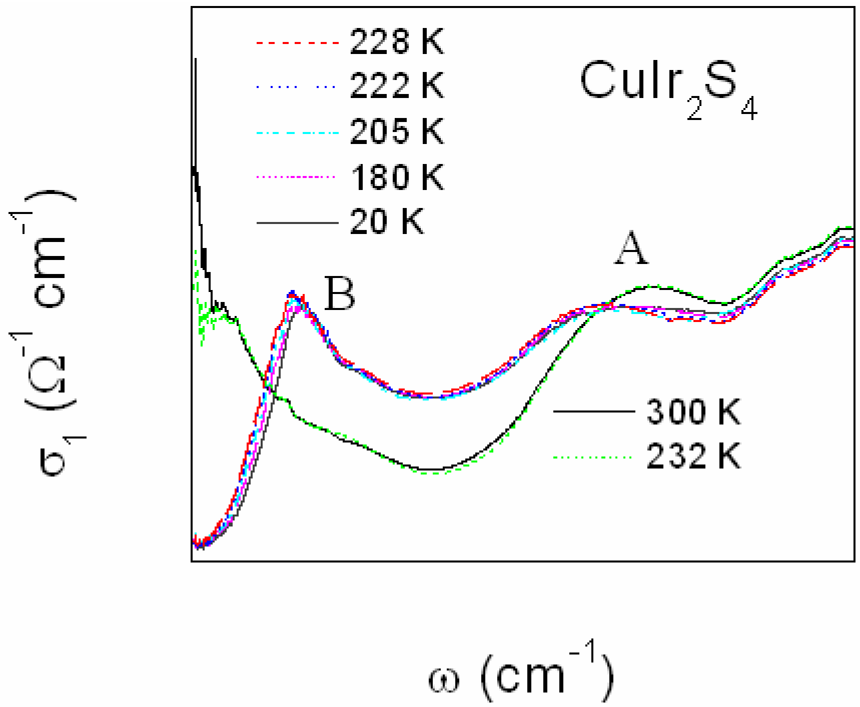
Room temperature spectra



Drude like response at low frequency

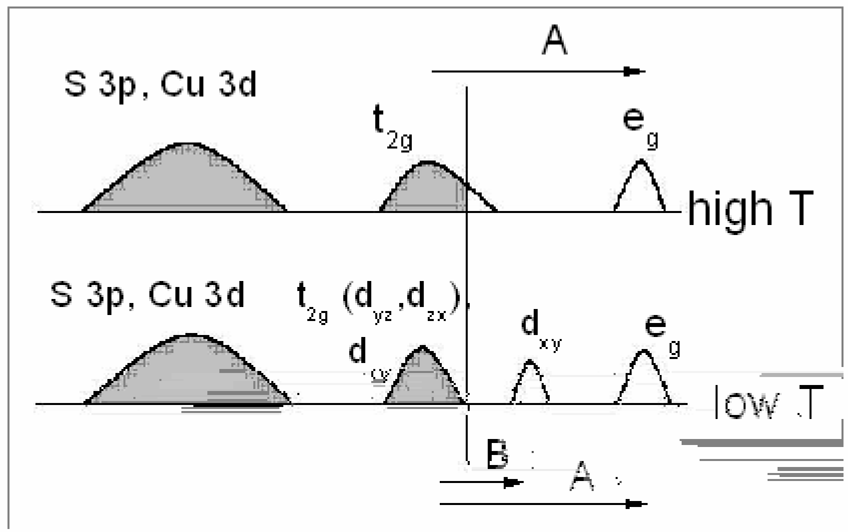

6000
4000
2000
0
0



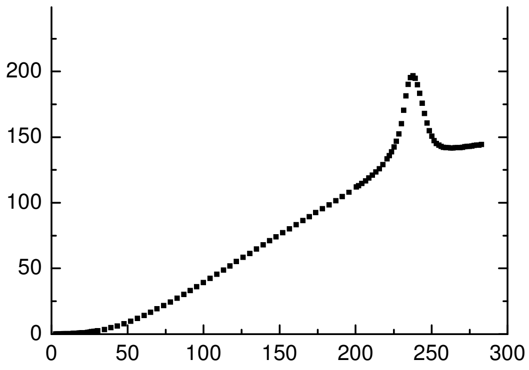


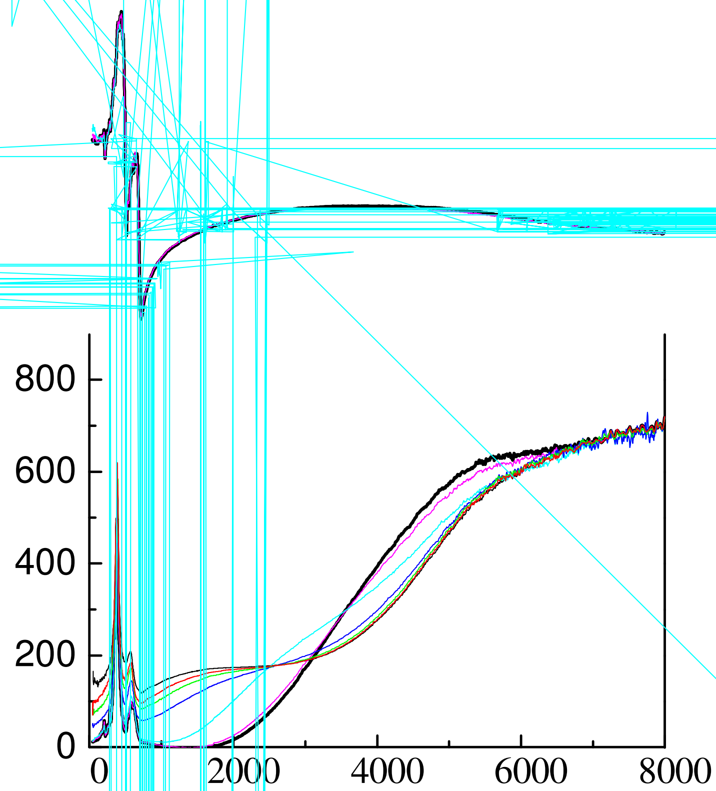
yz, zx bands fully occupied

xy orbital band splitted



MgTi2O4




800
600
400
200
0
0
2000
4000
6000
8000

TRANSITION METAL OXIDES

Travels in one dimension

The discovery that electrons in $Tl_2Ru_2O_7$ lose their three-dimensional nature at low temperatures and arrange in chains, opens up a new direction in research into transition metal oxides.

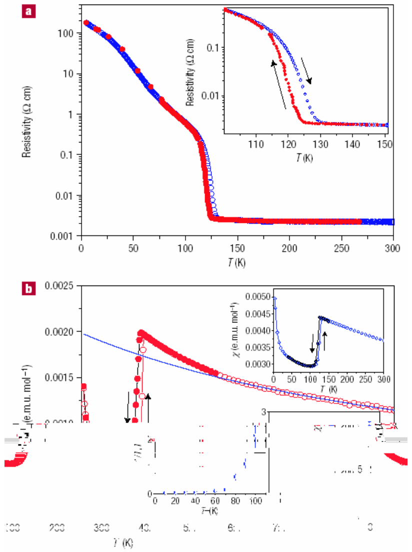
JEROEN VAN DEN BRINK

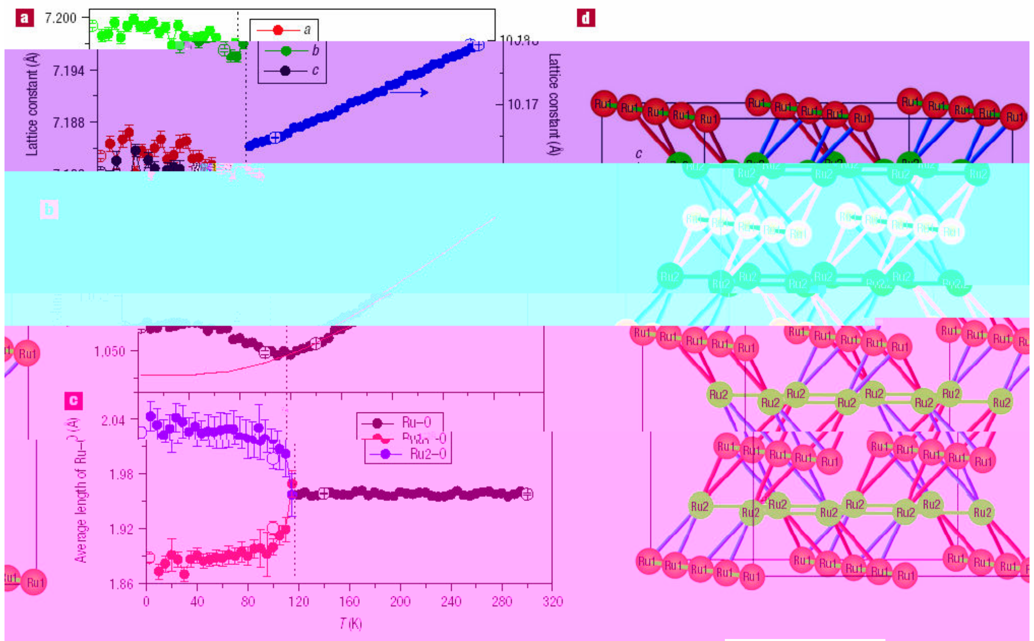
Figure 1 Orbital ordering in $Tl_2Ru_2O_7$. Driven by orbital degrees of freedom, electrons in the three-dimensional crystal (background) self-organize into one-dimensional chains (foreground).

Nature Materials (issue of June, 2006)

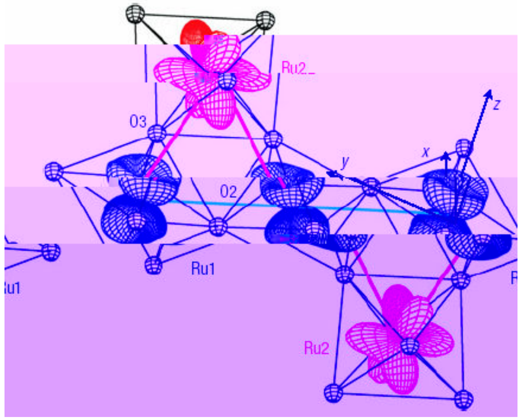
Spin gap in $Tl_2Ru_2O_7$ and the possible formation of Haldane chains in three-dimensional crystals

SEONGSU LEE[1], J.-G. PARK[1,2]*, D. T. ADROJA[3], D. KHOMSKII[4], S. STRELTSOV[5], K. A. McEWEN[6], H. SAKAI[7], K. YOSHIMURA[7], V. I. ANISIMOV[5], D. MORI[8], R. KANNO[8] AND R. IBBERSON[3]





$t_{2g}^3 \uparrow t_{2g}^1 \downarrow$



Neutron experiment: spin gap ~ 11 meV

Below T_{MI}, Ru1 and Ru2 ions exist

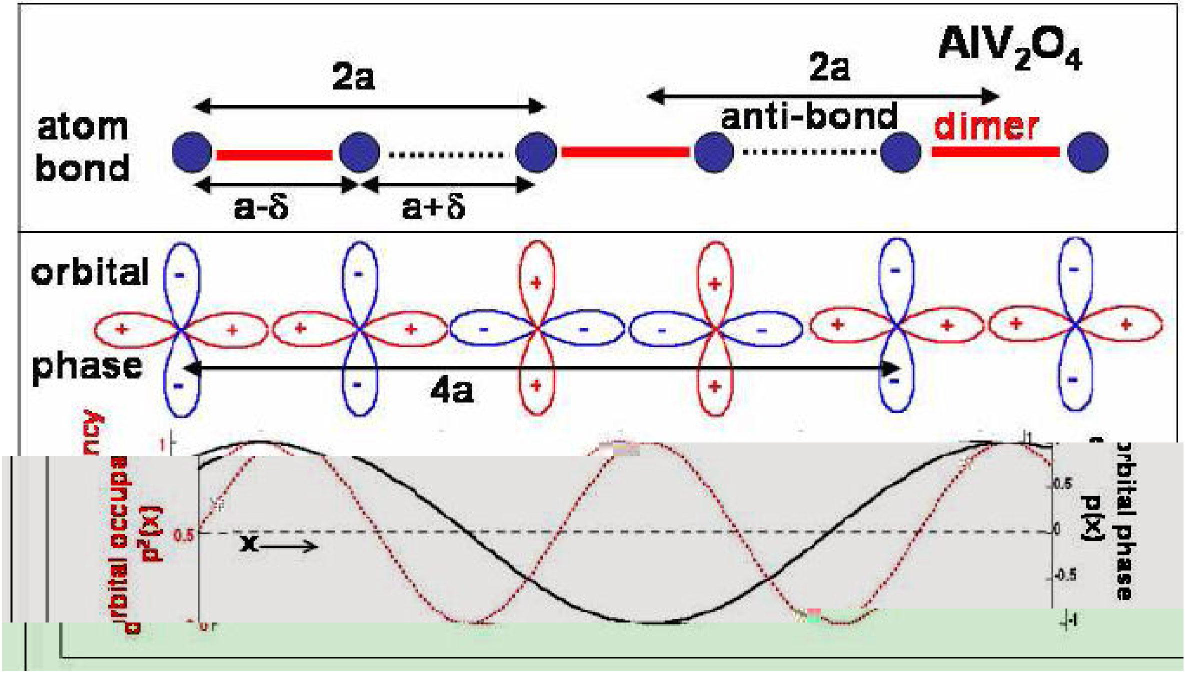
both Ru1 and Ru2 as low-spin Ru^{4+} with $S = 1$

Zig-zap 1D Haldane chain with s=1

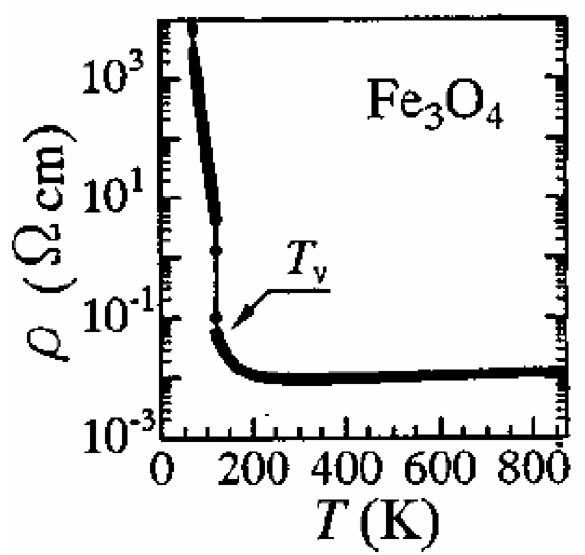
Croft-12-7-06.doc 1

Universality in one dimensional orbital wave ordering in spinel and related compounds: an experimental perspective

M. Croft, V. Kiryukhin, Y. Horibe, and S-W. Cheong
Rutgers Center for Emergent Materials and Department of Physics and Astronomy, Rutgers University, Piscataway, NJ 08854

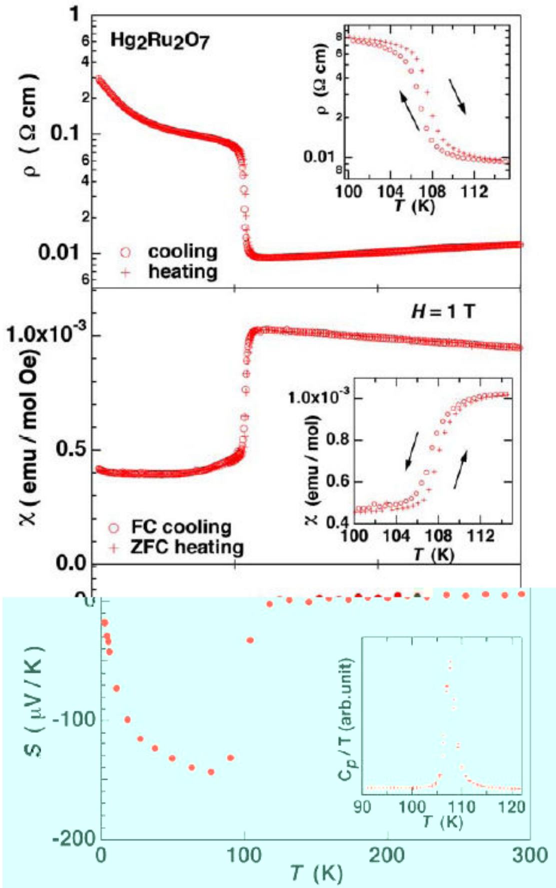


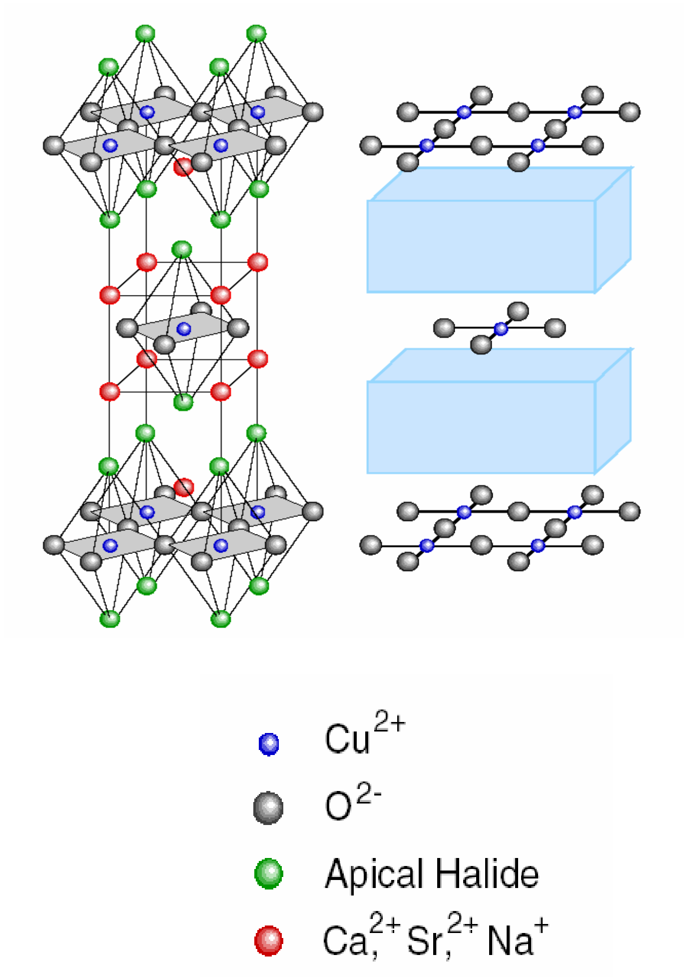
Verwey transition in Fe3O4



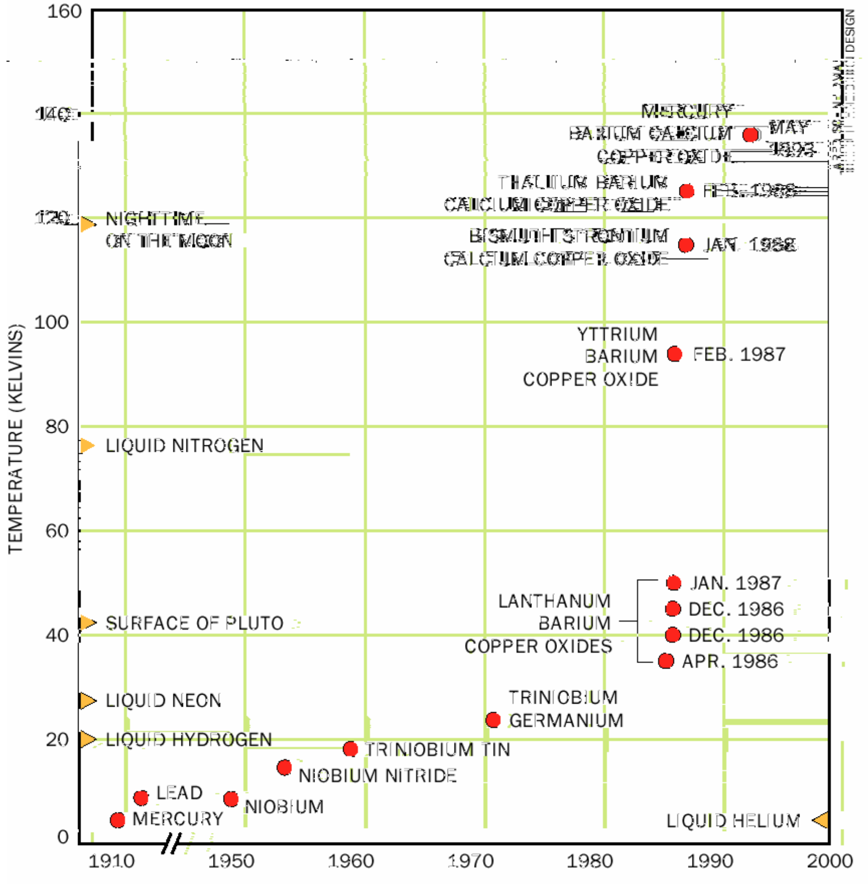
Metal-insulator Transition in a Pyrochlore-type Ruthenium oxide, $Hg_2Ru_2O_7$

[redacted]
Peter A. Sharma[1], Yoshihiko Okamoto[1,2], Aiko Nakao[1], [redacted] Ayako Yamamoto[1,2,*],
ji Niitaka[1,2], Daisuke Hashizume[1], and Hidenori Takagi[1,2,3] [redacted] Hiroko Aruga Katori[1,2], Se



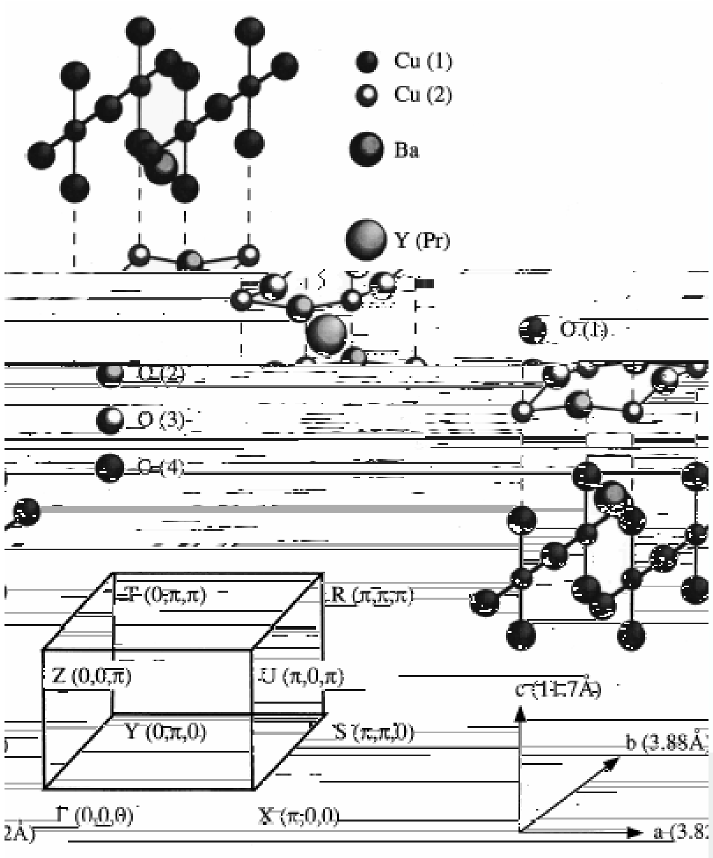


Cu^{2+}
O^{2-}
Apical Halide
Ca^{2+}, Sr^{2+}, Na^{+}

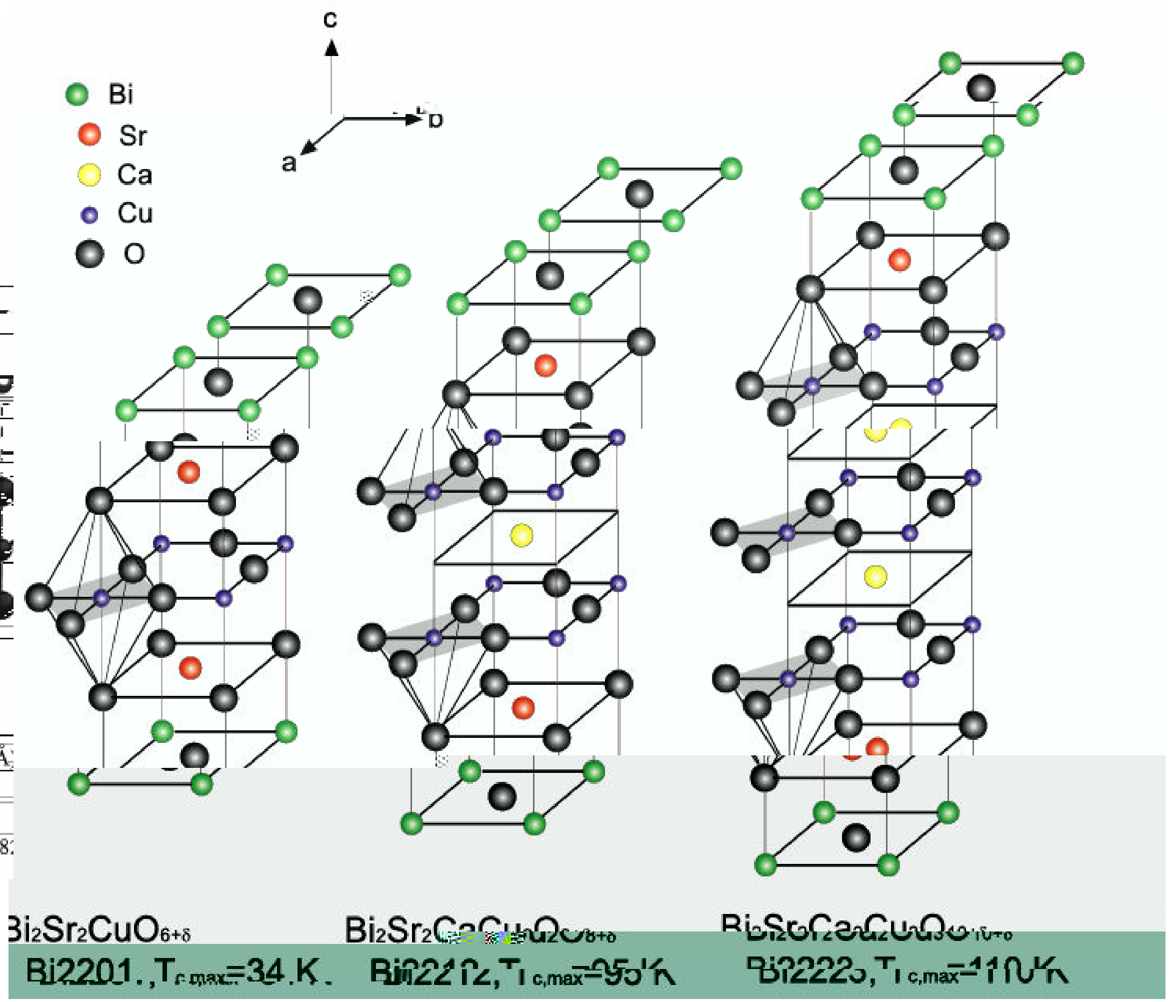


TEMPERATURE (KELVINS)
160
140
120
100
80
60
40
20
0
1910
1950
1960
1970
1980
1990
2000
MERCURY
BARIUM CALCIUM
COPPER OXIDE
MAY
THALLIUM BARIUM
CALCIUM COPPER OXIDE
BISMUTH STRONTIUM
CALCIUM COPPER OXIDE
JAN. 1988
NIGHTTIME
ON THE MOON
YTTRIUM
BARIUM
COPPER OXIDE
FEB. 1987
LIQUID NITROGEN
LANTHANUM
BARIUM
COPPER OXIDES
JAN. 1987
DEC. 1986
DEC. 1986
APR. 1986
SURFACE OF PLUTO
LIQUID NEON
TRINIOBIUM
GERMANIUM
LIQUID HYDROGEN
TRINIOBIUM TIN
NIOBIUM NITRIDE
LEAD
NIOBIUM
MERCURY
LIQUID HELIUM

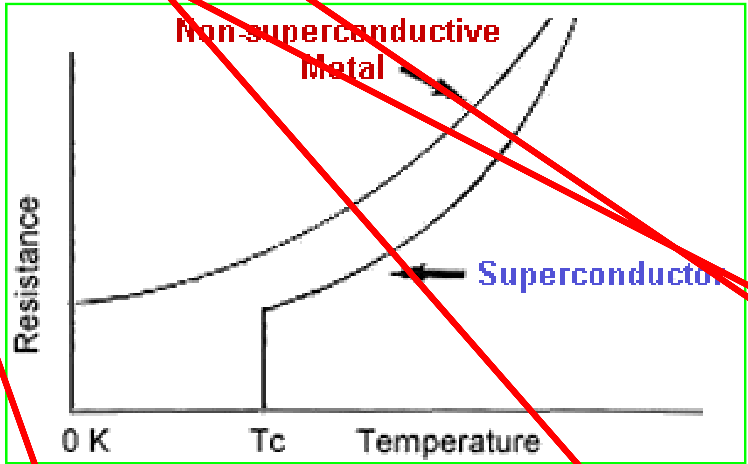
Structure of high-Tc cuprates

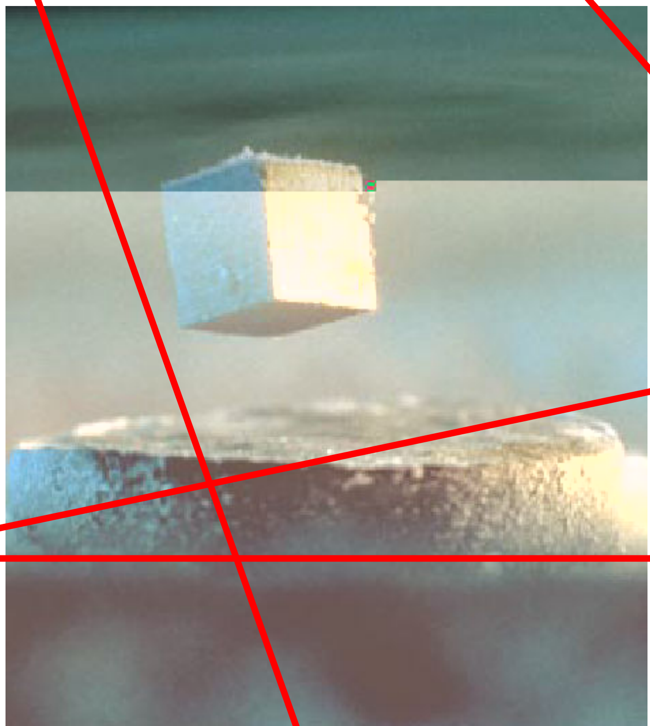


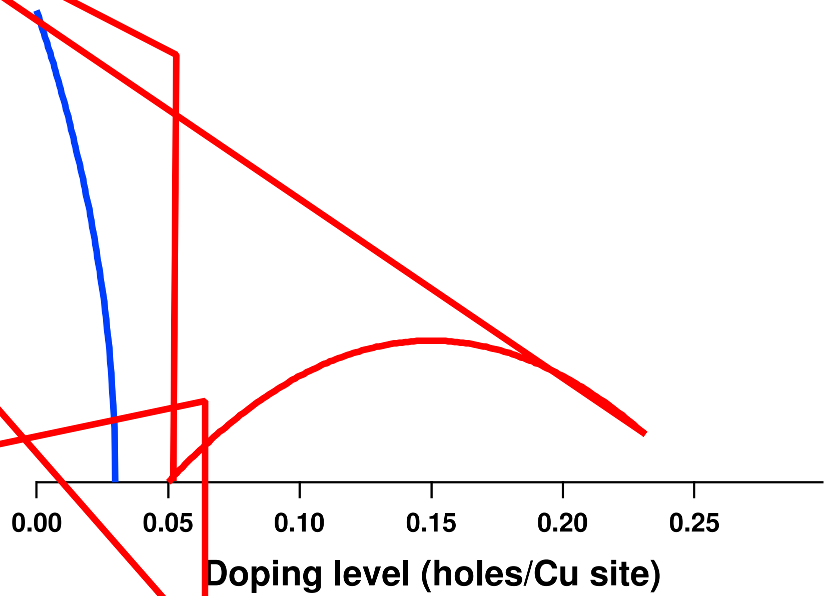
$YBa_2Cu_3O_{7-\delta}$

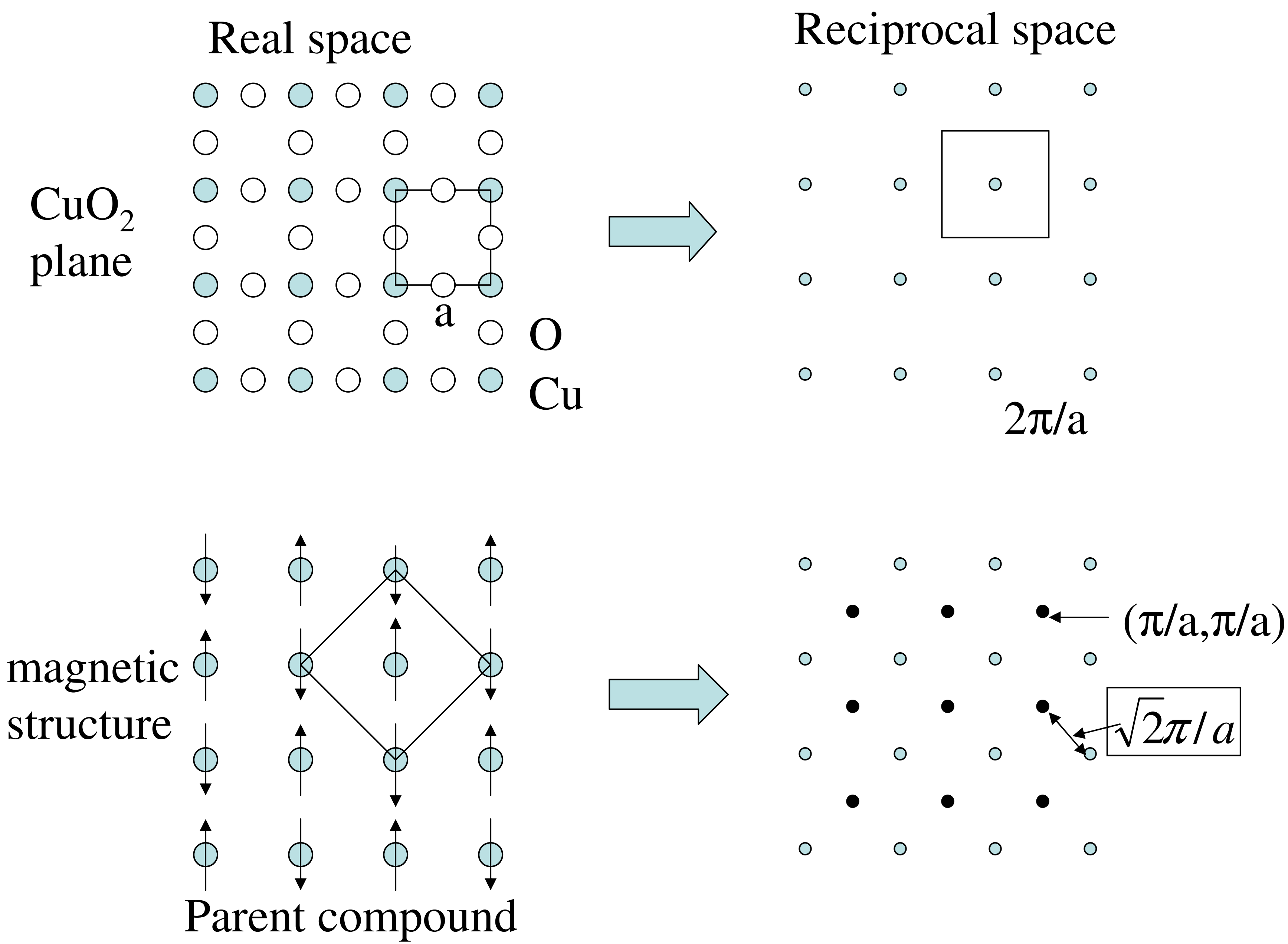


Superconductivity



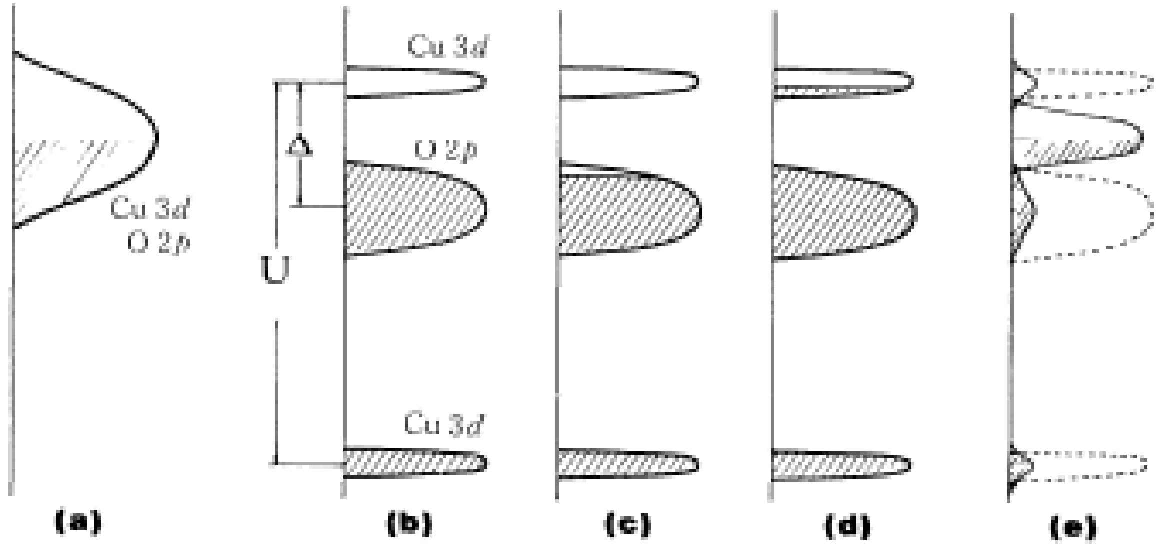


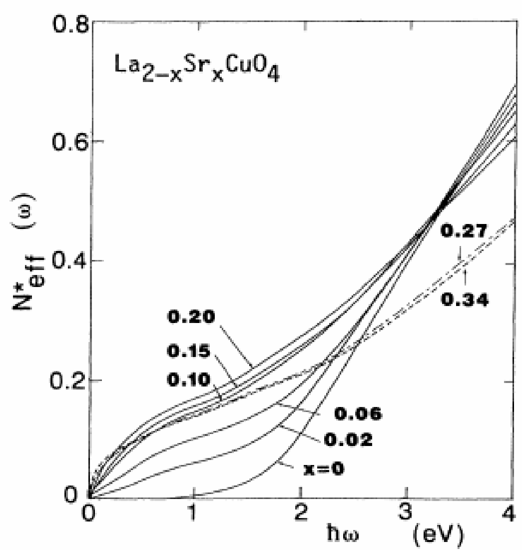


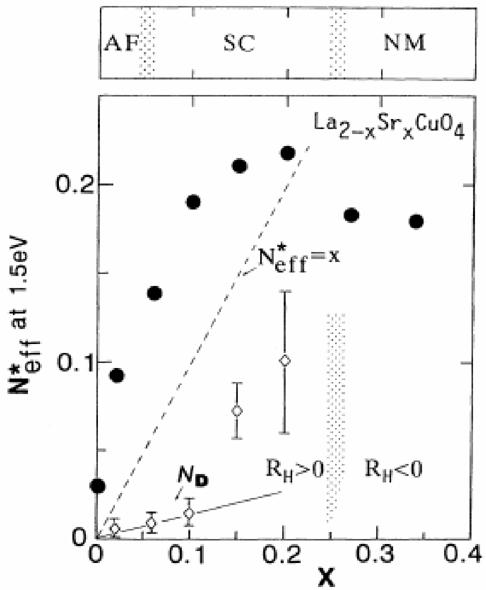

Real space
Reciprocal space
CuO_2 plane
a
O
Cu
$2\pi/a$
magnetic structure
$(\pi/a,\pi/a)$
$\sqrt{2}\pi/a$
Parent compound

Neutron scattering provides a lot information about spin excitations:

- 3D Bragg peaks at (π, π) for parent compound (Long range order),
- Incommensurate peaks away from the (π, π) point in doped compounds spin fluctuation,
- **~40 meV resonance at (π, π) below T_c.**


Cu 3d
O 2p
Cu 3d
O 2p
U
Δ
Cu 3d
(a)
(b)
(c)
(d)
(e)


$La_{2-x}Sr_xCuO_4$
N^*_{eff} (ω)
ħω (eV)
0.20
0.15
0.10
0.06
0.02
x=0
0.27
0.34


AF
SC
NM
$La_{2-x}Sr_xCuO_4$
$N^*_{eff}=x$
N^*_{eff} at 1.5eV
N_D
$R_H>0$
$R_H<0$
X

M e c n e ec n n e ec c c e

- Mode coupling effect in ARPES and tunneling
- Mode coupling effect in IR spectra of conventional superconductor
- Feature in IR spectra of high-Tc superconductors

Extraction the boson (phonon) spectral function

BCS theory for conventional superconductors

$$\Delta = |V| \frac{1}{N} \sum \frac{\Delta}{2E_k}$$ Tc equation

$$\frac{2\Delta}{k_B T_c} = 3.53$$ **n e y** $$\frac{\Delta C}{\gamma T_c} = 1.43$$

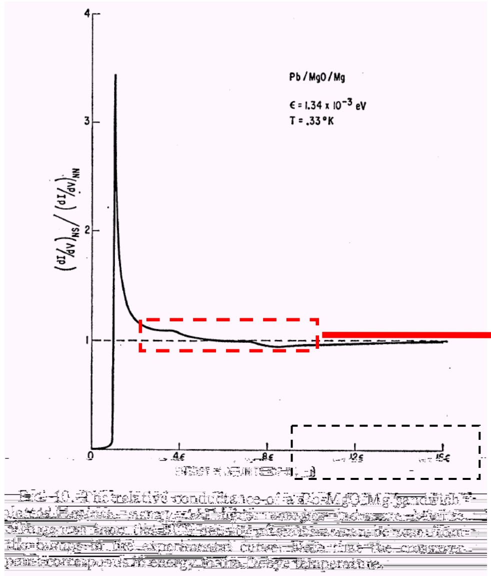
Eliashberg Theory

Extension of BCS formalism to include dynamical electron-phonon interaction

$$\Delta(k,\omega) = \mathcal{F}[V_{k,k'}(\omega,\omega')]$$ ← A function of the interaction

e n Can we invert the theory to extract the potential uniquely from a knowledge of Δ(k,ω) ?

I. Giaever, H.R. Hart, Jr., and K. Megerle, PRB 126, 941 (1962)



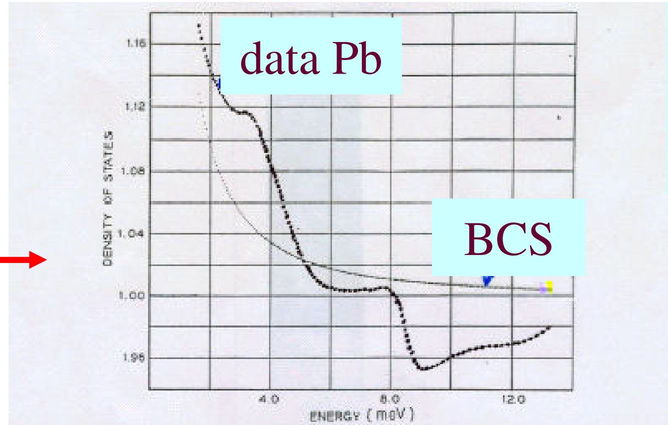
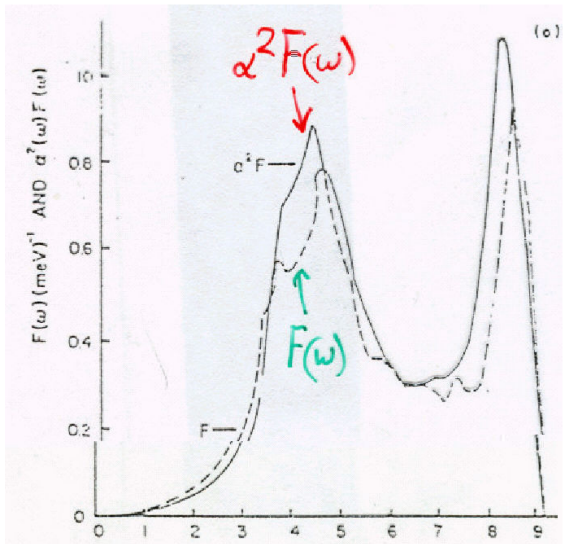


Fig. 23. Electronic density of states $N(E)$ for lead vs. $E-\Delta_0$ obtained from the data of Fig. 19. The smooth curve is the BCS density of states.

McMillan and Rowell, Superconductivity, ed. By R.D. Parks (1969)

requires Eliashberg theory:

- phonon dynamics (retardation) taken into account $[\alpha^2 F(\Omega)]$
- gap is a function of frequency $\Delta(\omega) = \mathcal{F}[\{\alpha^2 F(\Omega)\}, \mu^*]$
- density of states is modified: $\frac{dI}{dV} \propto N(\omega) = N(\epsilon_F)\mathrm{Re}\{\frac{\omega}{\sqrt{\omega^2 - \Delta^2(\omega)}}\}$



RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 51, NUMBER 22 1 JUNE 1995-II

Phonon structure in the tunneling conductance of $Bi_2Sr_2CaCu_2O_8$

D. Shimada, Y. Shiina, A. Mottate, Y. Ohyagi, and N. Tsuda*

Department of Applied Physics, Science University of Tokyo, 1-3 Kagurazaka, Shinjuku-ku, Tokyo 162, Japan

(Received 17 March 1995)

Clear phonon structures were observed in the tunneling conductance of a $Bi_2Sr_2CaCu_2O_8$-GaAs junction ... definitely exclude a *d*-wave state.

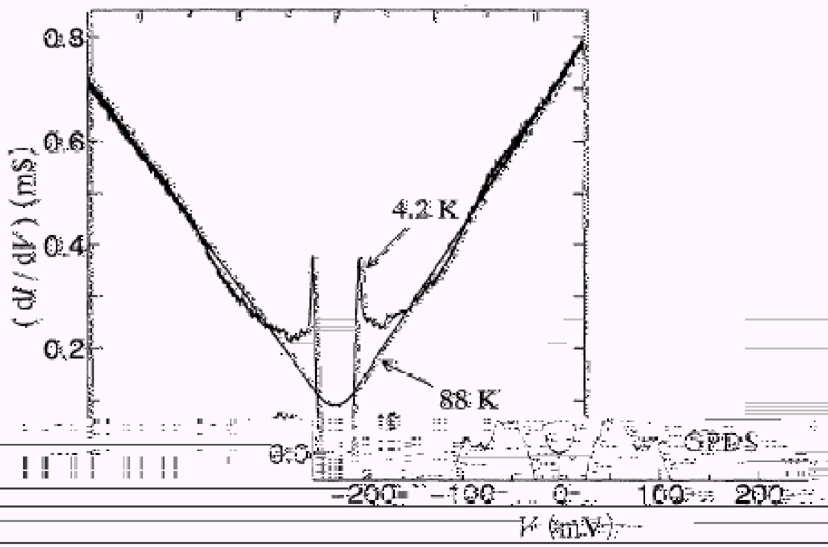


FIG. 2. The normalization procedure was illustrated. The subtracted conductances at 4.2 and 88 K were plotted together with the GPDS of B2212 (Ref. 14). These subtracted conductances were normalized. See the text.

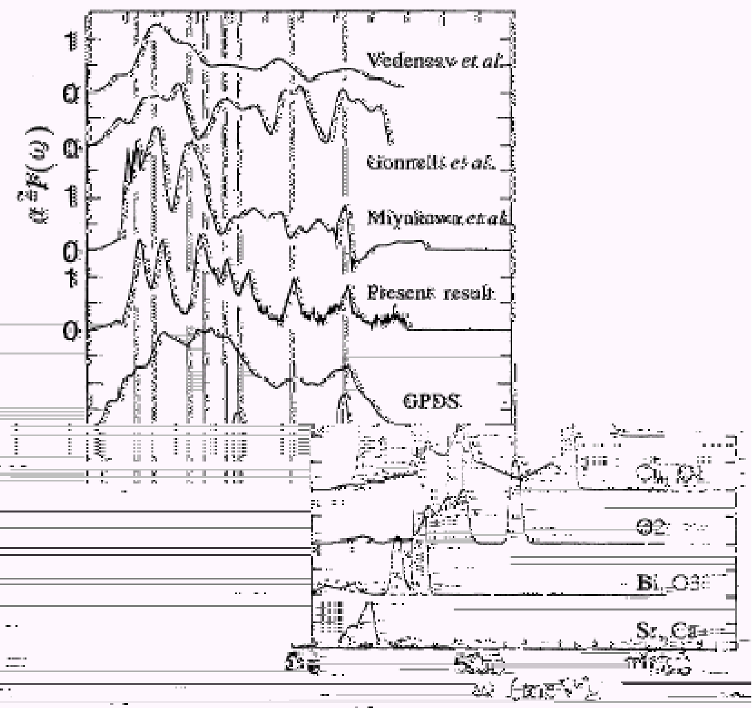


FIG. 4. Spectral functions obtained by Vedeneev et al. ...

RAPID COMMUNICATIONS

PHYSICAL REVIEW B **68**, 180504(R) (2003)

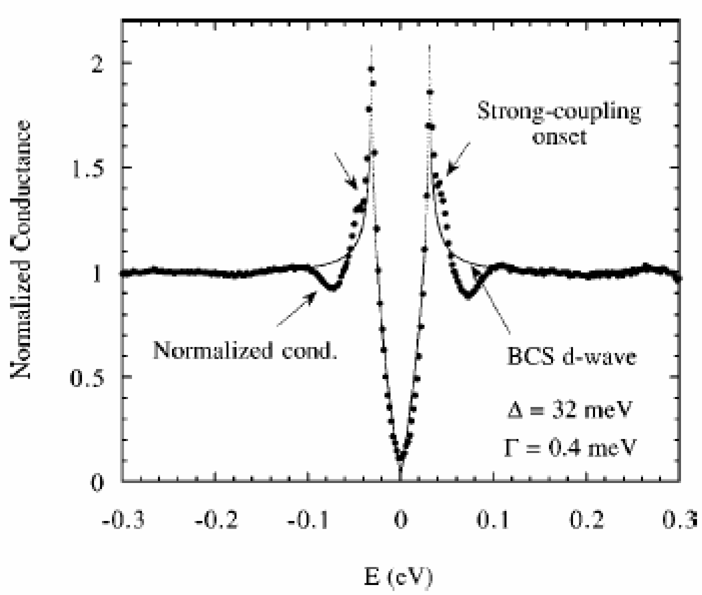
Tunneling spectroscopy of $Bi_2Sr_2CaCu_2O_{8+\delta}$: Eliashberg analysis of the spectral dip feature

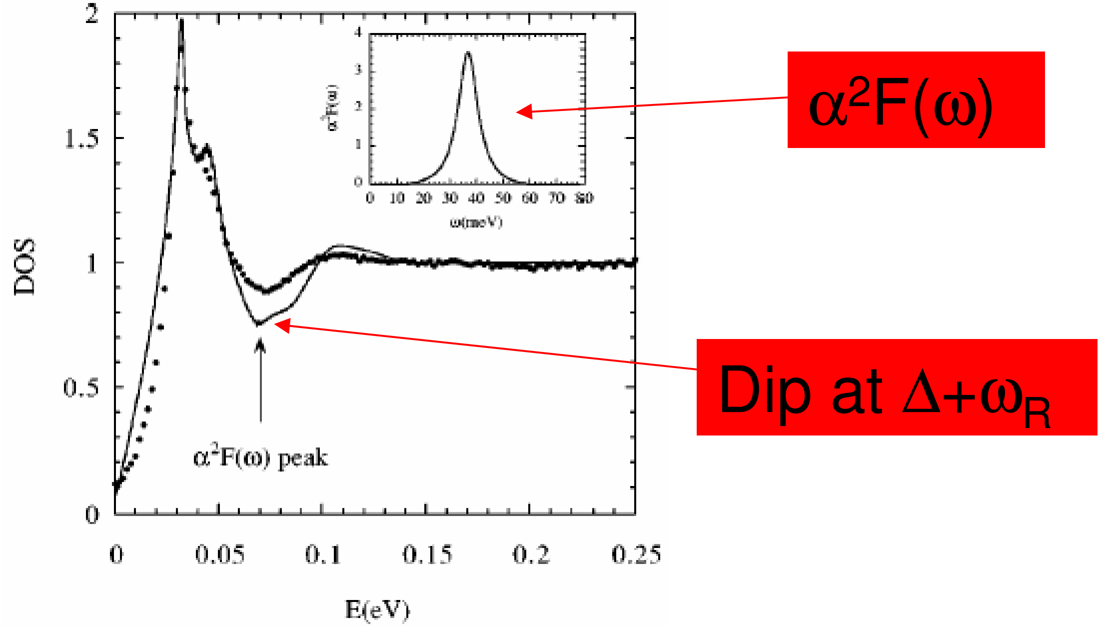
J. F. Zasadzinski,[1,2] L. Coffey,[1] P. Romano,[3] and Z. Yusof[2]

[1]Physics Division, Illinois Institute of Technology, Chicago, Illinois 60616, USA

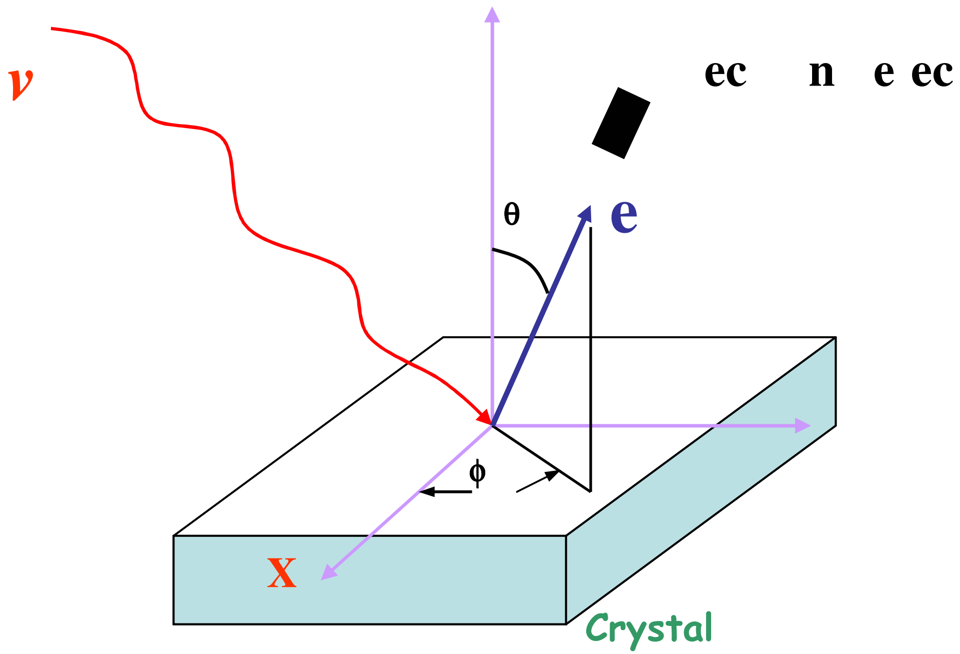
(Received 2 September 2003; published 17 November 2003)

Eliashberg strong-coupling theory extended to a d-wave symmetric gap function is used to fit a published tunneling spectrum of $Bi_2Sr_2CaCu_2O_{8+\delta}$ near optimal doping. The shape, location, and strength of the high-bias spectral dip feature is adequately reproduced using a single-peak $\alpha^2F(\omega)$ centered at 36.5 meV. $\alpha^2F(\omega)$ also self-consistently determines the measured gap value $\Delta = 32$ meV. Possible origins of the bosonic spectrum that gives rise to high-T_c superconductivity are discussed.





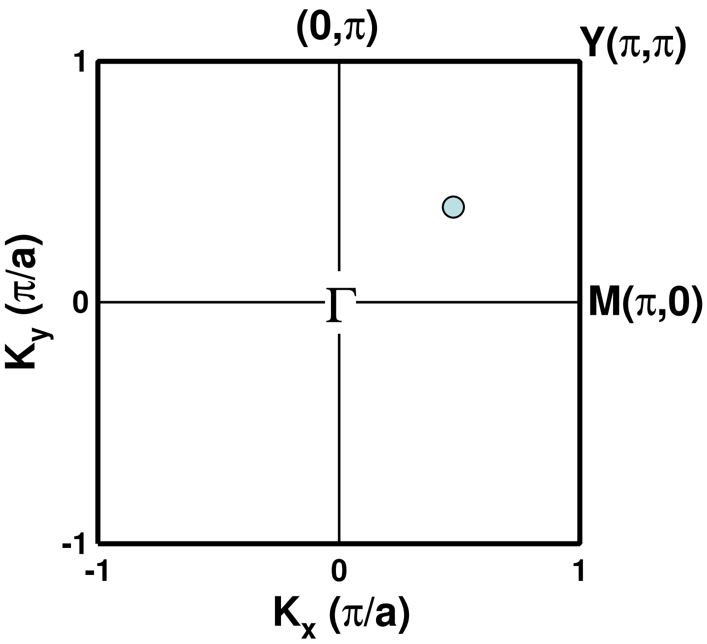
An e e e e n ec c y *ARPES*

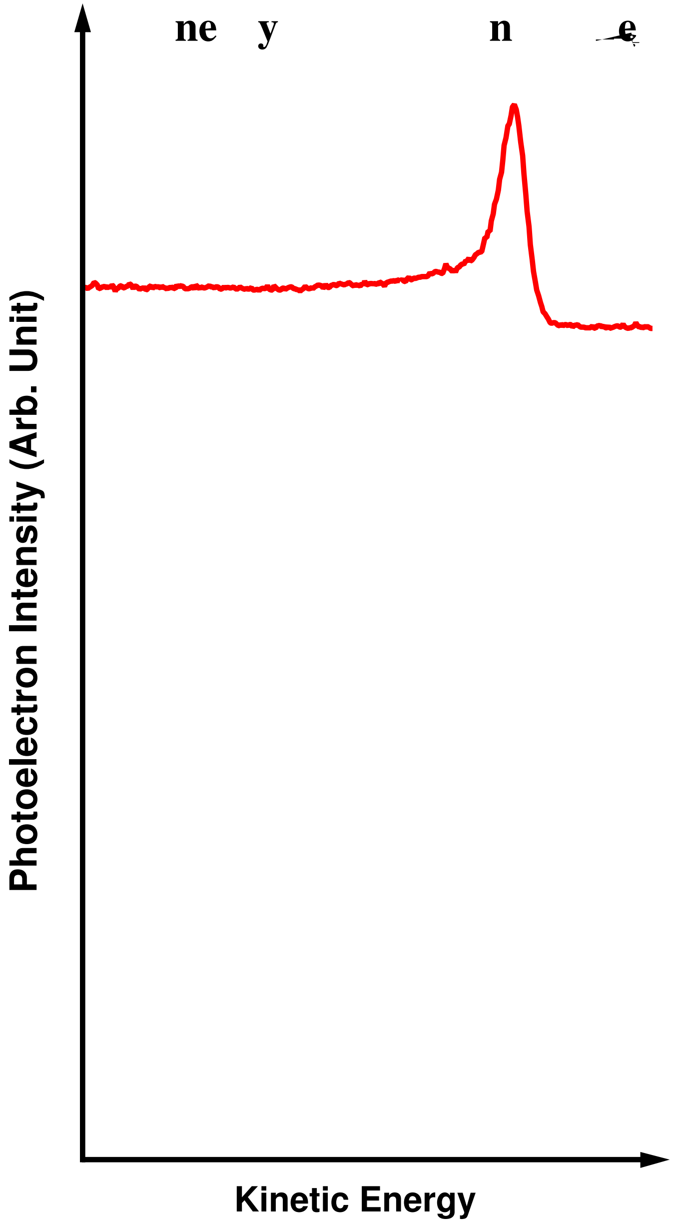


Energy Conservation: B ν − n−Φ

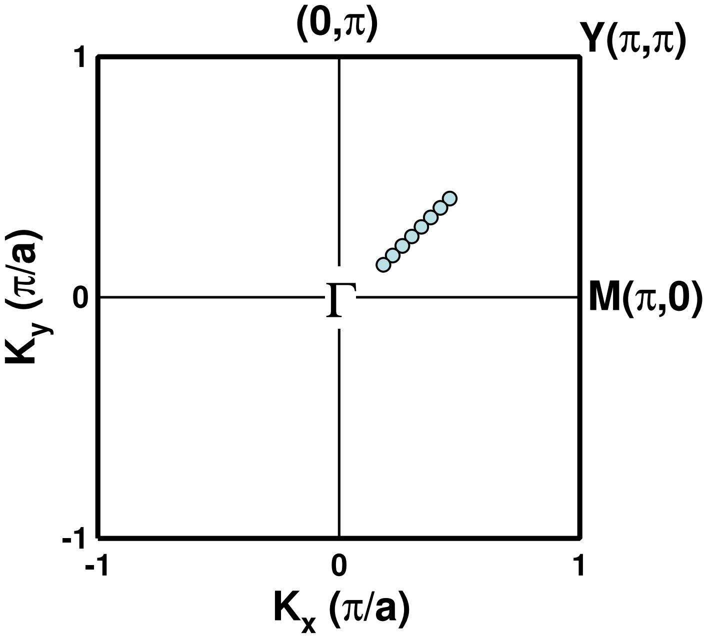
Momentum Conservation:

A B n M n n e ce

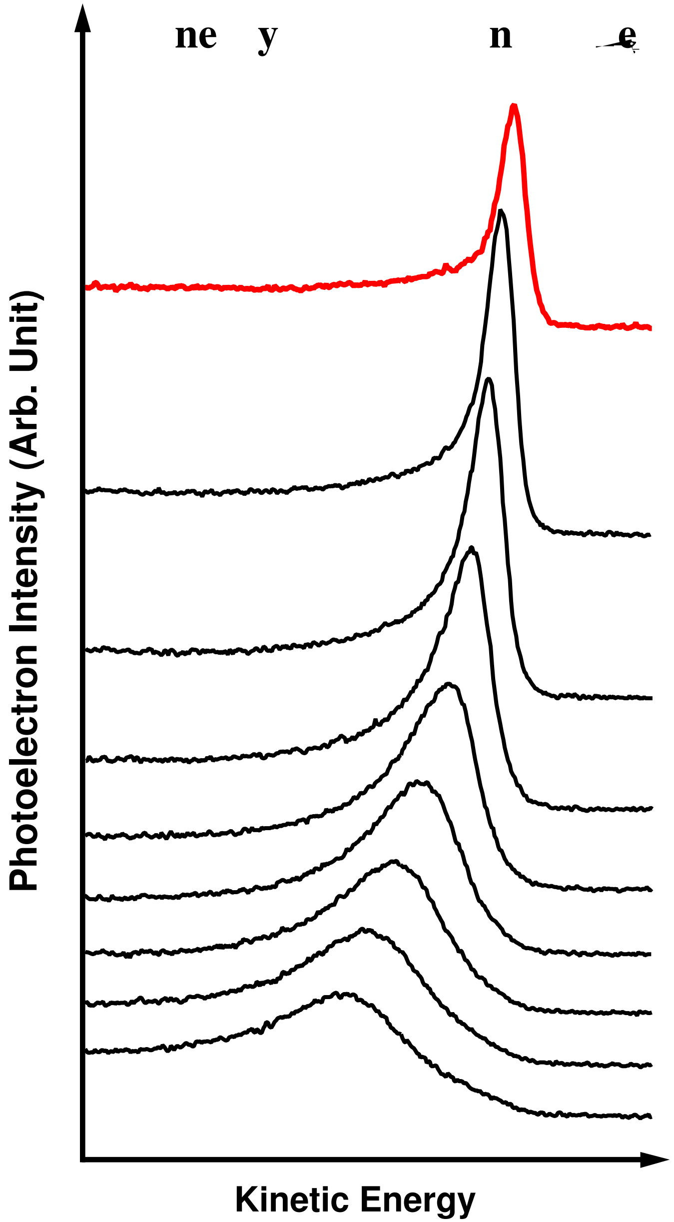

(0,π)
Y(π,π)
M(π,0)
Γ
1
0
-1
-1
0
1
K_y (π/a)
K_x (π/a)


Photoelectron Intensity (Arb. Unit)
Kinetic Energy

A B n M n n e ce

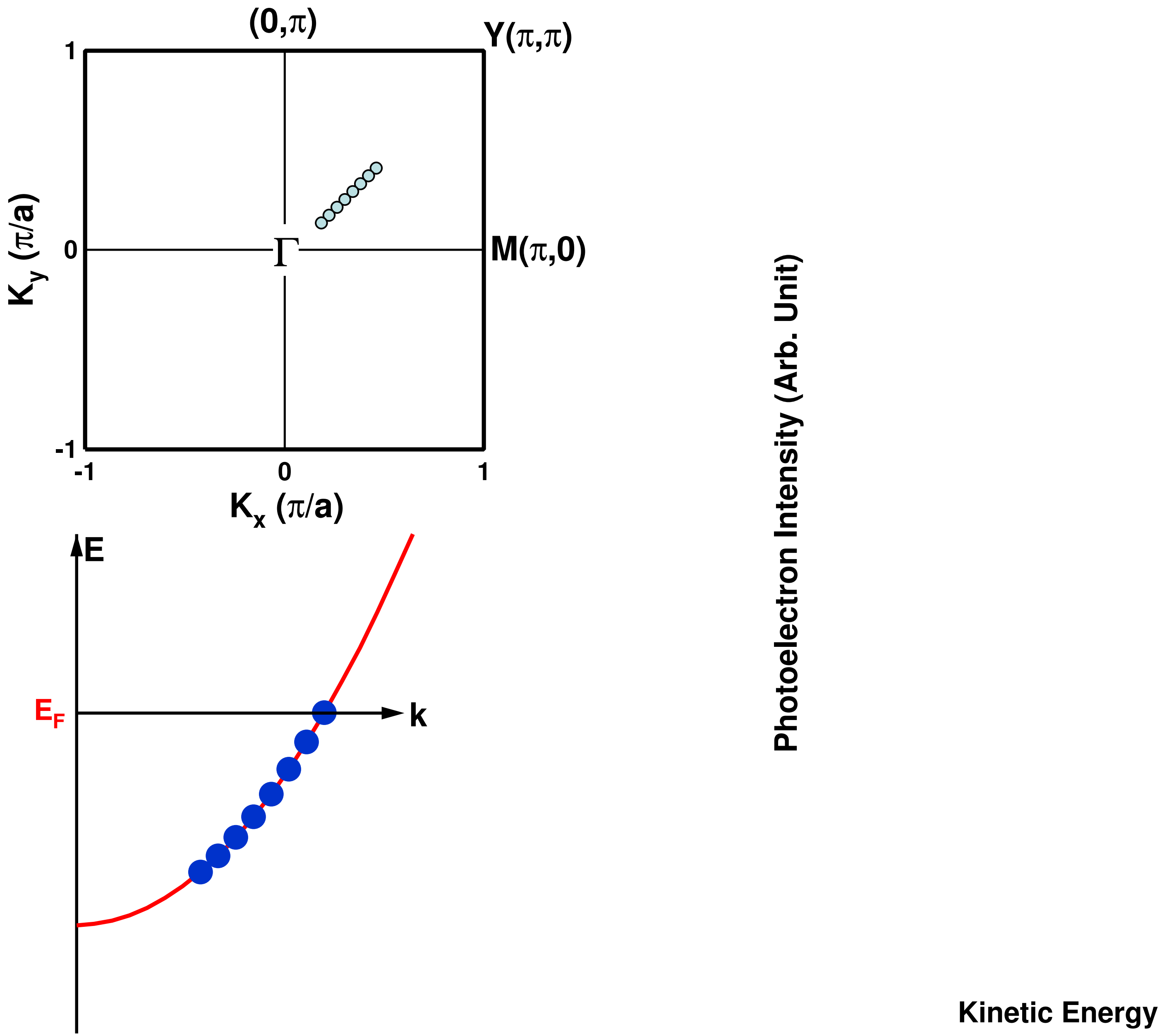


(0,π)
Y(π,π)
M(π,0)
Γ
1
0
-1
-1
0
1
Ky (π/a)
Kx (π/a)



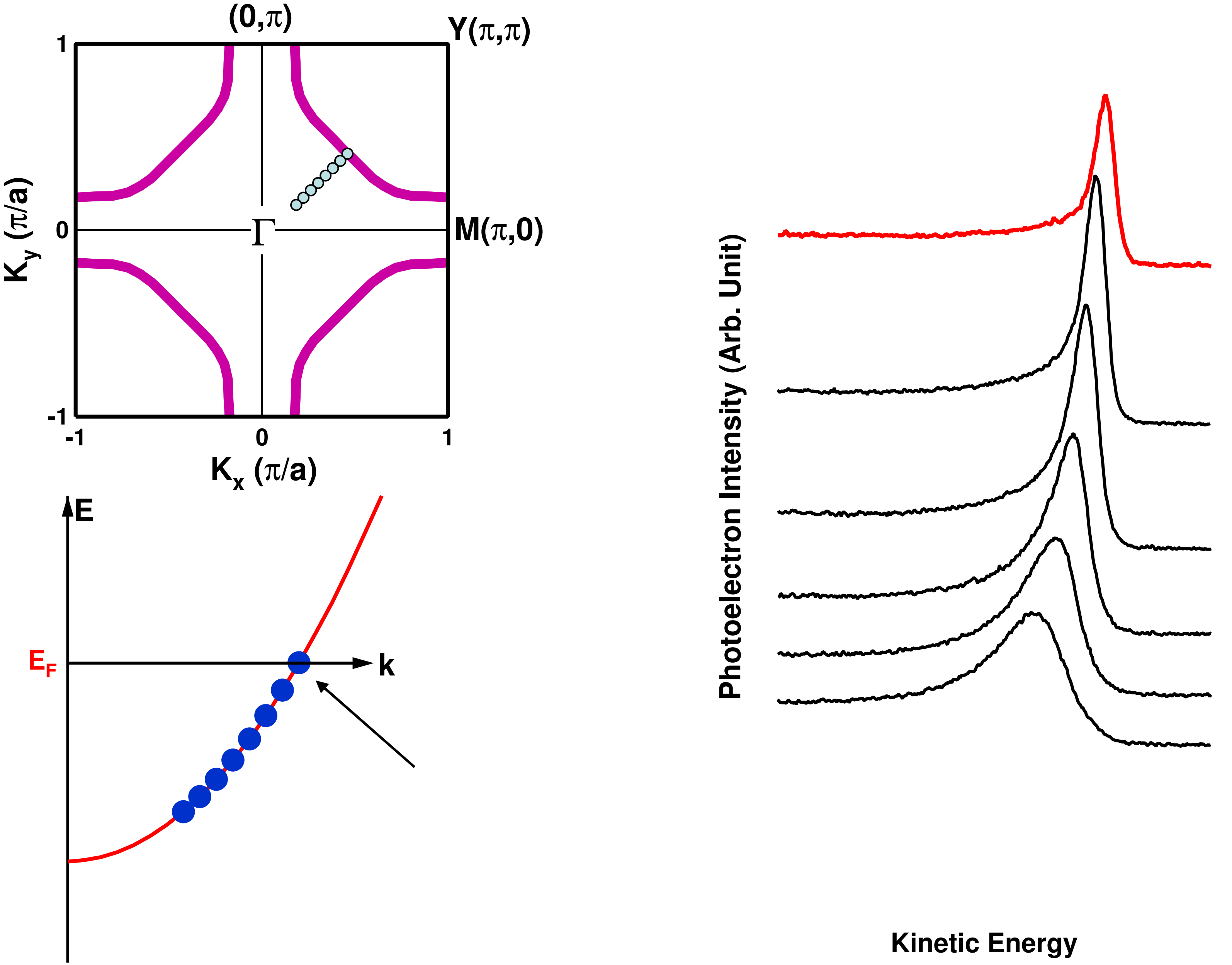
ne y
n
e
Photoelectron Intensity (Arb. Unit)
Kinetic Energy

A B n M n n e ce



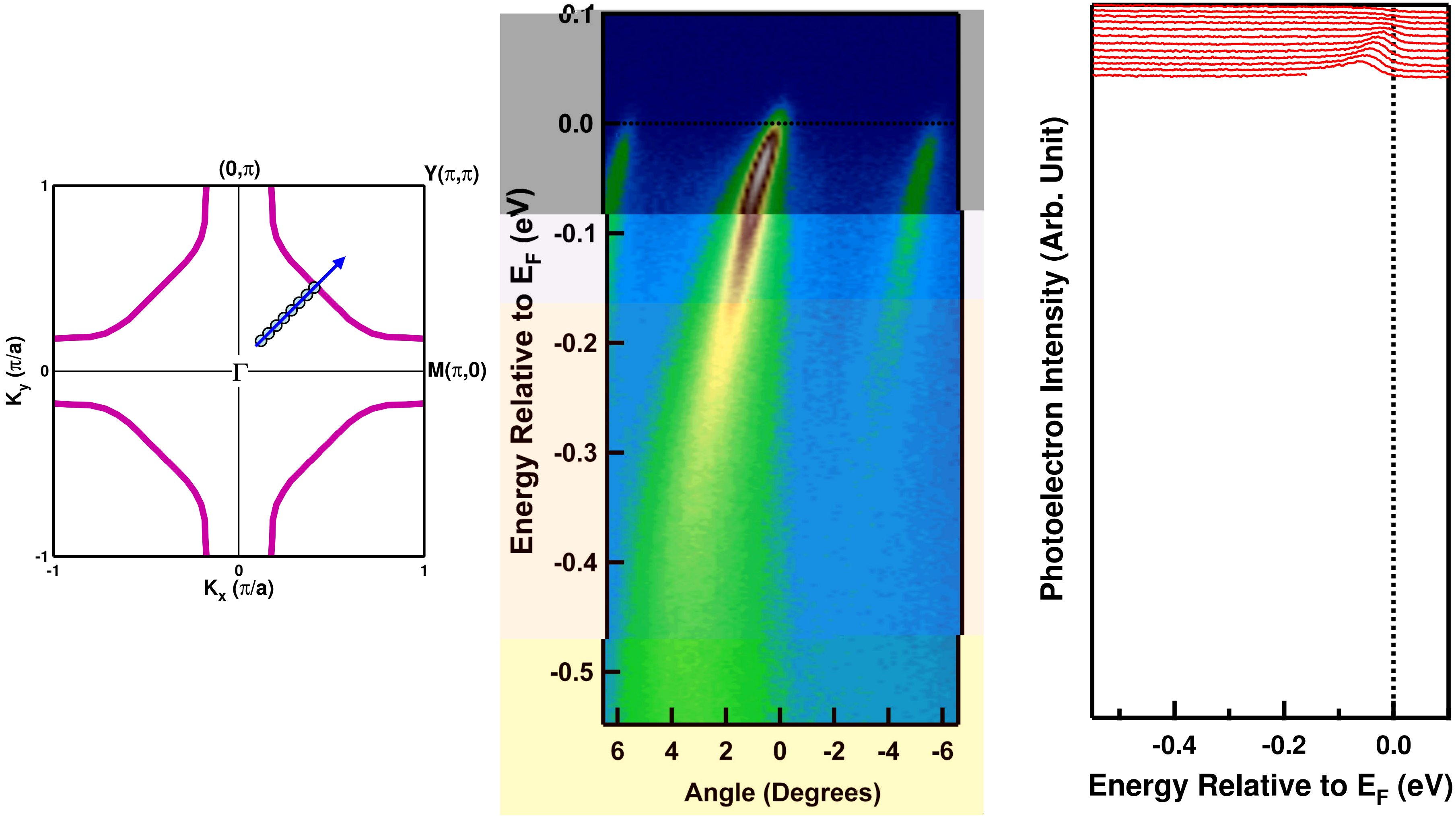
(0,π)
Y(π,π)
M(π,0)
Γ
1
0
-1
-1
0
1
K_y (π/a)
K_x (π/a)
E
E_F
k
Photoelectron Intensity (Arb. Unit)
Kinetic Energy

A B n M n n e ce

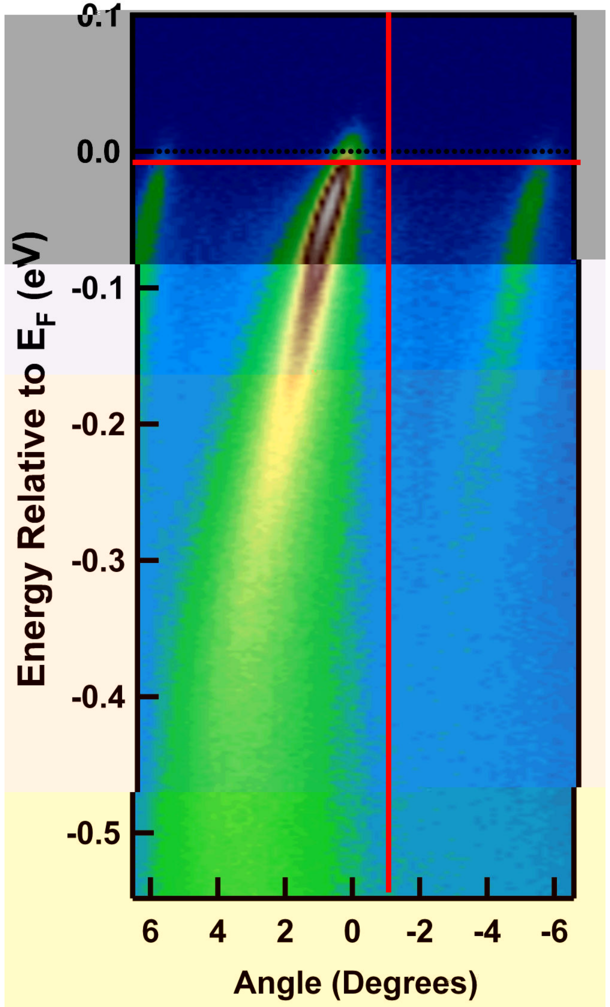


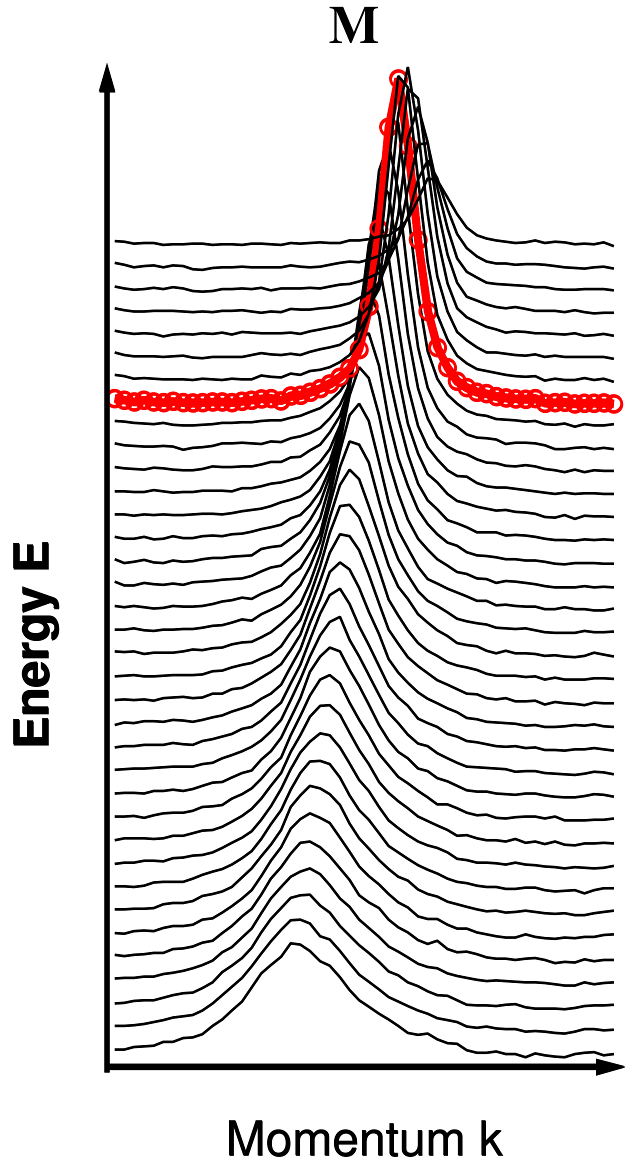
(0,π)
Y(π,π)
M(π,0)
Γ
1
0
-1
-1
0
1
K_y (π/a)
K_x (π/a)
E
E_F
k
Photoelectron Intensity (Arb. Unit)
Kinetic Energy

e A A – M e An e ec n



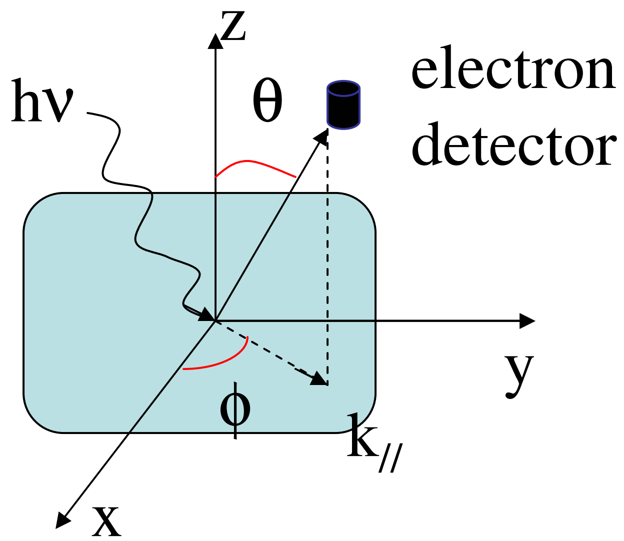
ec κ c n ec n e ne y M en n e





photoemission

Detected electrons ∝ N(ω)•**f(ω)**



$$\because N(\omega) = \frac{1}{2\pi}\sum_k A(k,\omega)$$

A c n n ∝ A ω • ω

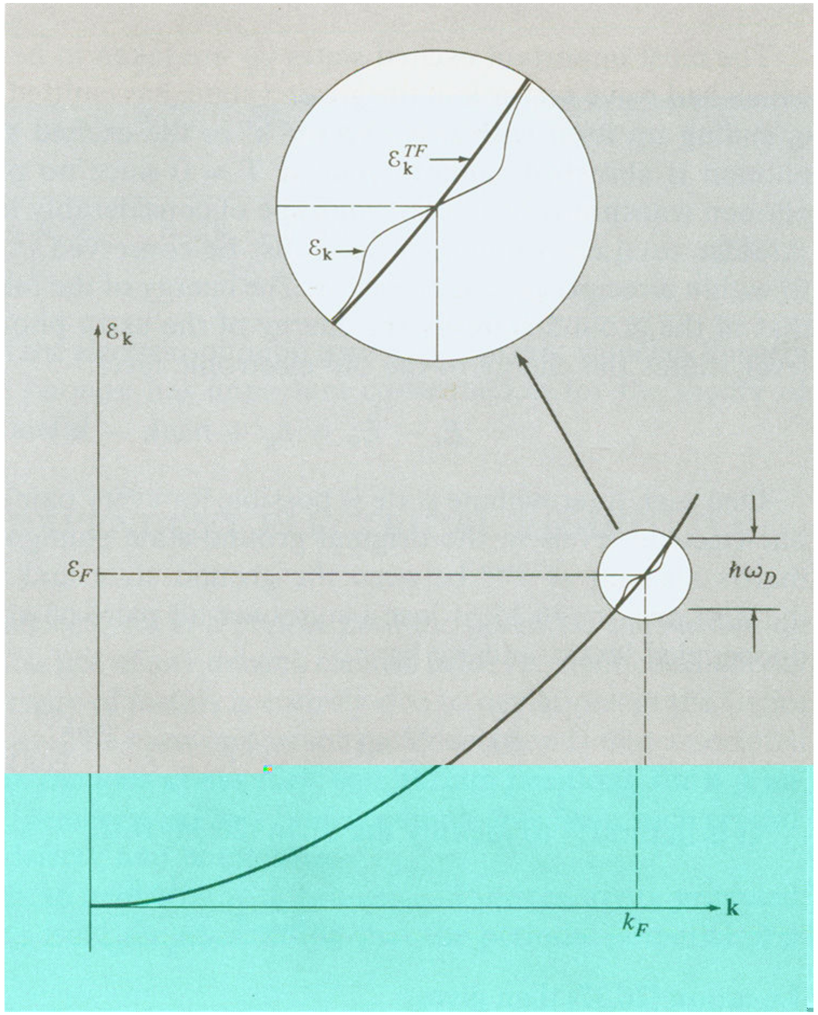
$$\because A(k,\omega) = (-1/\pi)\,\mathrm{Im}G(k,\omega), \qquad G(k,\omega) = \frac{1}{\omega - \varepsilon(k) - \sum(k,\omega)}$$

$$\therefore A(k,\omega) = \frac{1}{\pi}\frac{\mathrm{Im}\sum(\omega,k)}{[\omega - \varepsilon_k - \mathrm{Re}\sum(\omega,k)]^2 + [\mathrm{Im}\sum(\omega,k)]^2}$$

PEAK POSITION: Dispersion e c y ec e e c

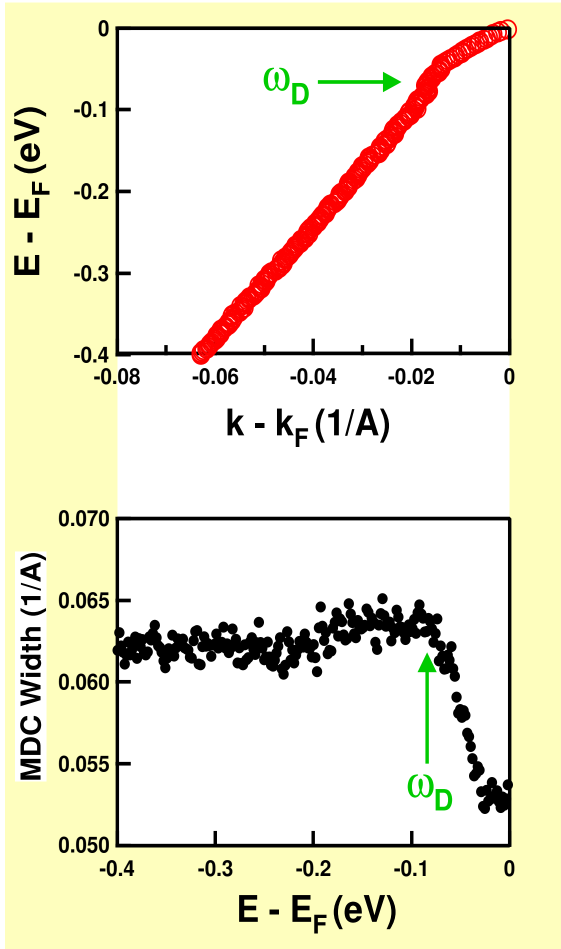
PEAK WIDTH: ImΣ or 1/τ scattering rate

M n e n M ny B y ec B n en z n



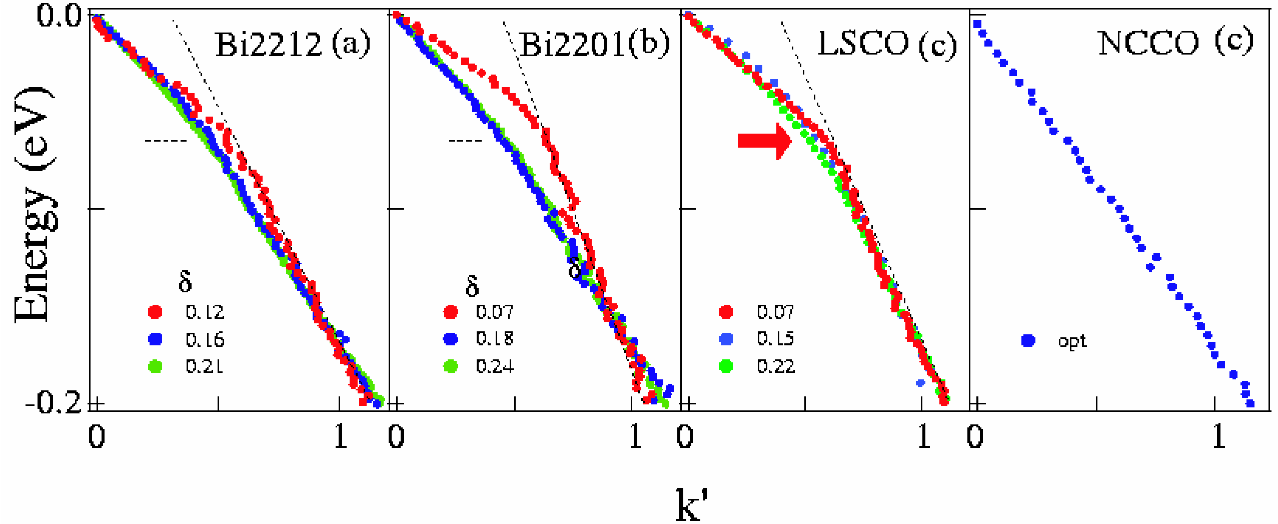
A c Me n e y c

Be ce e



en e e e L
L e e B 6
n e y

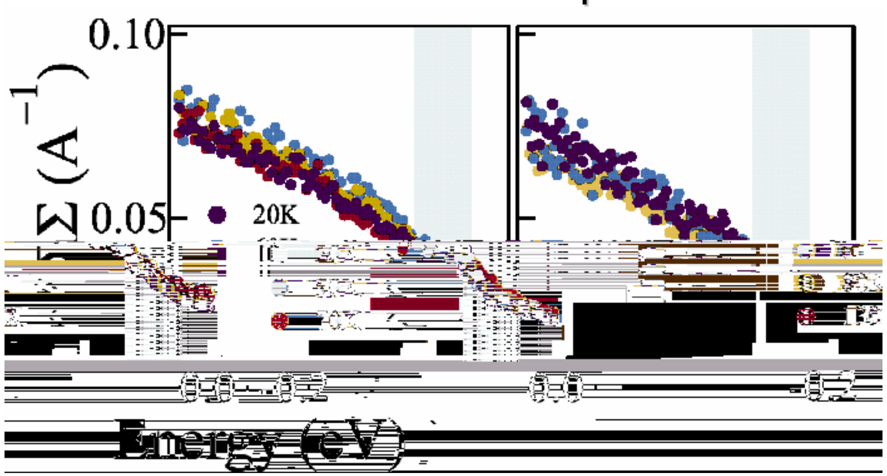
A. Lanzara, et al., Nature 412, 510 (2001)

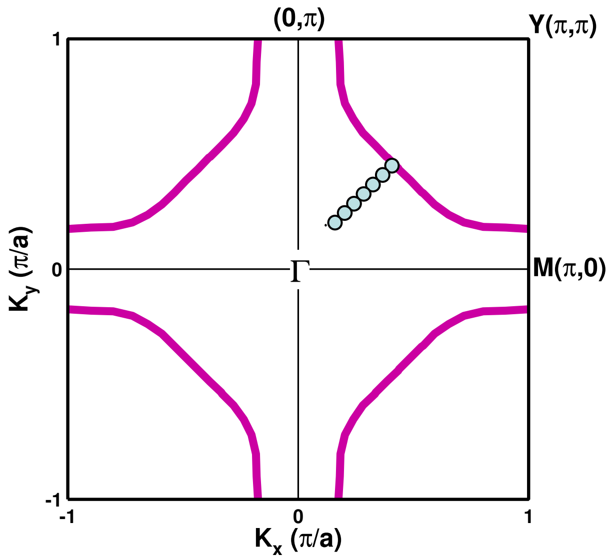


The kink is observed both below and above Tc in all hole-type cuprates

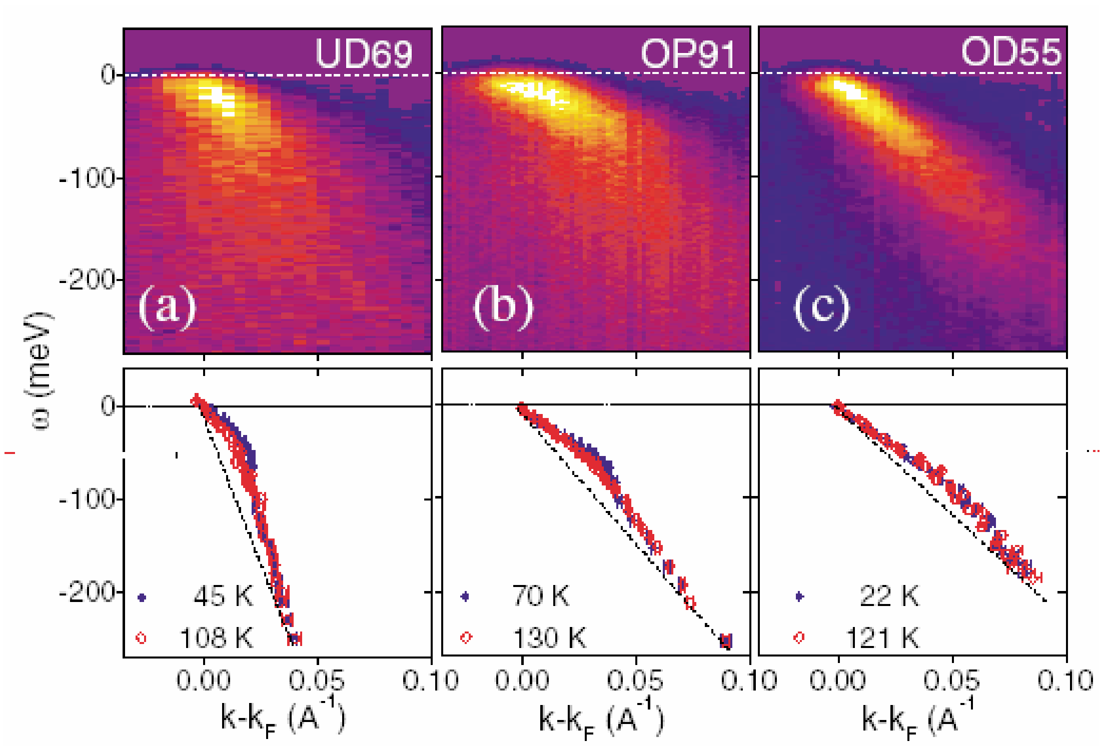
Drop in the ImΣ

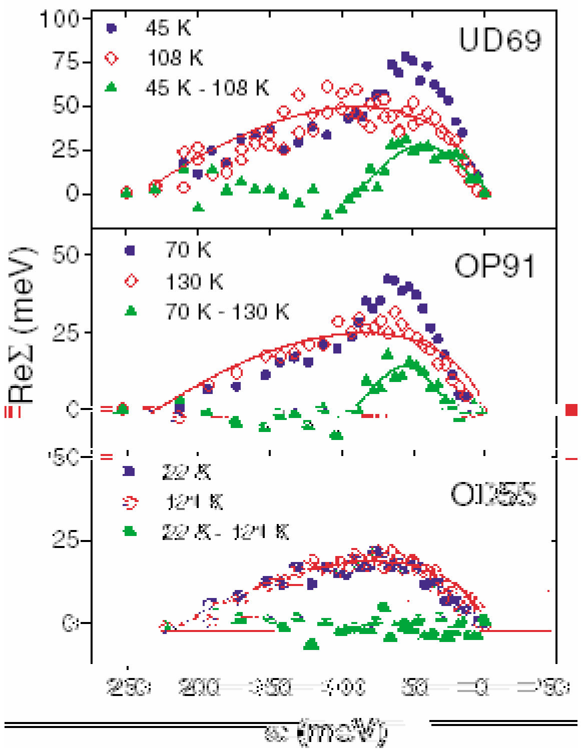
UD-Bi2201 opt-Bi2212

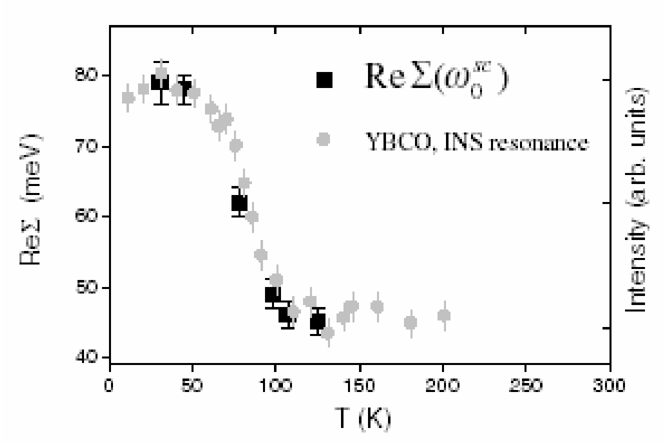


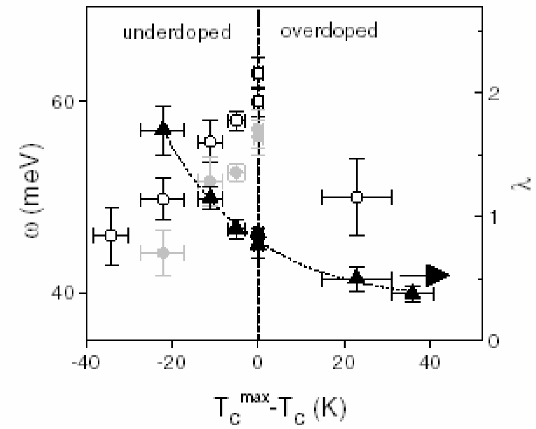


P. D. Johnson, et al., PRL 87, 177007 (2001)

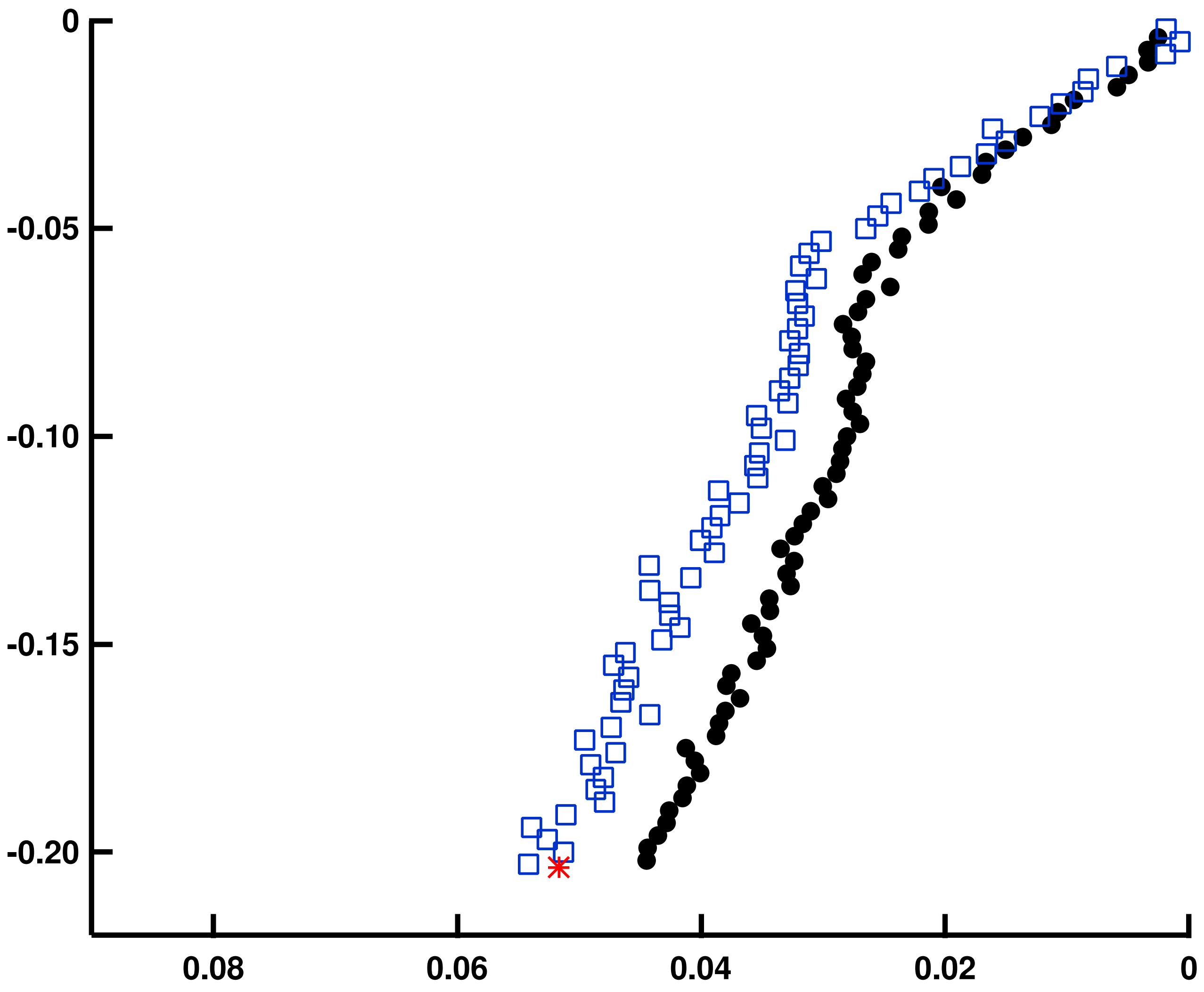


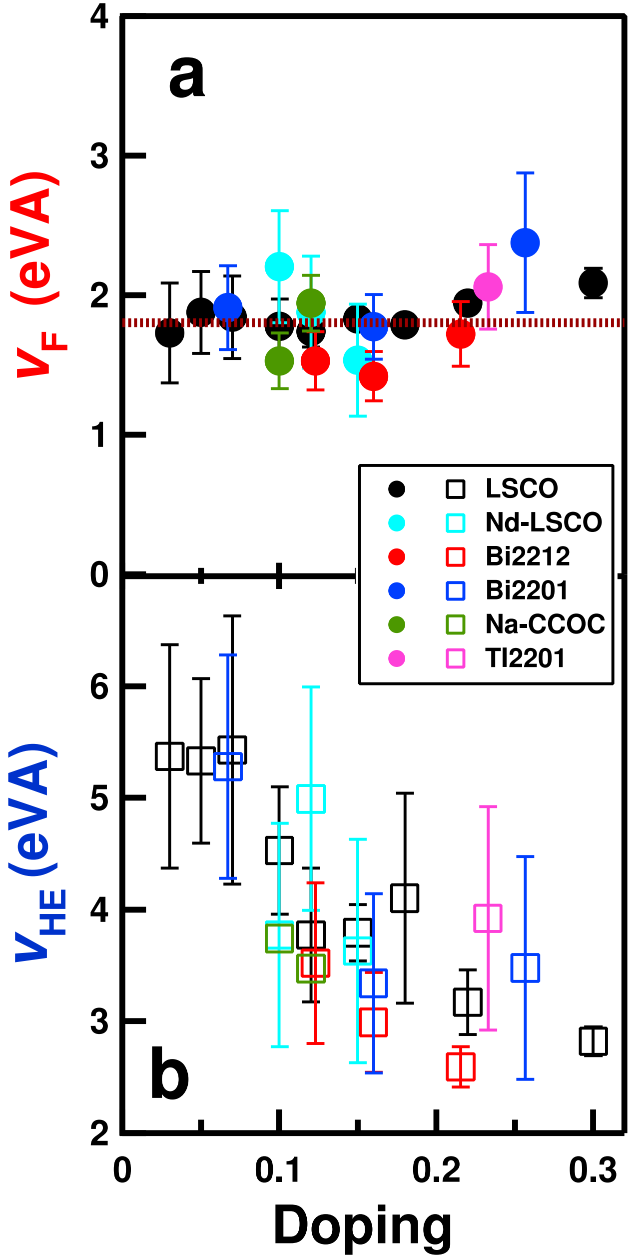






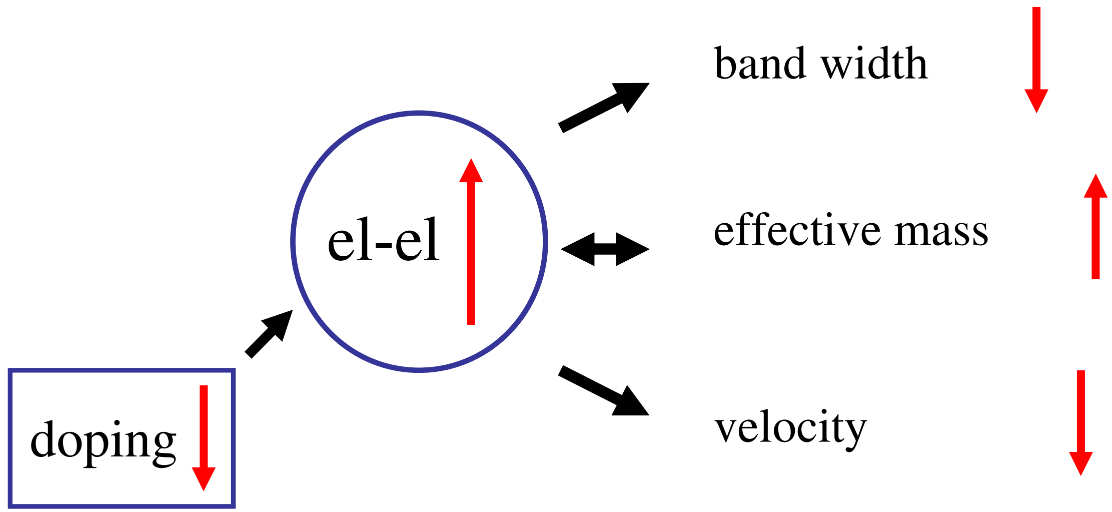
$$\lambda = -(\partial \operatorname{Re}\Sigma / \partial\omega)_{E_F}$$


0
-0.05
-0.10
-0.15
-0.20
0.08
0.06
0.04
0.02
0



Observation of universal Fermi velocity is unexpected.

Doping Dependence of High-Energy Velocity is Anomalous



ꭗ c n B n c ec nc n eΣ

In metals, the real part of self-energy is related to the bosonic spectral function by:

$$\mathrm{Re}\,\Sigma(k,\varepsilon,T)=\int_0^\infty d\omega\,\alpha^2F(\omega;\varepsilon,k)\,K\left(\frac{\varepsilon}{kT},\frac{\omega}{kT}\right)$$

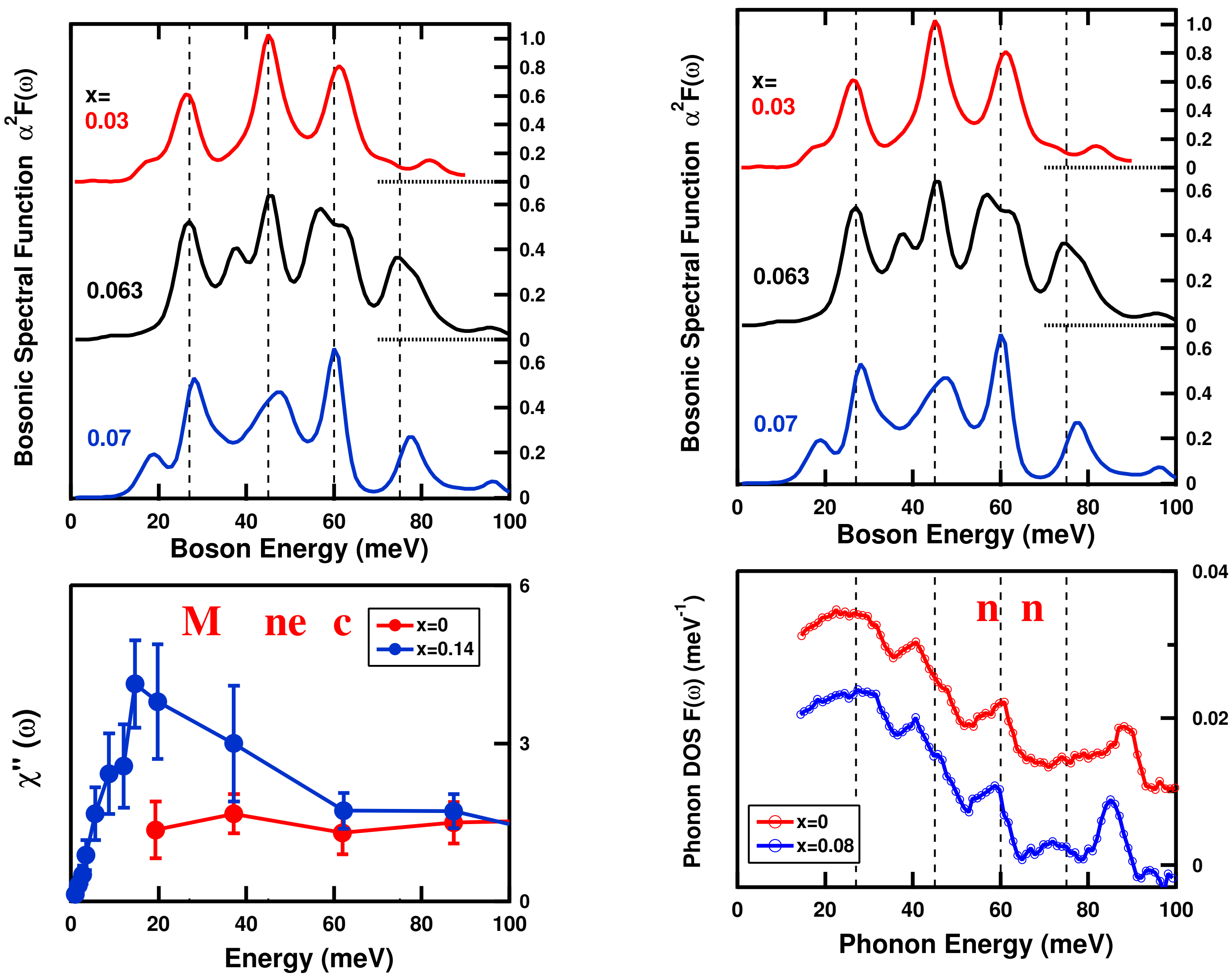
where

$$K(y,y')=\int_{-\infty}^{\infty}dx\,\frac{2y'}{x^2-y'^2}f(x+y)$$

with f(x) being the Fermi-Dirac distribution Function

Mꭗ n y Me ⇒ α ω

n e c e ec nc n n n c e



e
e
n n

y en e
L 6 6

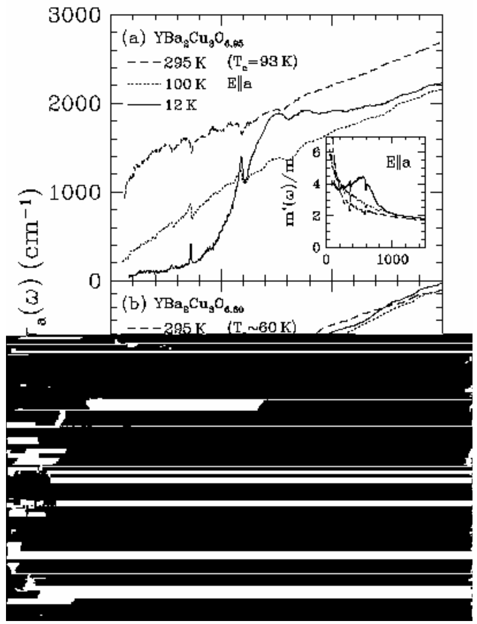
Mc eeney e
L

YBCO

C C Homes

D N Basov

T. Timusk



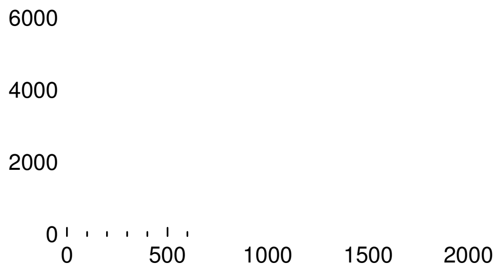
R(ω)

⇒ $\sigma_1(\omega)$

⇒ $1/\tau(\omega)$

Tl-2212 thin
film T_c=108 K

N. L. Wang et al.,
PRB03

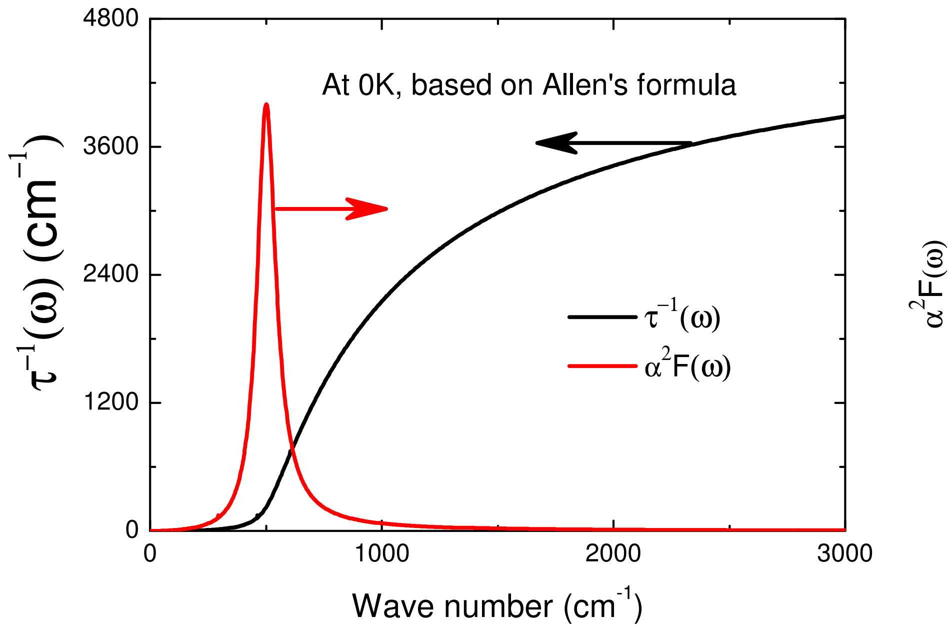


The electron-boson (phonon) interaction

$$1/\ \ (\ \ ) = \frac{2}{\omega}\int_0^\infty d\Omega(\omega-\Omega)\alpha_{tr}^2(\Omega)F(\Omega)$$

T=0 K

P.B.Allen 1971

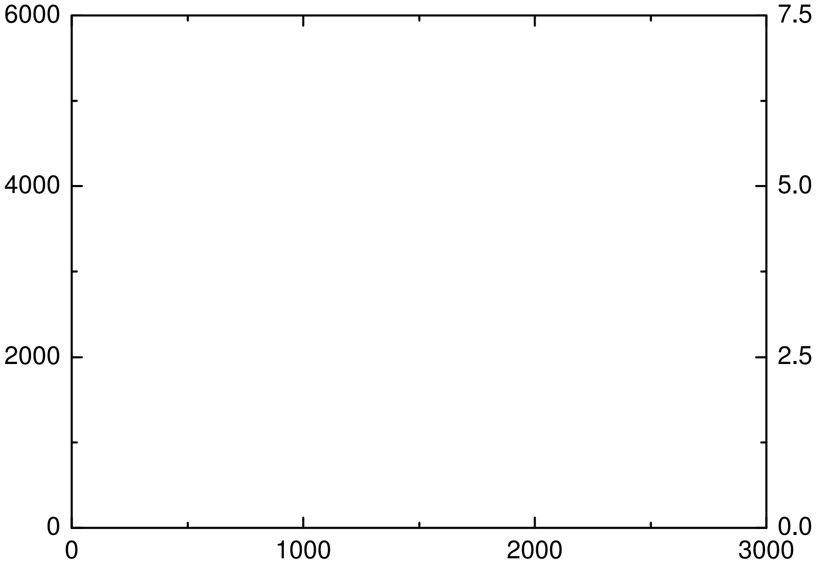


$$\alpha^2F(\omega) = \frac{\omega_p^2\omega^2}{(\omega_0^2-\omega^2)^2+\gamma^2\omega^2}$$

ω_0=500 cm-1

γ=100 cm-1

ω_p^2=50000 cm-2


6000
4000
2000
0
7.5
5.0
2.5
0.0
0
1000
2000
3000

Inversion of reflectance is a VERY ill-defined problem, but the "image" of $\alpha^2F(\Omega)$ is in the data.

Marsiglio et al., Phys. Lett. A **245**, 172 (1998)

normal state !

$$\sigma(\nu) = \frac{\omega_P^2}{4\pi}\frac{i}{\nu}\int_0^\nu d\omega \frac{1}{\nu + \frac{i}{\tau} - \Sigma(\nu - \omega + i\delta) - \Sigma(\omega + i\ldots}$$

where

igh precision (Pb)

n's" inversion — use perturbation theory

requires hi

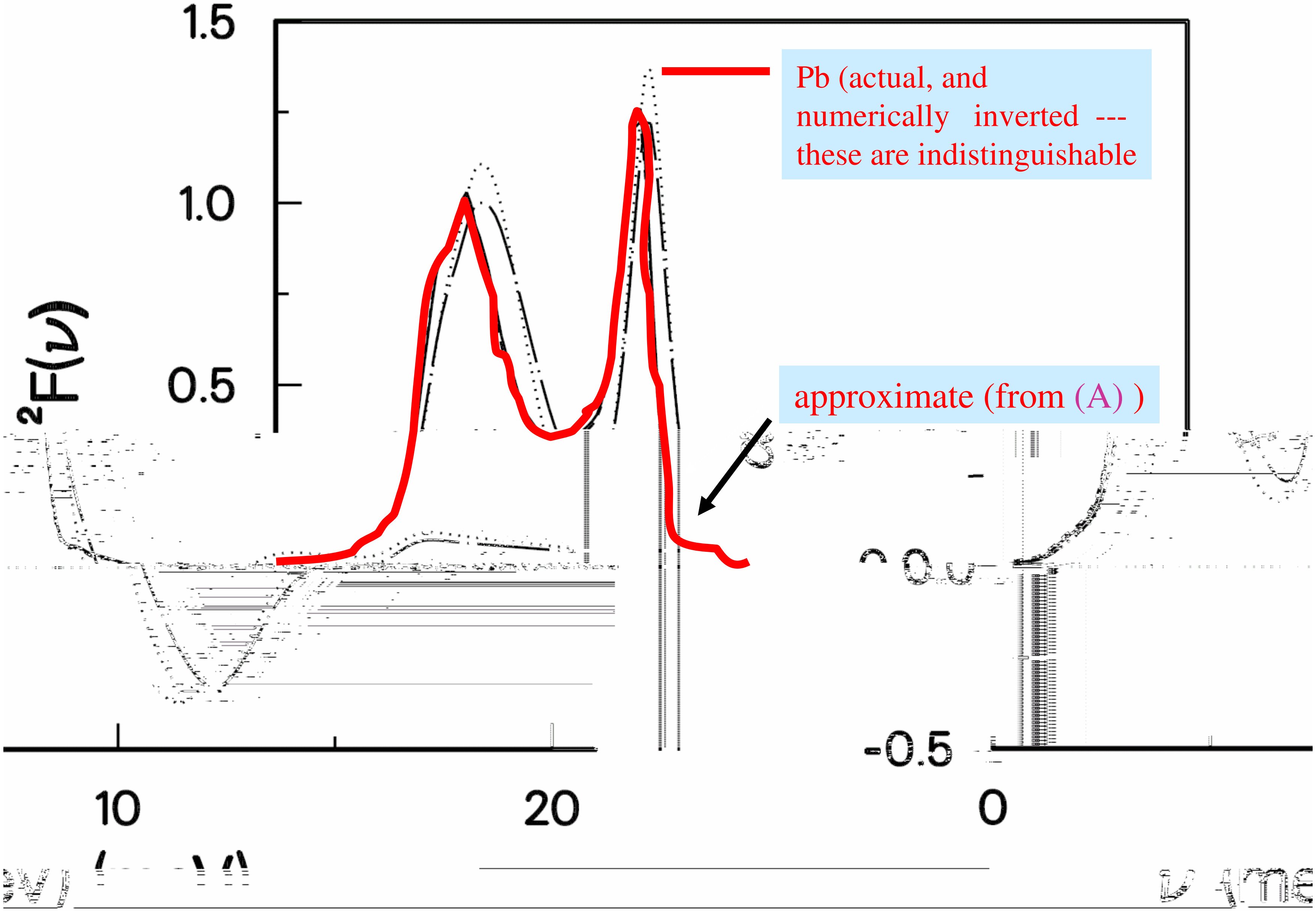
"Poor ma

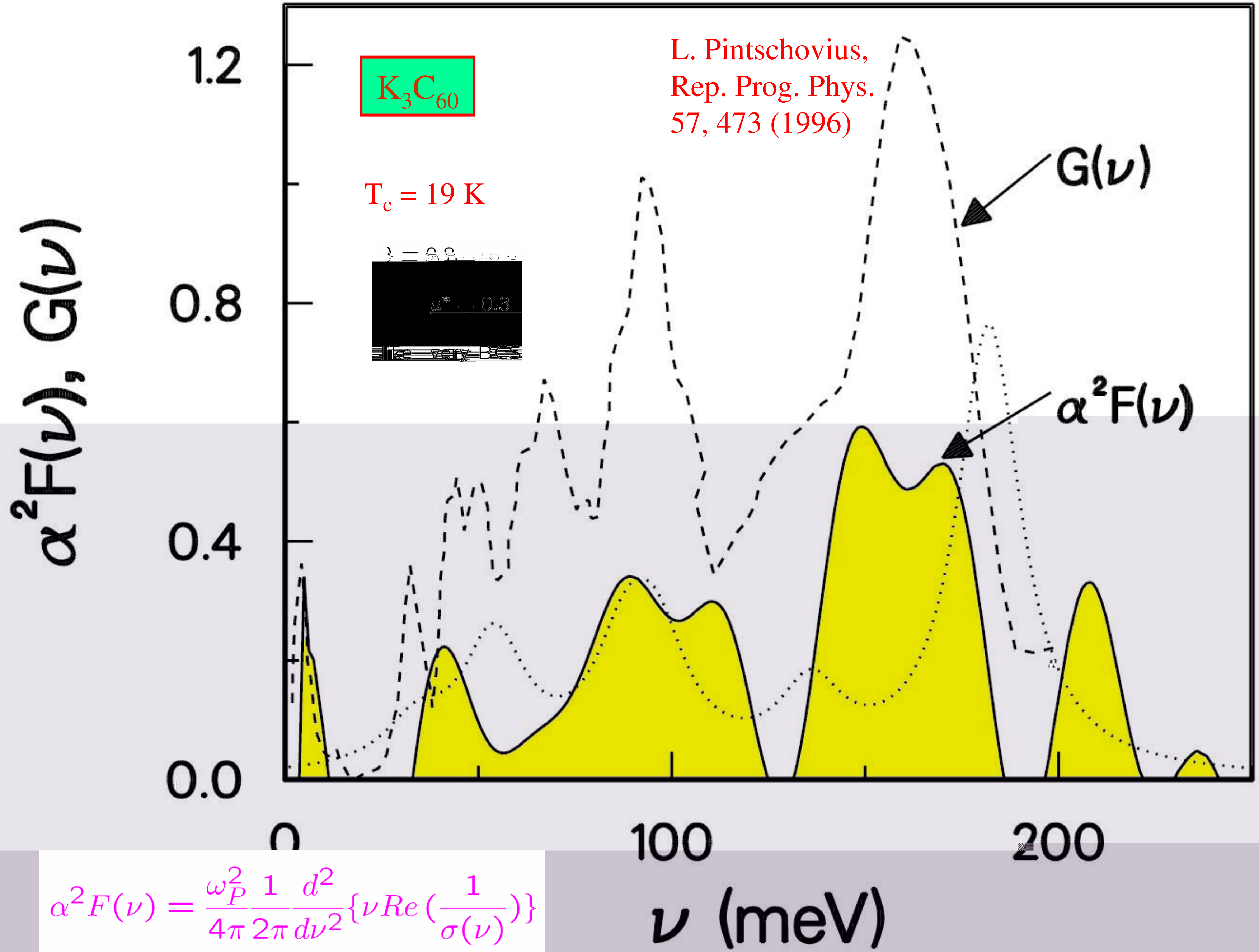
Find:

or

$$W(\omega) = \frac{1}{2\pi}\frac{d^2}{d\omega^2}[\omega\frac{1}{\tau(\omega)}]$$

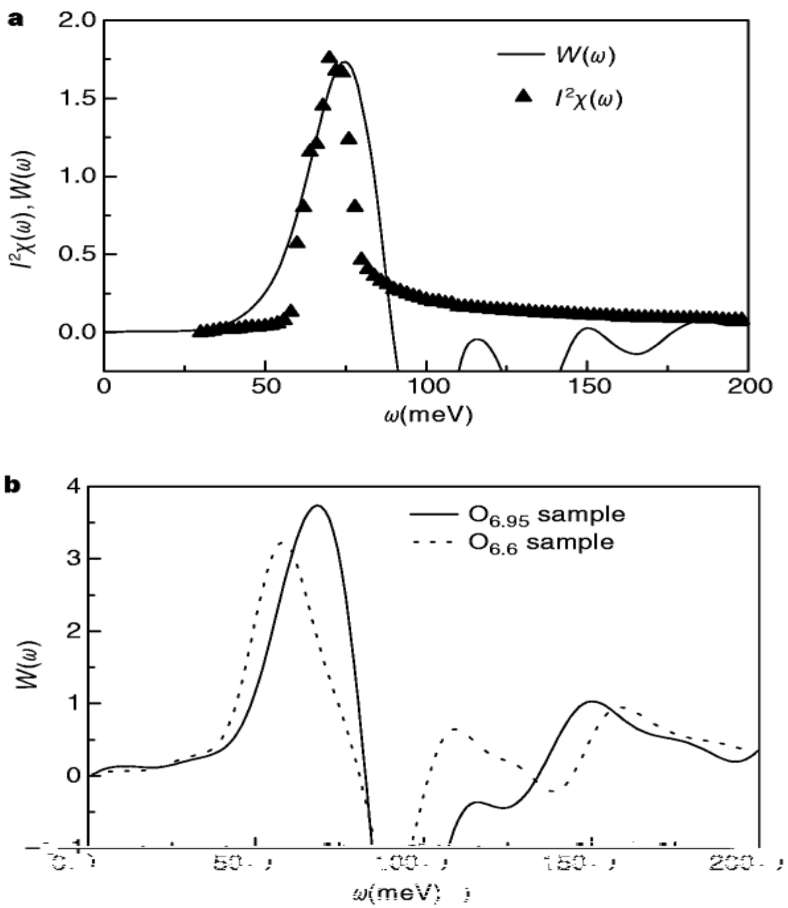
$$\text{(A)} \quad \alpha^2 F(\nu) = \frac{\omega_P^2}{4\pi}\frac{1}{2\pi}\frac{d^2}{d\nu^2}\{\nu Re\,(\frac{1}{\sigma(\nu)})\}$$





$$\alpha^2 F(\nu) = \frac{\omega_P^2}{4\pi}\frac{1}{2\pi}\frac{d^2}{d\nu^2}\{\nu Re\,(\frac{1}{\sigma(\nu)})\}$$

Coupling to 41 meV mode



J.P. Carbotte, E. Schachinger and D.N. Basov, Nature 401, 354(1999)

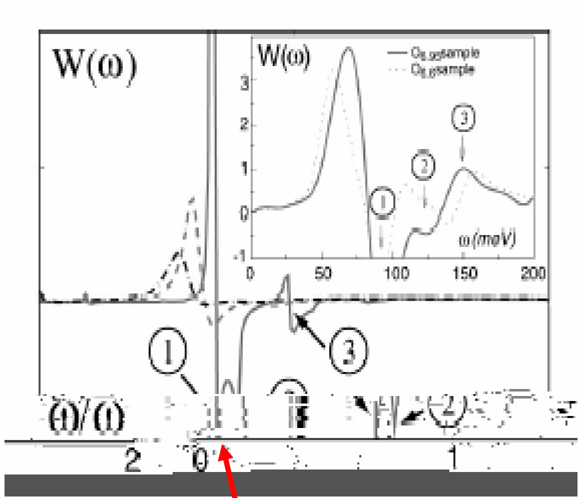
$$W(\omega) = \frac{1}{2\pi}\frac{d^2}{d\omega^2}[\omega\frac{1}{\tau(\omega)}]$$

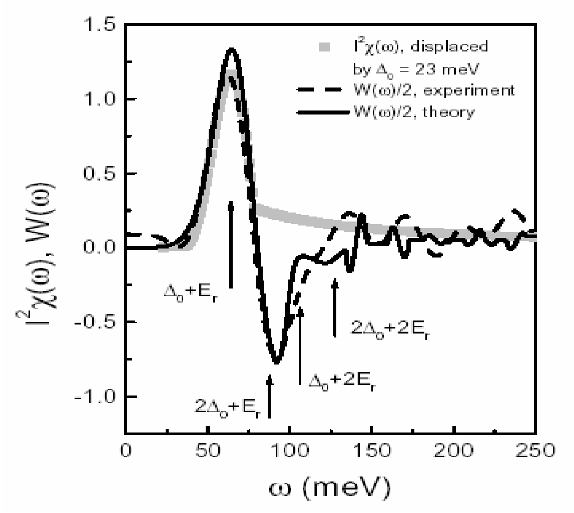
The peak in W(ω): Δ + Ω

Because of d-wave pairing, the peak is shifted by Δ (not 2Δ!)

A. Abanov, et al. Phys. Rev. B 63, 180510 (R) (2001)

Schasinger and Carbotte, PRB 03





$$W(\omega) = \frac{1}{2\pi} \frac{d^2}{d\omega^2} [\omega \frac{1}{\tau(\omega)}]$$

2Δ + Ω

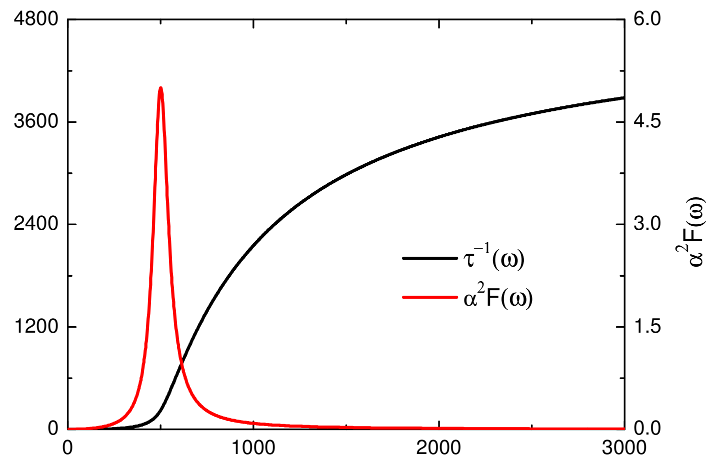
The peak in W(ω): Δ + Ω

Because of d-wave pairing, the peak is shifted by Δ (not 2Δ!)

problem

the bosonic spectral function can not be negative. The negative values are linked with the overshoot in $1/\tau(\omega)$.

A mode is unable to cause a overshoot in $1/\tau$



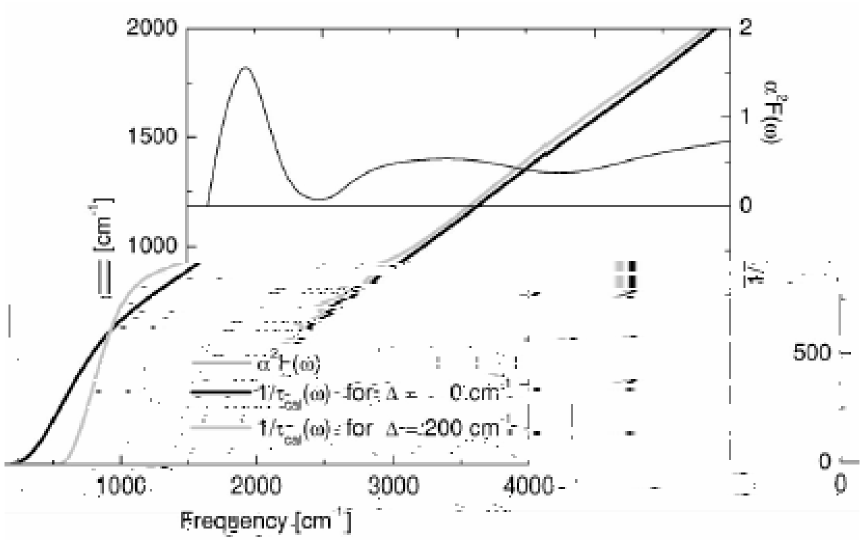
S. V. Dordevic, et al. PRB 71, 104529 (2005)

Allen's formula for the scattering rate in the superconducting state

$$1/\tau(\omega)=\frac{2\pi}{\omega}\int_0^{\omega-2\Delta} d\Omega(\omega-\Omega)\alpha^2F(\Omega)\,E\left[\sqrt{1-\frac{4\Delta^2}{(\omega-\Omega)^2}}\right]$$

P.B.Allen 1971

E(x) is the second kind elliptic integral



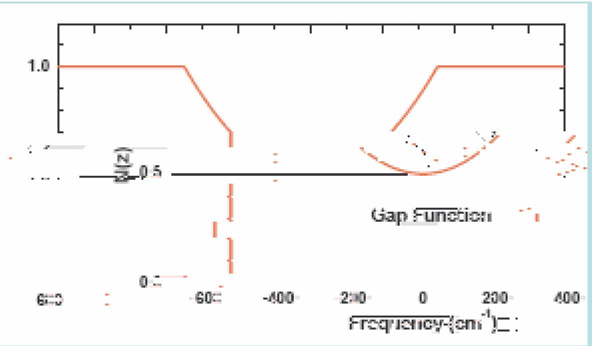
odel spectral function $\alpha^2F(\omega)$ (thin line) is used to
;cattering rate $1/\tau_{cal}(\omega)$ from Eq. (13). For $\Delta=0$ the
attering rate resembles $1/\tau(\omega)$ of underdoped
(Fig. 7). However, for finite values of the gap the
ıttering rate resembles $1/\tau(\omega)$ of optimally doped
: there is an *overshoot* following the suppressed re-

FIG. 9. M
calculate the s
calculated sc
$YBa_2Cu_3O_{6.60}$
calculated sca
$YBa_2Cu_3O_{6.95}$
gion (Fig. 7).

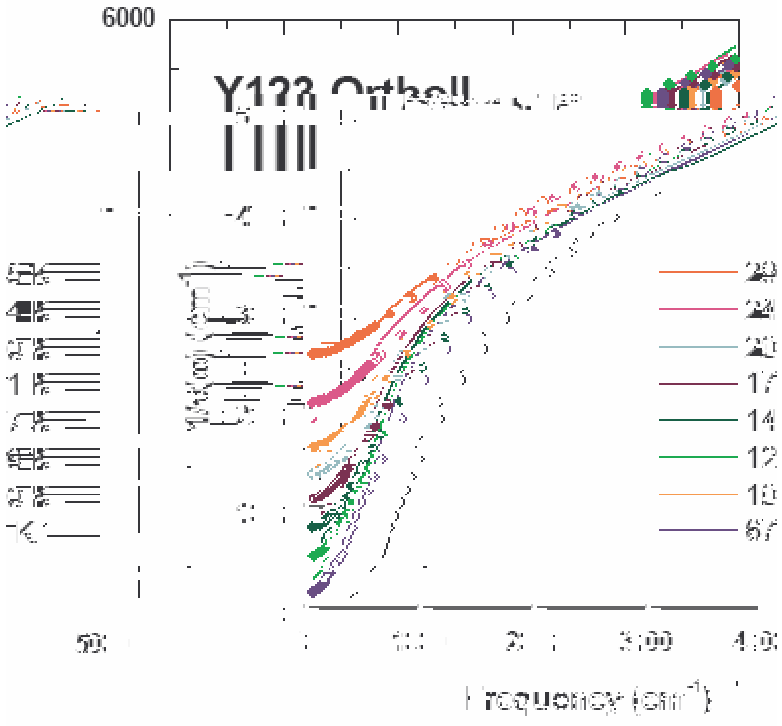
J. Hwang, T. Timusk, et al. cond-mat/0505302

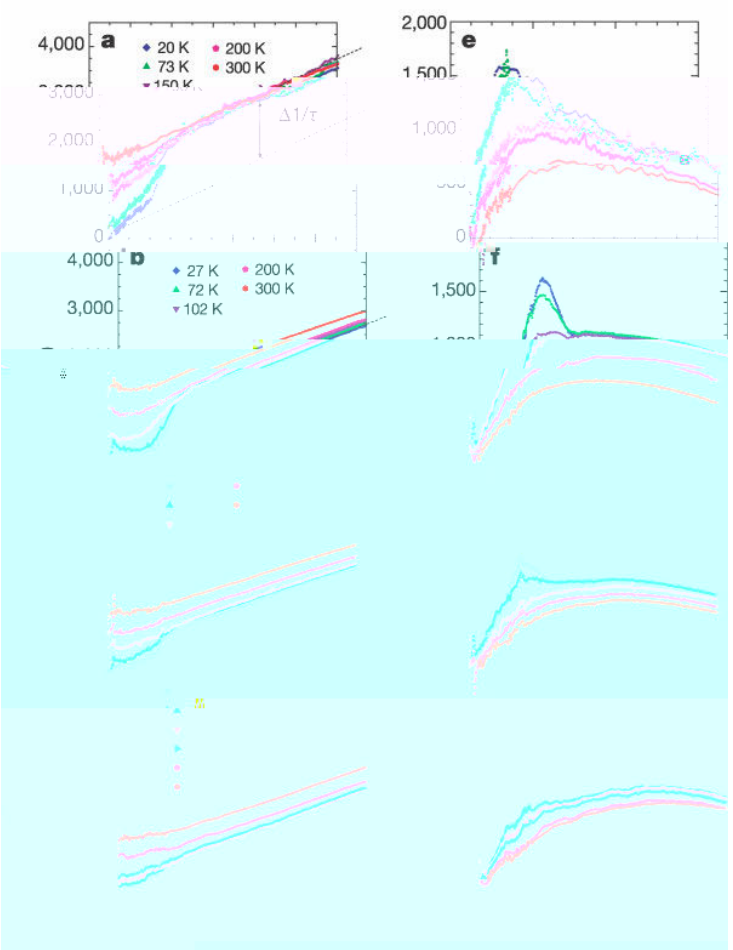
$$\frac{1}{\tau(\omega,T)} = \frac{\pi}{\omega}\int_0^{+\infty} d\Omega\,\alpha^2F(\Omega)\int_{-\infty}^{+\infty} dz[N(z-\Omega)+N(-z+\Omega)]$$
$$[n_B(\Omega)+1-f(z-\Omega)][f(z-\omega)-f(z+\omega)]$$

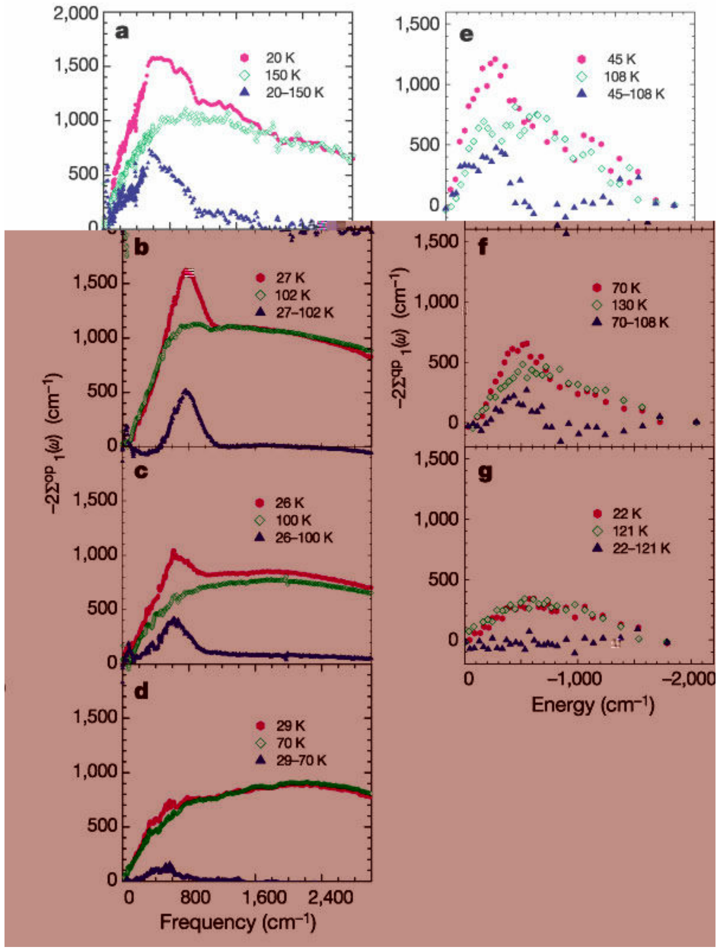
$$N(z) = [N(0)+(1-N(0))\frac{z^2}{\Delta^2}]\theta(\Delta-|z|)+\theta(|z|-\Delta)$$



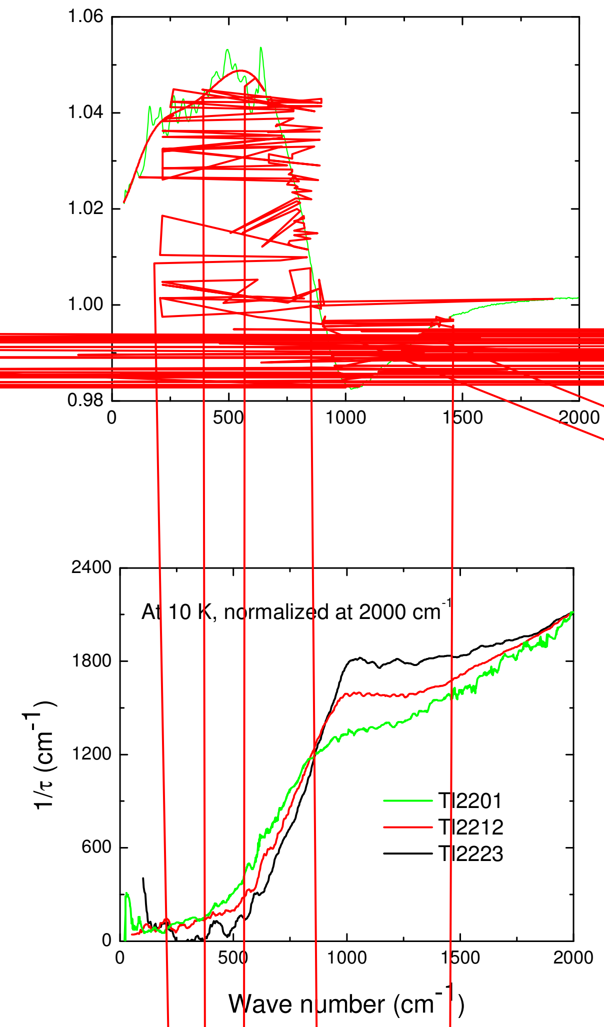
$$\begin{aligned}
\alpha^2F(\Omega) &= \mathrm{PK}(\Omega)+\mathrm{BG}(\Omega)\\
\mathrm{PK}(\Omega) &= \frac{A}{\sqrt{2\pi}(d/2.35)}e^{-(\Omega-\Omega_{PK})^2/[2(d/2.35)^2]}\\
\mathrm{BG}(\Omega) &= \frac{I_s\Omega}{\Omega_0^2+\Omega^2}
\end{aligned}$$

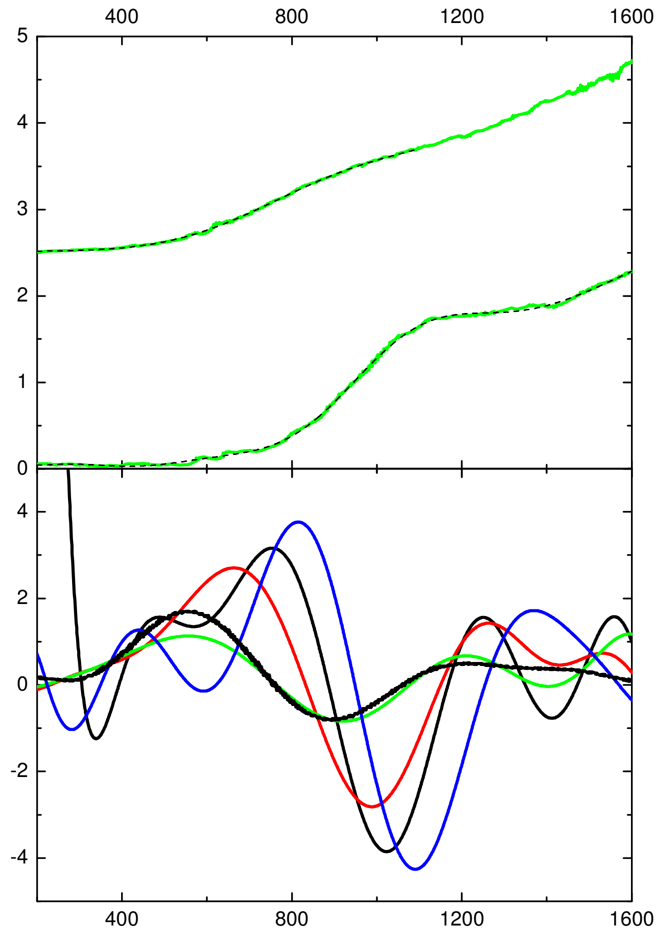






Hwang, Timusk, Gu,
Nature 427, 714 (2004)


1.06
1.04
1.02
1.00
0.98
0
500
1000
1500
2000
2400
1800
1200
600
0
At 10 K, normalized at 2000 cm^{-1}
Tl2201
Tl2212
Tl2223
1/τ (cm^{-1})
Wave number (cm^{-1})



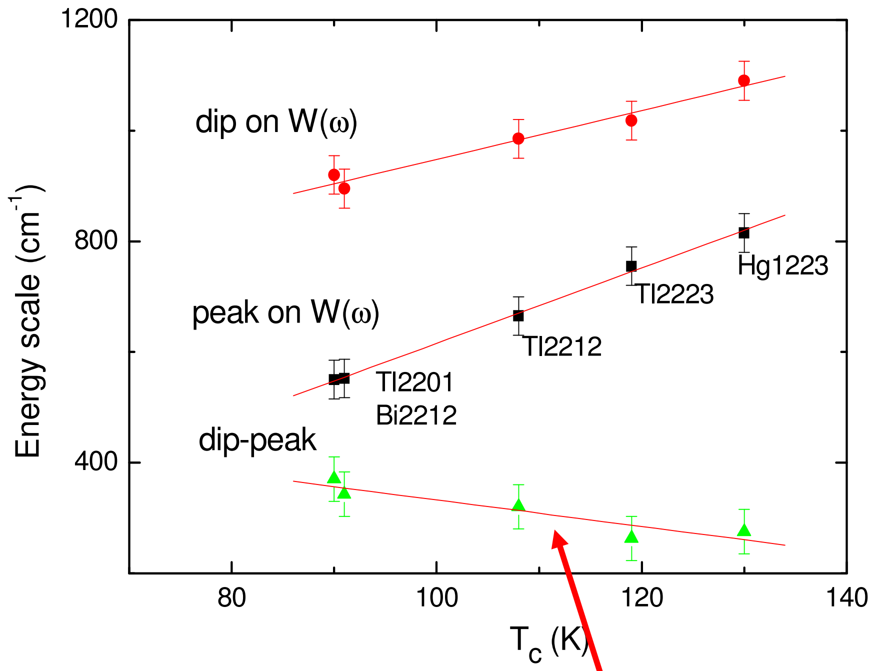
400
800
1200
1600
5
4
3
2
1
0
4
2
0
-2
-4
400
800
1200
1600

$2\Delta+\Omega \propto T_c$

or $T_c=k(2\Delta+\Omega)$

the scaling behavior means that not only the gap amplitude is proportional to Tc, but the boson mode energy is also proportional to Tc.

challenge phonon origin of bosonic mode

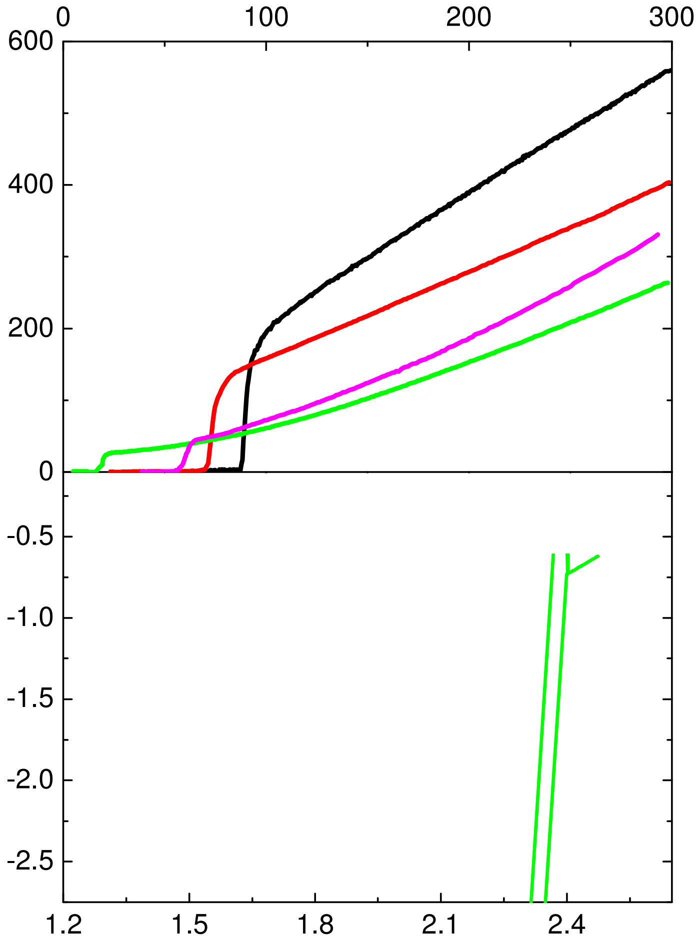


According to Carbotte et al., dip - peak=Δ

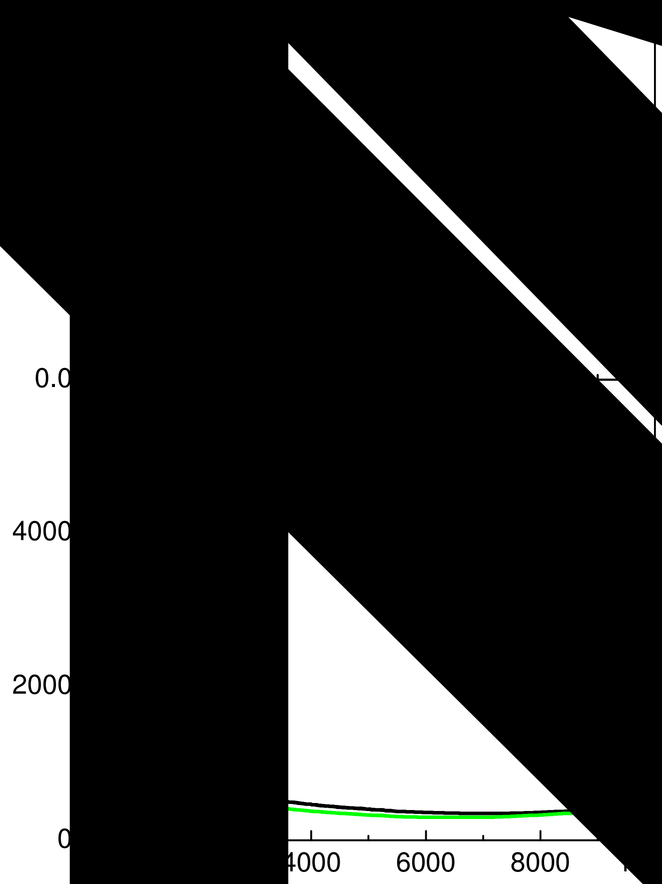
Not reasonable!

challenge the established model

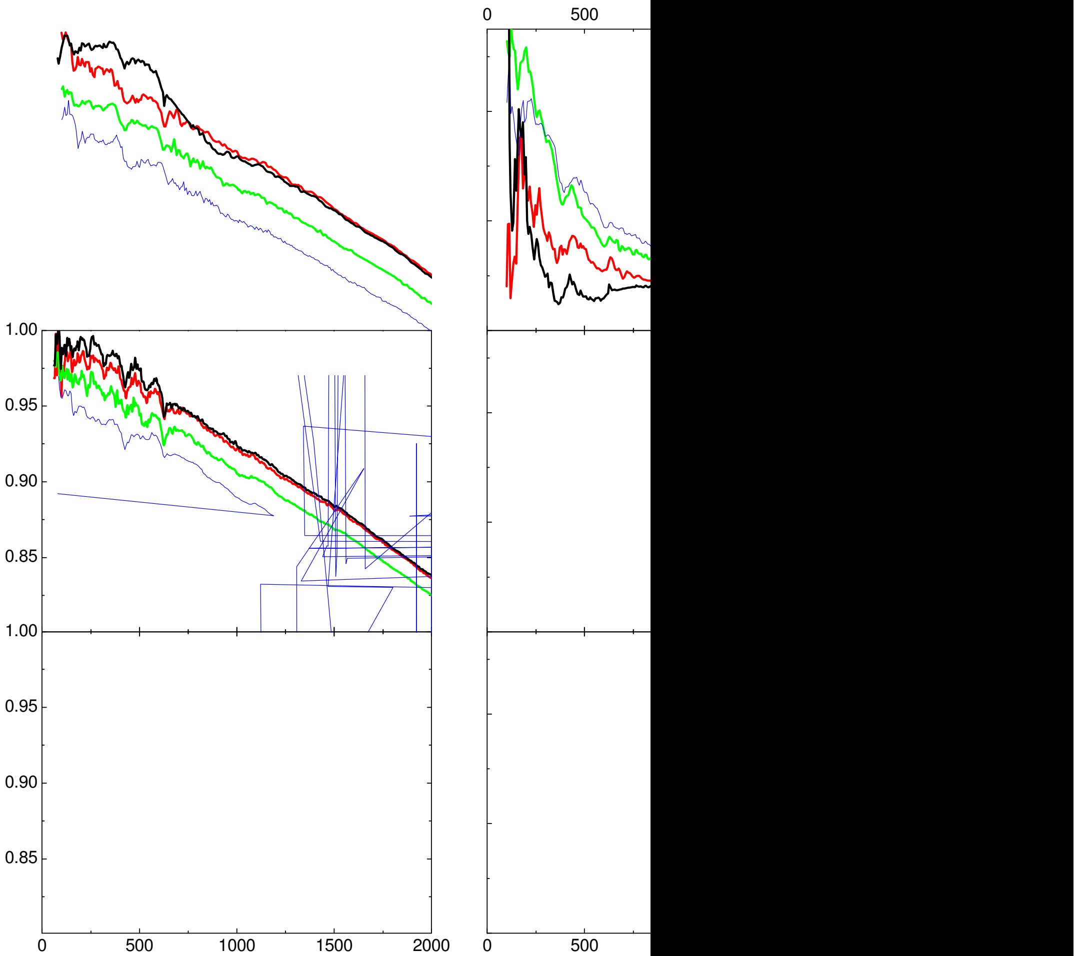
Y. C. Ma and N. L. Wang, PRB 72, 104518 (2005).

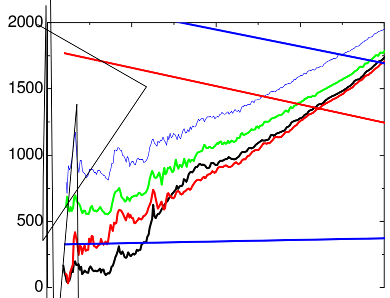


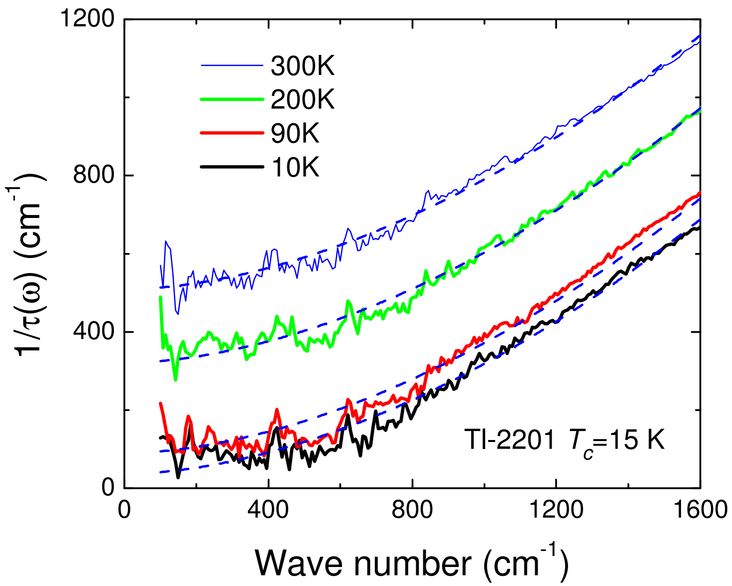
0
100
200
300
600
400
200
0
-0.5
-1.0
-1.5
-2.0
-2.5
1.2
1.5
1.8
2.1
2.4

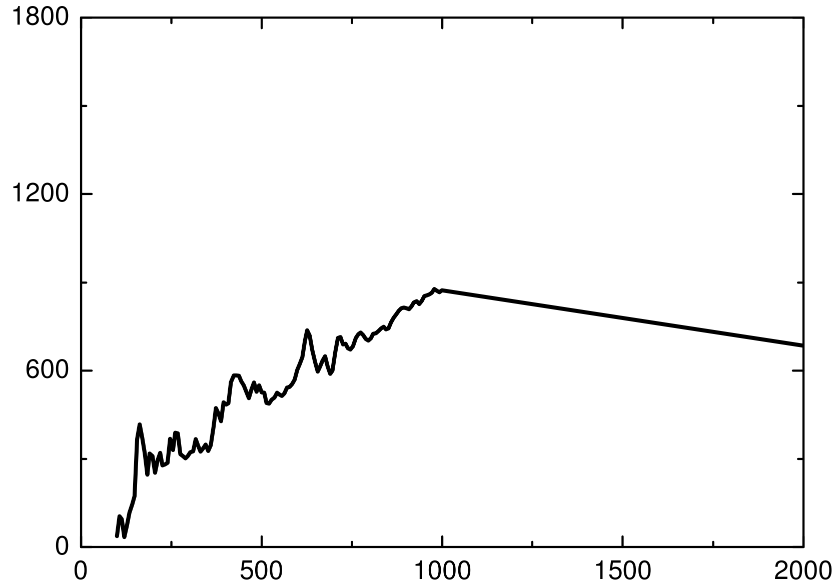


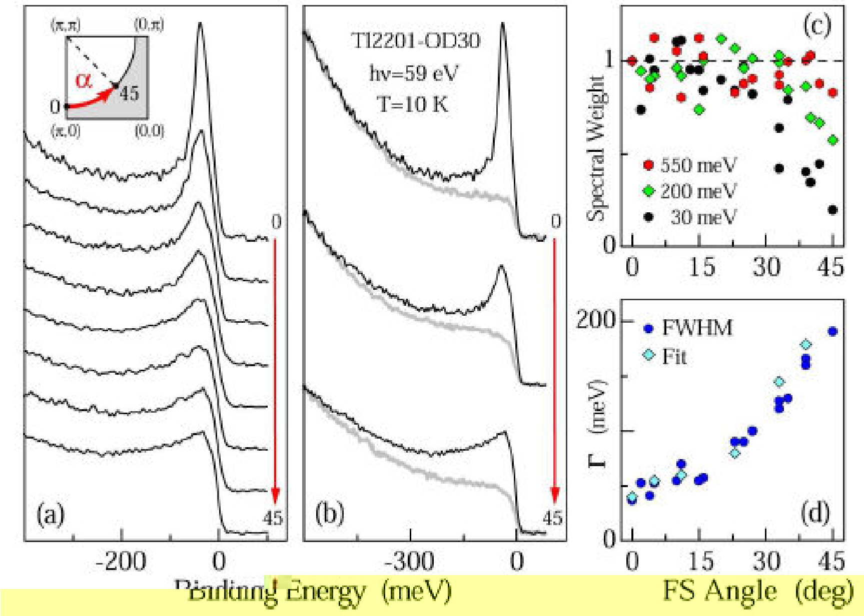
0.0
4000
2000
0
4000
6000
8000


1.00
0.95
0.90
0.85
1.00
0.95
0.90
0.85
0
500
1000
1500
2000
0
500
0
500

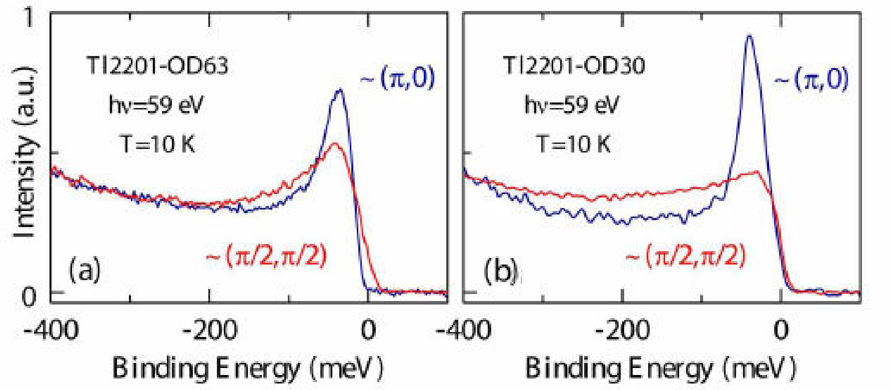

2000
1500
1000
500
0


300K
200K
90K
10K
Tl-2201 T_c=15 K
1/τ(ω) (cm^{-1})
Wave number (cm^{-1})
0
400
800
1200
1600
0
400
800
1200


0
600
1200
1800
0
500
1000
1500
2000



M. Plate et al., PRL 95, 077001 (2005)



Antinodal quasiparticle lifetime strongly increase, and becomes longer than that near nodal region.

nodal quasiparticle peak becomes even broader in heavily overdoped sample than in intermediately overdoped sample

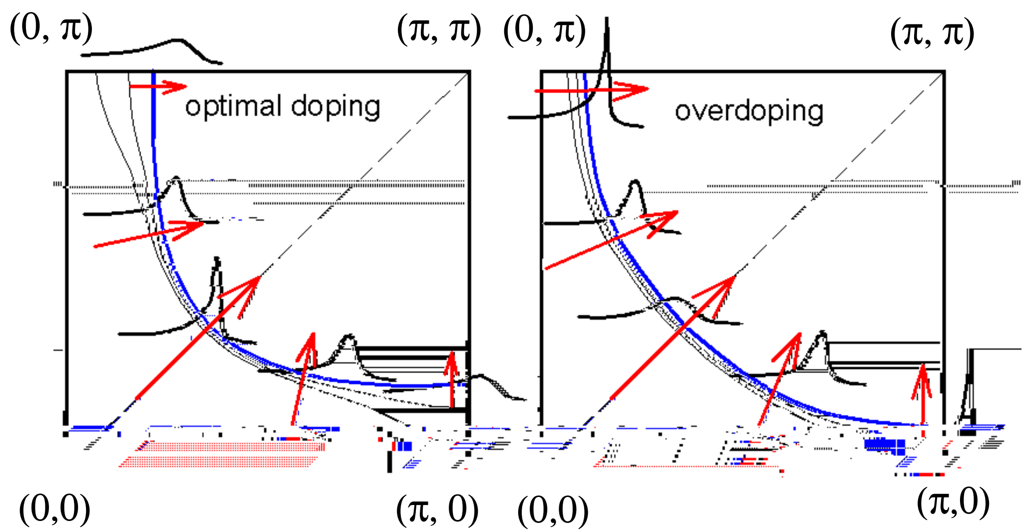
Naively, one can ascribe the reduction of the optical scattering rate to the increase of the lifetime of antinodal quasiparticles

However, the lifetime increase of the antinodal quasiparticles is not the sole reason.

$$\frac{1}{\tau(\omega)} = \frac{\omega_p^2}{4\pi}\mathrm{Re}\left(\frac{1}{\sigma(\omega)}\right)$$

υ_k appears as a weighted factor in the integration.The larger the υ_k and the smaller the τ^{-1}, the larger contribution it has to the transport.

$$\sigma(\omega) = -\frac{e^2}{4\pi^3\hbar}\int \frac{\vec{v}_k\vec{v}_k}{v_k}\frac{dS_F}{1/\tau - i\omega}$$



The change of the Fermi velocity arising from the shape change of Fermi surface with doping, especially near the antinodal region, also contribute to the transport.