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Angle Resolved photoemission spectroscopy.

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Angle resolved photoemission: Interacting electrons

Part III

Papers: S. Hüfner et al., J. Electron Spectroscopy Rel. Phenom. 100 (1999)
A. Damascelli et al., Rev. Modern Phys. (2005)
F. Reinert et al., New J. Phys. 7 (2005)
X.J. Zhou et al., J. Electron Spectroscopy Rel. Phenom. 126 (2002)

Thanks to: A. Damascelli, X. Shen, R. Claessen, Ph. Hofmann and E. Rotemberg from whose I have taken slides and figures

Outline

- Interacting electrons: many-body physics
- Single particle spectral density function $A(k, \omega)$
- The self-energy
- The "kinky" physics: electron-phonon interactions
- 1D System: Luttinger liquid. Spinon and holon dispersion
- Mott-Hubbard insulator
- Fullerenes

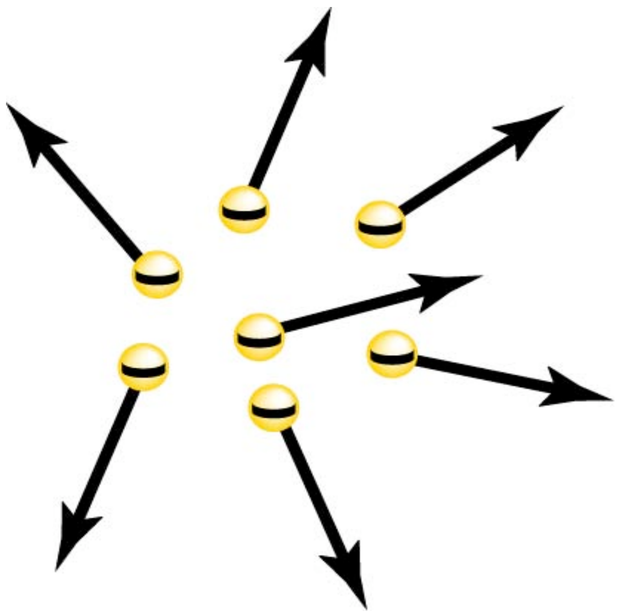
Interaction effects between electrons: “Many-body Physics”

Many body effects are due to the interactions between the electrons and each other, or with excitations inside the crystal :

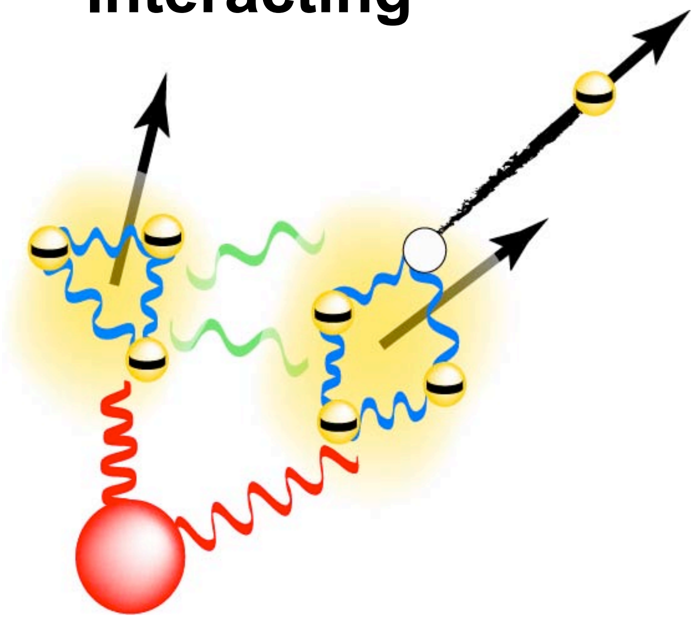
1) A “many-body” problem: intrinsically hard to calculate and understand

2) Responsible for many surprising phenomena:
Superconductivity, Magnetism, Density Waves, ...

Non-Interacting



Interacting



Interacting Electrons: many-body physics

$$\sum_{j=1}^{N} A(r_j)\cdot p_j = A\cdot p$$

$$I(E_{kin}) = \frac{2e^2\pi}{m^2\hbar}\sum_f \left|\langle N,f|A\cdot p|N,i\rangle\right|^2 \rho\left(E_f^N\right)\delta\left(E_f^N - E_i^N - h\nu\right)$$

$$I(E_{kin}) = \sum_f |M_{fi}|^2 \rho\left(E_f^N\right)\delta\left(E_f^N - E_i^N - h\nu\right)$$

The final state relevant for photoemission must contain a free electron with wave vector **k** and energy E_{kin}.

$$I(E_{kin}) = \frac{2e^2\pi}{m^2\hbar}\sum_x \left|\langle k, N-1, x|A\cdot p|N,i\rangle\right|^2 \rho\left(E_x^{N-1}\right)\rho\left(E_{kin}\right)\delta\left(E_{kin} + E_x^{N-1} - E_i^N - h\nu\right)$$

Now the sum is over all the possible final excited states x of the (N-1)-electrons system left behind by the photoelectron. The essential step in simplifying this expression consists in the factorization of the final state wave function $|k, N\text{-}1, x\rangle$ as the product of the photoelectron ϕ_k and the ϕ_x(N-1) electrons wave functions.

In second quantization $|k, N-1, x\rangle \approx \phi_k \phi_x (N-1) = c_k^+ |N-1, x\rangle$

This involves two assumptions:

1) Sudden approx.: The photoelectron decuples immediately from the photohole left behind and carries no information on the relaxation of the (N-1) system

2) We neglect inelastic losses of the photoelectron on its travel inside the crystal

$$I(E_{kin}) = \frac{2e^2\pi}{m^2\hbar} \sum_{j=1}^{N} |M_{k,kj}|^2 \sum_x |\langle N-1, x | c_{kj} | N, i\rangle|^2 \rho(E_x^{N-1}) \rho(E_{kin}) \delta(E_{kin} + E_x^{N-1} - E_i^N - h\nu)$$

where

$$|N, i\rangle = \frac{1}{N} c_{kj}^+ c_{kj} |N, i\rangle \qquad M_{k,kj} = \frac{1}{N} c_k A(r_j) p_j c_{kj}^+ = \frac{1}{N} \langle k | A(r_j) p_j | kj\rangle$$

Transition probability for interacting electrons

$$I(E_{kin}) = \frac{2e^2\pi}{m^2\hbar}\sum_{j=1}^{N}\left|M_{k,kj}\right|^2\sum_{x}\left|\langle N-1,x\left|c_{kj}\right|N,i\rangle\right|^2\rho\left(E_x^{N-1}\right)\rho\left(E_{kin}\right)\delta\left(E_{kin}+E_x^{N-1}-E_i^N-h\nu\right)$$

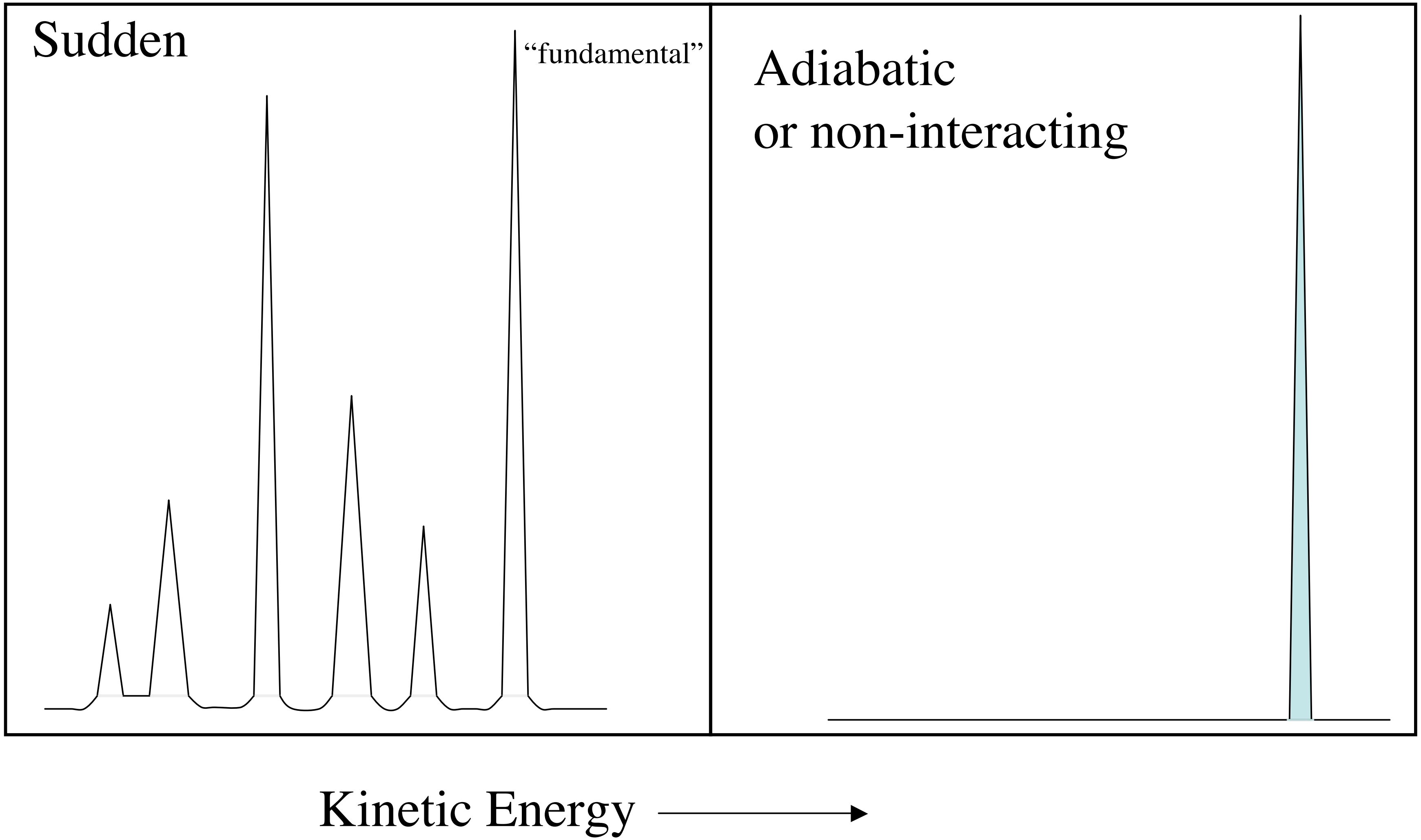
c_{kj} destroys an electron with momentum kj from the initial state $|N,i\rangle$

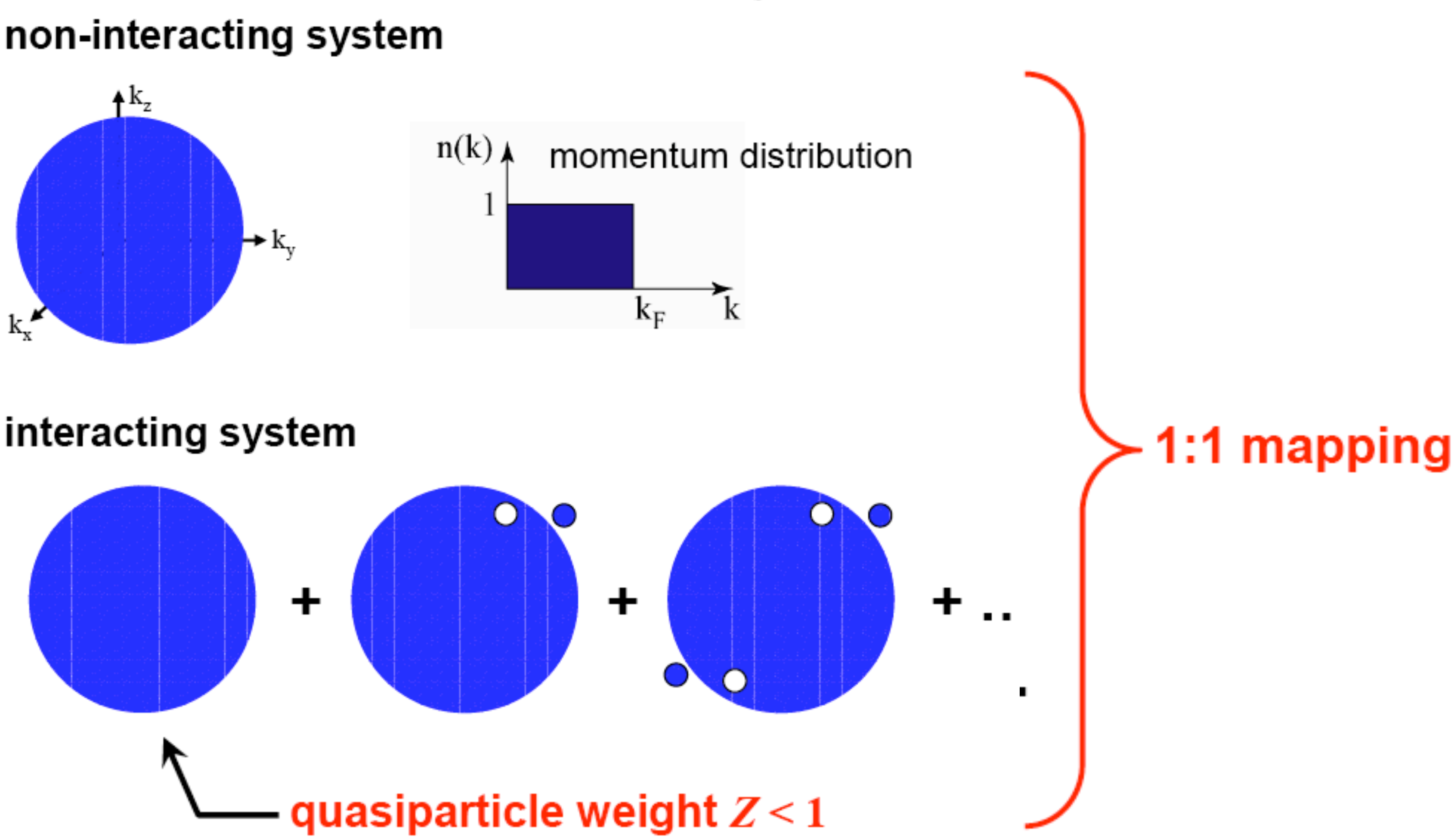
$|N\text{-}1,x\rangle$ is an eigenstate of the (N-1) Hamiltonian,
while the (N-1) wave function $c_{kj}|N,i\rangle$ is not

We can write $E_i^N - E_x^{N-1} = (E_i^N - E_0^{N-1}) - (E_x^{N-1} - E_0^{N-1}) = \varepsilon_0^i - \Delta\varepsilon_x$

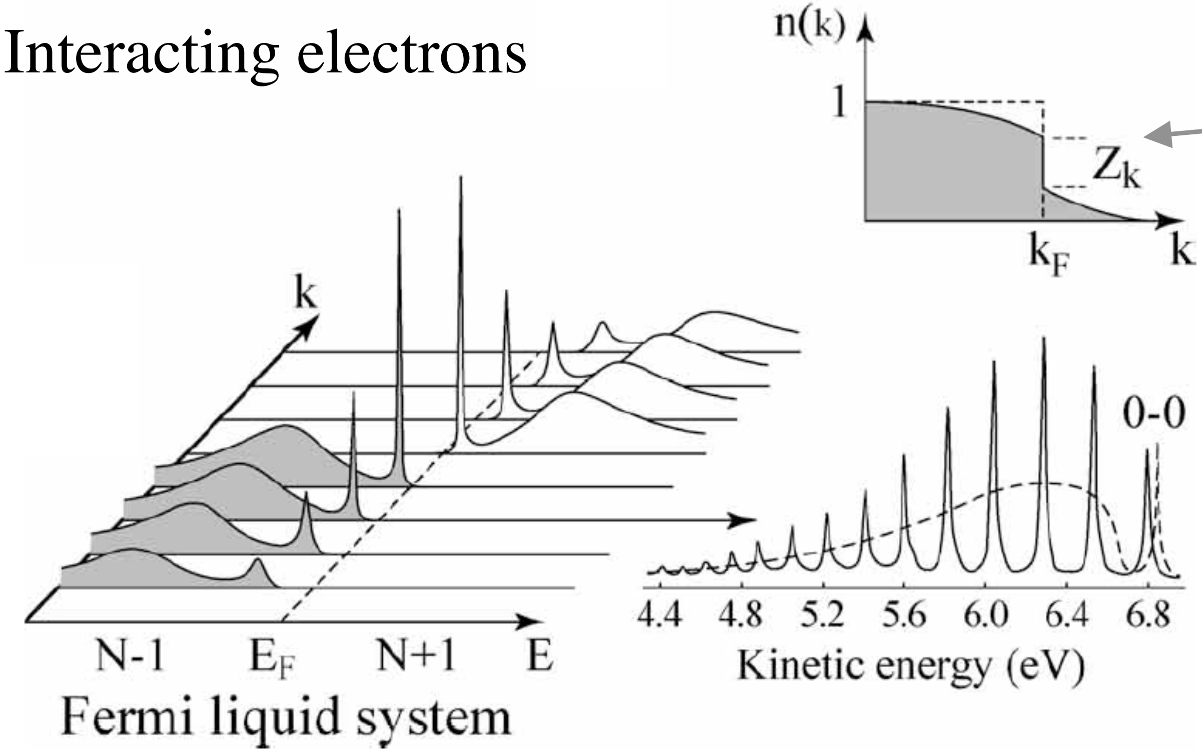
Interpretation: The photon absorption suddenly creates an (N-1)-electron state $c_{kj}|N,i\rangle$ that is not an eigenstate of the (N-1) Hamiltonian (frozen state). The spectrum is the projection of this frozen states over the "fully relaxed" eigenstates $|N\text{-}1,x\rangle$ of the (N-1) Hamiltonian. We call "fundamental peak" (or "elastic peak", or "coherent peak") the transition leaving the (N-1)-system in the ground state $|N\text{-}1,0\rangle$ that correspond to a photoelectron with kinetic energy $E_{kin} = (E_i^N - E_0^{N-1}) + h\nu = \varepsilon_0^i + h\nu$
The spectrum also exhibits peaks at lower kinetic energies by quantities $-\Delta\varepsilon_x$ when the system is left in an excited $|N\text{-}1,x\rangle$ state.

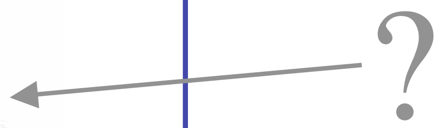
Interacting electrons



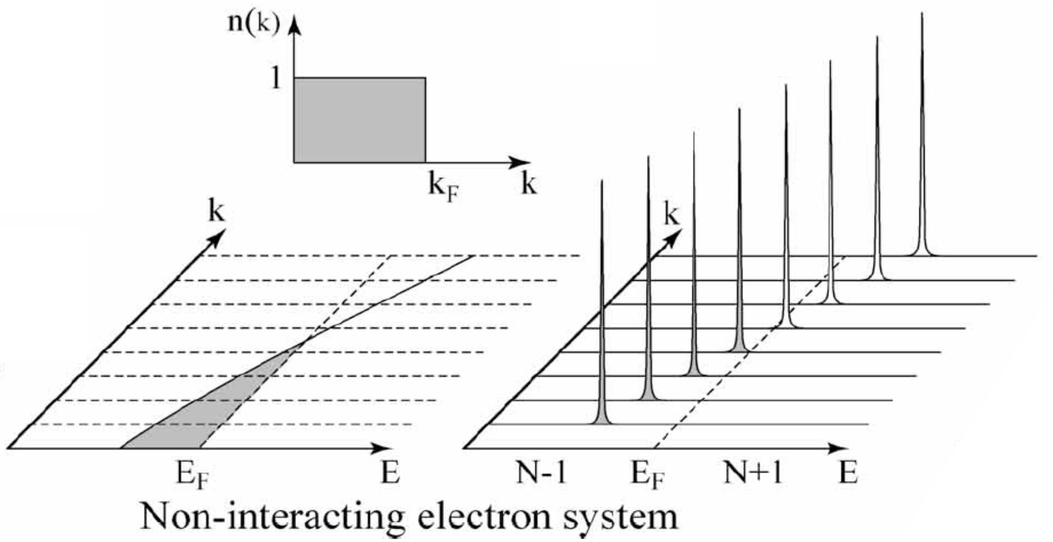

non-interacting system
k_z
k_y
k_x
n(k)
momentum distribution
1
k_F
k
interacting system
+
+
+ . . .
1:1 mapping
quasiparticle weight $Z < 1$

Interacting electrons





Still no information on the lifetime of the states (width of the peaks)



A bit of math and the quasi-particles

It is useful to introduce the one-electron removal Green function formalism:

$$G(kj,\omega j) = \sum_x \frac{\left|\langle N-1,x|c_{kj}|N,i\rangle\right|^2}{\omega j - E_x^{N-1} + E_i^N - i\eta}$$

η can be infinitesimally small

c_{kj} destroys an electron with momentum kj and energy ωj from the initial state $|N,i\rangle$

… and the corresponding spectral density function $A(kj,\omega j)=(1/\pi)\mathrm{Im}G(kj,\omega j)$

In the limit $\eta \to 0$:

$$A(kj,\omega j) = \frac{1}{\pi}\sum_x \left|\langle N-1,x|c_{kj}|N,i\rangle\right|^2 \delta\left(\omega j - E_x^{N-1} + E_i^N\right) = \frac{1}{\pi}\mathrm{Im}\,G(kj,\omega j)$$

Comparing to:

$$I(E_{kin}) = \frac{2e^2\pi}{m^2\hbar}\sum_{j=1}^{N}\left|M_{k,kj}\right|^2 \sum_x \left|\langle N-1,x|c_{kj}|N,i\rangle\right|^2 \rho\left(E_x^{N-1}\right)\rho\left(E_{kin}\right)\delta\left(E_{kin} + E_x^{N-1} - E_i^N - h\nu\right)$$

We have $$I(E_{kin}) = \frac{2e^2\pi^2}{m^2\hbar}\sum_{j=1}^{N}\left|M_{k,kj}\right|^2 A(kj,\omega j)$$

Where $A(kj,\omega j) \neq 0$ only when $\omega j = h\nu - E_{kin} = \left|E_i^N - E_x^{N-1}\right|$

Rewriting in terms of the electron binding energy ω, considering the momentum conservation and including the Fermi-Dirac distribution:

$$I(k,\omega) = I_{if}(k,\mathbf{A},\nu)\,A(k,\,\omega)\;\mathrm{fd}(\omega,\,T)$$

Proportional to Matrix elements

Spectral function

Fermi-Dirac

This is the most important result: in the sudden approx. the photoemission spectrum is proportional to the single particle spectral density function *A(k, ω)*

This relationship has been obtained in the limit η→0 (η is the peak width), i.e. the peaks are Dirac's δ. It can be extended to "real systems" where the width Γ is finite.

$$G(k,\omega) = \sum_x \frac{\left|\langle N-1,x|c_k|N,i\rangle\right|^2}{\omega - E_x^{N-1} + E_i^N - i\Gamma}$$

$$A(k,\omega) = \frac{1}{\pi}\operatorname{Im} G(k,\omega) = \frac{\Gamma}{\pi}\sum_x \frac{\left|\langle N-1,x|c_k|N,i\rangle\right|^2}{(\omega - E_x^{N-1} + E_i^N)^2 + \Gamma^2}$$

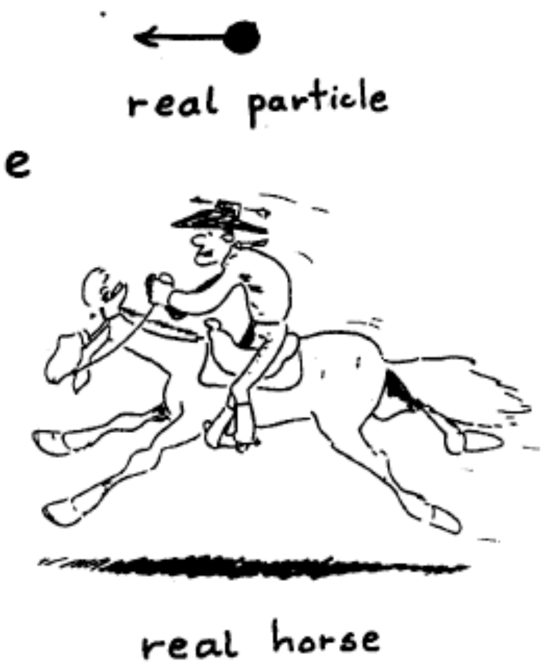
Quasi-particle: when one hole is added adiabatically forming an (N-1)-electron system the coulomb interaction is screened by the formation of an electron cloud around the hole. At equilibrium, the hole+the screening cloud is a quasi-particle.
An eigenstate $|N-1, x\rangle$ of the (N-1)-electron system can be obtained by adding a quasi-particle to the N-electron system (quasi-particle state).

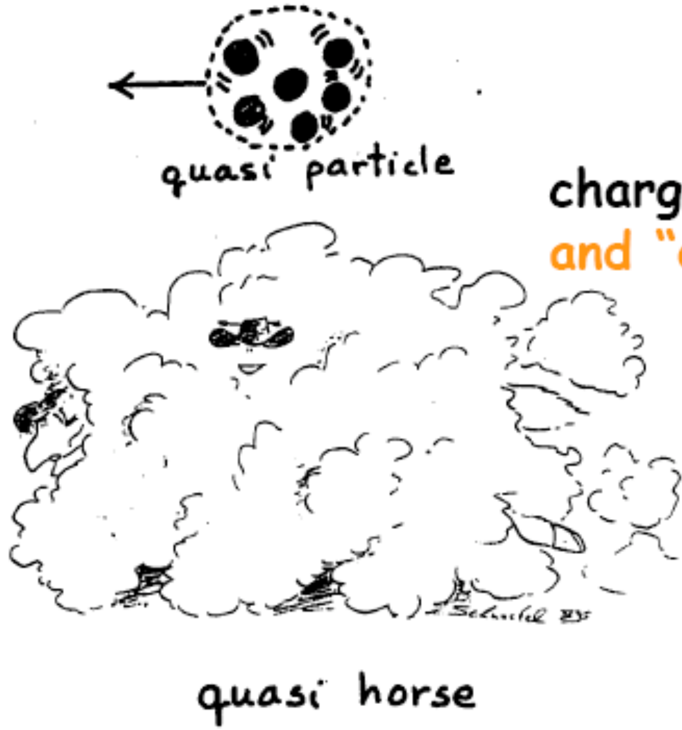
If instead we suddenly simply add a bare hole of momentum k (or we remove an electron of momentum k) we obtain the state $c_k|N,i\rangle$, that in general is not an eigenstate of the (N-1)-system, but it will have a finite overlap with the corresponding quasi-particle state.

The spectral density function A(k, ω) gives the probability that the original system plus the bare hole will be found in an exact eigenstate of the (N-1)-system

non-interacting electrons	**interacting** electrons

charge -e
spin 1/2





charge, spin
and "dressing"

band structure

$\varepsilon_0(\mathbf{k})$

quasiparticle band structure

$$\varepsilon(\mathbf{k}) = \varepsilon_0(\mathbf{k}) + \Sigma(\mathbf{k}, \varepsilon)$$

self-energy

$$G(k,\omega) = \overbrace{\frac{|\langle N-1,i|c_k|N,i\rangle|^2}{\omega - \varepsilon(k) - i\Gamma}}^{Z_k} + \sum_{x\neq i} \frac{|\langle N-1,x|c_k|N,i\rangle|^2}{\omega - \varepsilon_x(k) - i\Gamma} = G_{coh}(k,\omega) + G_{incoh}(k,\omega)$$

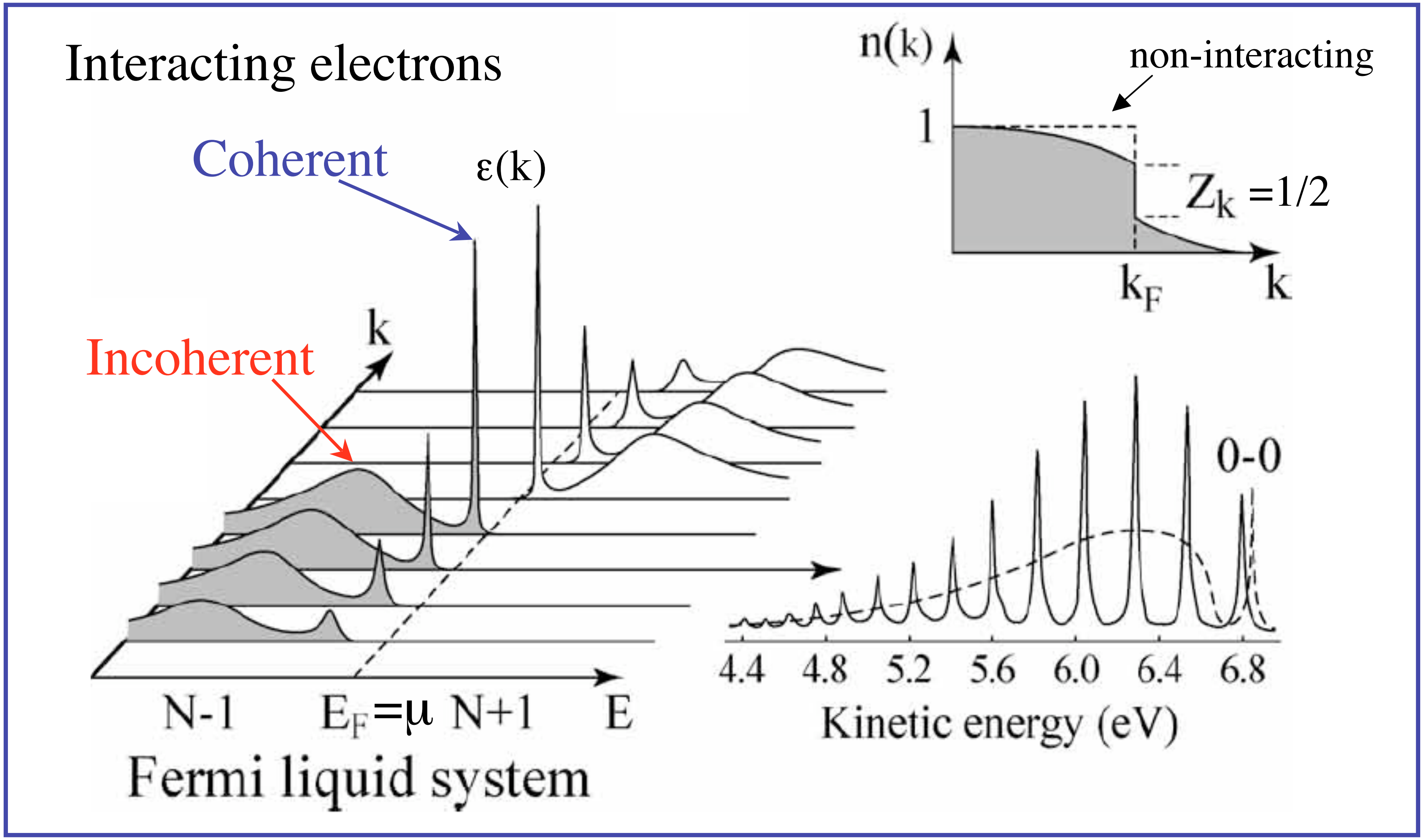
$$A(k,\omega) = -\frac{1}{\pi}\,\mathrm{Im}\,G(k,\omega) = \frac{\Gamma}{\pi}\frac{|\langle N-1,i|c_k|N,i\rangle|^2}{(\omega-\varepsilon(k))^2+\Gamma^2} + \frac{\Gamma}{\pi}\sum_{x\neq i}\frac{|\langle N-1,x|c_k|N,i\rangle|^2}{(\omega-\varepsilon_x(k))^2+\Gamma^2}$$

$$= A(k,\omega)_{coh.} + A(k,\omega)_{incoh}$$

Where $\varepsilon(k)$ is the quasi-particle energy referred to the Fermi level $\mu=0$

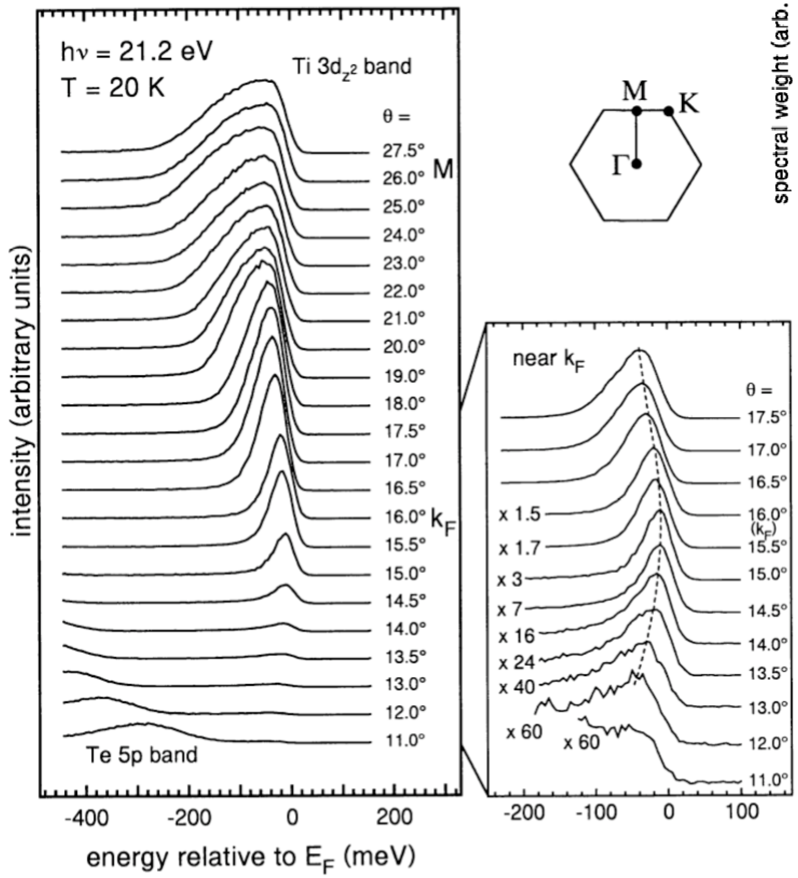
As $\varepsilon(k) \rightarrow \mu$, $\Gamma \propto (\varepsilon - \mu)^2 \rightarrow 0$

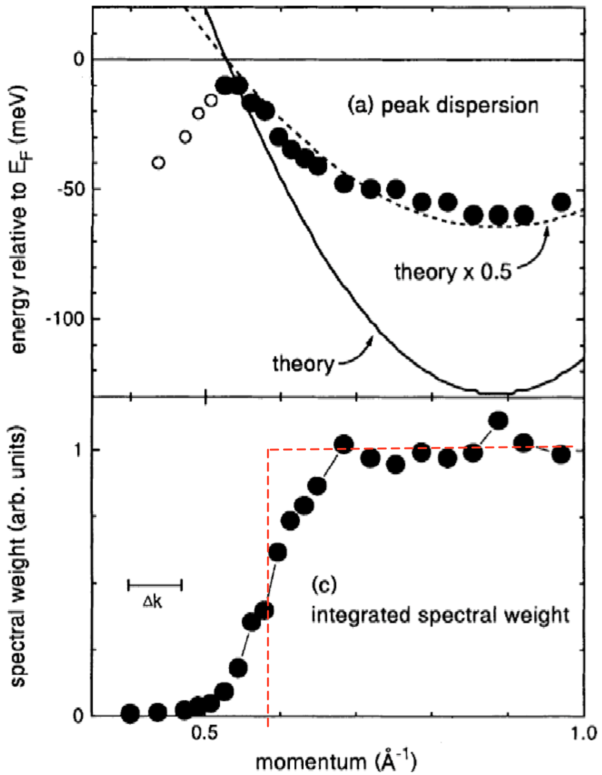
The quasi-particle is well-defined only at (or very close to) the Fermi level, where its lifetime $1/\Gamma \rightarrow \infty$

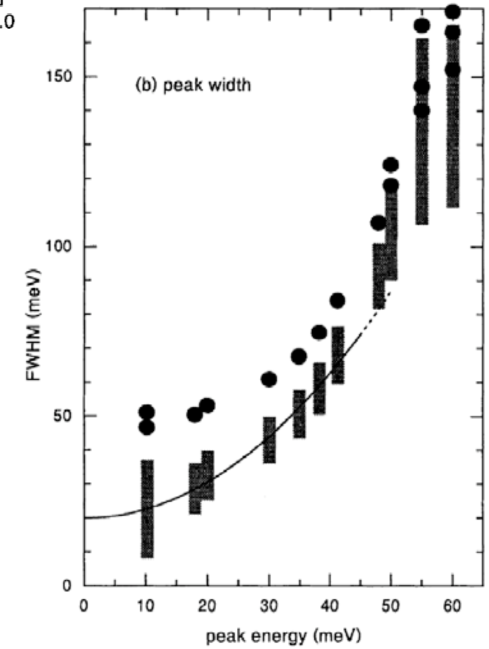


$$A(k,\omega)=\frac{\Gamma}{\pi}\frac{Z_k}{(\omega-\varepsilon(k))^2+\Gamma^2}+\frac{\Gamma}{\pi}\sum_{x\neq i}\frac{\left|\langle N-1,x|c_k|N,i\rangle\right|^2}{(\omega-\varepsilon_x(k))^2+\Gamma^2}=A(k,\omega)_{coh.}+A(k,\omega)_{incoh}$$

Example: $TiTe_2$







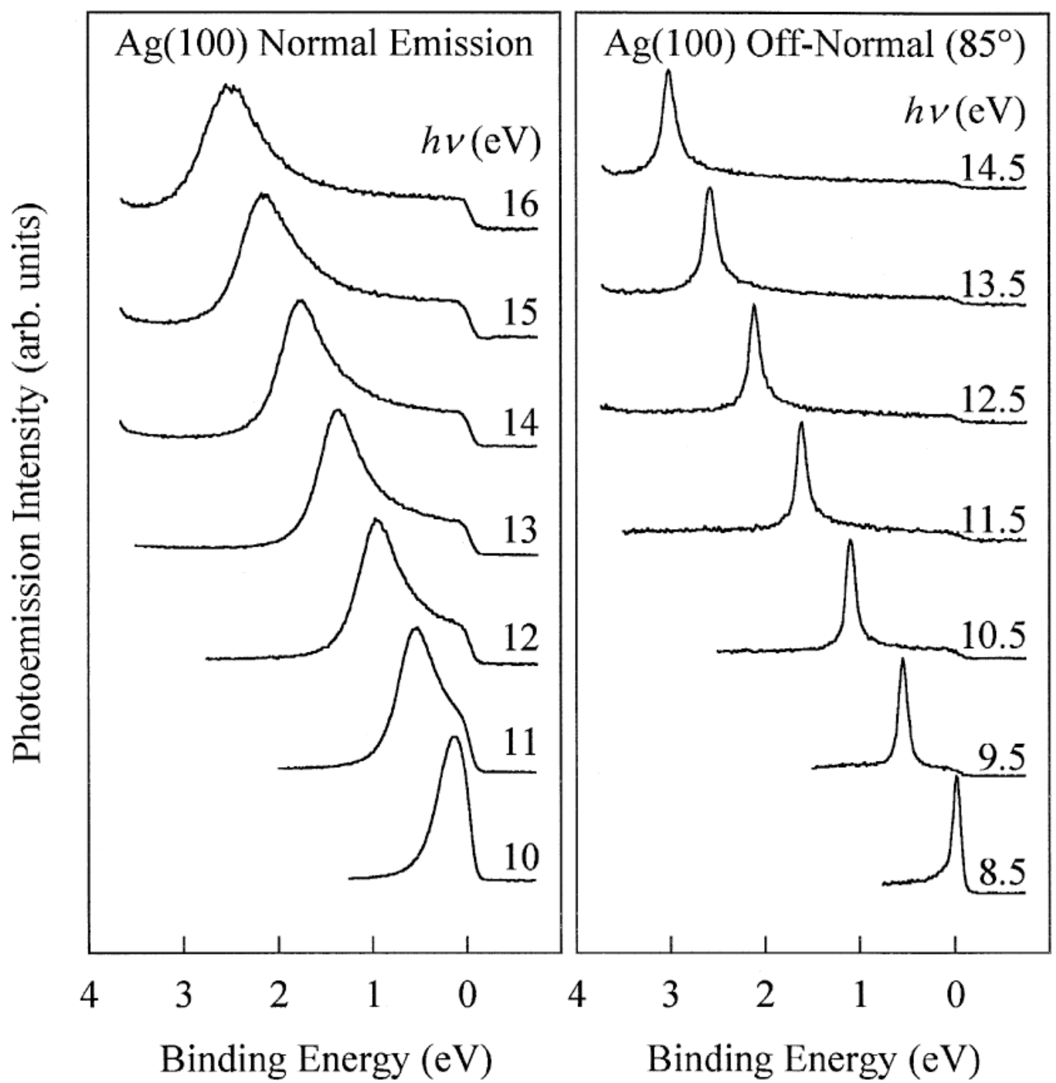
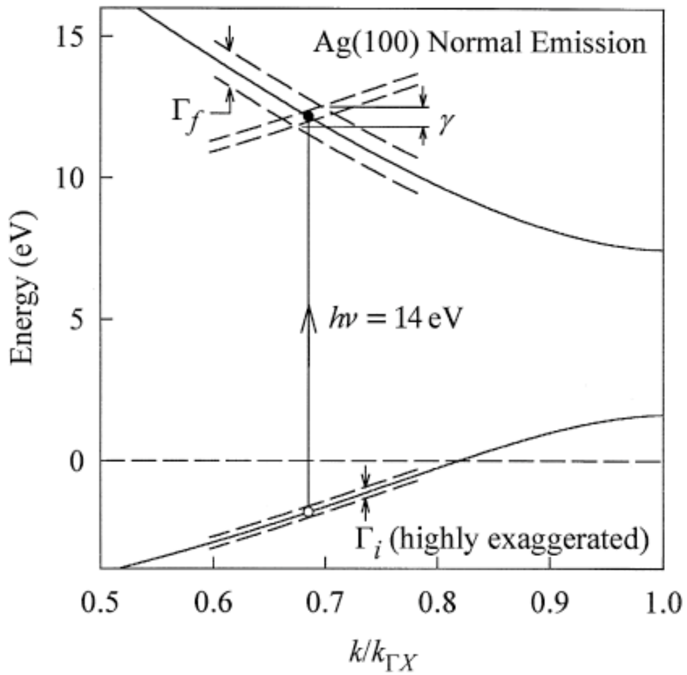


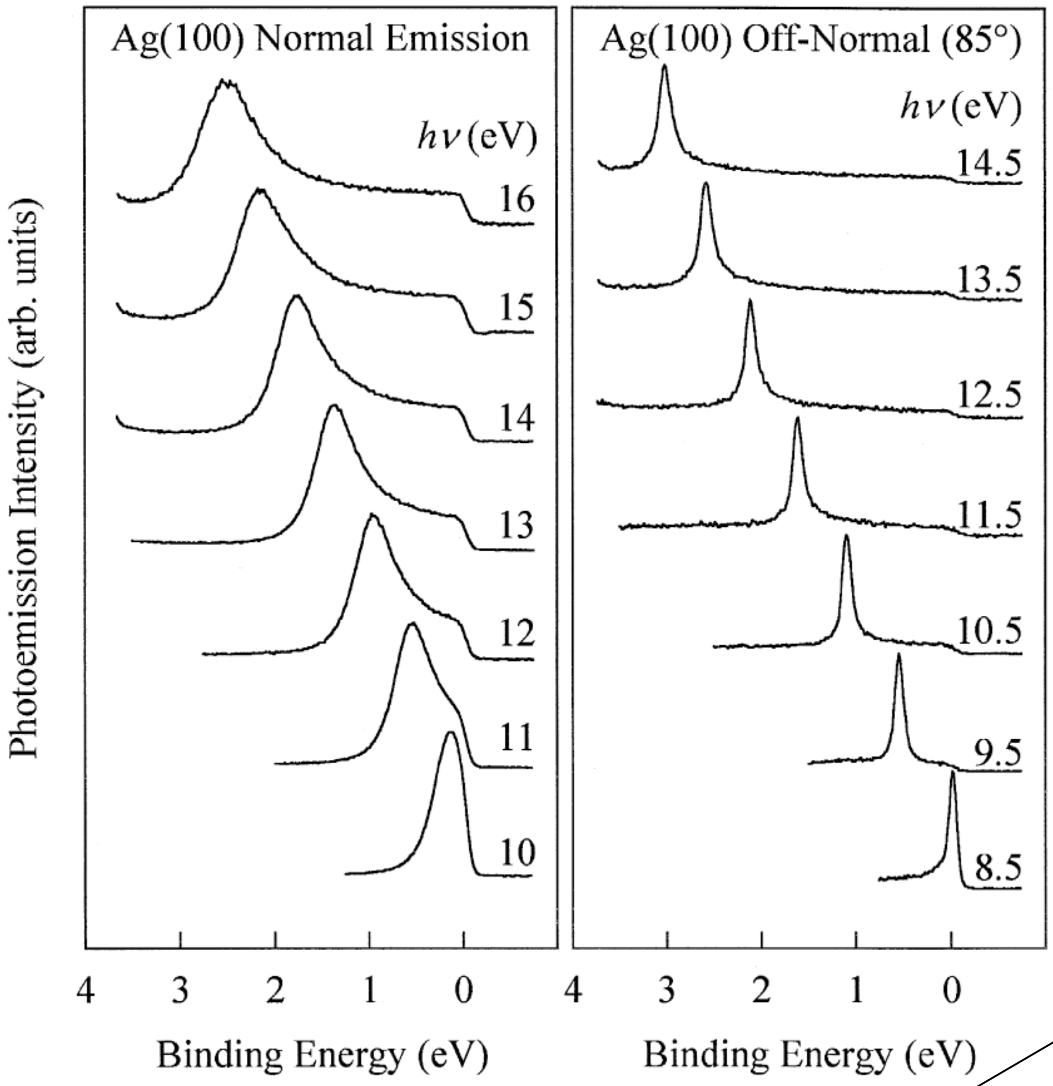
Fig. 1. Angle resolved photoemission spectra taken with a normal emission geometry (left panel) and a grazing emission geometry (right panel). The photon energies are indicated in the figure.

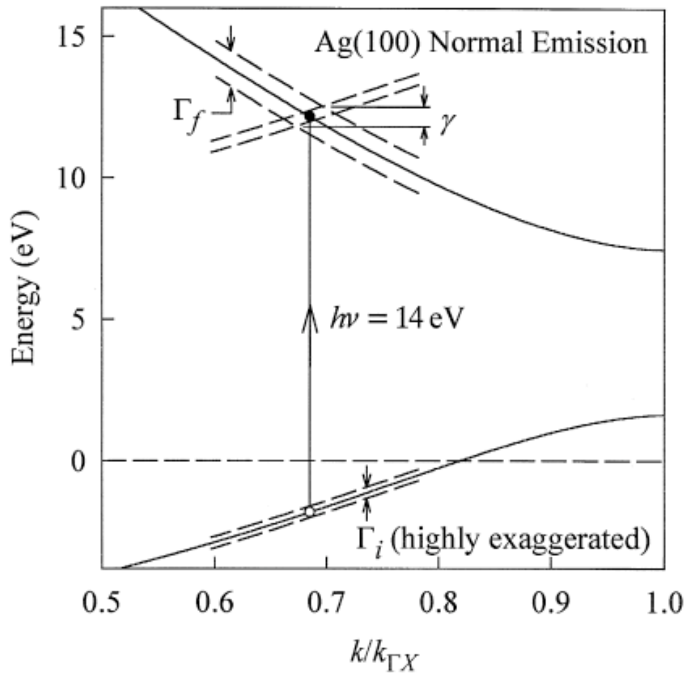


The total width γ (overlapping region) depends on the slopes, or group velocities.

γ is dominated by Γ_f (much larger than Γ_i).

Difficult to obtain the true quasiparticle inverse lifetime.

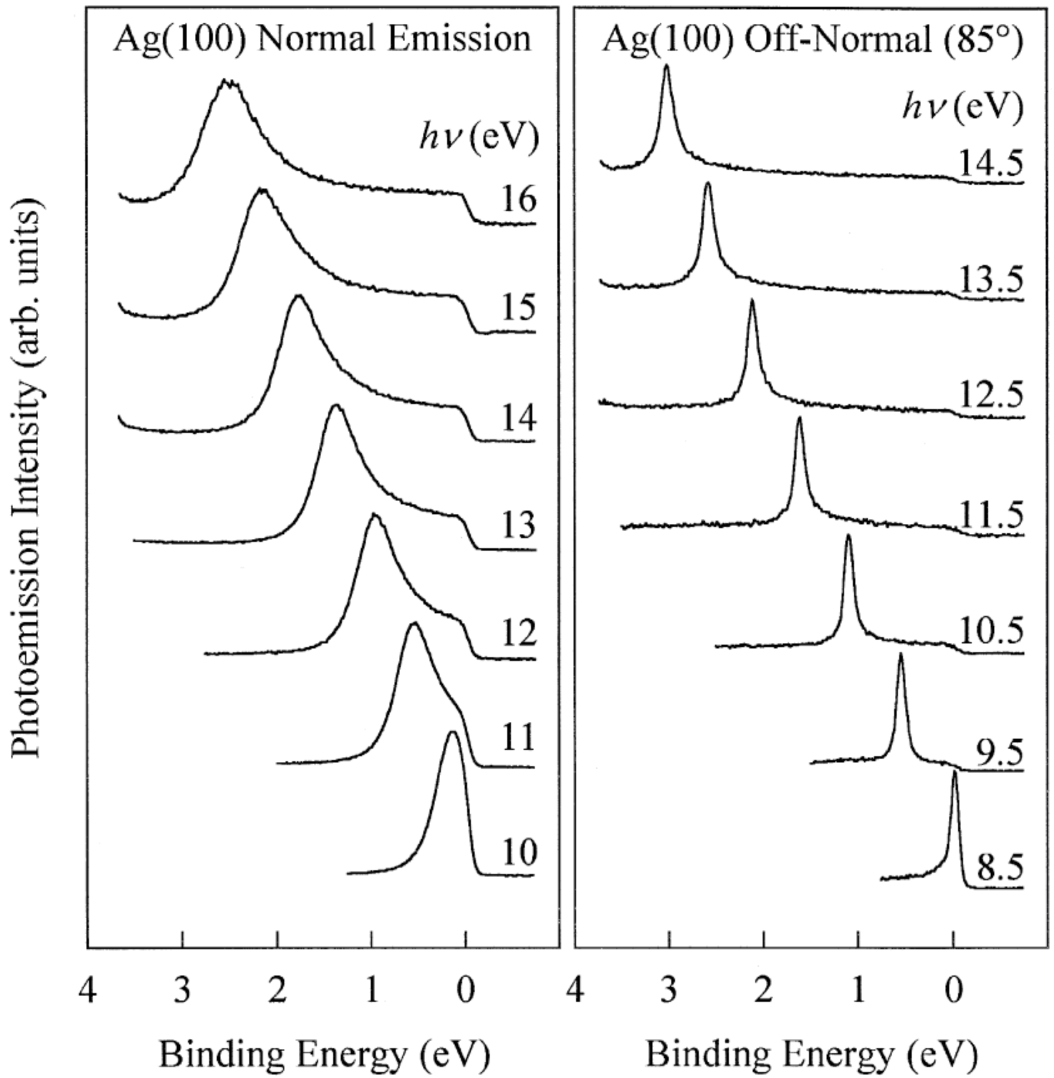


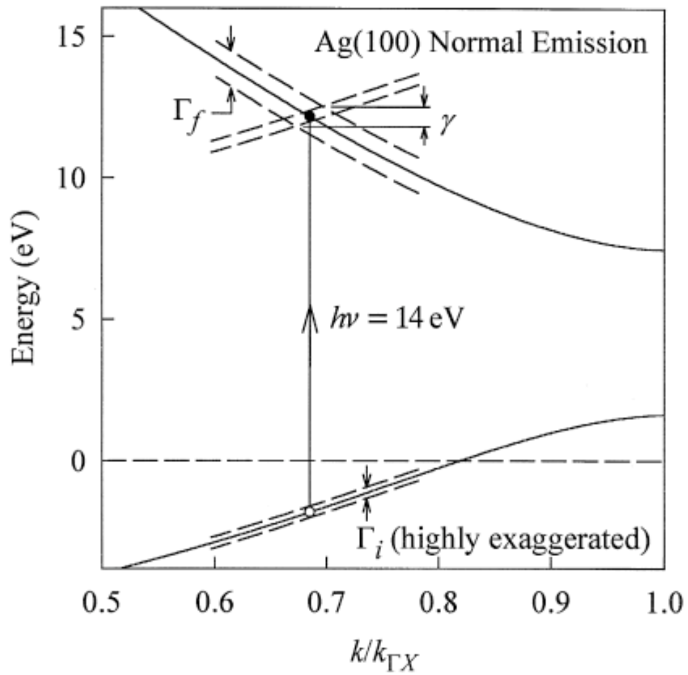


$$\gamma = \frac{\dfrac{\Gamma_{\mathrm{i}}}{|v_{\mathrm{i}\perp}|} + \dfrac{\Gamma_{\mathrm{f}}}{|v_{\mathrm{f}\perp}|}}{\left|\dfrac{1}{v_{\mathrm{i}\perp}} - \dfrac{1}{v_{\mathrm{f}\perp}}\right|}$$

Normal emission

Interesting when $v_{\mathrm{i}}=v_{\mathrm{f}}$ and $v_{\mathrm{i}}/v_{\mathrm{f}}=0$





When $v_i/v_f=0$ $\gamma = C\cdot\Gamma_i$

$$C = \left|1 - \frac{m v_{i\|}\sin^2\theta}{\hbar k_\|}\right|^{-1}$$

Grazing emission →

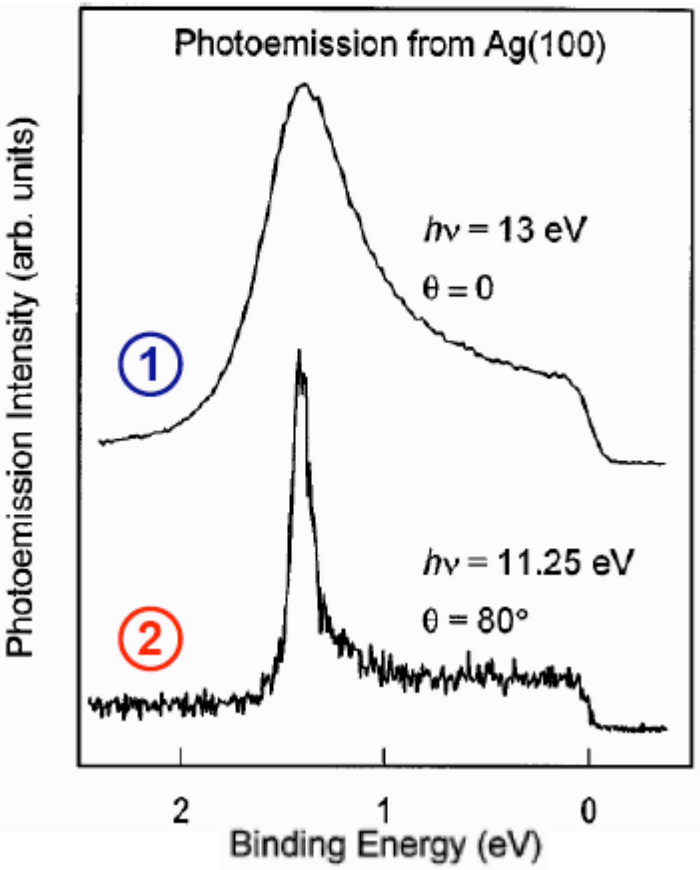
$$\gamma = \frac{\dfrac{\Gamma_i}{|v_{i\perp}|} + \dfrac{\Gamma_f}{|v_{f\perp}|}}{\left|\dfrac{1}{v_{i\perp}}\left(1 - \dfrac{m v_{i\|}\sin^2\theta}{\hbar k_\|}\right) - \dfrac{1}{v_{f\perp}}\left(1 - \dfrac{m v_{f\|}\sin^2\theta}{\hbar k_\|}\right)\right|}$$

ARPES: FWHM and Inverse Lifetime

FWHM of an ARPES peak

$$\Gamma = \frac{\frac{\Gamma_i}{|v_{i\perp}|} + \frac{\Gamma_f}{|v_{f\perp}|}}{\left| \frac{1}{v_{i\perp}} \left[1 - \frac{m v_{i\|} \sin^2 \vartheta}{\hbar k_\|} \right] - \frac{1}{v_{f\perp}} \left[1 - \frac{m v_{f\|} \sin^2 \vartheta}{\hbar k_\|} \right] \right|}$$

Hansen *et al.*, PRL **80**, 1766 (1998)



① if $E_i \simeq E_F$

→ $\Gamma_i \longrightarrow 0$ → $\boxed{\Gamma \propto \Gamma_f}$

② if $|v_{i\perp}| \simeq 0$

→ $$\Gamma = \frac{\Gamma_i}{\left| 1 - \frac{m v_{i\|} \sin^2 \vartheta}{\hbar k_\|} \right|} \equiv C\,\Gamma_i$$

if $v_{i\|} < 0$, large; θ large; $k_\|$ small

→ $C < 1$, and $\boxed{\Gamma < \Gamma_i}$

The self-energy

It is useful to express the effects of the electron interactions in terms of the "electron self energy" defined as:

$$\Sigma(k,\omega) = \Sigma_1(k,\omega) + i\Sigma_2(k,\omega)$$

$\Sigma(\mathbf{k},\omega)$: the *"self-energy"* - captures the effects of interactions

$$\Gamma = \Sigma_2$$

$$\varepsilon(k) = \varepsilon_0(k) + \Sigma_1(k,\omega) = Z_k \varepsilon_0(k)$$

$$Z_k = \left(1 - \frac{\partial \Sigma_1}{\partial \omega}\right)^{-1}_{\omega = \varepsilon_0(k)}$$

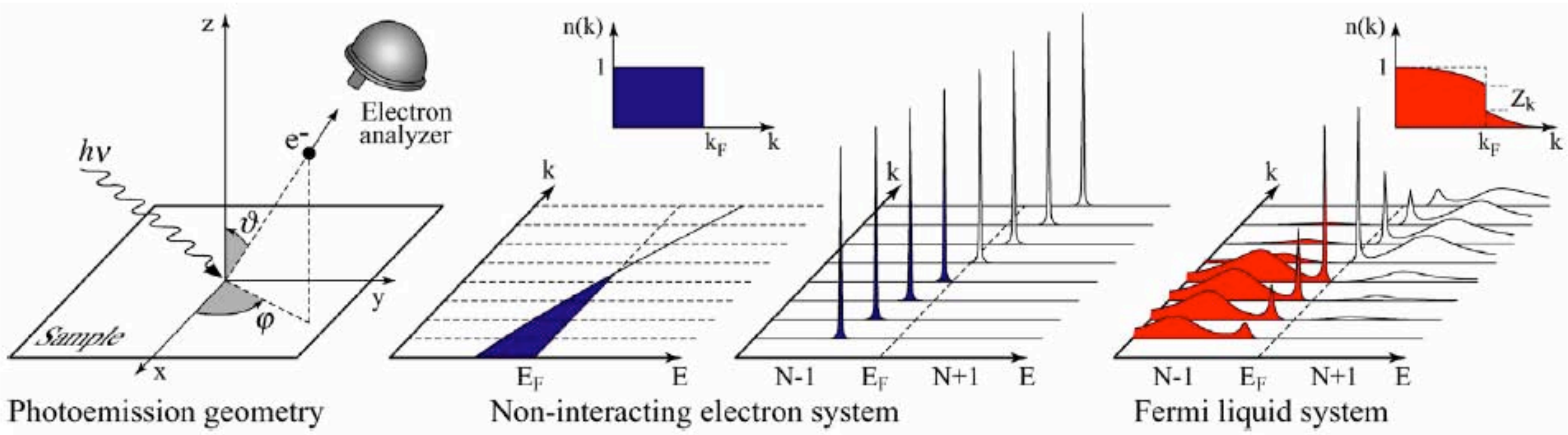
… rewriting G(k,ω) and A(k,ω):

$$G(k,\omega) = \frac{Z_K}{\omega - \left[\varepsilon_0(k) + \Sigma(k,\omega)\right]} + G_{inch.}(k,\omega)$$

$$A(k,\omega) = \frac{\Sigma_2}{\pi} \frac{Z_k}{\left[\omega - \varepsilon_0(k) - \Sigma_1\right]^2 + \Sigma_2^2} + A_{inch.}(k,\omega)$$

$$\lambda = \left(-\frac{\partial \Sigma_1}{\partial \omega}\right)_{\omega = E_F}$$

Coupling constant



non-interacting

$$A(\vec{k},\omega) = -\frac{1}{\pi}\operatorname{Im}\frac{1}{\omega - \varepsilon_{\vec{k}} + 0^+}$$

$$= \delta(\omega - \varepsilon_{\vec{k}})$$

Fermi liquid

$$A(\vec{k},\omega) = -\frac{1}{\pi}\operatorname{Im}\frac{1}{\omega - \varepsilon_{\vec{k}} - \Sigma(\vec{k},\omega) + 0^+}$$

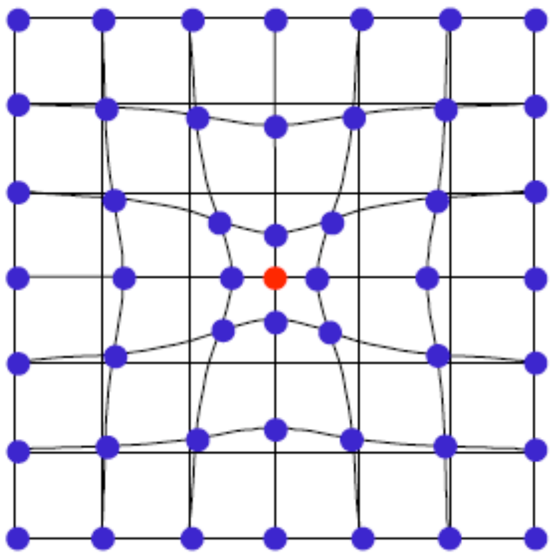
$$= -\frac{1}{\pi}\operatorname{Im}\frac{Z_{\vec{k}}}{\omega - E_{\vec{k}} - i\Gamma_{\vec{k}}} + A_{inc}$$

→ **energy renormalization:** $E_{\vec{k}} = \varepsilon_{\vec{k}} + \operatorname{Re}\Sigma = Z_k \cdot \varepsilon_{\vec{k}}$

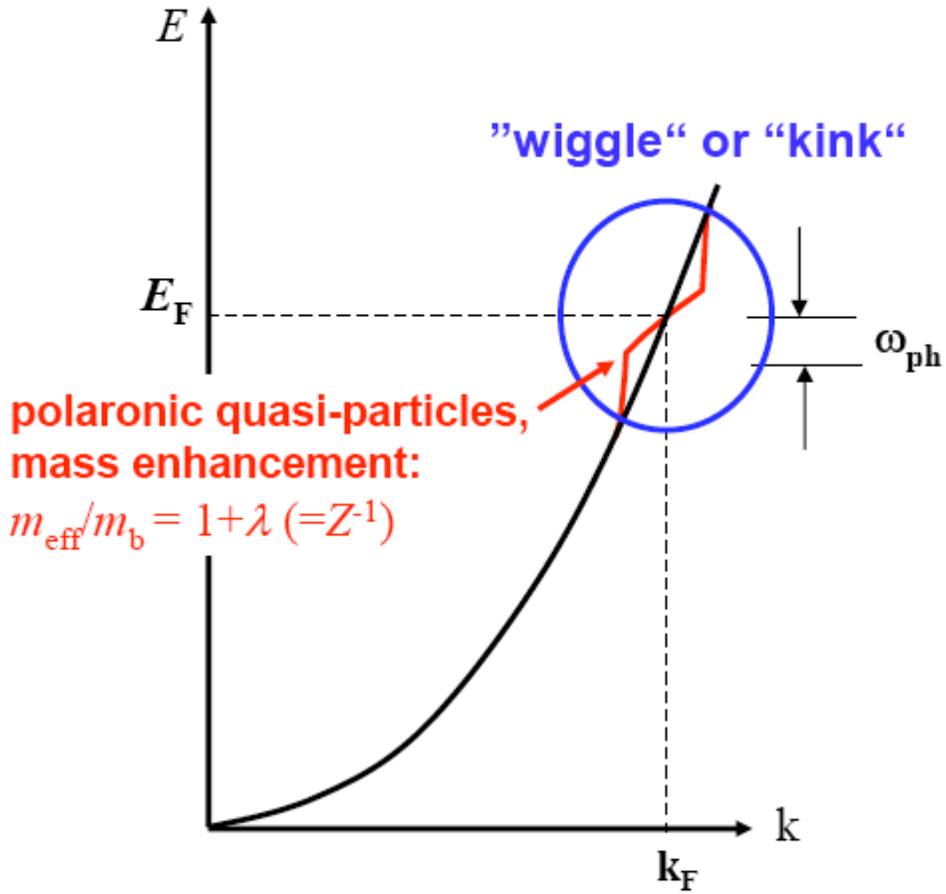
→ **lifetime broadening:** $\Gamma_{\vec{k}} = \operatorname{Im}\Sigma$

→ **quasiparticle weight:** $Z_{\vec{k}} = (1 - \frac{\partial\Sigma}{\partial\omega})^{-1} \le 1$

The “Kinky” physics



• Clear-cut case of a quasiparticle picture
• The quasiparticle mass near E_F is renormalized and the density of state increased



electron + (dynamical) lattice polarization
= polaronic quasiparticle

Electron-phonon coupling

$$A(k,\omega) = \frac{\Sigma_2}{\pi} \frac{Z_k}{\left[\omega - \varepsilon_0(k) - \Sigma_1\right]^2 + \Sigma_2^2} + A_{inch.}(k,\omega)$$

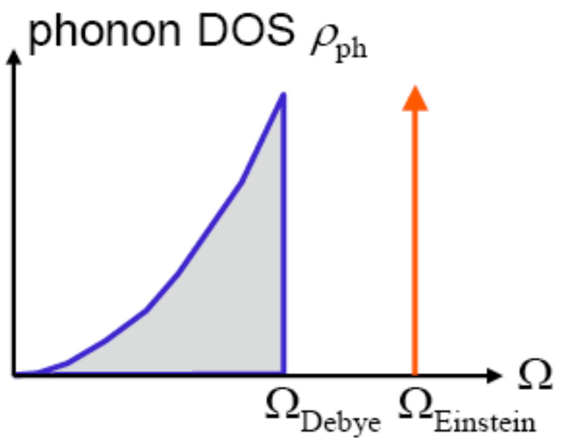
Spectral function: excitation spectrum

electronic self-energy

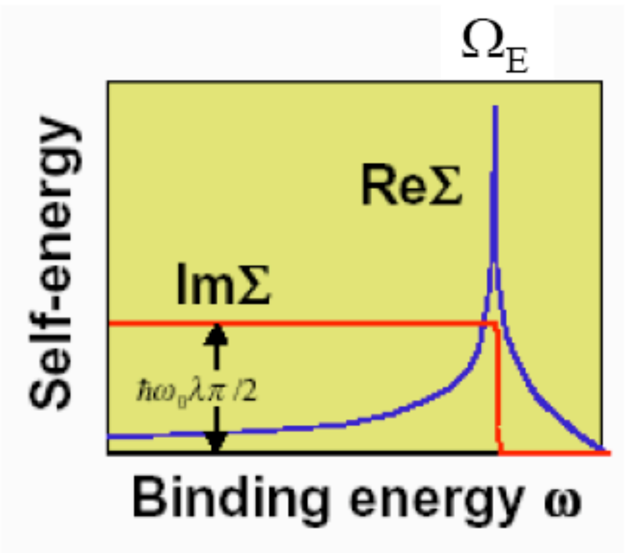
$$\mathrm{Im}\Sigma(\omega) \propto \int_0^{\omega} \alpha^2 F(\Omega) d\Omega = \lambda \int_0^{\omega} \rho_{ph}(\Omega) d\Omega$$

λ - electron-phonon coupling constant

$\mathrm{Re}\Sigma(\omega)$ **from Kramers-Kronig relation**

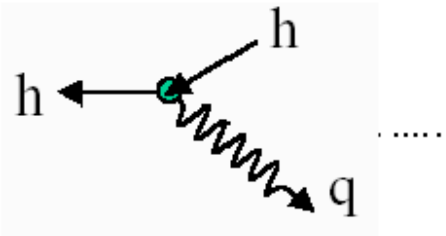


example: Einstein model:



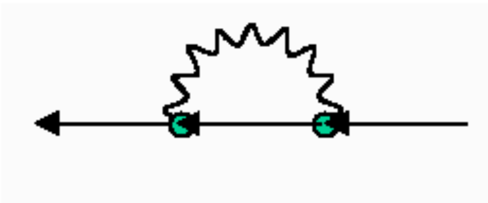
$$|\varepsilon_{\vec{k}} - E_F| > \omega_0$$

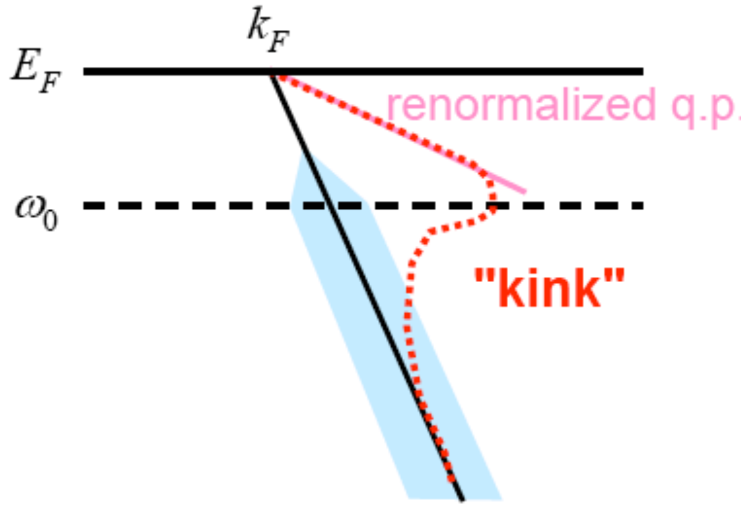
hole emits (decays into) *real* phonon



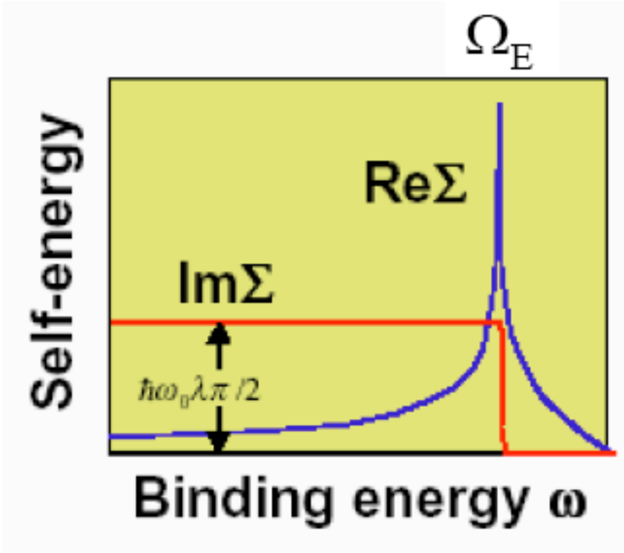
$$|\varepsilon_{\vec{k}} - E_F| < \omega_0$$

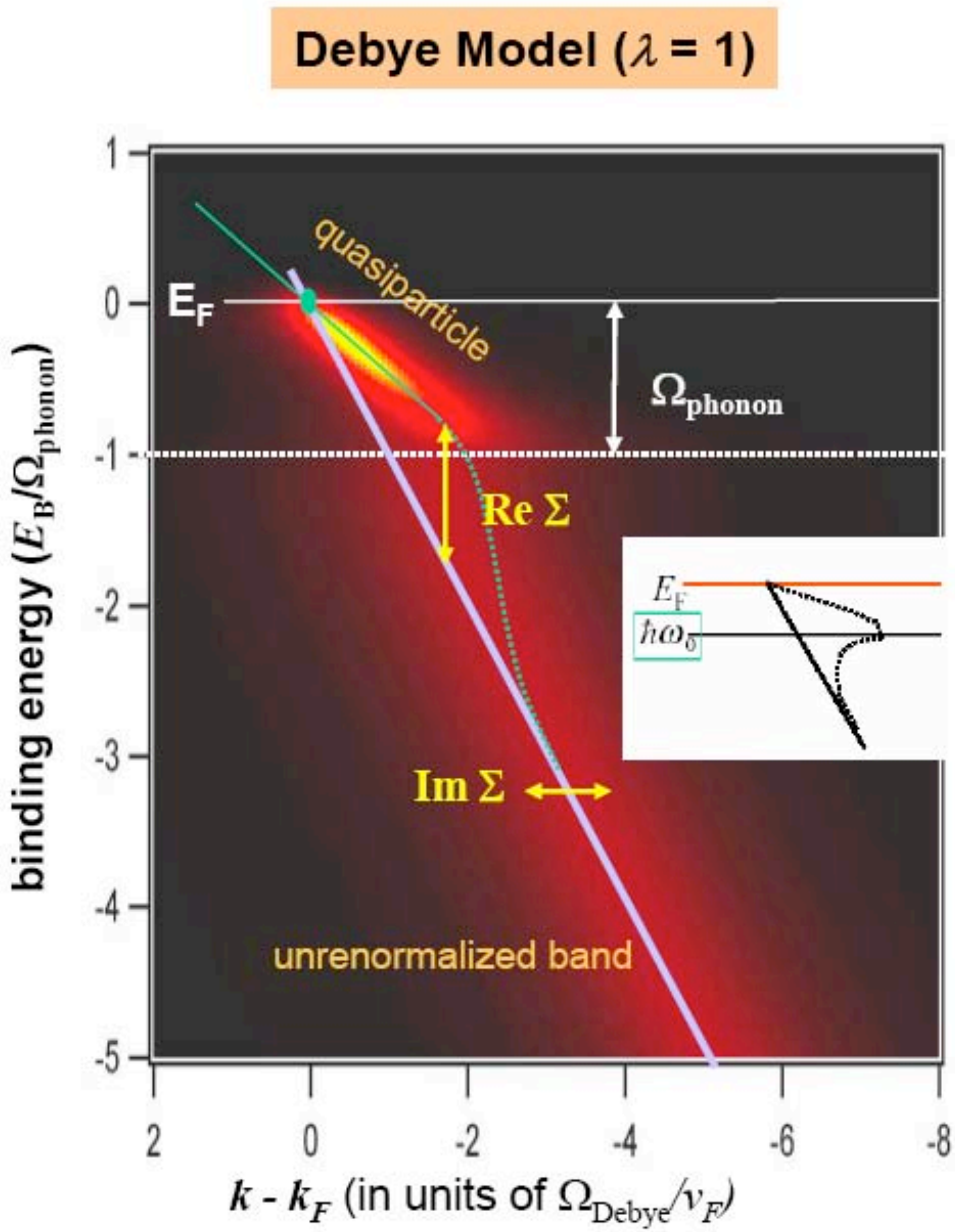
hole emits and reabsorbs phonon, dressed with cloud of *virtual* phonons

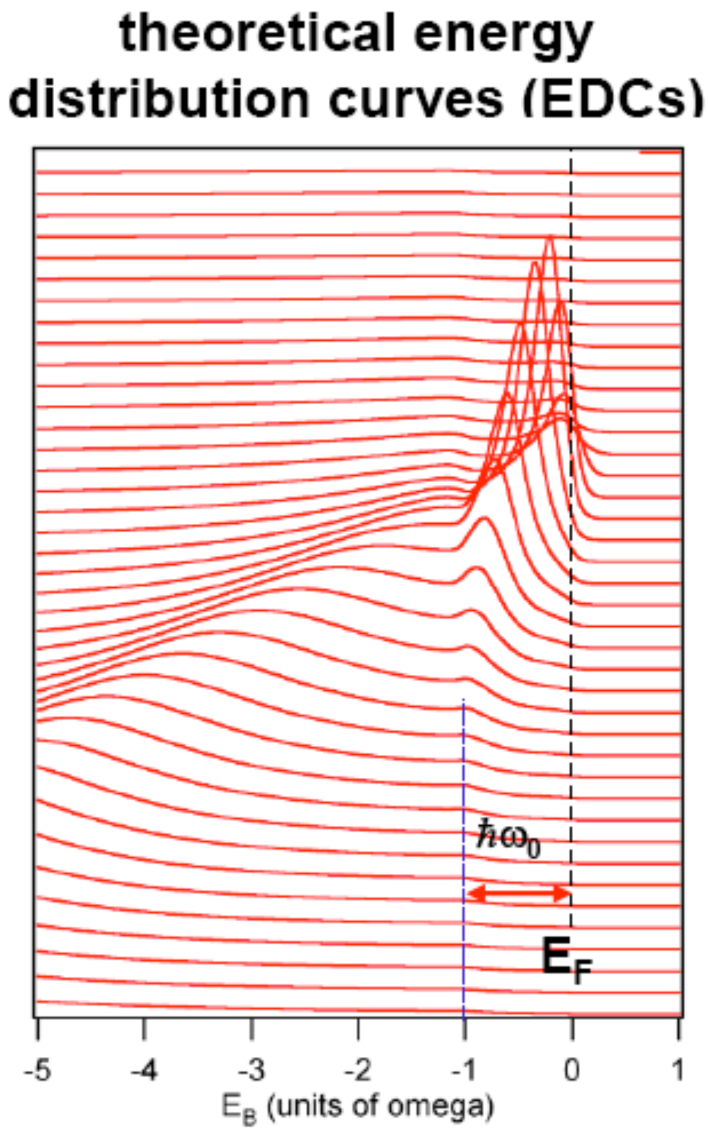




example: Einstein model:



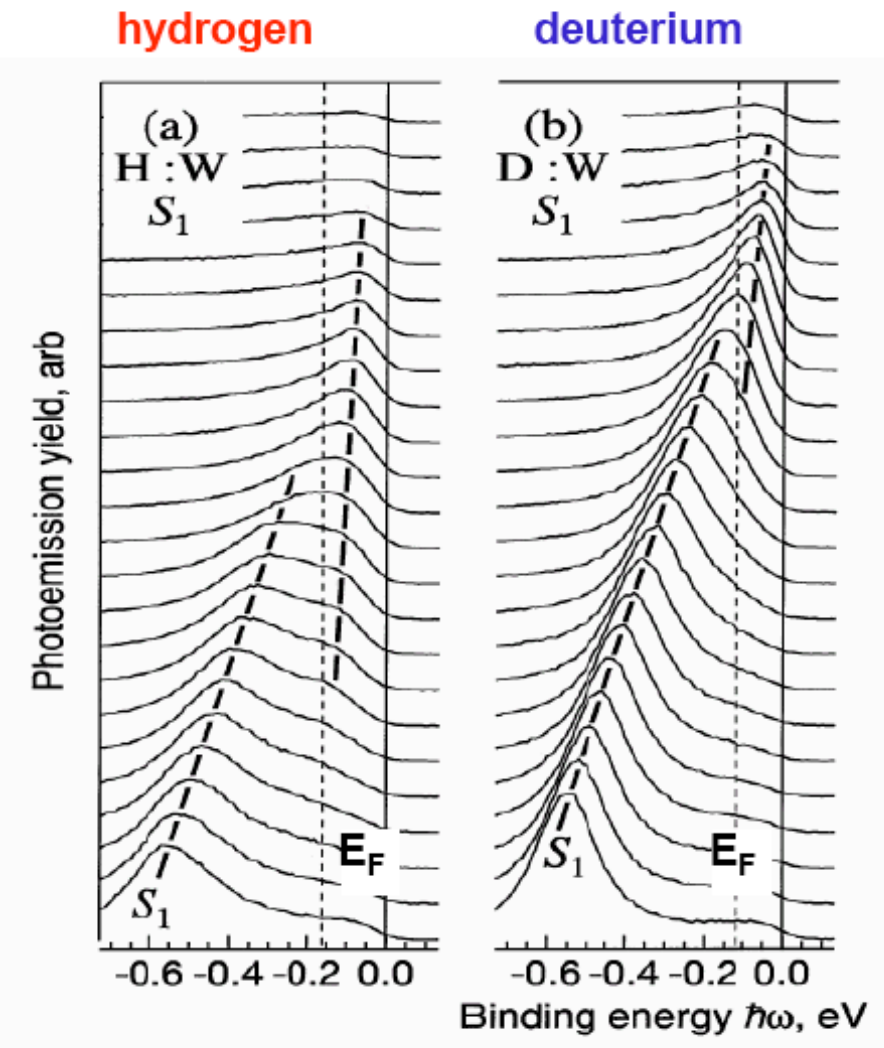

Debye Model (λ = 1)
quasiparticle
E_F
Ω_{phonon}
Re Σ
Im Σ
E_F
$\hbar\omega_0$
unrenormalized band
binding energy (E_B/Ω_{phonon})
1
0
-1
-2
-3
-4
-5
2
0
-2
-4
-6
-8
$k - k_F$ (in units of Ω_{Debye}/v_F)

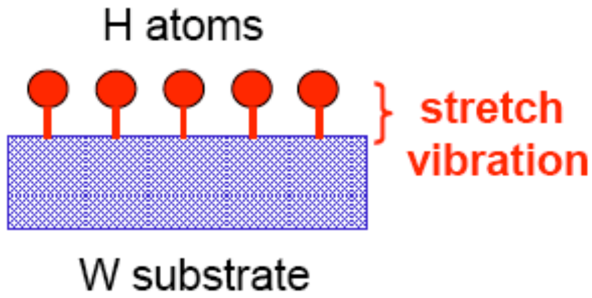

theoretical energy distribution curves (EDCs)
$\hbar\omega_0$
E_F
-5
-4
-3
-2
-1
0
1
E_B (units of omega)

Coupling to adsorbate vibrations on a surface

hydrogen adsorbed on W(110) – an Einstein-type system

*E. Rotenberg, J. Schäfer et al., PRL **84**, 2925 (2000)*





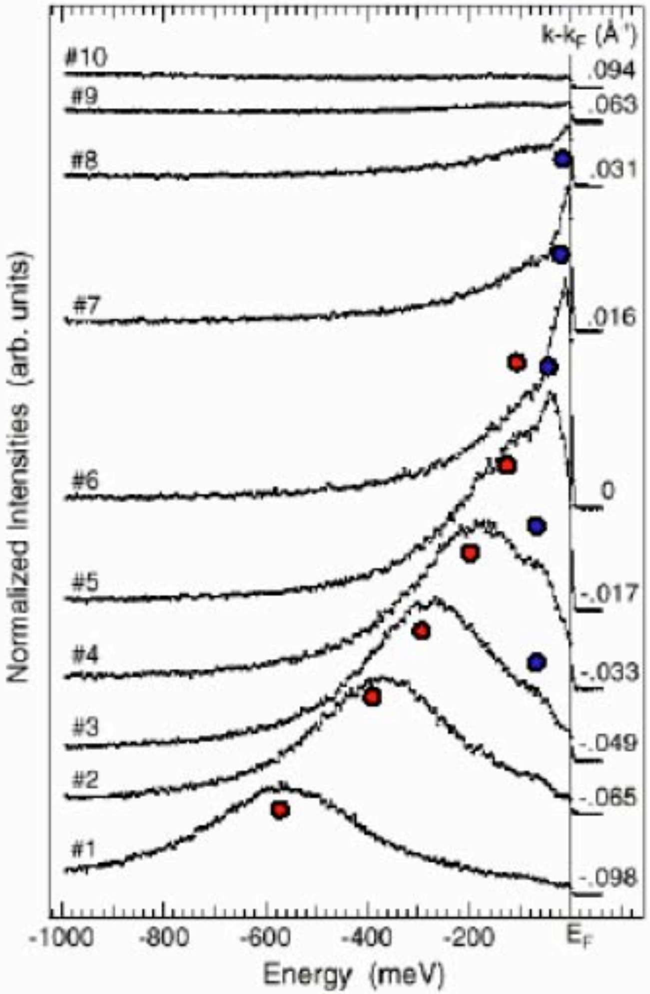
quantitative analysis:

- **energy scale:** ω_0 = 160 meV for H,
  115 meV for D (isotope effect $1/\sqrt{2}$)
- **coupling constant:** λ = 1.4 for H/W(110)

- **significant mass renormalization**
- **isotope effect H → D**
  $(\omega_0 \sim 1/\sqrt{M})$

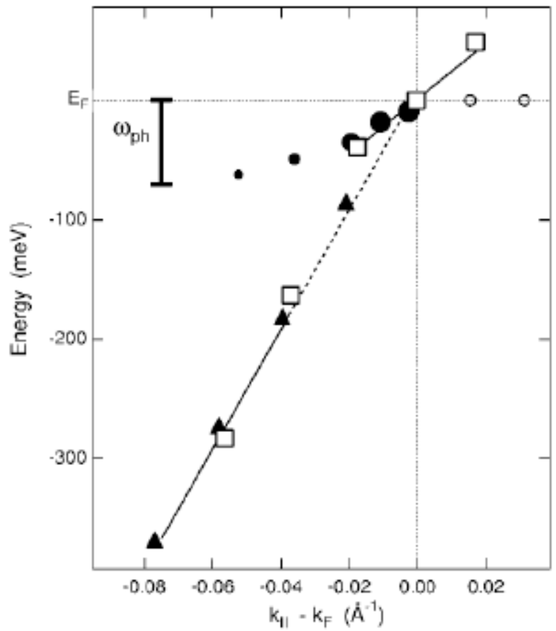
Intrinsic electron-phonon coupling on a surface: Debye model

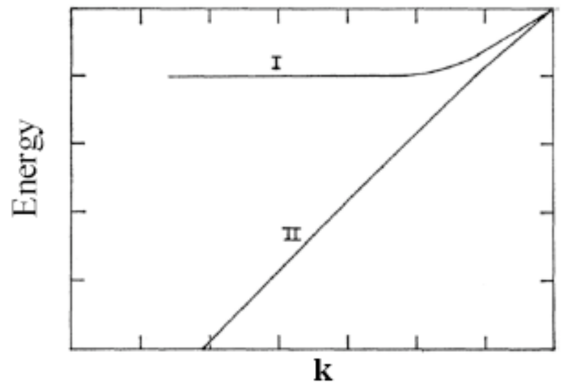
Be(0001) T=12K



Hengsberger et al, PRL 83,592 (1999).

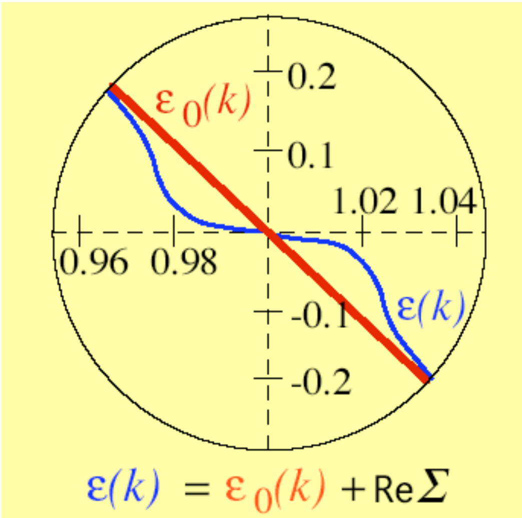
Theory and Experiment





S. Engelsberg and J.R. Schrieffer, **PR** 131, 993 (1963)

How to get λ?: real part of Σ



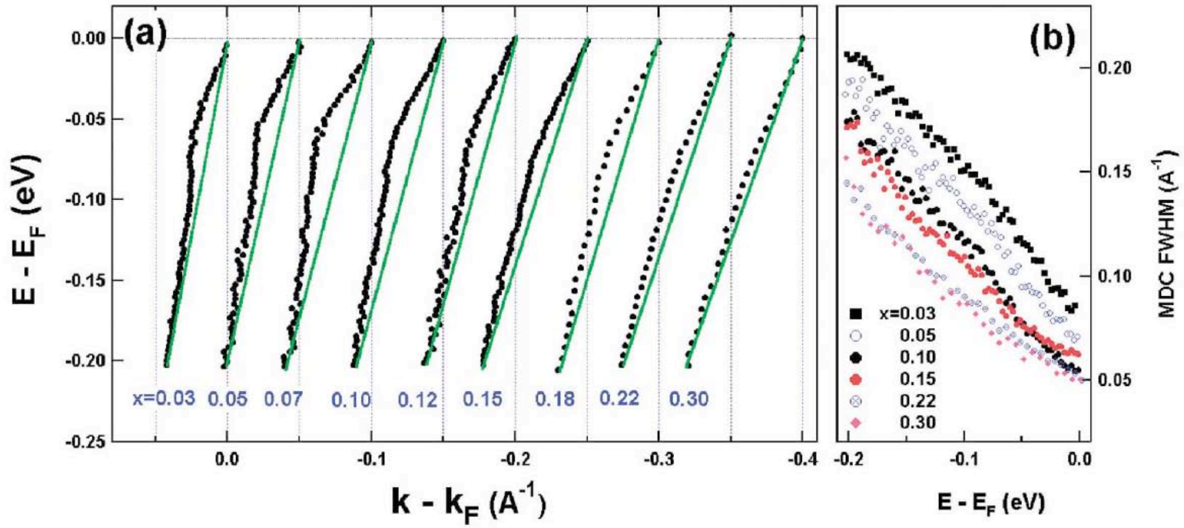


Fig. 13. Dispersion (a) and MDC width (FWHM)(b) of LSCO samples ($x = 0.03$~0.30) measured along the nodal direction, as determined from fitting MDCs. For clarity, the dispersion in (a) is offset horizontally along the momentum axis. The green lines in (a) connect the points in dispersion at E_F and 0.2 eV which approximately represents the bare band; they also serve as guides to the eye to identify the kink in dispersion. The MDC width (b) shows an overall decrease with increasing doping. A slight drop in MDC width is discernible at a binding energy of ~80 meV, particularly obvious for lower doping samples.

$$\lambda = \frac{d\Re\Sigma}{d\epsilon}\Big|_{\epsilon_F}$$

but this may also be caused by something else....

- yields directly λ when measured at 0 K.
- the effect has to be large in order to be observable
- the un-renormalized dispersion has to be known

How to get λ?: imag. part of Σ

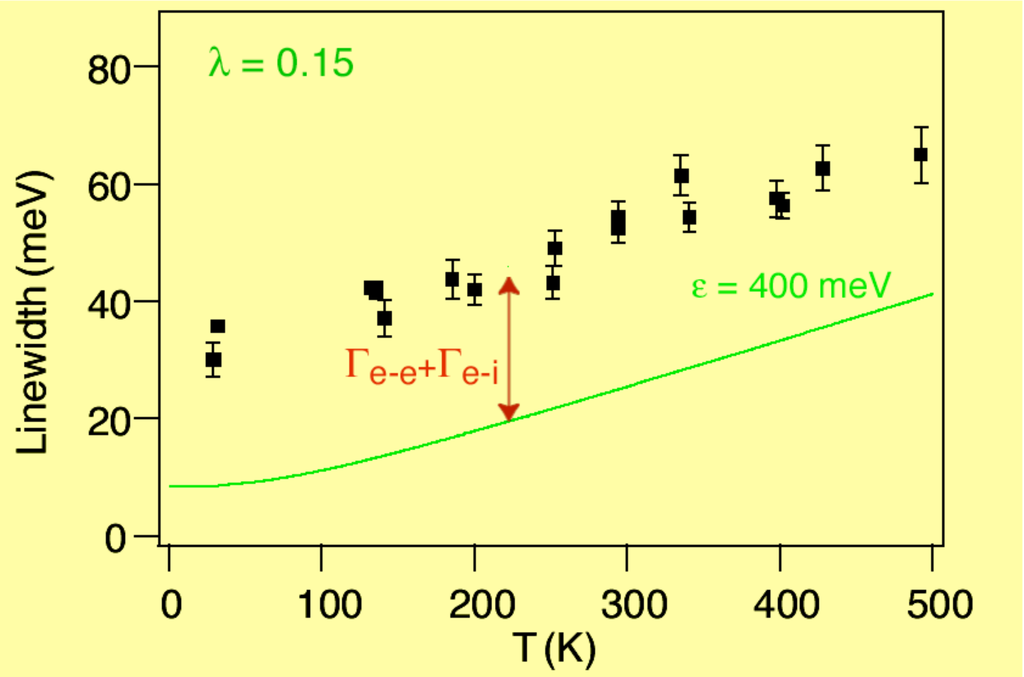
EDC linewidth $\Gamma = \Gamma_{e-e}(T) + \Gamma_{e-i}(T) + \Gamma_{e-ph}(T)$

$$\Gamma_{e-ph}(T) = 2\pi\hbar \int_0^{\omega_m} d\omega' \alpha^2 F(\omega')[1 - f(\omega - \omega') + 2n(\omega') + f(\omega + \omega')] \simeq 2\pi\lambda k_B T$$

$$\alpha^2 F(\omega) = \lambda(\frac{\omega}{\omega_D})^2 \quad , \omega < \omega_D$$

$$\alpha^2 F(\omega) = 0, \omega > \omega_D$$

- In most cases, the temperature dependence of the lifetime is dominated by the electron-phonon coupling.
- The T-dependence of the linewidth can be used to extract λ.
- The T-dependence is **independent of binding energy** (not too close to the Fermi level).
- several practical problems when the binding energy is very close to the Fermi level



B.A. McDougall, T. Balasubmaranian and E. Jensen PRB 51, 13891 (1995).

How to get λ?: imag. part of Σ

EDC linewidth $\Gamma = \Gamma_{e-e}(\cancel{T}) + \Gamma_{e-i}(\cancel{T}) + \Gamma_{e-ph}(T)$

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$$\alpha^2 F(\omega) = \lambda(\frac{\omega}{\omega_D})^2 \quad , \omega < \omega_D$$
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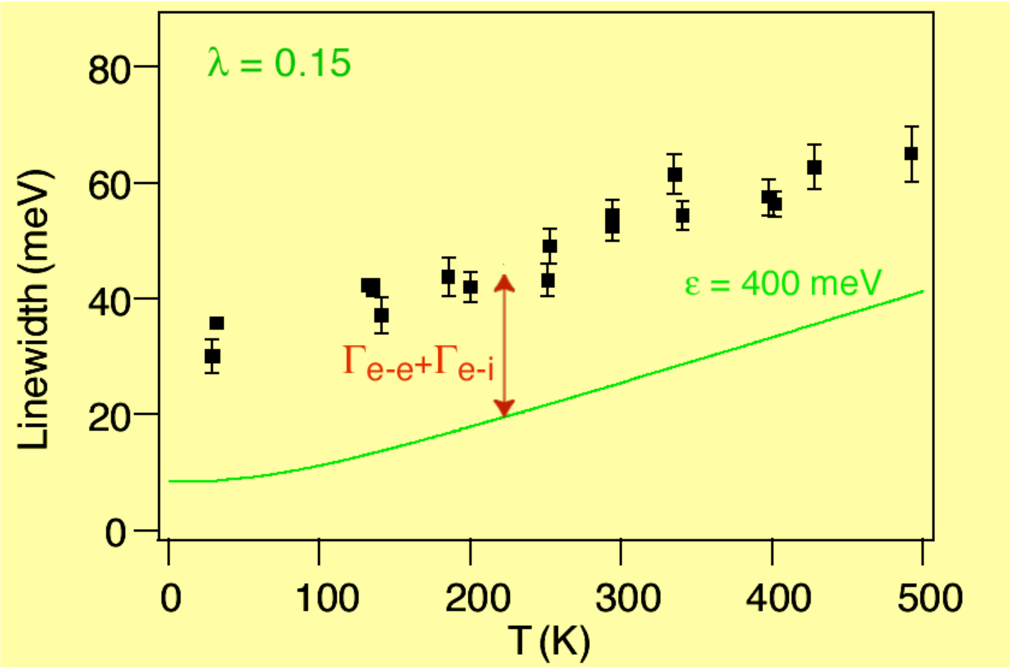
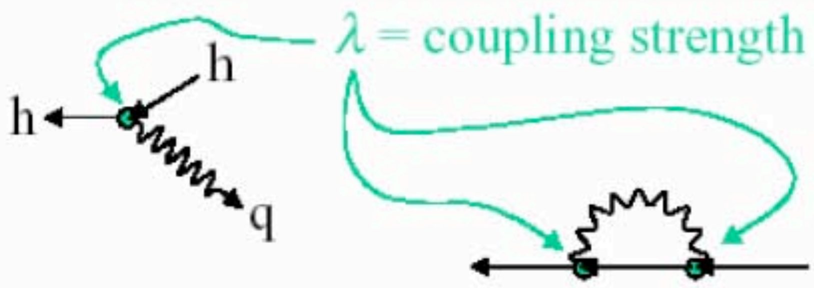
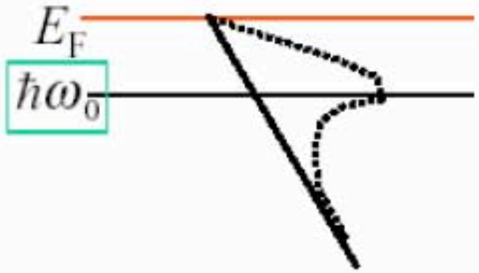


B.A. McDougall, T. Balasubmaranian and E. Jensen PRB 51, 13891 (1995).

Electron-phonon coupling constant and superconductivity





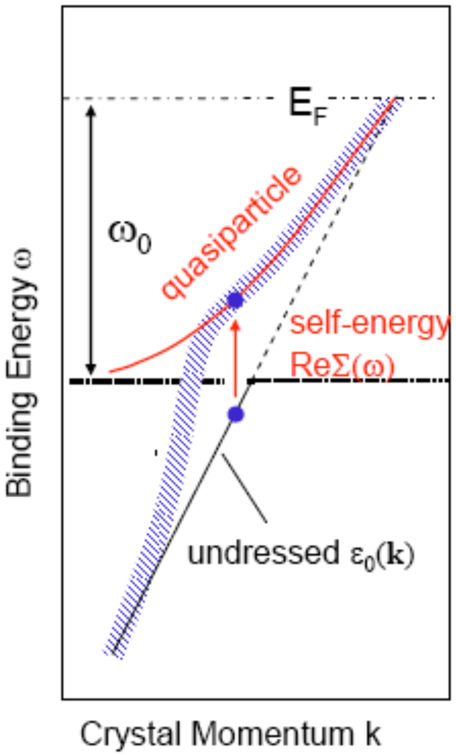
Strong-coupling theory of superconductivity

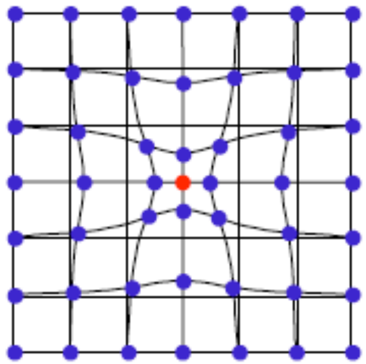
	Matl	λ	w0 [K]	Tc(theory)	Tc(expt)
	W	0.28	390	0.01	0.012
	Mo	0.41	460	0.84	0.92
	Be	0.24	1000	**0.02**	0.026
3-D	Hg	1	72	3.56	4.16
	Pb	1.12	105	6.25	7.19
	Nb	0.82	277	9.20	9.22
	Pd	0.15	274	0.00	not SC
	PdH	0.75	475	12.67	10
2-D	H:W	0.5-1.4	1932	**50-150**	?
	Be surf	1.15	1000	**70.21**	?

$$T_c \propto \omega_0 \exp(-\frac{1}{\lambda})$$

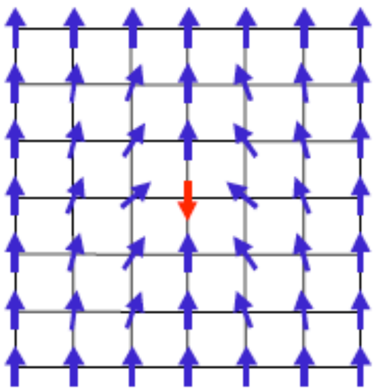
table by Eli Rotenberg

Coupling to other bosons

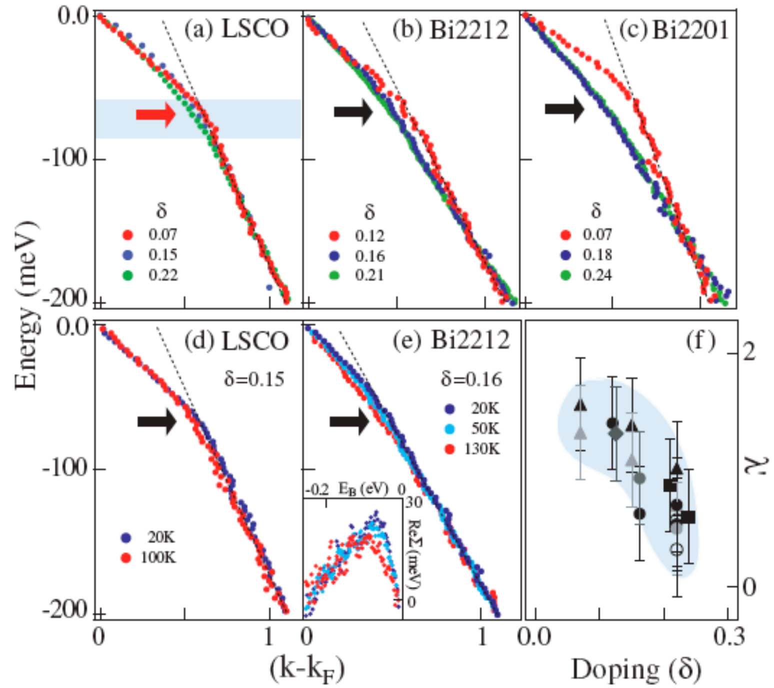




e-ph



e-spin

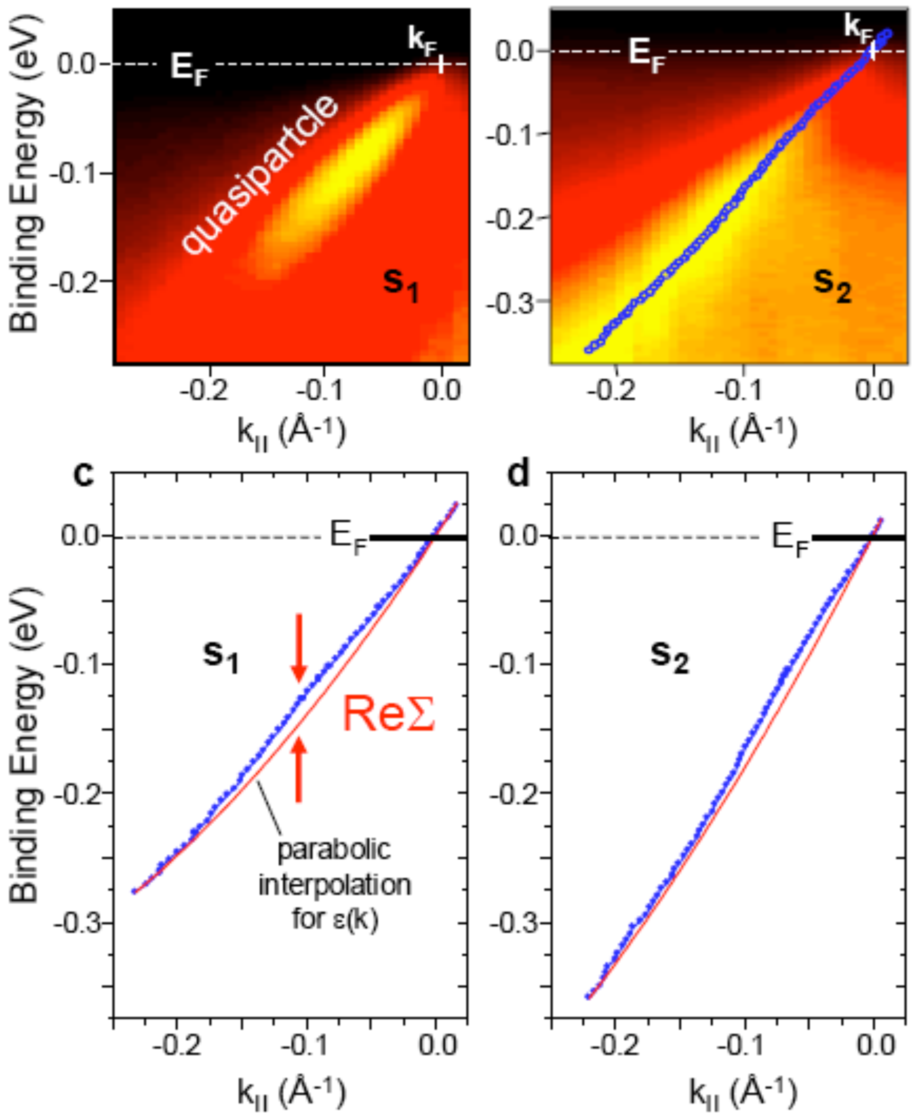


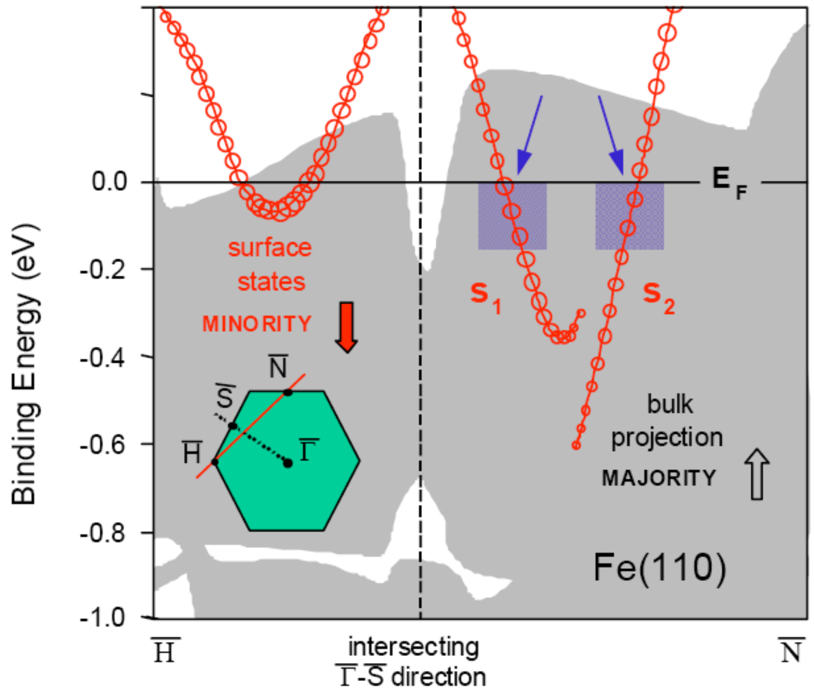
formation of quasiparticles by coupling to spin excitations ?

kink observed in the cuprates :

- Cooper-pairing mediated by spin fluctuations ?
- problem: energy scales for phonons and magnetic modes very similar

Fe(001) surface state: dispersion and lifetime width



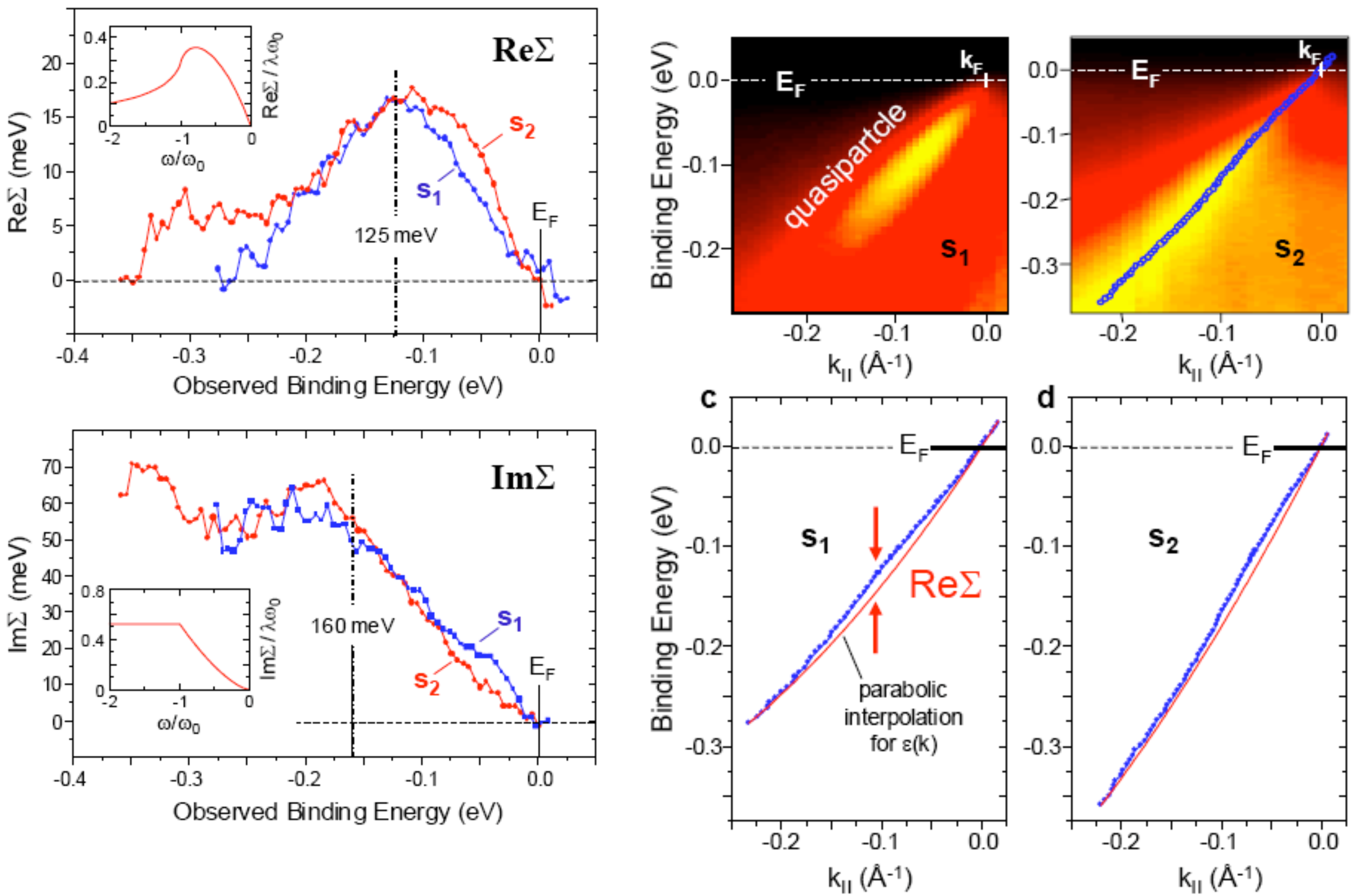


self-energy $\Sigma(\omega)$ derived from momentum distribution curves (MDCs)

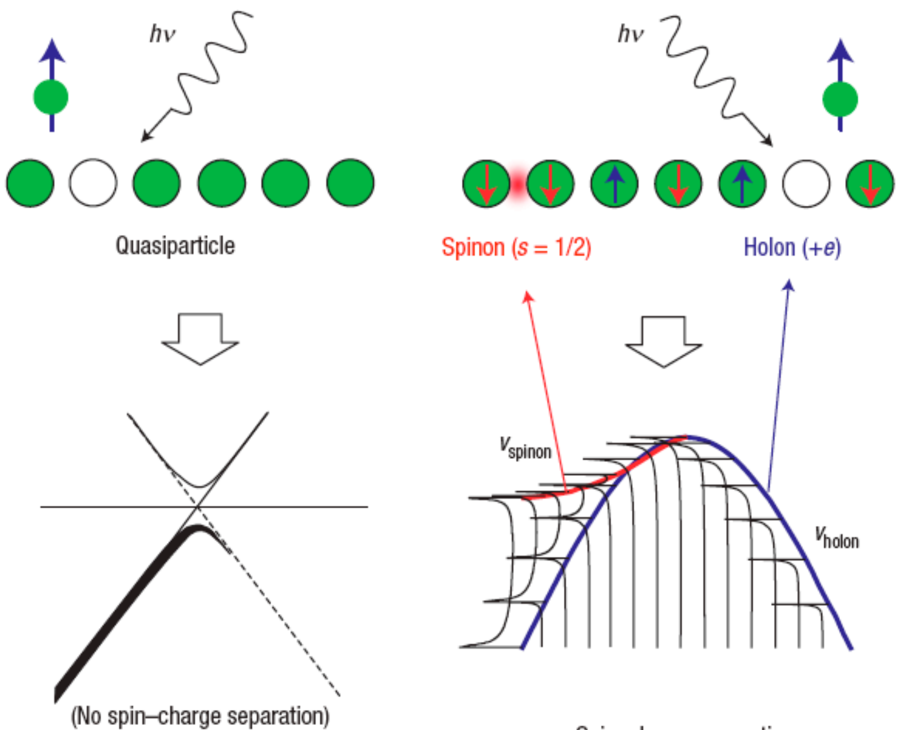
peak maximum $\rightarrow \varepsilon_k + \mathrm{Re}\,\Sigma(\omega)$

renormalization @ 100-200 meV

(>> ω_{Debye} ~ 30 meV)


ReΣ
ReΣ (meV)
ReΣ / λω0
ω/ω0
125 meV
s1
s2
EF
Observed Binding Energy (eV)
ImΣ
ImΣ (meV)
ImΣ / λω0
160 meV
Binding Energy (eV)
kF
quasiparticle
k|| (Å-1)
c
d
parabolic
interpolation
for ε(k)

1D System: breakdown of the Fermi liquid
Spinon and holon dispersion

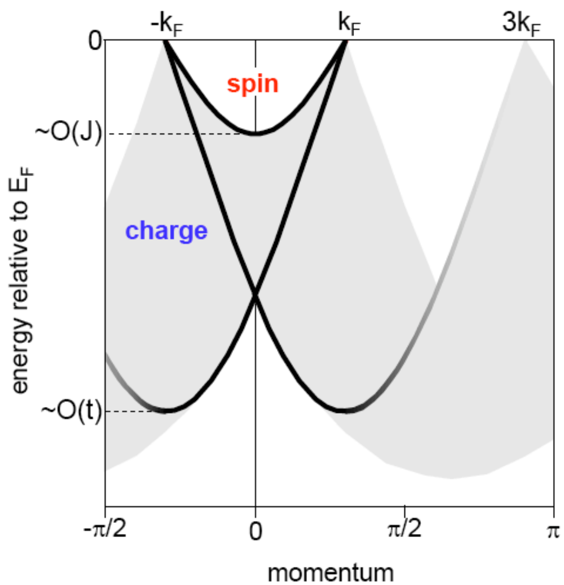


Band picture + spin density wave

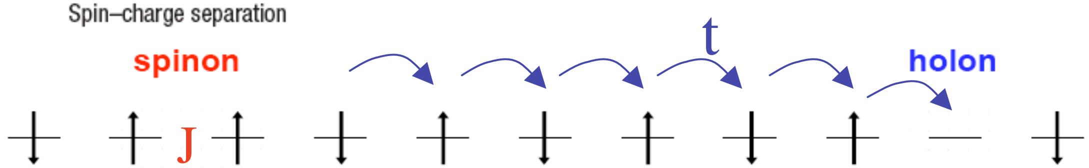
Spin–charge separation

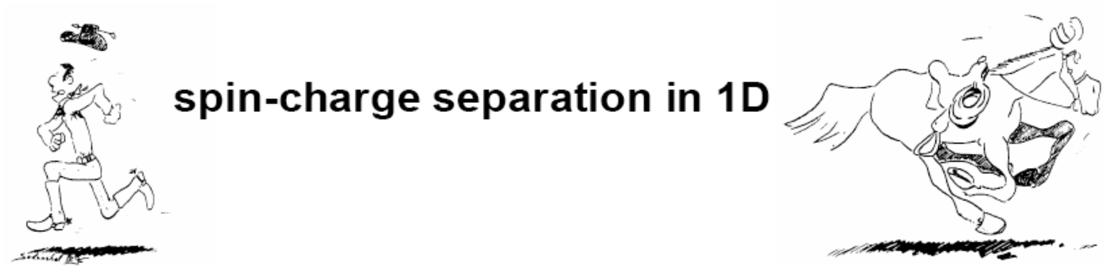
t - hopping integral

$J \propto t^2/U$ - magnetic exchange



U >> t
strong
coupling





K. Penc et al. (1996): tJ-model
J.M.P. Carmelo et al. (2002 / 2003): Bethe ansatz
E. Jeckelmann et al. (2003): dynamical DMRG

Distinct spinon and holon dispersions in photoemission spectral functions from one-dimensional $SrCuO_2$

B.J. Kim at al., Nature Physics 2 (2006)

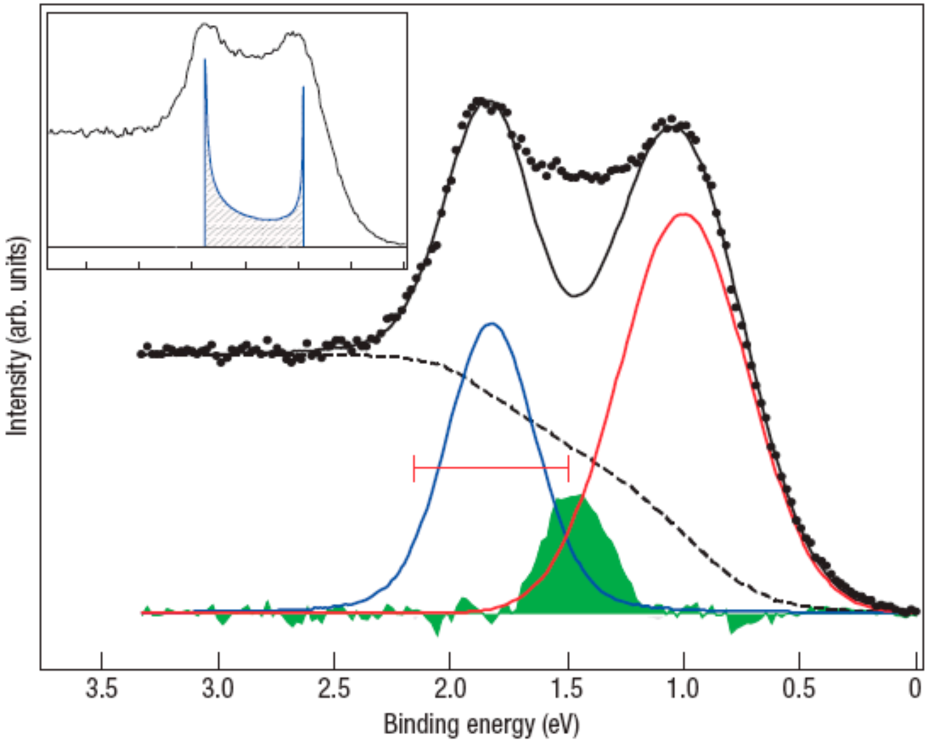
$$H = t \sum_{<ij>,\sigma} c^{+}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

t – hopping integral

U – local Coulomb energy

$J \propto t^2/U$ - magnetic exchange energy

strong coupling $U >> t$



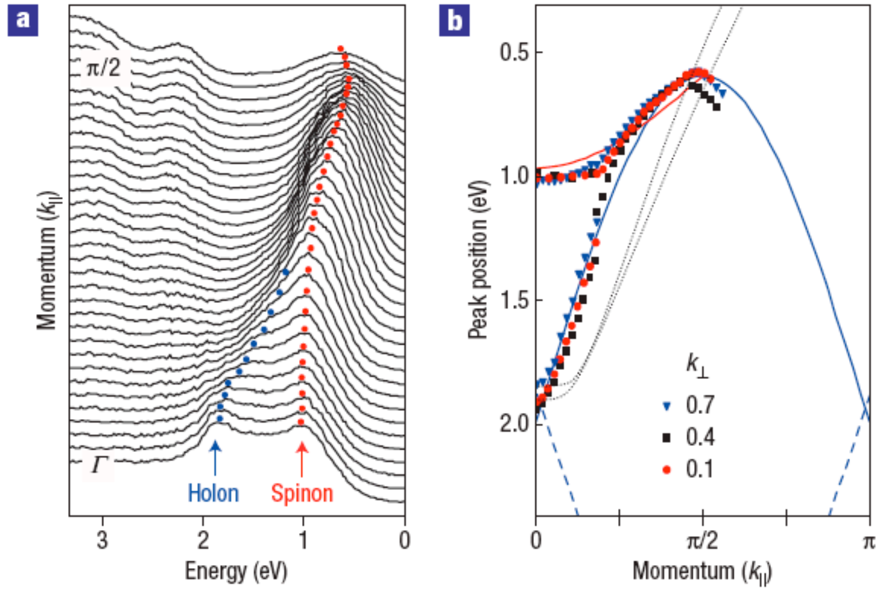
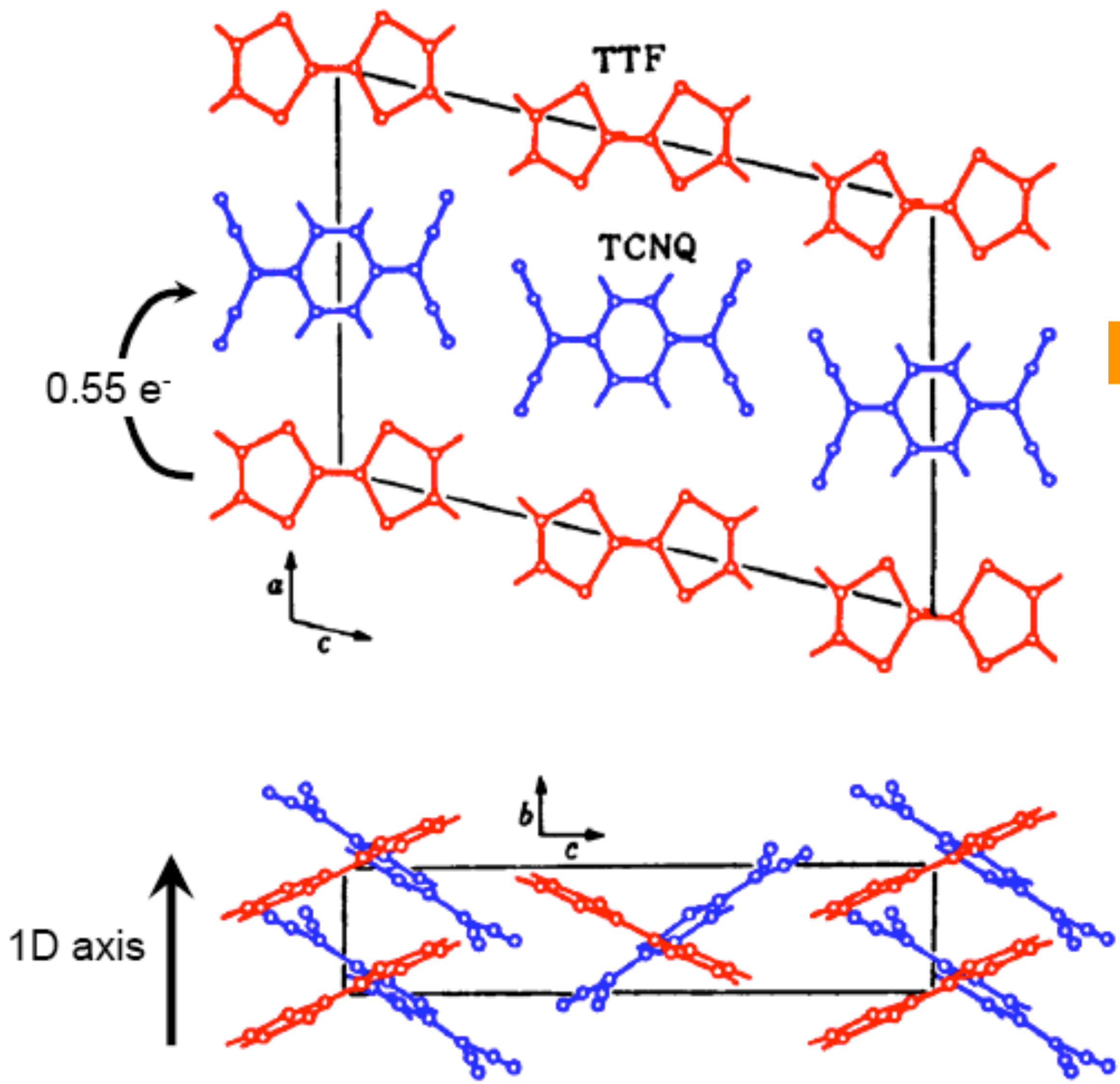


Figure 3 EDCs and dispersions. a, EDCs for $k_{||}$ between Γ and 0.6π at $k_\perp = 0.7$ Å^{-1}. Each EDC is curve-fitted to find the peak positions. Two peaks were used in the region between $k_{||} = \Gamma$ and $\pi/4$, whereas a single peak was used for the rest. The results are marked by red and blue circles. **b**, Experimental (symbols) and theoretical (solid and dashed lines) dispersions. The theoretical dispersions are obtained by taking the nearest-neighbour hopping of $t = 0.65$ eV and the exchange coupling of $J = 0.23$ eV. Dispersions from the band theory are also shown as two dotted lines[22].

TTF-TCNQ: an organic 1D metal



strongly anisotropic conductivity
$\sigma_b/\sigma_a \approx \sigma_b/\sigma_c \sim 1000$

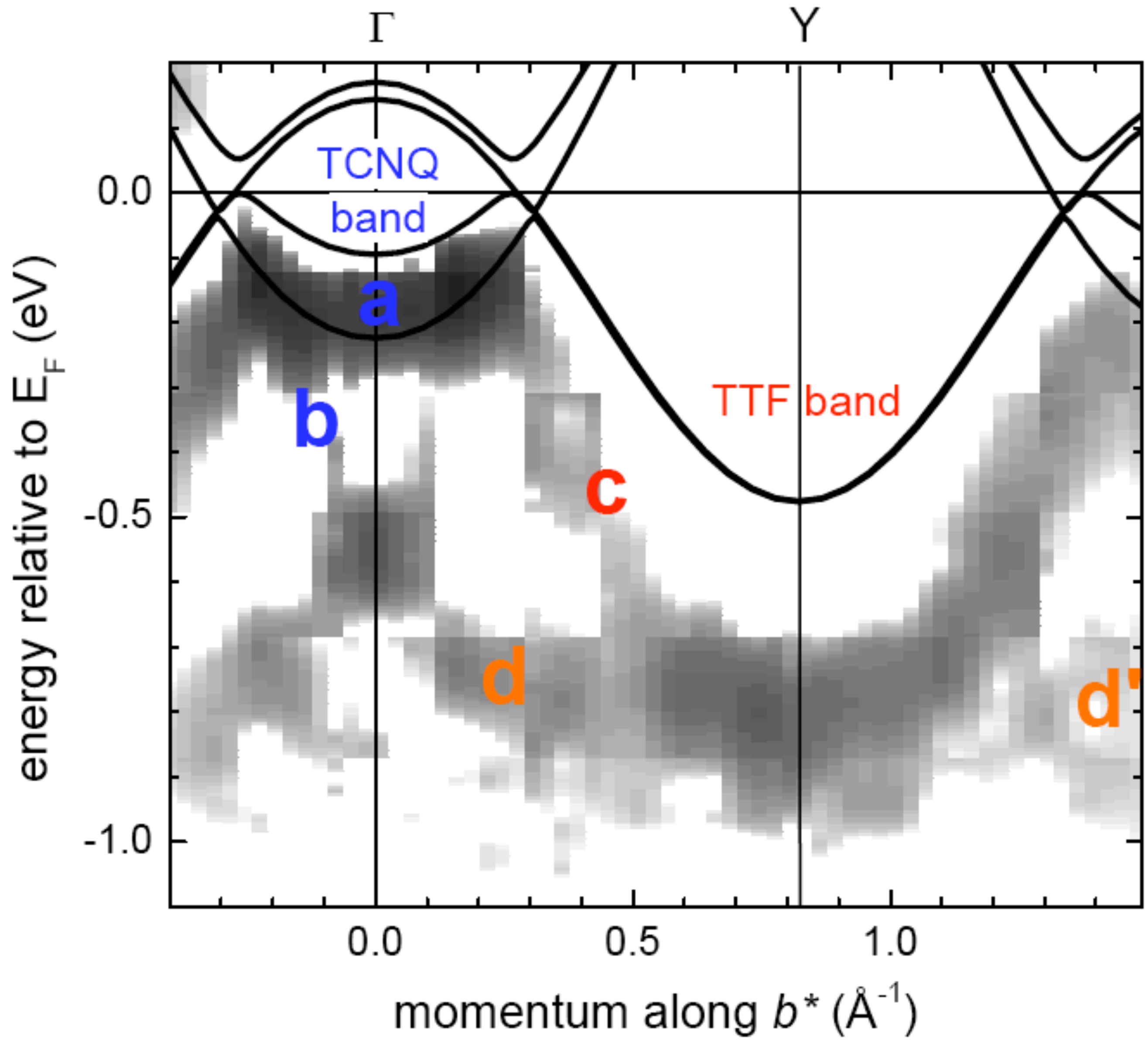
Peierls instability @ $T_P = 54$ K,
incommensurate CDWs on
TCNQ stacks

electronic correlation effects:

- $4k_F$-fluctuations (on TTF stacks ?) observed up to 300 K
- enhanced magnetic susceptibility
- enhanced NMR relaxation rate

$\Rightarrow$ **estimate for Hubbard model parameters:**

U ~ 4t ~ 1 eV



$-d^2I/dE^2$ vs. **k**

experimental band width doubled relative to theory

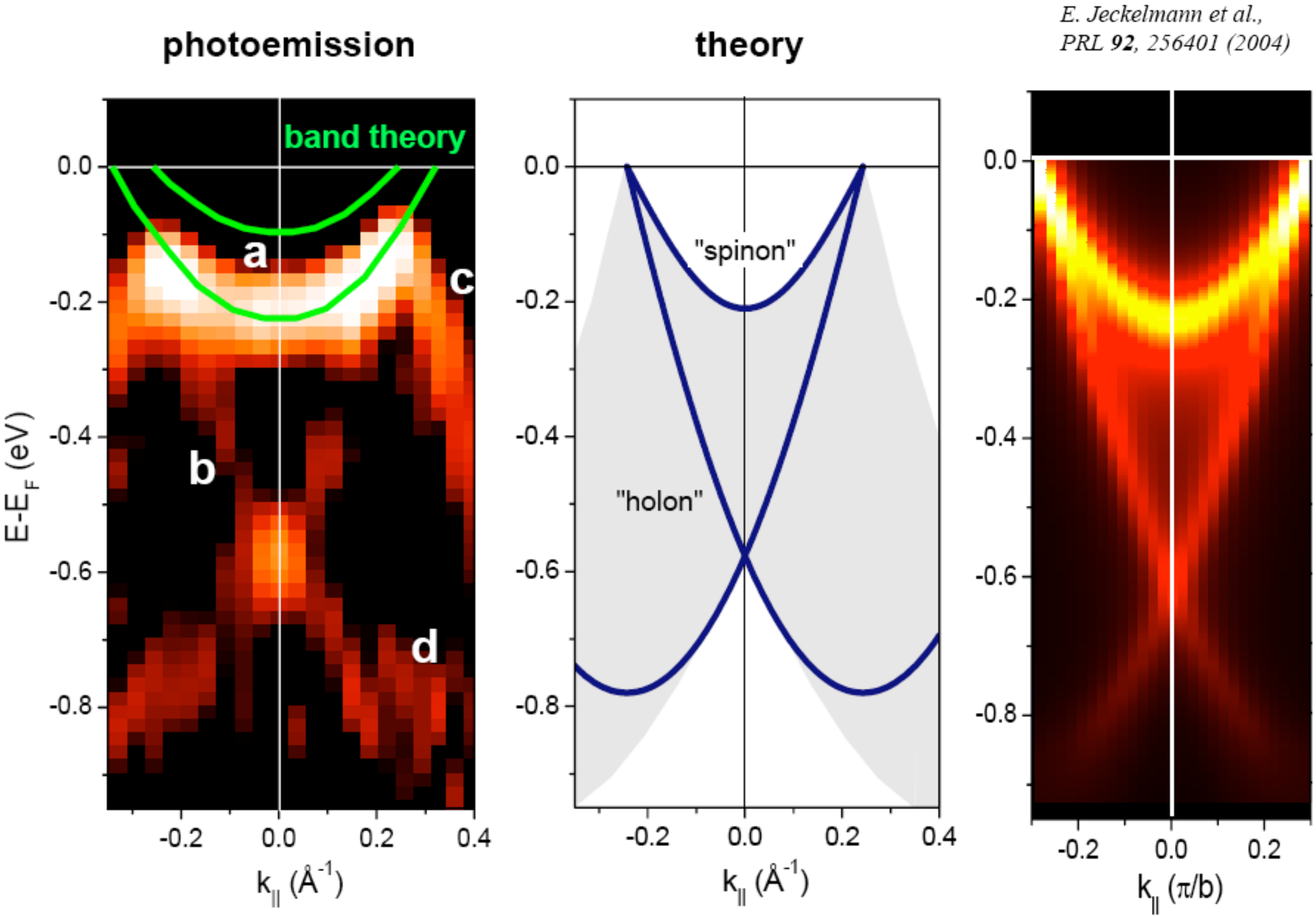
→ **molecular surface relaxation**

PRB ***67****, 125402 (2003)*

spectral structure (d) not explained by band theory

→**1D correlation effects**

PRL ***88****, 096402 (2002);*
PRB ***68****, 125111 (2003)*

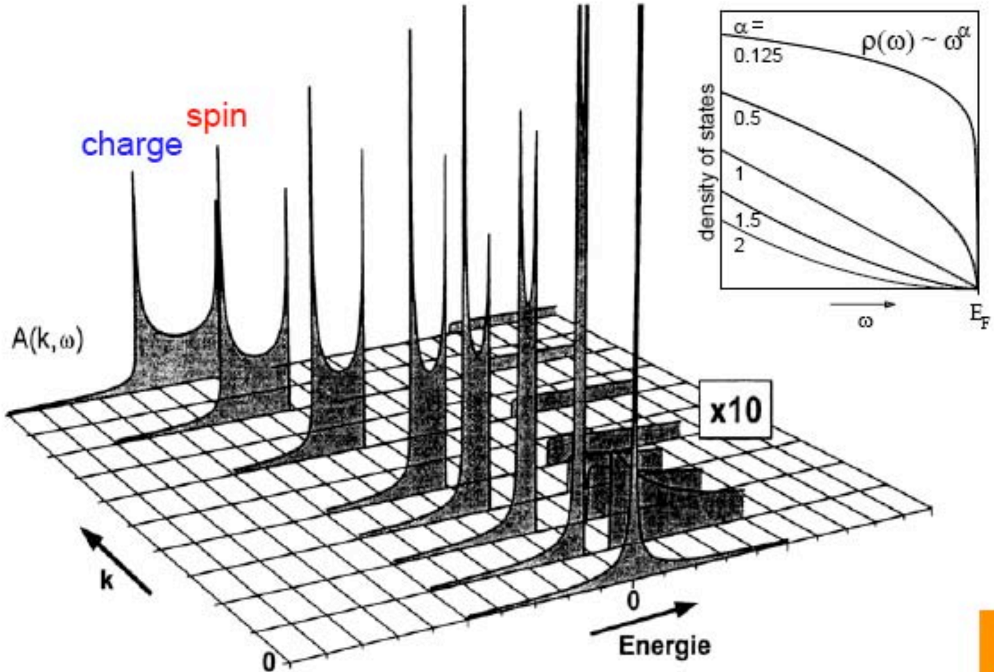


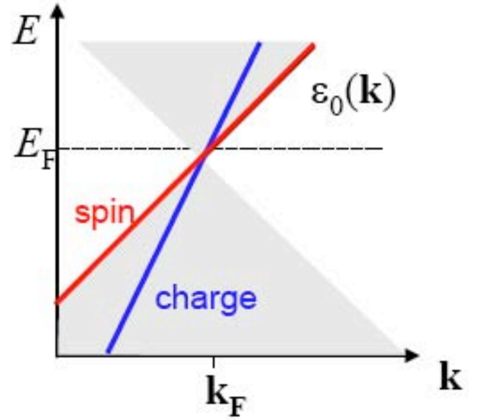
photoemission
band theory
a
b
c
d
E-E_F (eV)
k_|| (Å^-1)
theory
"spinon"
"holon"
k_|| (Å^-1)
E. Jeckelmann et al.,
PRL 92, 256401 (2004)
k_|| (π/b)

1D System: breakdown of the Fermi liquid
The Tomonaga-Luttinger liquid

Tomonaga-Luttinger model:

spectral function $A(\mathbf{k},\omega)$



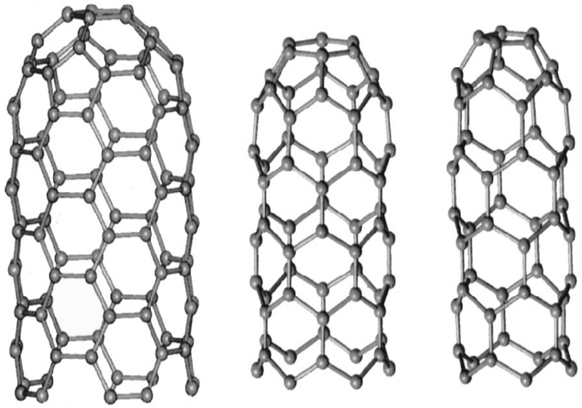


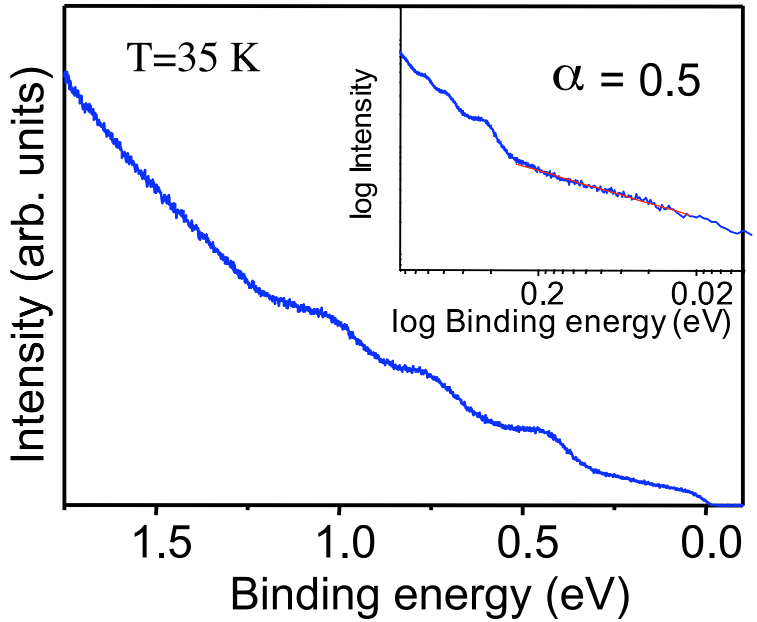
- **spin-charge "separation"**
- **failure of the quasiparticle concept**
- **power law onset in DOS (no Fermi edge !)**

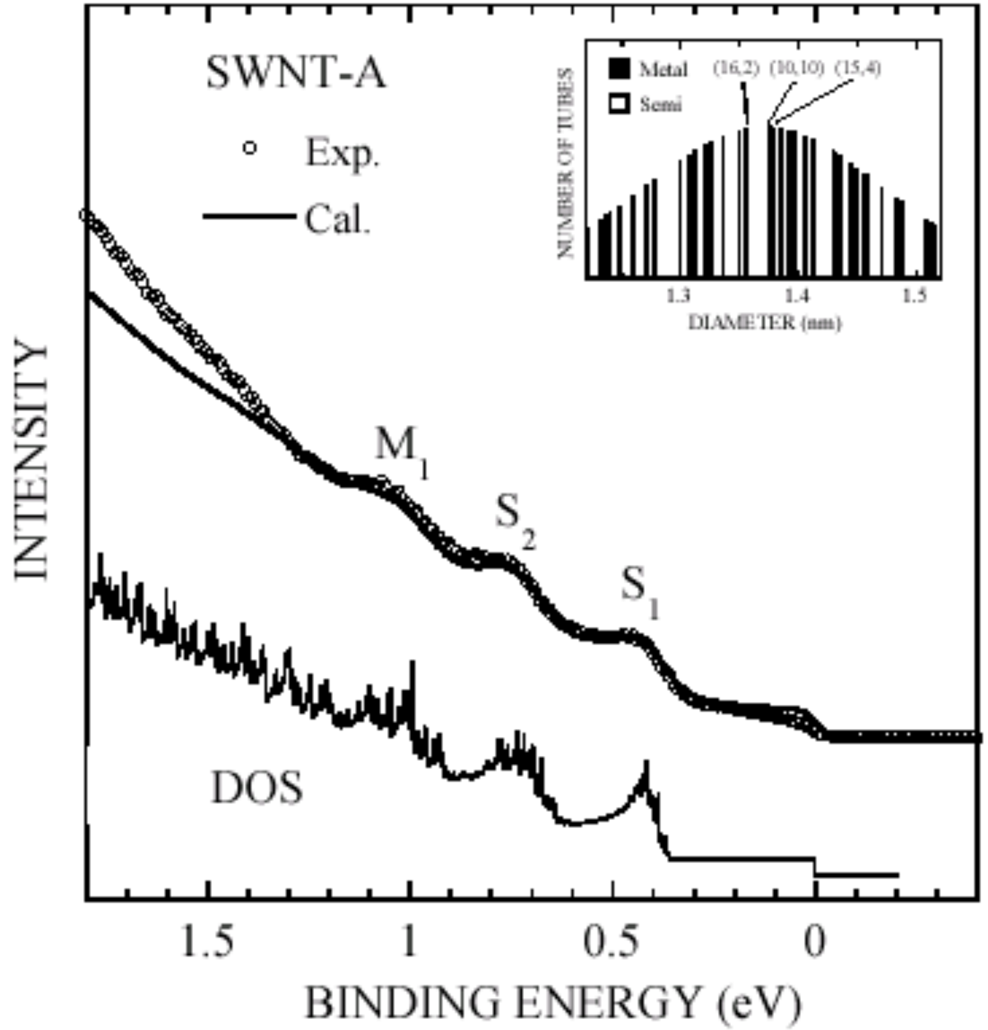
generic low-energy physics of interacting 1D metals: LUTTINGER LIQUID

Voit (1995)
Schönhammer and Meden (1995)

SWCNTs: an example of Tomonaga-Luttinger liquid

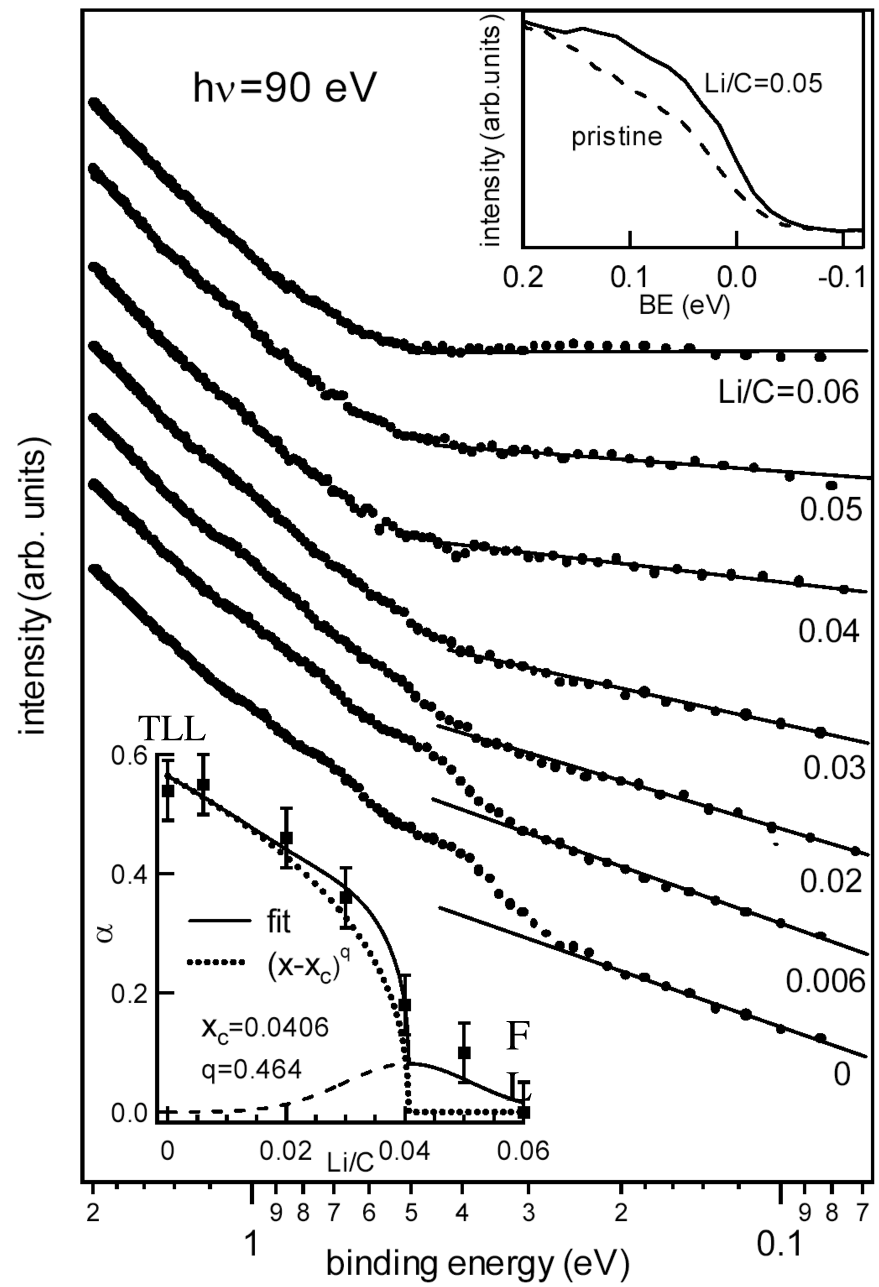






H. Ishii et al, Nature, 426, 540 (2003)

log-log plot



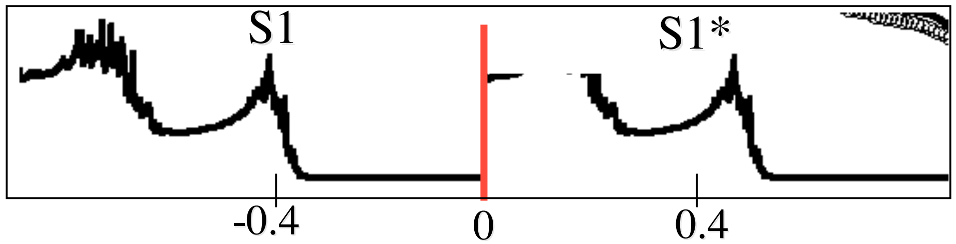
Transition from a Tomonaga-Luttinger liquid to a Fermi liquid

$n(E) \propto |E-E_F|^{\alpha}$, where $\alpha=(g+g^{-1}-2)/8$ depends on the size of the Coulomb interaction and *g* is the Luttinger parameter

$\alpha \sim 0.53\pm0.05$ for pristine SWCNTs in agreement with other estimations

$\alpha=0$ Fermi liquid

R. Larciprete, S. Lizzit, L. Petaccia, A. Goldoni, PRB 71, (2005)

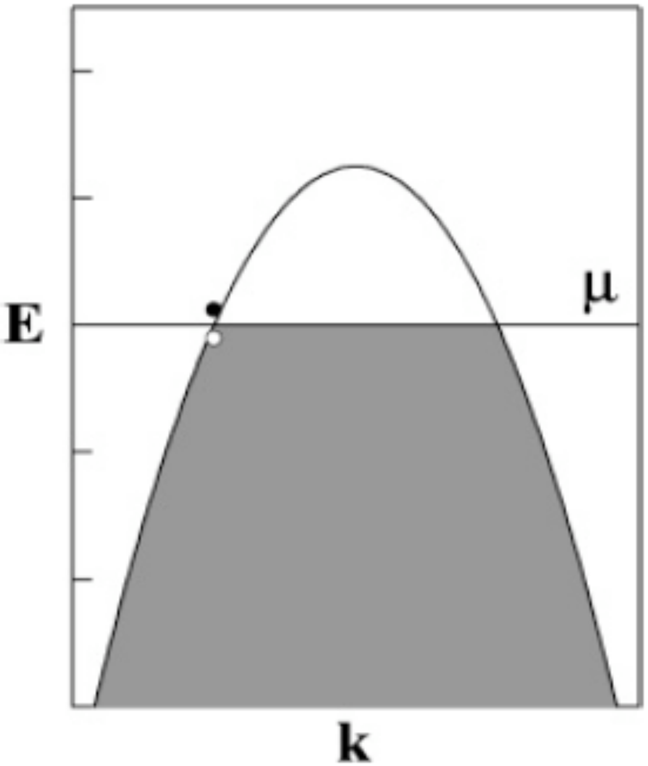


Mott-Hubbard insulator

Non-interacting Limit

- metallic
- bandwidth ~ 8*t* ~ 3 eV

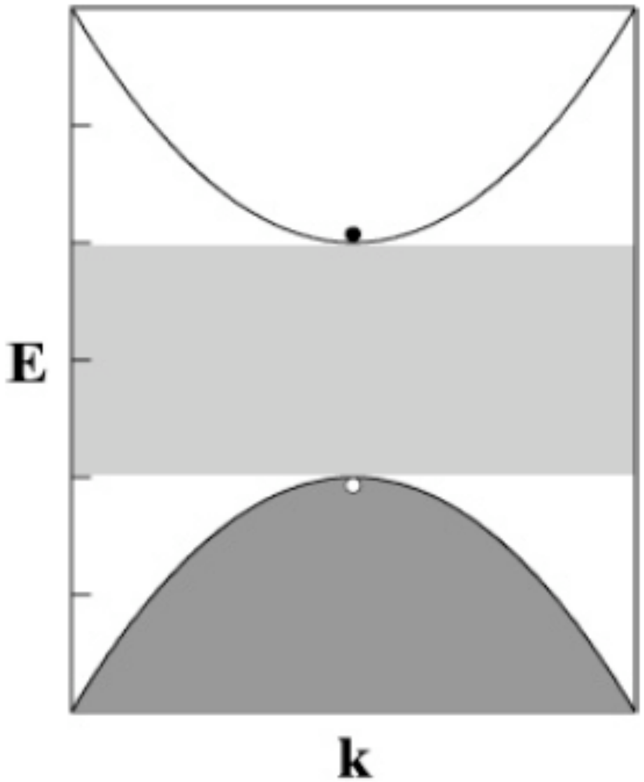
Metal



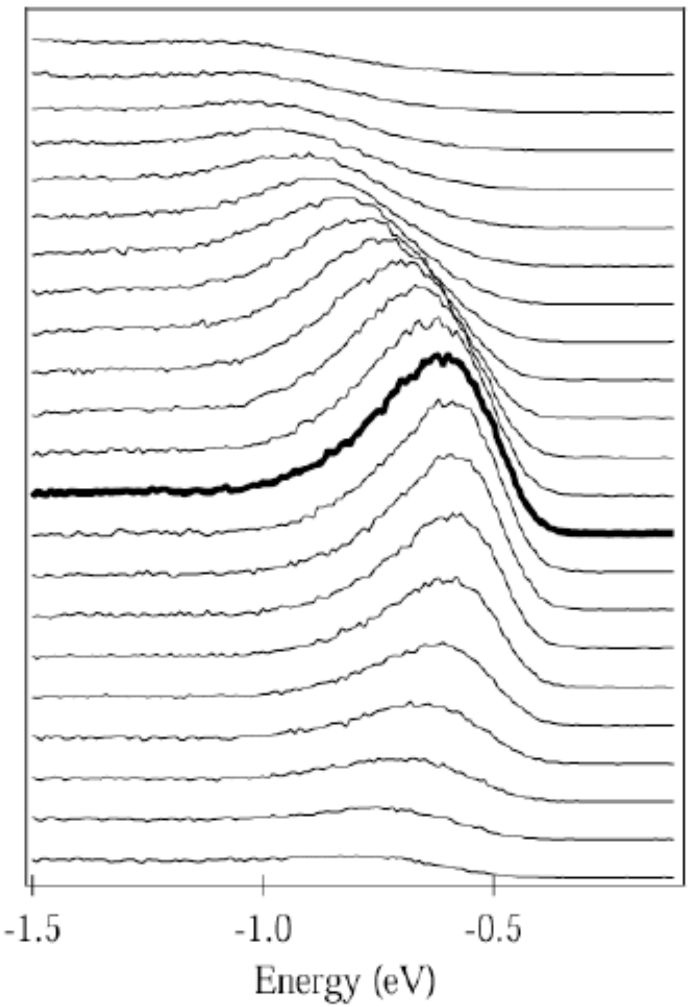
Strongly Interacting (Mott) Limit

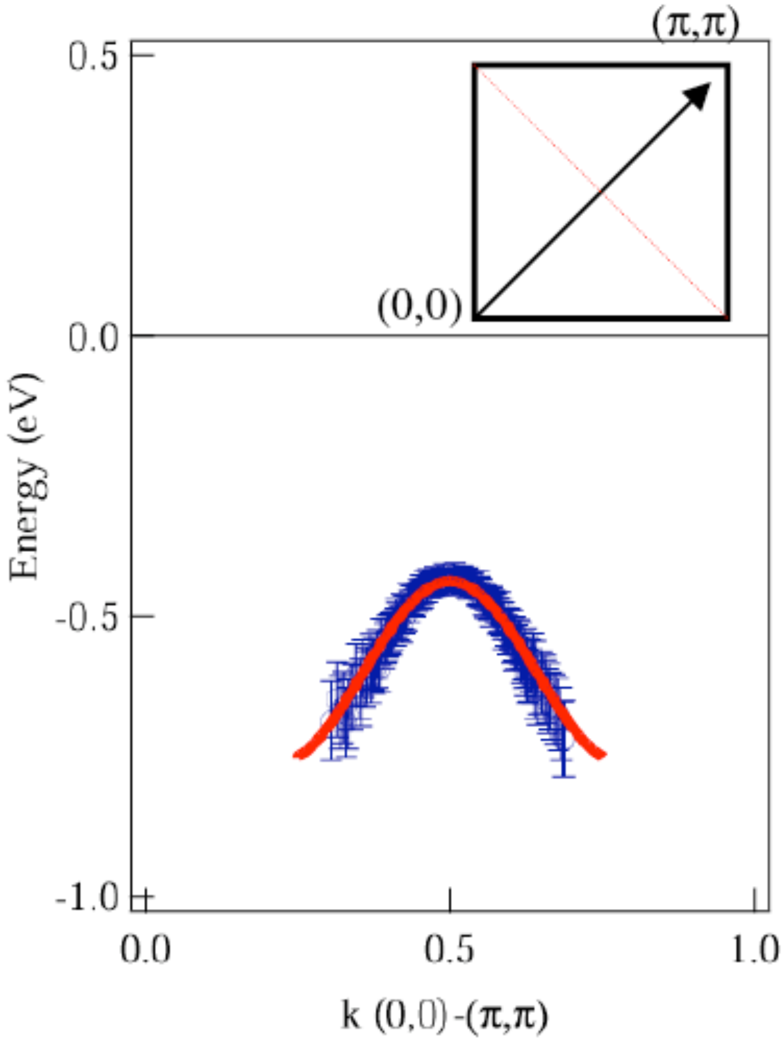
- insulating (Δ ~ 2 eV)
- antiferromagnetic
- bandwidth ~ 2*J* ~ 0.3 eV

Insulator

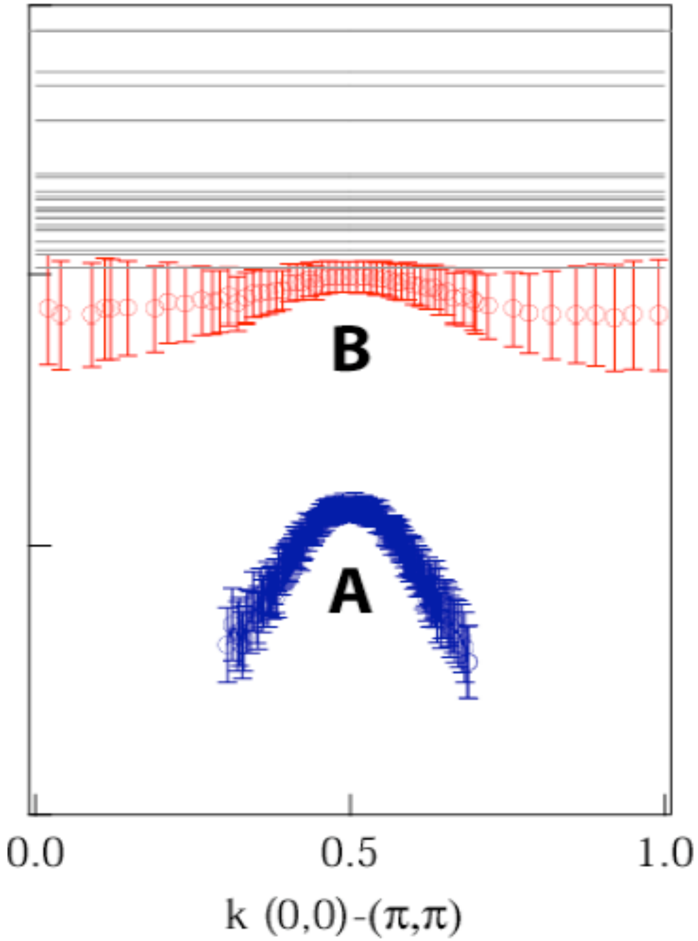


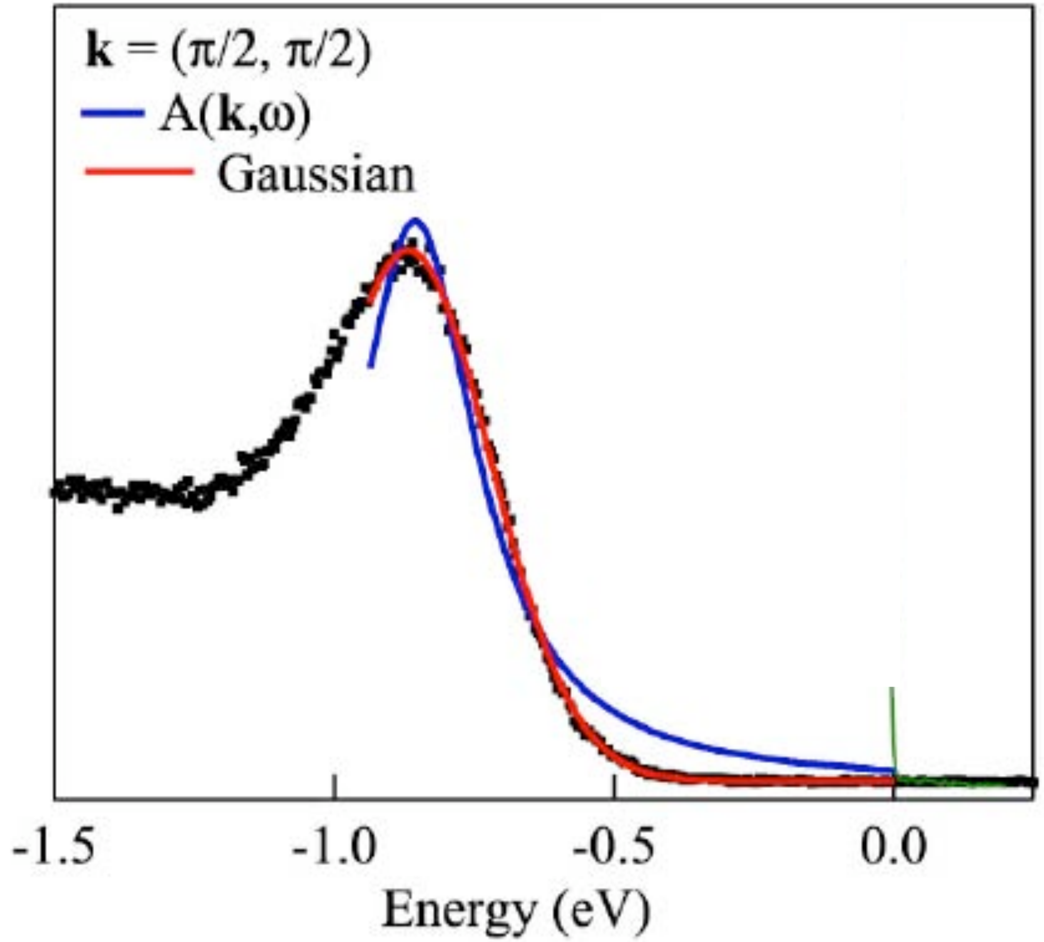
$Ca_{2-x}Na_xCuO_2Cl_2$: at x=0 Mott-Hubbard insulator





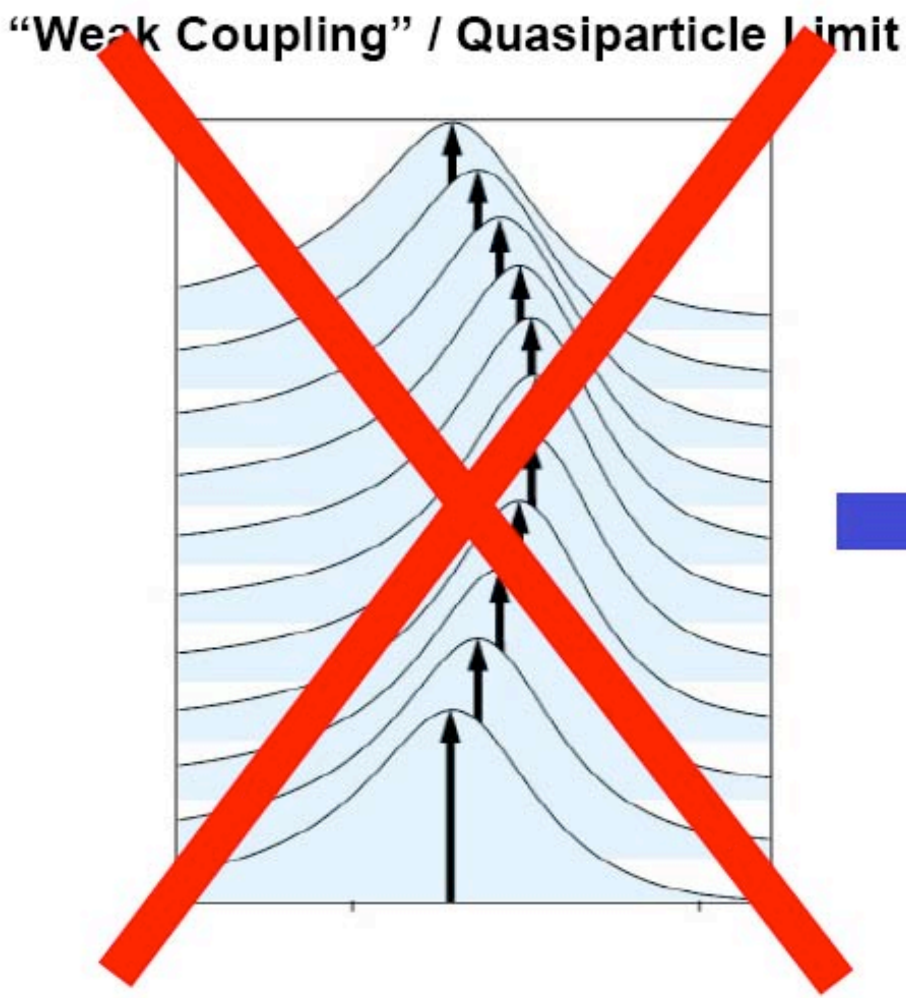
- Dispersion of peak intensity follows *t-J* model well
- Suggests quasiparticle excitations from *t-J* model are appropriate
- However, this is not the end of the story....

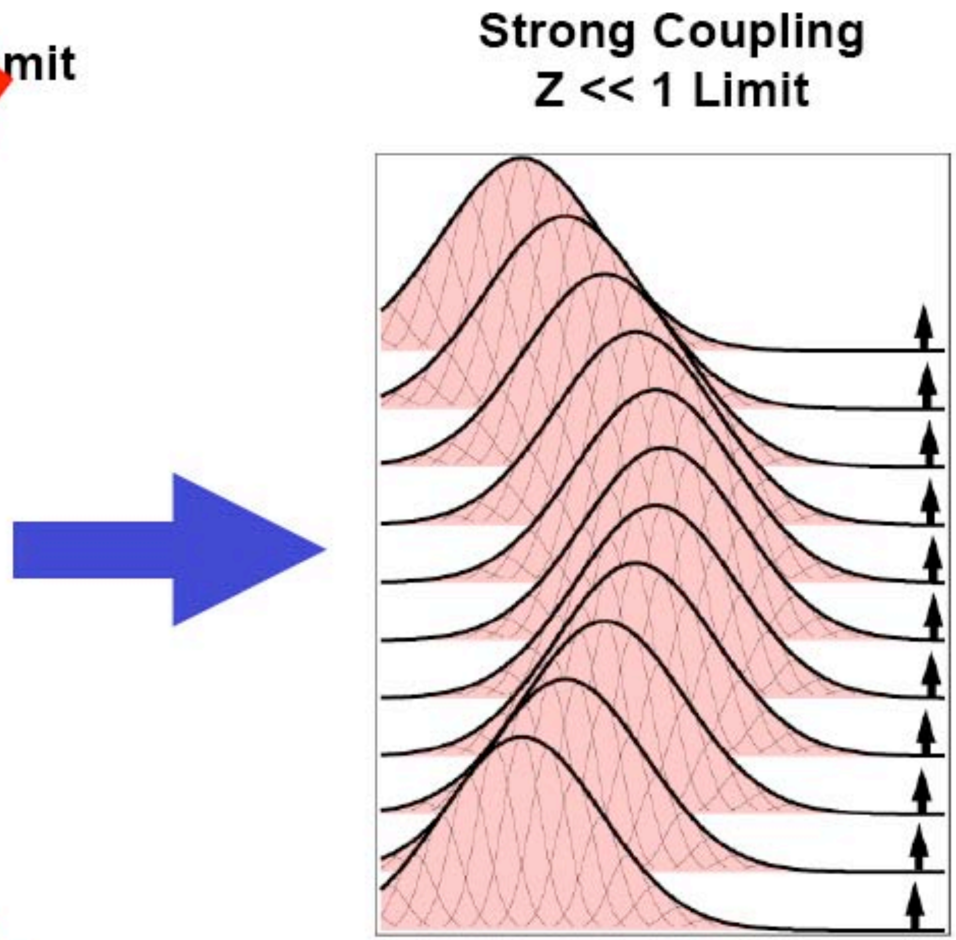




$$A(\mathbf{k},\omega) \propto \frac{\mathrm{Im}\Sigma(\mathbf{k},\omega)}{[\omega - \varepsilon_k - \mathrm{Re}\Sigma(\mathbf{k},\omega)]^2 + [\mathrm{Im}\Sigma(\mathbf{k},\omega)]^2}$$

- Spectral function formalism **FAILS** to qualitatively describe lineshape
- Linewidth far too broad

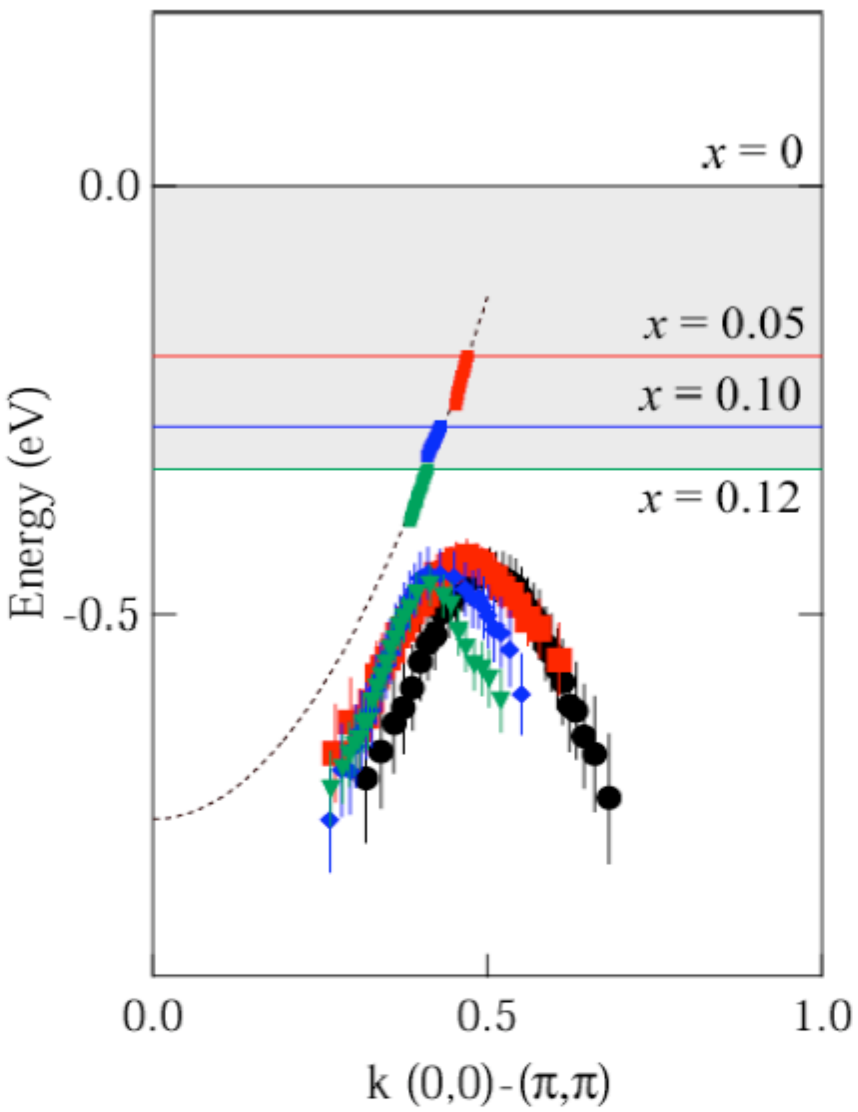


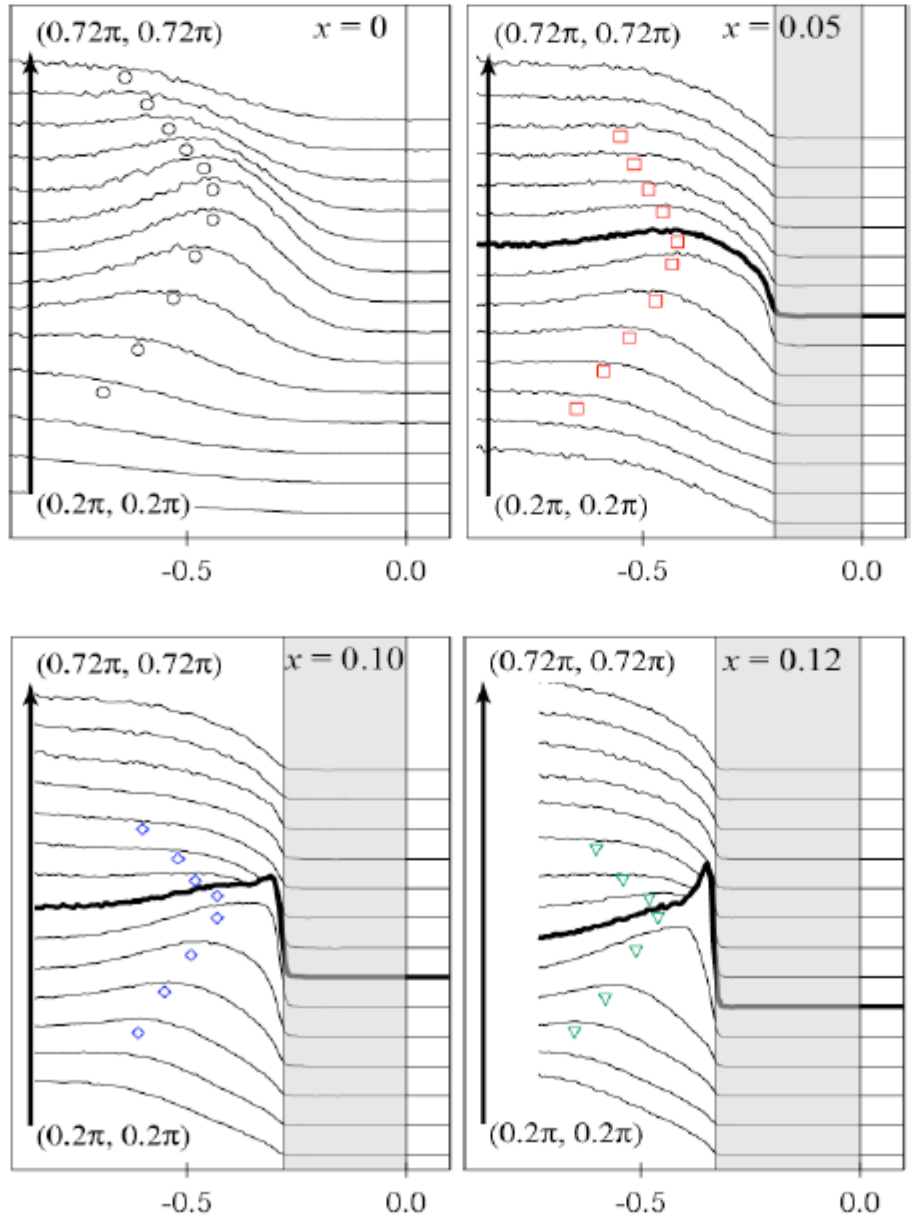


Polaron formation

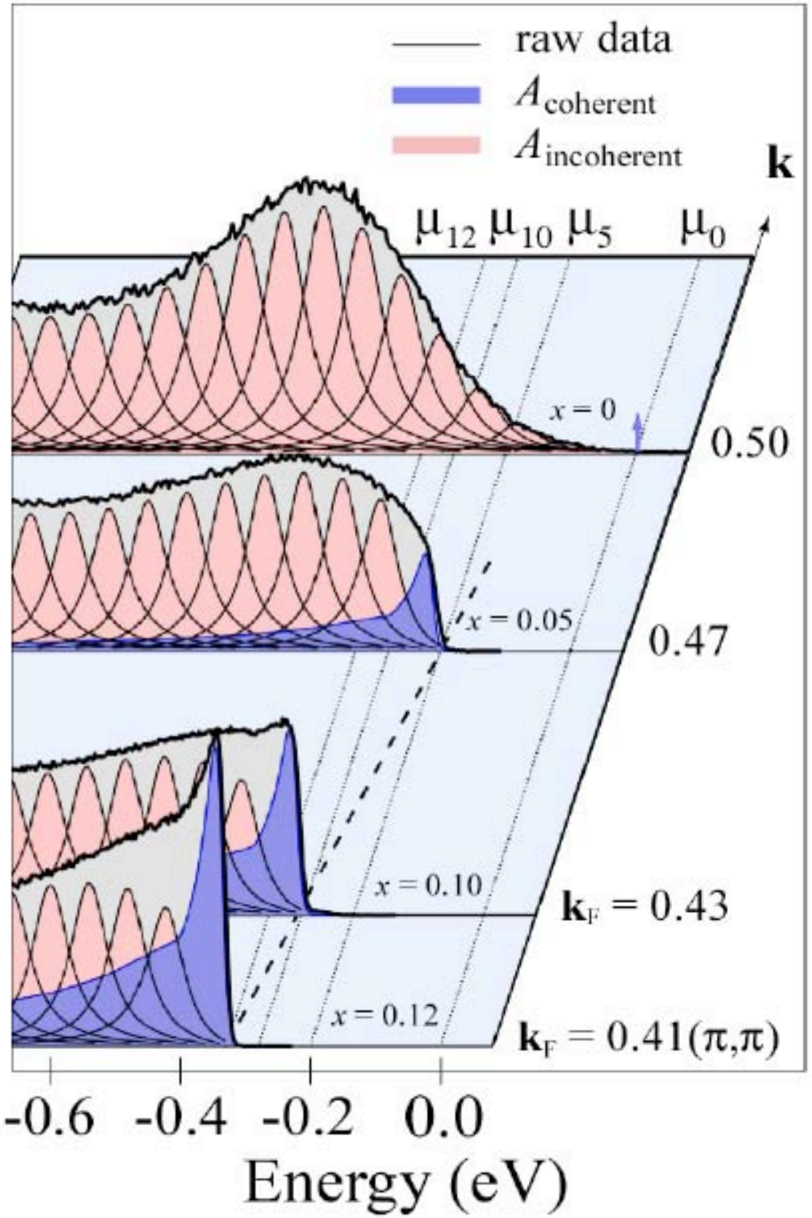
- Consistent with extreme width
- Explains anomalous lineshape
- Justifies positions of chemical potential
- Vast majority of spectral weight in *incoherent* transitions

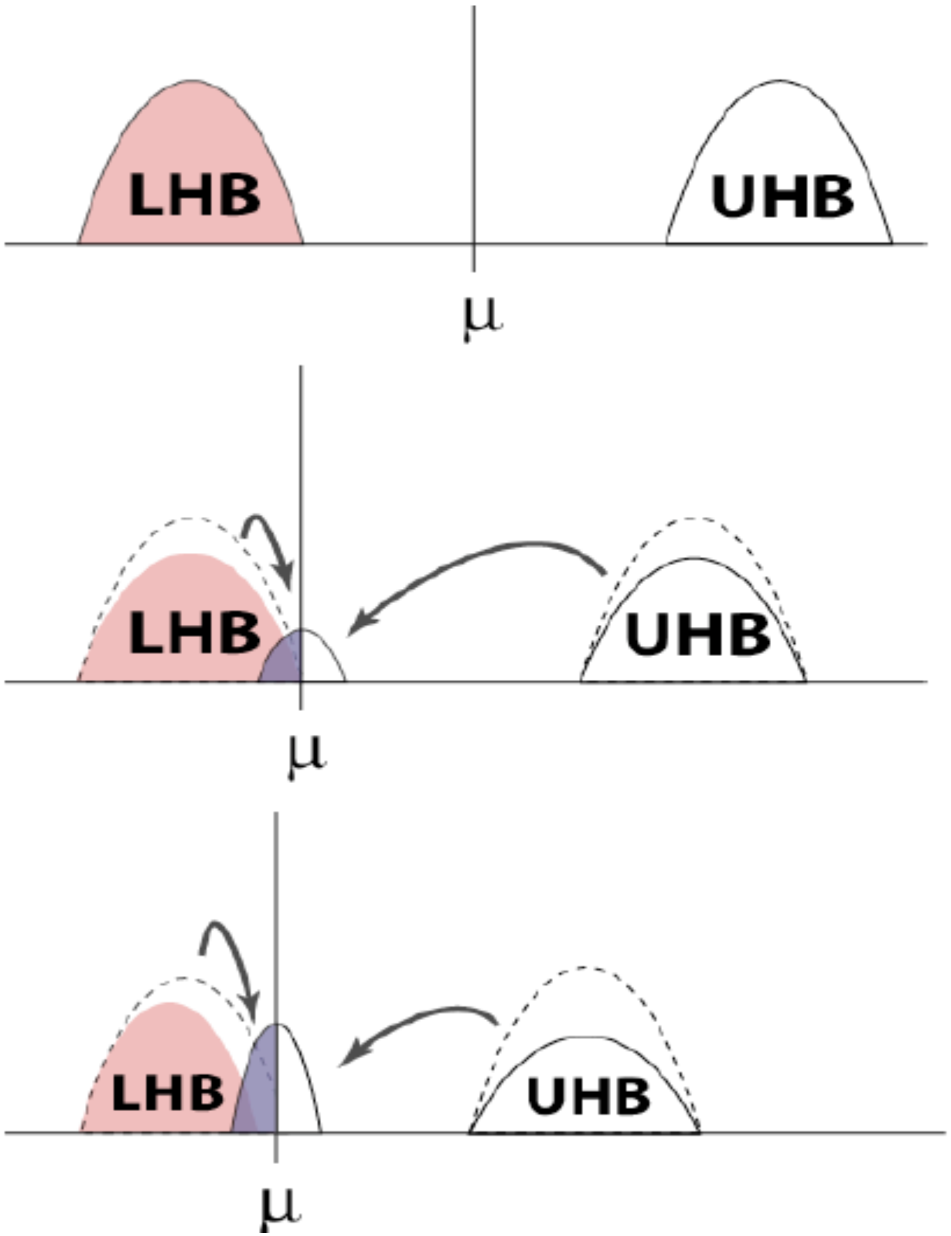
$Ca_{2-x}Na_xCuO_2Cl_2$: doping dependence

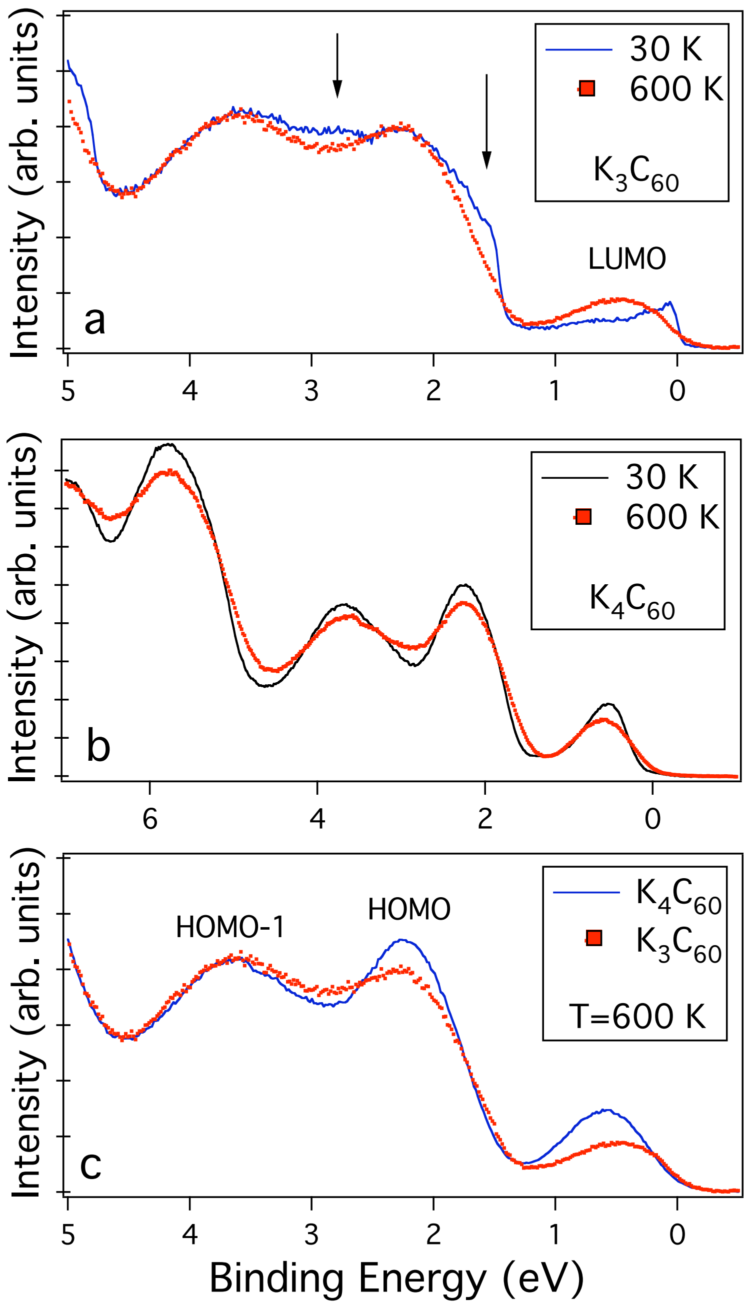




$Ca_{2-x}Na_xCuO_2Cl_2$: doping dependence

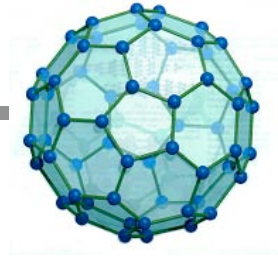






A. Goldoni, L. Sangaletti, S.L. Friedmann, Z.-X. Shen, M. Peloi, F. Parmigiani, G. Comelli and G. Paolucci, J. Chem. Phys. 113, 8266 (2000)

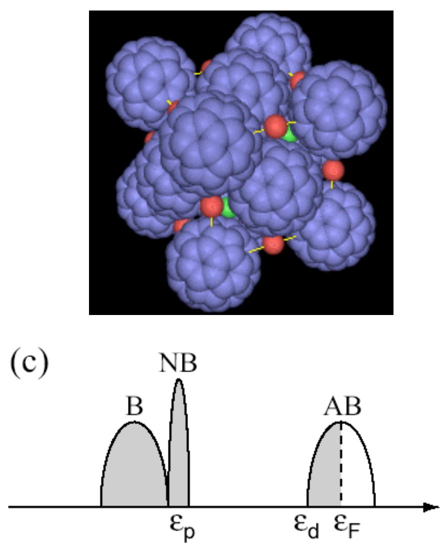
Fullerenes

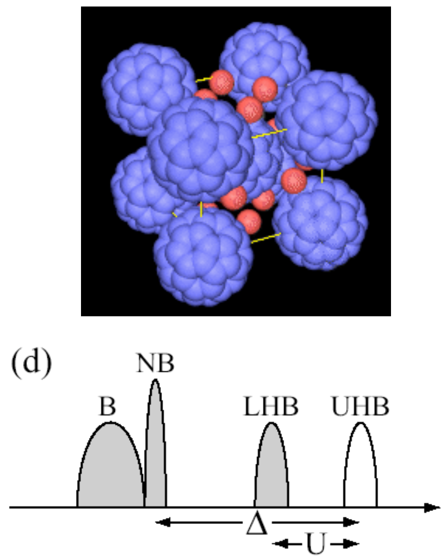


Strongly correlated metal

Strong correlations U ~ 1 - 1.3 eV
Small band dispersion W ~ 0.5 - 0.6 eV
Orbital degeneracy (HOMO 5 fold, LUMO 3 fold)
Small Fermi energy ~ 0.25 eV
Phonon spectrum up to 0.2 eV
Jahn-Teller distortions in charged C_{60}
E_{JT}~ 0.03-0.18 eV for C_{60}^{n-}

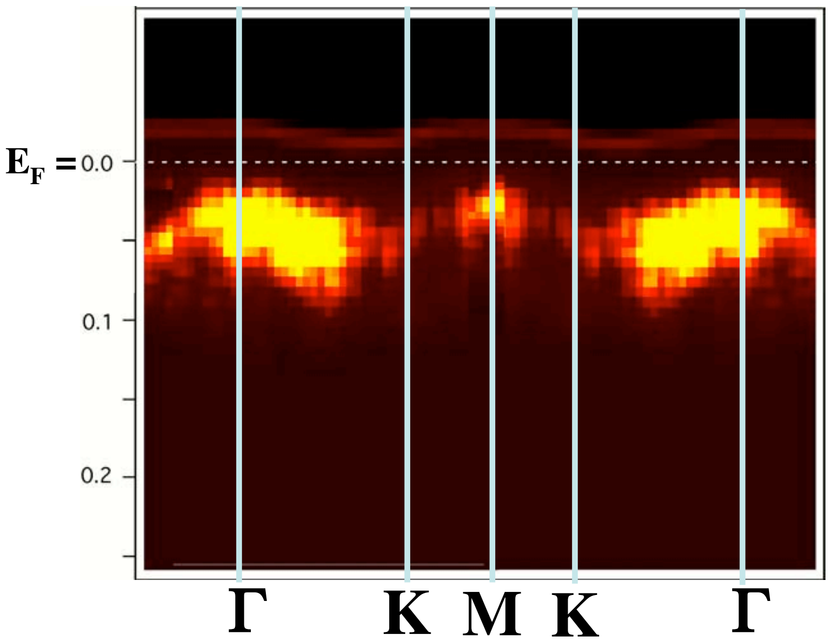
Mott-Hubbard insulator

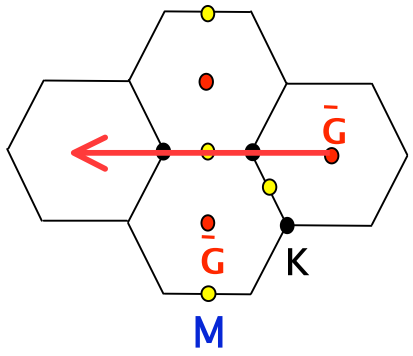


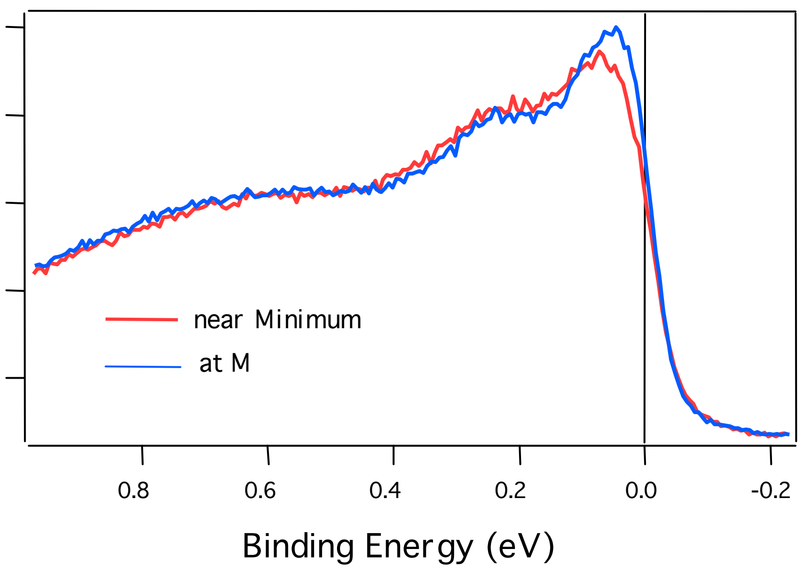


Band dispersion of $K_3C_{60}(111)$

Dispersion < 100 meV







Spectrum dominated by phonon and plasmon excitations; quasi-particle coherent peak confined near E_F