International Seminar and Workshop on

Strong Correlations and ARPES: Recent Progress in Theory and Experiment

5. April 2005

Spectral densities of strongly correlated electron systems

Green's function: $$G_\nu(\mathbf{k},\omega) = \frac{1}{\omega - \varepsilon_\nu(\mathbf{k}) - \Sigma_\nu(\mathbf{k},\omega)}$$

quasiparticle pole:

$$G(\mathbf{k},\omega) = \frac{Z}{\omega - \varepsilon_{\mathrm{qp}}(\mathbf{k}) - \mathrm{i}\gamma_{\mathrm{k}}\,\mathrm{sgn}\,\omega} + G_{\mathrm{inc}}(\mathbf{k},\omega)$$

Here: special focus on $G_{\mathrm{inc}}(\mathbf{k},\omega)$

Aim: to show that $G_{\mathrm{inc}}(\mathbf{k},\omega)$ consists of excitations involving

internal degrees of freedom of the correlation hole

- with dispersions
- simplest example: shadow band

Formalism:

retard. Green fct.
$$G_\sigma(\mathbf{k},t) = -i\Theta(t)\left\langle \psi_0 \left| \left[c_\sigma(\mathbf{k},t), c_\sigma^+(\mathbf{k}) \right]_+ \right| \psi_0 \right\rangle$$

notation:
$$(A \mid B)_+ = \left\langle \psi_0 \left| \left[A^+, B \right]_+ \right| \psi_0 \right\rangle$$

choice of operators which generate the correlation hole:
$$c_\sigma^+(i), A_n(i) \Rightarrow \{A_\nu(i)\}$$
$$\Longrightarrow \{A_\nu(\mathbf{k})\}$$

Green's function matrix:
$$G_{\mu\nu}(\mathbf{k},t) = -i\Theta(t)\left(A_\mu(\mathbf{k},t) \middle| A_\nu(\mathbf{k}) \right)_+$$

with:
$$LO = [H,O]_- = i\frac{dO}{dt} \Longrightarrow O(t) = e^{iLt}O$$

$$G_{\mu\nu}(\mathbf{k},z) = \left(A_\mu \middle| \frac{1}{z-L} A_\nu \right)_+$$

formal solution

$$\left[z\underline{\underline{1}} - \left(\underline{\underline{L}} + \underline{\underline{M}}(z)\right)\underline{\underline{\chi}}^{-1}\right]\underline{\underline{G}}(z) = \underline{\underline{\chi}}$$

with matrix elements

$$L_{\mu\nu} = \left(A_\mu \middle| L A_\nu\right)_+$$

$$M_{\mu\nu} = \left(A_\mu \middle| LQ \frac{1}{z - QLQ} QLA_\nu\right)_+$$

$$\chi_{\mu\nu} = \left(A_\mu \middle| A_\nu\right)_+$$

Q projects onto space perpendicular to A_ν : $\quad Q = 1 - \sum_{\mu\nu} \left|A_\mu\right)_+ \chi^{-1}_{\mu\nu} \left(A_\nu\right|$

remain within space spanned by $\{A_\nu\}$ ⟹ $\underline{\underline{M}}(z) = 0$

⟹ matrix equation has dimensions $N_A \times N_A \quad ; \quad N_A = \# A_\nu$

Applications: 1- band Hubbard model

$$H = -t\sum_{\langle ij\rangle\sigma}\left(c^{+}_{i\sigma}c_{j\sigma} + h.c.\right) + U\sum_{i} n_{i\uparrow}n_{i\downarrow}$$

$$A_1(i) = c^{+}_{i\sigma}\ , A_2(i) = c^{+}_{i\sigma}\delta n_{i-\sigma} \qquad \delta n_{i-\sigma} = n_{i-\sigma} - \langle n_{i-\sigma}\rangle$$

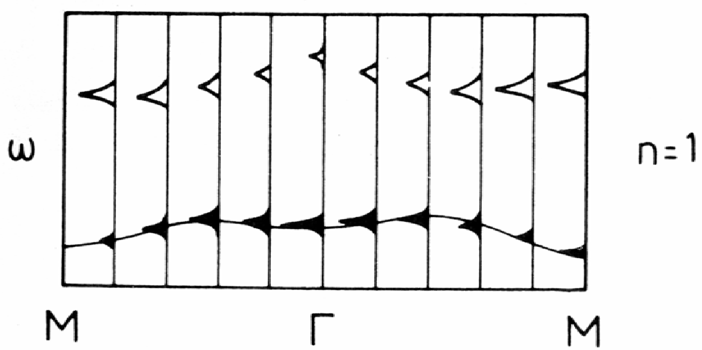
$$A_1(\mathbf{k}) = c^{+}_{\mathbf{k}\sigma}\ ,\ A_2(\mathbf{k}) = \frac{1}{\sqrt{N_0}}\sum_{i} e^{i\mathbf{k}\mathbf{R}_i}c^{+}_{i\sigma}\delta n_{i-\sigma}$$

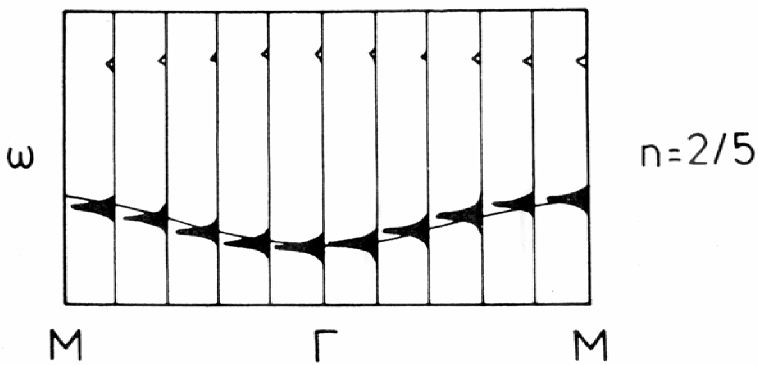
solve 2 x 2 matrix

$$G_{11}(\mathbf{k},z) = \frac{1-n/2}{z-\varepsilon(\mathbf{k})\left(1-n/2\right)} + \frac{n/2}{z-U-\varepsilon(\mathbf{k})n/2}$$

Hubbard I approximation , lower + upper Hubbard band

filling $n = \frac{2}{5}$ → shadow band


ω
n=1
M
Γ
M


ω
n=2/5
M
Γ
M

Application: Ni (paramgnetic):

5-band Hubbard model:

$$H = \sum_{\mathbf{k}\nu\sigma} \varepsilon_\nu(\mathbf{k}) n_{\nu\sigma}(\mathbf{k}) + \frac{1}{2} \sum_{\ell\sigma\sigma'} \sum_{ijmn} V_{ijmn} c^+_{i\sigma}(\ell) c^+_{m\sigma'}(\ell) c_{n\sigma'}(\ell) c_{j\sigma}(\ell)$$

i,j,m,n = orbit. indices , ℓ = site index

$$V_{ijmn} = U_{im}\delta_{ij}\delta_{mn} + J_{ij}\left(\delta_{in}\delta_{jm} + \delta_{im}\delta_{jn}\right)$$

$$U_{im} = U + 2J - 2J_{im}$$

$J_{im} =$ exchange matrix (anisotropies)

choise of $\left\{A_\nu\right\}$

$$A^{(0)}_\nu(\mathbf{k}) = c^+_{\nu\uparrow}(\mathbf{k})$$

$$A^{(1)}_{ij}(\ell) = \begin{cases} c^+_{i\uparrow}(\ell)\delta n_{i\downarrow}(\ell) & i = j \\ c^+_{i\uparrow}(\ell)\delta n_j(\ell) & i \neq j \end{cases}$$

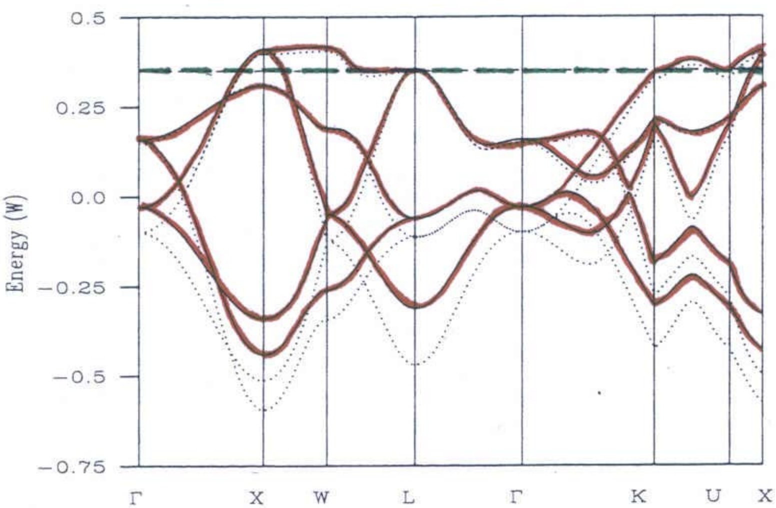
$$A^{(2)}_{ij}(\ell) = c^+_{i\uparrow}(\ell) s^z_j(\ell) + c^+_{i\downarrow}(\ell) s^+_j(\ell)$$

$$A^{(3)}_{ij}(\ell) = c^+_{j\downarrow}(\ell) c^+_{j\uparrow}(\ell) c_{i\downarrow}(\ell)$$

$$A^{(\alpha)}_{ij}(\mathbf{k}) = \frac{1}{\sqrt{N_0}} \sum_\ell A^{(\alpha)}_{ij}(\ell) e^{i\mathbf{k}\mathbf{R}_\ell}$$

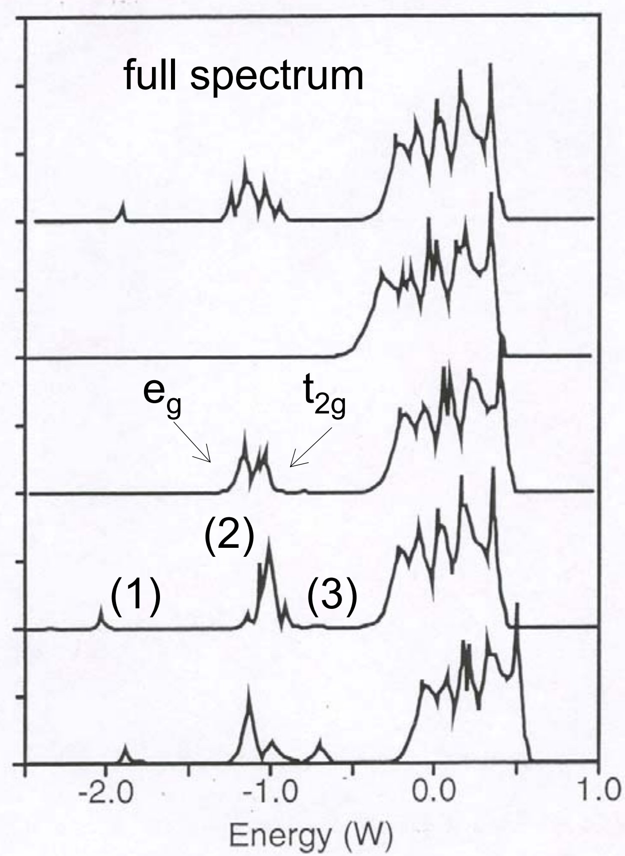
total #: 1 + 25 + 20 + 20 = 66

Results for paramagnetic Ni



reduction of bandwidth

n_d=9.4



(1) ^1S
(2) ^1G; ^1D
(3) ^3P; ^3F

U = 0.56
J = 0.22
ΔJ = 0.031

HF result

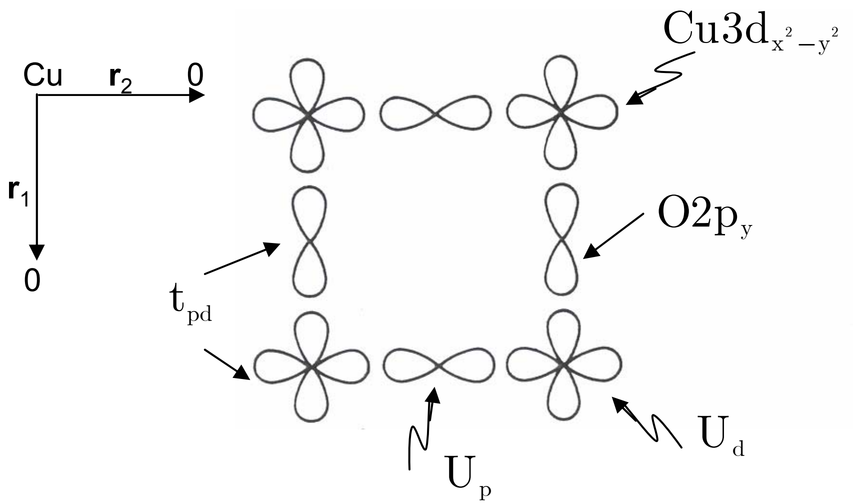
J = ΔJ = 0

J = 0.22

full spectr. but with Ω = 1

(Unger, Igarashi)

Application: CuO planes



1 hole per CuO_2

$\varepsilon_p - \varepsilon_d = 3.6\,\mathrm{eV}$

$t_{pd} = 1.3\,\mathrm{eV}$

$U_d = 10.5\,\mathrm{eV}$

$U_p = 4\,\mathrm{eV}$

3 band Hubbard Hamiltonian (hole representation)

$$H = \sum_{m\mathbf{k}\sigma} \varepsilon_{\mathbf{m}}(\mathbf{k})\, p^+_{m\mathbf{k}\sigma} p_{m\mathbf{k}\sigma} + U_p \sum_j n_{p\uparrow}(j) n_{p\downarrow}(j)$$
$$+ \varepsilon_d \sum_{\mathbf{k}\sigma} \mathbf{d}^+_{\mathbf{k}\sigma} d_{\mathbf{k}\sigma} + U_d \sum_i n_{d\uparrow}(i) n_{d\downarrow}(i)$$
$$+ 2t_{pd} \sum_{m\mathbf{k}\sigma} \left(\phi_{\mathbf{mk}} p^+_{m\mathbf{k}\sigma} d_{\mathbf{k}\sigma} + \phi^*_{m\mathbf{k}} d^+_{\mathbf{k}\sigma} p_{m\mathbf{k}\sigma} \right)$$

with

$$\varepsilon_m(\mathbf{k}) = \varepsilon_p \pm 2t_{pp} \left[\cos \mathbf{k}(\mathbf{r}_1 + \mathbf{r}_2) - \cos \mathbf{k}(\mathbf{r}_1 - \mathbf{r}_2)\right]$$

$$\phi_{m\mathbf{k}} = \frac{-i}{\sqrt{2}} \left[\sin \mathbf{k}\mathbf{r}_1 \pm \sin \mathbf{k}\mathbf{r}_2\right] \qquad m = 1, 2$$

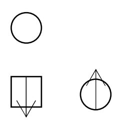
choice of variables $\{A_\nu\}$:

$$A_p(i) = p^+_\uparrow(i) \quad , \quad A_d(j) = d^+_\uparrow(j)$$

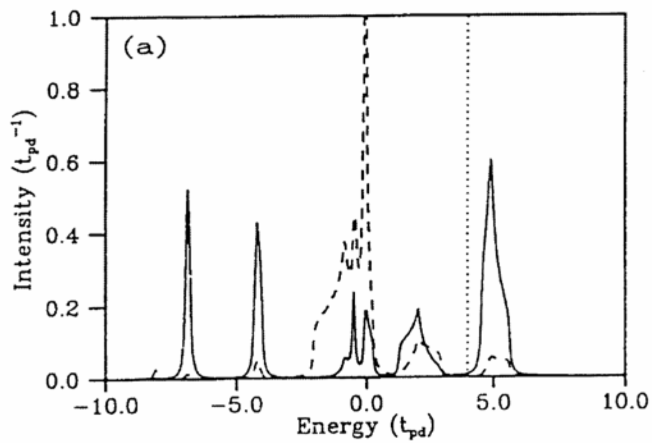
$$\bar{A}_p(i) = p^+_\uparrow(i)\delta n_{p\downarrow}(i) \quad , \quad \bar{A}_d(j) = d^+_\uparrow(j)\delta n_{d\downarrow}(j)$$

$A_a(i,\delta) = p^+_\uparrow(i) n_{d\downarrow}(i+\delta)$ AF , $A_f(i,\delta) = p^+_\downarrow(i) S^+_d(i+\delta)$ spin flip

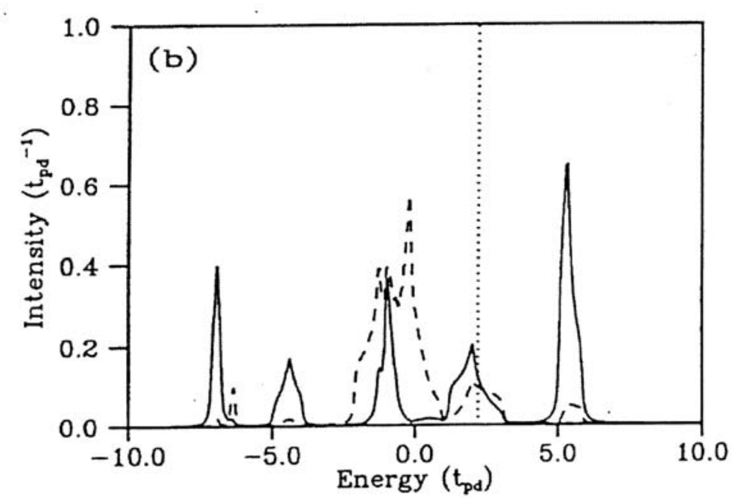
$A_c(i,\delta,\delta') = p^+_\uparrow(i) p^+_\downarrow(i+\delta') d_\downarrow(i+\delta)$ charge transfer $d \rightarrow p$



for each **k** point 9 x 9 matrix

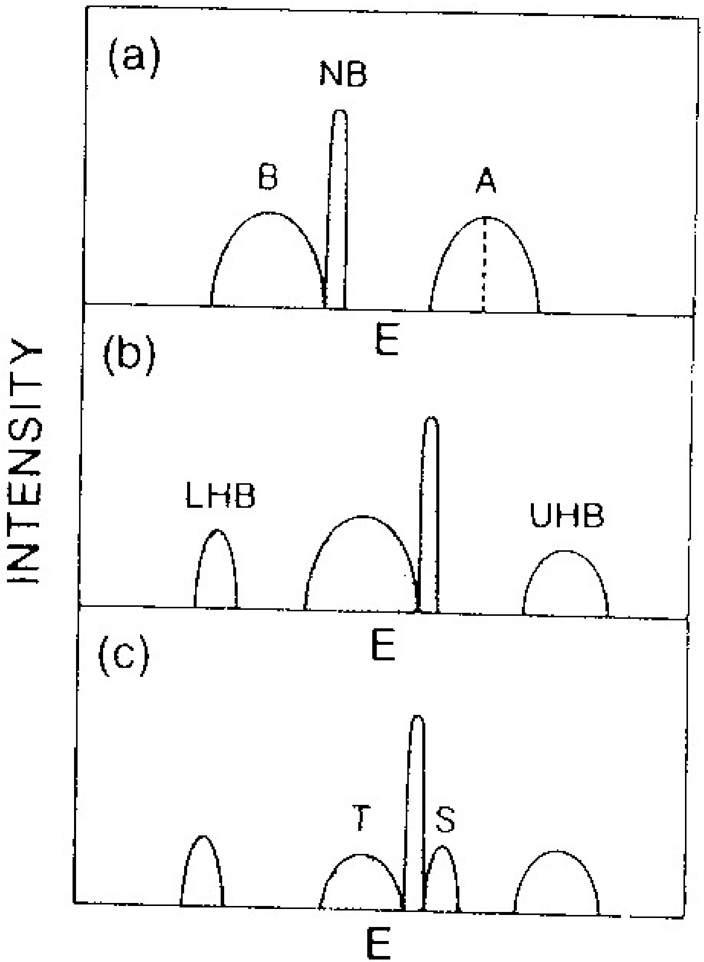


half-filling

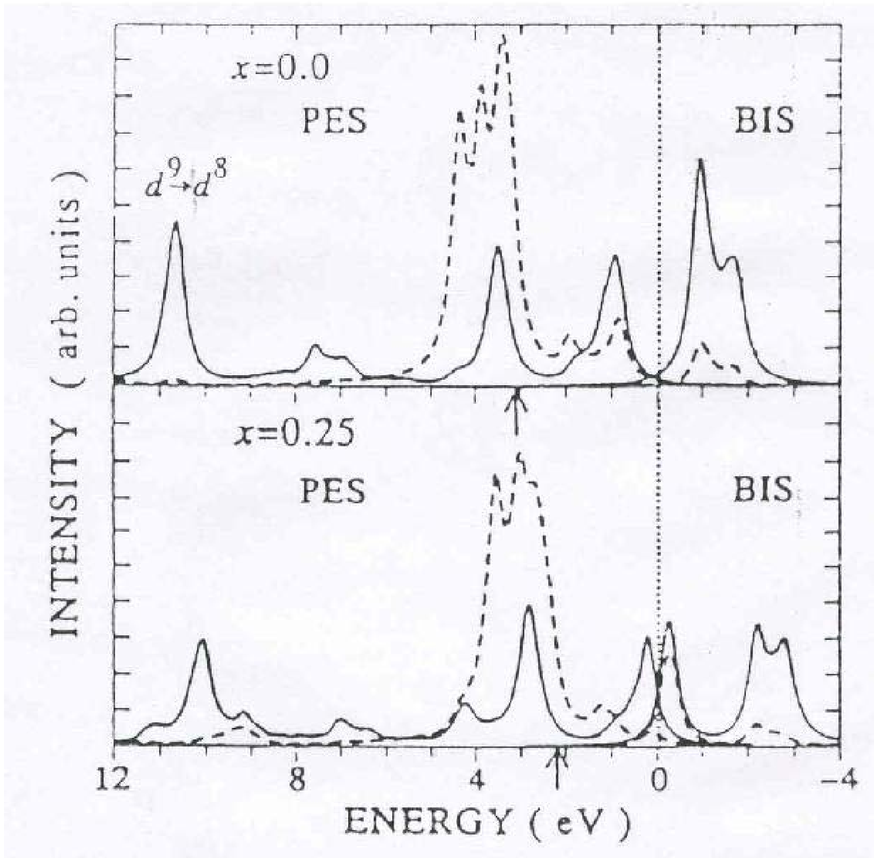


25 % holes

P. Unger



schematic spectral density



exact diagonalization of $(CuO)_4$ cluster

(Tohyama + Maekawa)

Application: Marginal Fermi liquid behavior

Hubbard model: $$H = -t\sum_{\langle ij\rangle\sigma}\left(c^{+}_{i\sigma}c_{j\sigma} + \mathrm{h.c.}\right) + U\sum_{i} n_{i\uparrow}n_{i\downarrow} = H_0 + H_1$$

⟹ $A(\mathbf{k}) = c^{+}_{\mathbf{k}\sigma}$ *but* keeping memory fct.

$$G(\mathbf{k},z) = \frac{1}{z - \varepsilon(\mathbf{k}) - U^2 M(\mathbf{k},\omega)}$$

projection method combined with CPA

Fourier transf. $$M_{ij}(z) = \left(c^{+}_{i\sigma}\delta n_{i-\sigma}\left|\frac{1}{z-\overline{L}}c^{+}_{j\sigma}\delta n_{j-\sigma}\right.\right) \qquad \overline{L} = QLQ$$

coherent potential: $\widetilde{H}(z) = H_0 + \widetilde{\Sigma}(z)\sum_i n_i$ with corresp. $\widetilde{L}(z)$

$$\overline{L} = Q\widetilde{L}Q + \sum_i L_I^{(i)}(z) \quad , \quad L_I^{(i)} = Q\left(U\delta n_{i\uparrow}\delta n_{i\downarrow} - \widetilde{\Sigma}(z)n_i\right)Q$$

expand $\frac{1}{z-\overline{L}}$ in terms of $L_I^{(i)}$ ⟶ scatter. problem

T maxtrix: decompose into $T = \sum_i T_i + \sum_{\langle ij \rangle} \delta T_{ij} + \sum_{\langle ijk \rangle} \delta T_{ijk} + \ldots$

limit yourself to two-particle cluster approximation: $T_i, \delta T_{ij}$

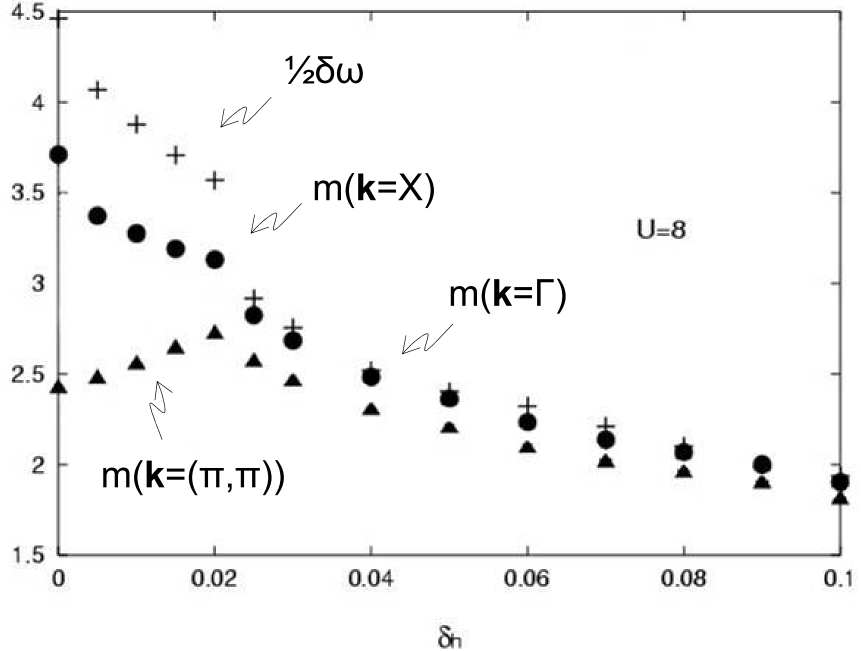
important: i and j may be far apart

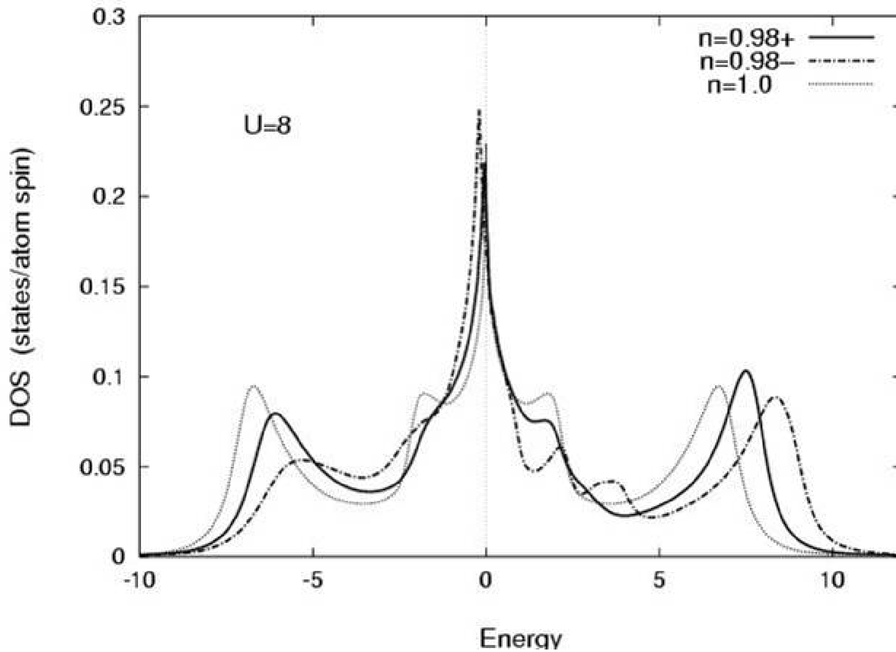
solve equat. with self-consist. coher. pot.

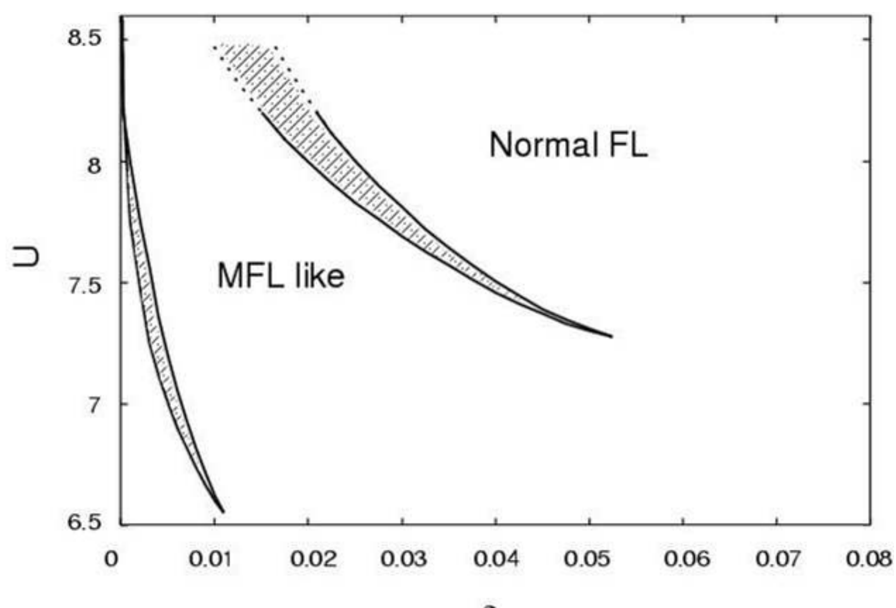
$$\widetilde{\Sigma}(z) = \frac{U^2}{N} \sum_{\mathbf{k}} M(\mathbf{k}, \omega)$$

$$m_{\mathbf{k}} = 1 - U^2 \, \mathrm{Re} \left. \frac{\partial M(\mathbf{k}, \omega)}{\partial \omega} \right|_{\omega = 0^+}$$

one finds $m_{\mathbf{k}} \sim \ln \delta\omega$


½δω
m(k=X)
m(k=Γ)
m(k=(π,π))
U=8
δh


n=0.98+
n=0.98–
n=1.0
U=8
DOS (states/atom spin)
Energy


Normal FL
MFL like
U

(Y. Kakehashi)