Generalized Dynamical Mean - Field Theory for Strongly Correlated Systems

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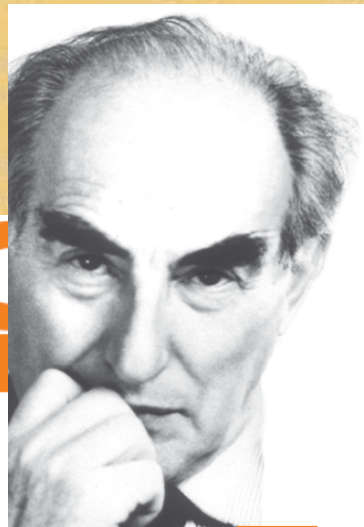
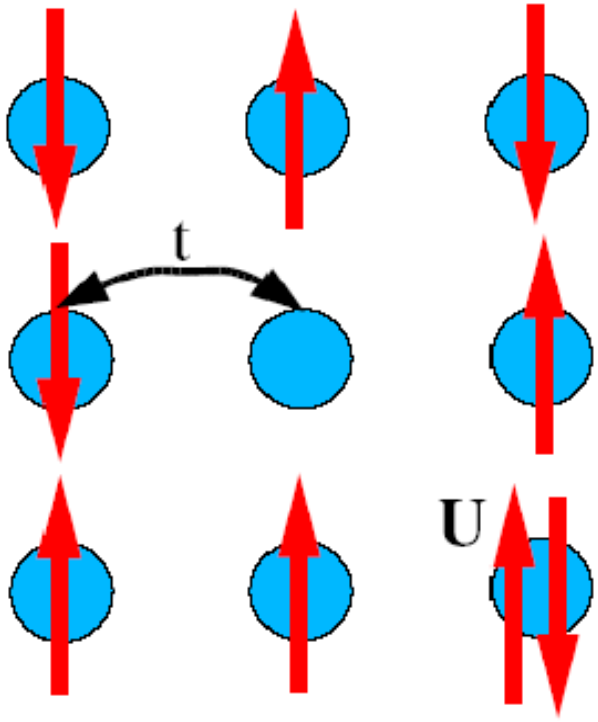
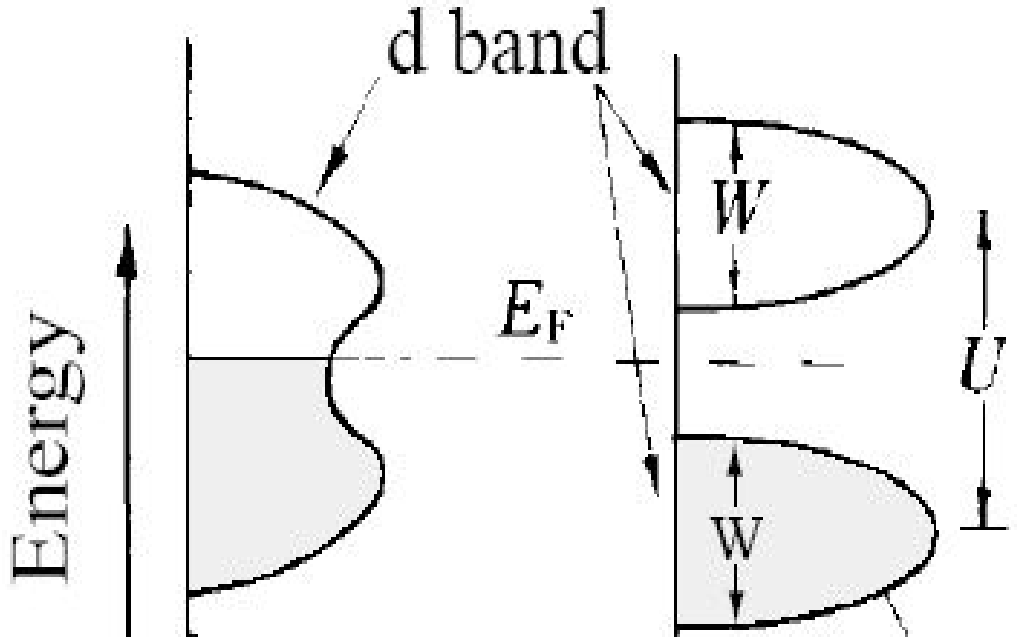


Hubbard model

J.Hubbard (1964)

$$H = -\sum_{ij,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$



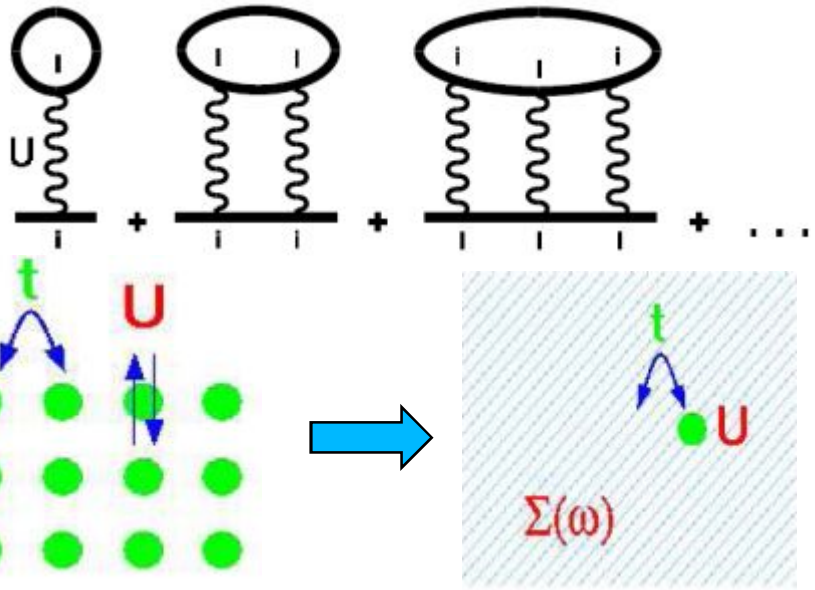


Correlated Metal Mott Insulator

Traditional DMFT approach

$$H = -\sum_{ij,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

J.Hubbard (1964)



In the limit of spatial dimensionality

$$d \to \infty$$

self - energy becomes ***local***, i.e.

$$\Sigma_{\mathbf{k}}(i\omega) \to \Sigma(i\omega)$$

Then the problem can be ***exactly*** (!) mapped on the equvalent problem of Anderson impurity, which is to be solved by some kind of "impurity solver" (QMC, CTQMC, NRG, NCA etc.)

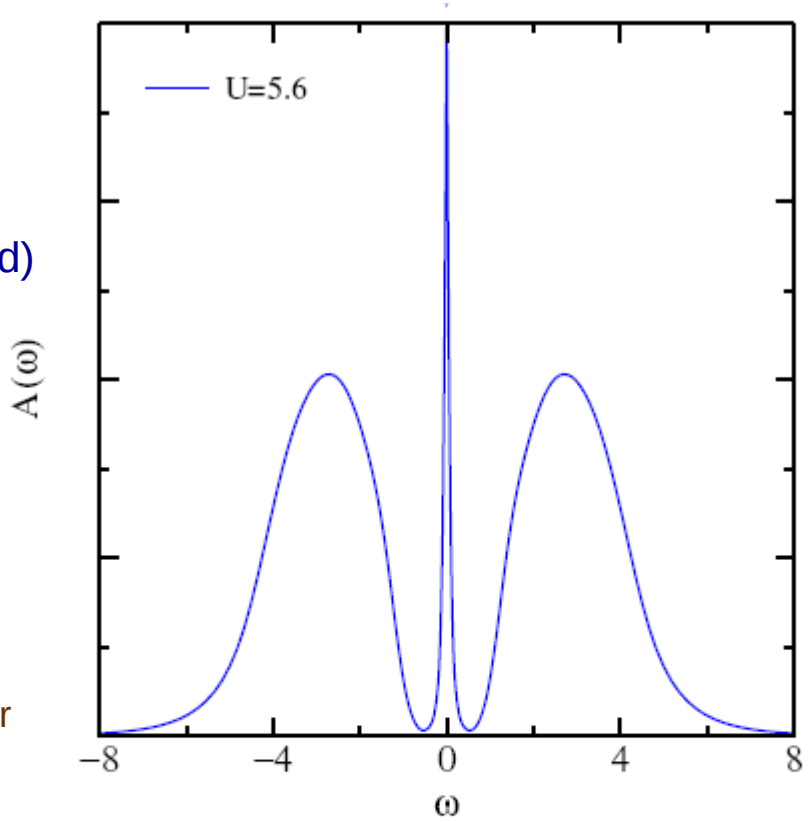
W.Metzner, D.Vollhardt, 1989, A.Georges, G.Kotliar, 1992, Th.Pruschke, M.Jarrell, 1992

The absence of **k** - dependence of electron self - energy is the basic shortcoming of the traditional DMFT, however only due to this fact we obtain an exact solution!

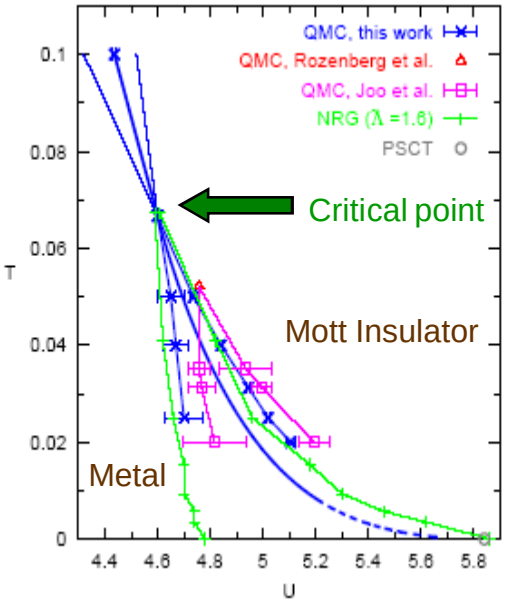
Numerical Results

$$N(\omega) = -\frac{1}{\pi}\mathrm{Im}G(\omega)$$

Standard DMFT results demonstrate formation of Hubbard bands and quasiparticle (Fermi - liquid) band at the Fermi level.



Metal - insulator transition at ***U=6***.



$W=2D=2Zt=4$

$U_c=1.5W=6$

Energies here in units of t for $Z=4$ (square lattice)

Metal – Fermi liquid

$$\Sigma(\omega) = (1-\frac{1}{Z})\omega - iB\omega^2 + \mathcal{O}(\omega^3)$$

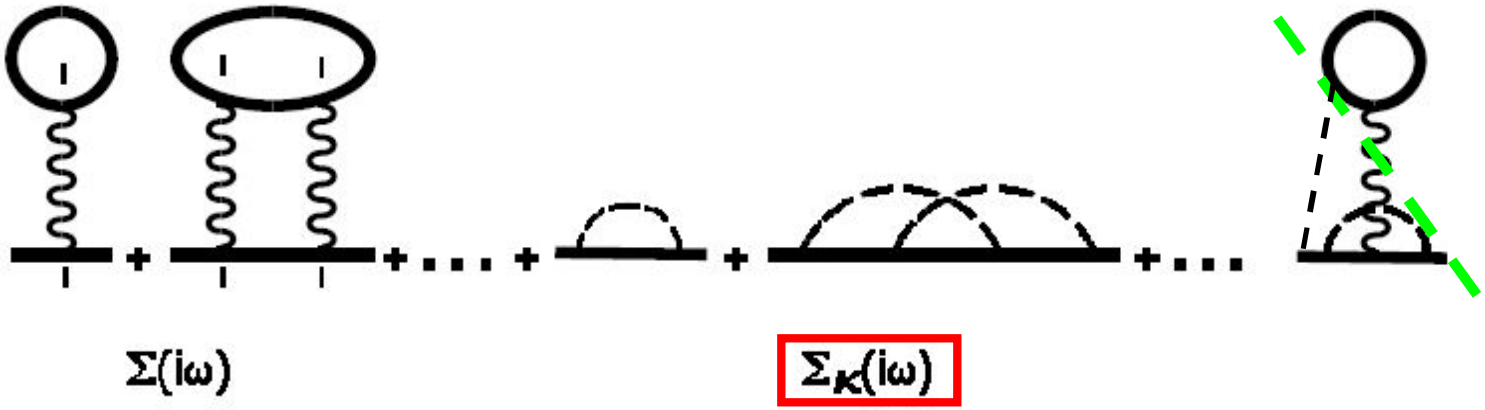
$$\frac{m^*}{m} = \frac{1}{Z} = 1 - \frac{\partial \mathrm{Re}\Sigma(\omega+i0^+)}{\partial\omega}\Big|_{\omega=0}$$

Basics of DMFT+Σ approach

- DMFT+Σ:

M.V.Sadovskii, I.A.Nekrasov, E.Z.Kuchinskii, Th.Pruschke, V.I.Anisimov (2005)

$$G_{\mathbf{k}}(i\omega) = \frac{1}{i\omega + \mu - \varepsilon(\mathbf{k}) - \Sigma(i\omega) - \Sigma_{\mathbf{k}}(i\omega)}$$



Σ_k - self-energy due to any “external” interaction!

DMFT+Σ calculation scheme:

1. Guess some initial value of *local* self – energy $\Sigma(i\omega)$, e.g. $\Sigma(i\omega) = 0$.

2. Construct $\Sigma_{\mathbf{p}}(i\varepsilon)$ within some (approximate) scheme, taking into account interactions with "external" interaction (impurity scattering in our case) which in general can depend on $\Sigma(i\omega)$ and μ.

3. Calculate local Green's function as:

$$G_{ii}(i\omega) = \frac{1}{N}\sum_{\mathbf{k}} \frac{1}{i\omega + \mu - \varepsilon(\mathbf{k}) - \Sigma(i\omega) - \Sigma_{\mathbf{k}}(i\omega)}$$

4. Define the "Weiss field" as:

$$\mathcal{G}_0^{-1}(i\omega) = \Sigma(i\omega) + G_{ii}^{-1}(i\omega)$$

5. Using some "impurity solver" calculate Green's function for the effective Anderson impurity, defined by Grassmanian functional integral:

$$G_d(\tau - \tau') = \frac{1}{Z_{\text{eff}}} \int Dc^+_{i\sigma} Dc_{i\sigma} c_{i\sigma}(\tau) c^+_{i\sigma}(\tau') \exp(-S_{\text{eff}})$$

with effective action for a fixed site ("impurity") i

$$S_{\text{eff}} = -\int_0^\beta d\tau_1 \int_0^\beta d\tau_2 c_{i\sigma}(\tau_1) \mathcal{G}_0^{-1}(\tau_1 - \tau_2) c^+_{i\sigma}(\tau_2) + \int_0^\beta d\tau U n_{i\uparrow}(\tau) n_{i\downarrow}(\tau)$$

and $Z_{\text{eff}} = \int Dc^+_{i\sigma} Dc_{i\sigma} \exp(-S_{\text{eff}})$, with $\beta = T^{-1}$, thus defining in fact the *new* value of $G_d^{-1}(i\omega)$.

6. Define the *new* value of local self – energy as:

$$\Sigma(i\omega) = \mathcal{G}_0^{-1}(i\omega) - G_d^{-1}(i\omega)$$

7. Using this new value as "initial" in step 1 continue the procedure until (and if) convergence is reached to obtain:

$$\boxed{G_{ii}(i\omega) = G_d(i\omega)}$$

Electron – phonon interaction and “kinks”

Electron – phonon interaction leads to a **“kink”** in electron dispersion within energy interval of $2\hbar\blacklozenge_D$ around the Fermi level.

Electron velocity: (A.B. Migdal, 1957)

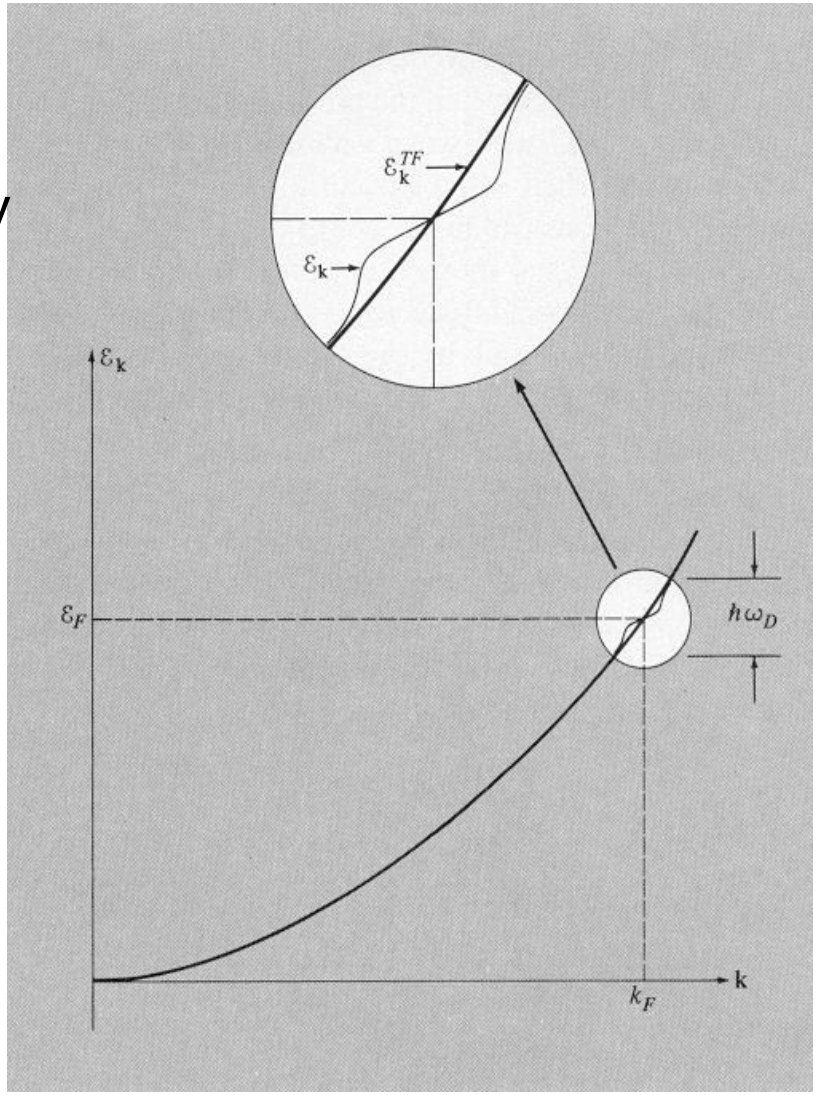
$$\mathbf{v}(\mathbf{k})=1/\hbar\cdot\partial\varepsilon_{\boldsymbol{k}}/\partial\mathbf{k}=\mathbf{v}^0(\mathbf{k})/(1+\lambda),$$

Effective mass *renormalization*:

$$m^*/m=1+\lambda$$

λ– dimensionles electron–phonon coupling

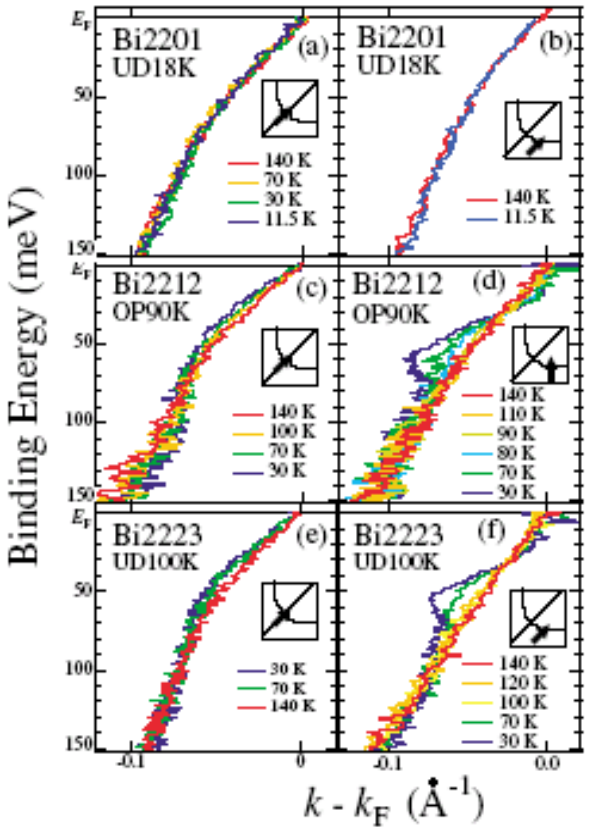
“Kinks” are now well observed in ARPES

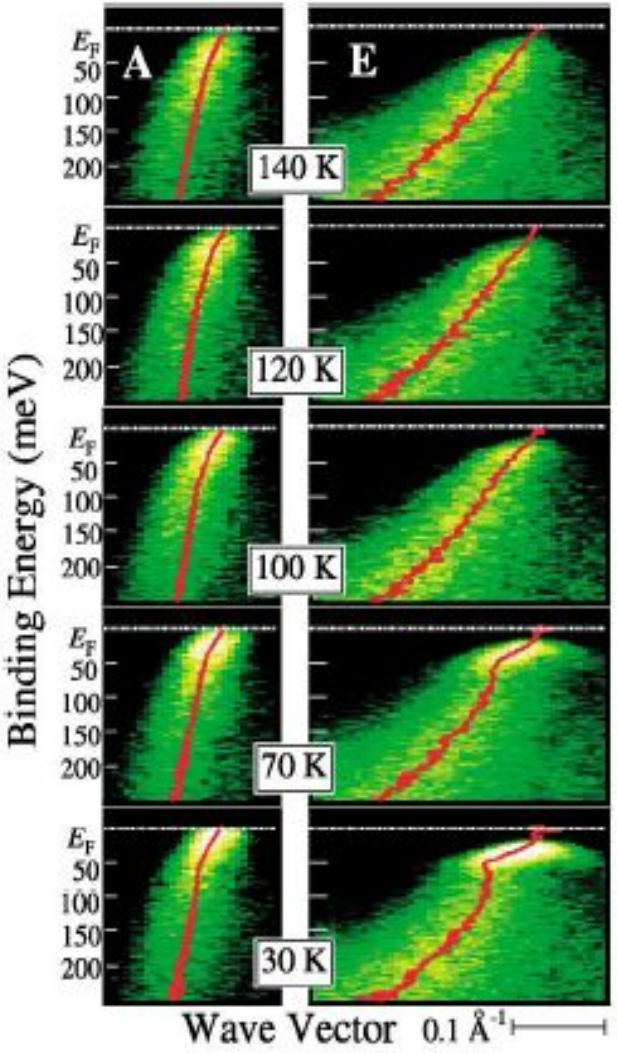


“Kinks” - Experimental

ARPES directly measures electron **spectral density** which allows to determine **quasiparticle** dispersion

~40-70 мэВ





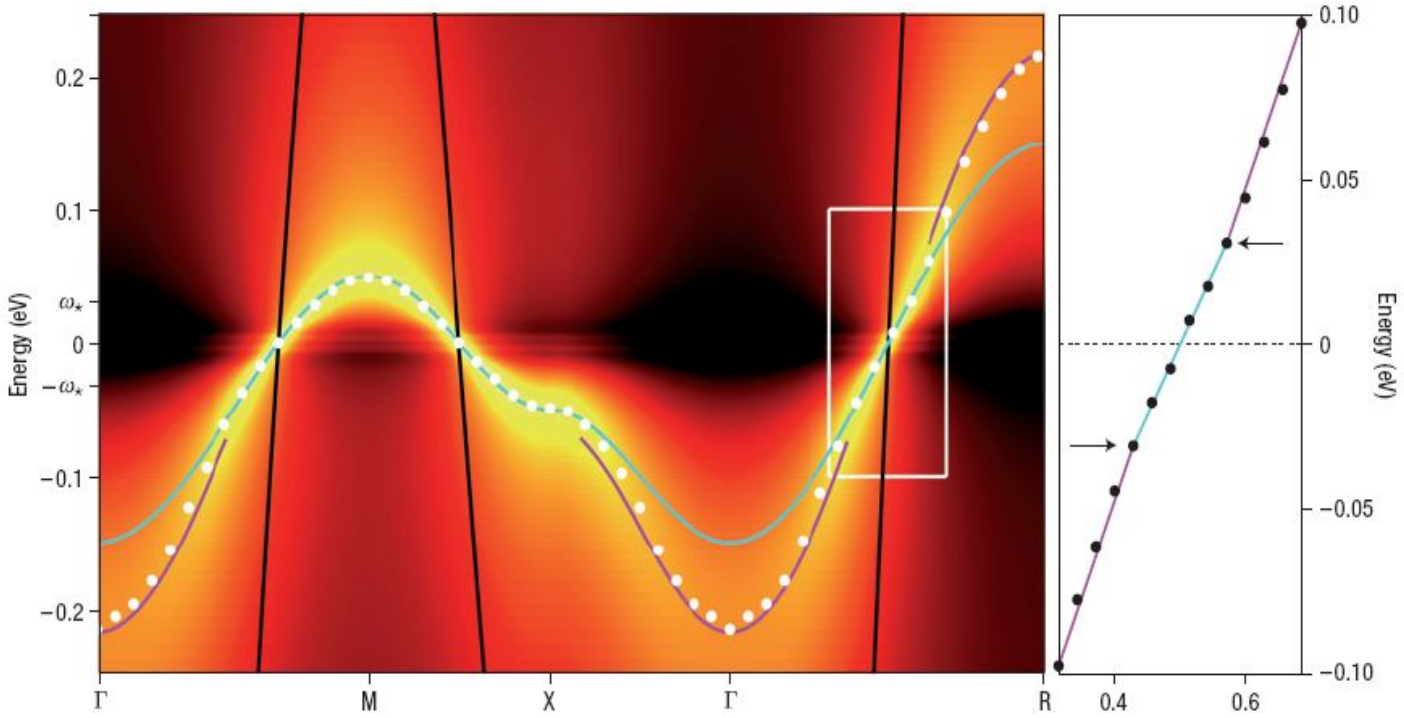
For HTSC cuprates “kink” energy

~ 40-70 meV, T_D~400-700K

Sato et al., PRL 91, 157003 (2004)

“Electronic kinks” in Hubbard model: DMFT

K.Buczuk, I.A.Nekrasov, D.Vollhardt et al. (2007)



Kinks in the dispersion relation, E_k, for a strongly correlated system. The intensity plot represents the spectral function $A(\mathbf{k}, \omega)$ (Hubbard model in DMFT, cubic lattice, interaction $U = 3.5$ eV, bandwidth $W = 3.46$ eV, $n = 1$, $Z_{FL} = 0.086$, $T = 5$ K). Close to the Fermi energy, the effective dispersion (white circles) follows the renormalized band structure, $E_k = Z_{FL}\epsilon_k$ (blue line). For $|\omega| > \omega_*$, the dispersion has the same shape but with a different renormalization, $E_k = Z_{QP}\epsilon_k - c\,\mathrm{sgn}(E_k)$ (pink line). Here $\omega_* = 0.03$ eV, $Z_{QP} = 0.135$ and $c = 0.018$ eV are all calculated (see the Supplementary Information) from Z_{FL} and ϵ_k (black line). A subinterval of Γ–R (white frame) is plotted on the right, showing kinks at $\pm\omega_*$ (arrows).

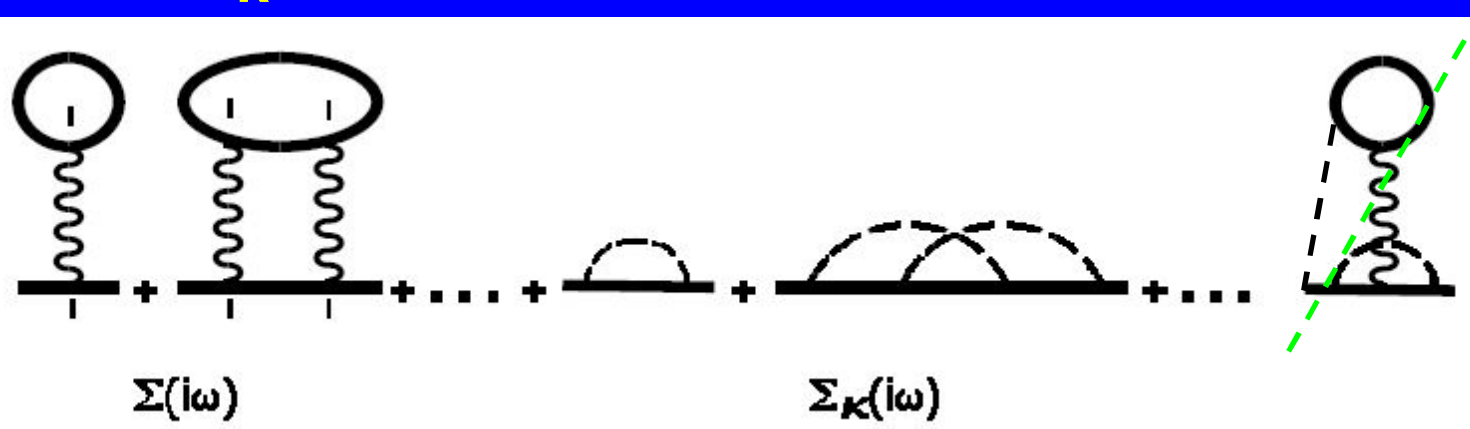
“Kink” energy

$$\omega_* = Z_{FL}(\sqrt{2} - 1)D$$

Fermi – liquid renormalization:

$$Z_{FL} = 1/(1 - \partial\,\mathrm{Re}\,\Sigma(\omega)/\partial\omega)|_{\omega=0} \equiv m/m^*$$

DMFT+Σ_k for Electron – Phonon Interaction



DMFT self-energy Electron – phonon self-energy

Migdal theorem – el-ph vertex corrections small as $\frac{\omega_D}{\varepsilon_F} \ll 1$

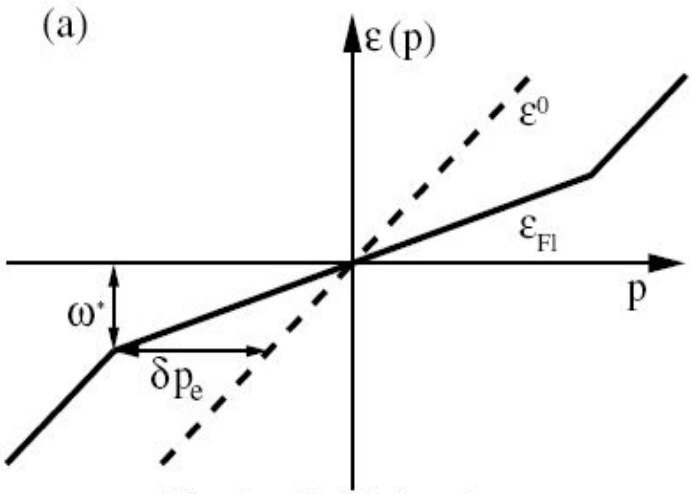
$$\Sigma_{ph}(\varepsilon, \mathbf{p}) = ig^2 \sum_{\omega,\mathbf{k}} \frac{\omega_0^2(\mathbf{k})}{\omega^2 - \omega_0^2(\mathbf{k}) + i\delta} \times \frac{1}{\varepsilon + \omega - \xi_{\mathbf{p}+\mathbf{k}} - \Sigma_{ii}(\varepsilon + \omega) - \Sigma_{ph}(\varepsilon + \omega, \mathbf{p} + \mathbf{k})}$$

$$\omega_0(\mathbf{k}) = \begin{cases} uk, & k < \frac{\omega_D}{u} \\ \omega_0, & k < k_0 \end{cases} .$$

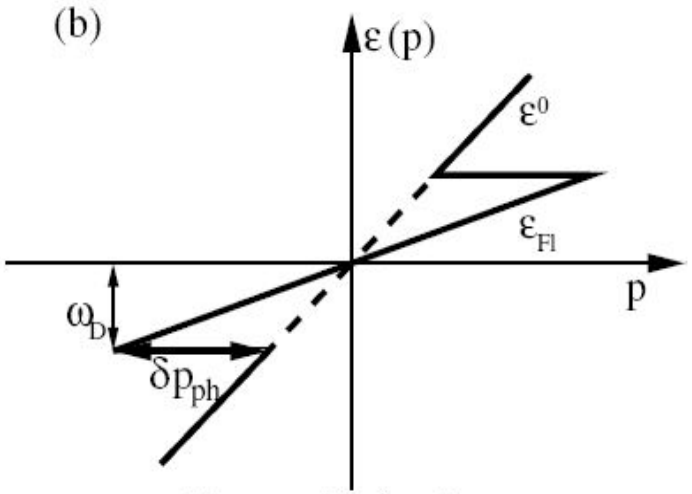
$\xi_{\mathbf{p}}$ – free (band) electrons

Here u is the sound velocity, ω_D, ω_0 are Debye and Einstein frequencies with cut-off k_0 of the order of Fermi momentum

DMFT+Σ : “Kinks” in Electron Dispersion



Electronic kink scheme



Phonon kink scheme

$$\omega^* = Z_{FL}(\sqrt{2}-1)D$$

$$\delta p_e = \frac{\omega^*}{v_F^*}\left(1-\frac{Z_{FL}}{Z_0}\right) \equiv \frac{\omega^*}{v_F^*}\lambda_e$$

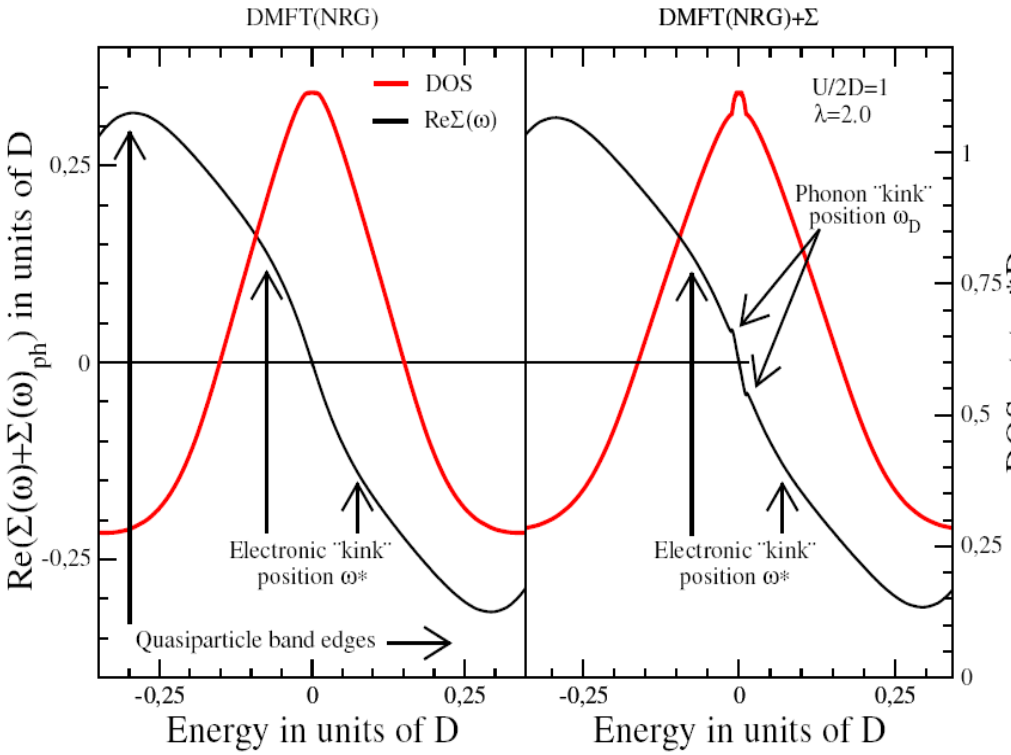
$$\delta p_{ph} = \frac{\omega_D}{v_F}\lambda$$

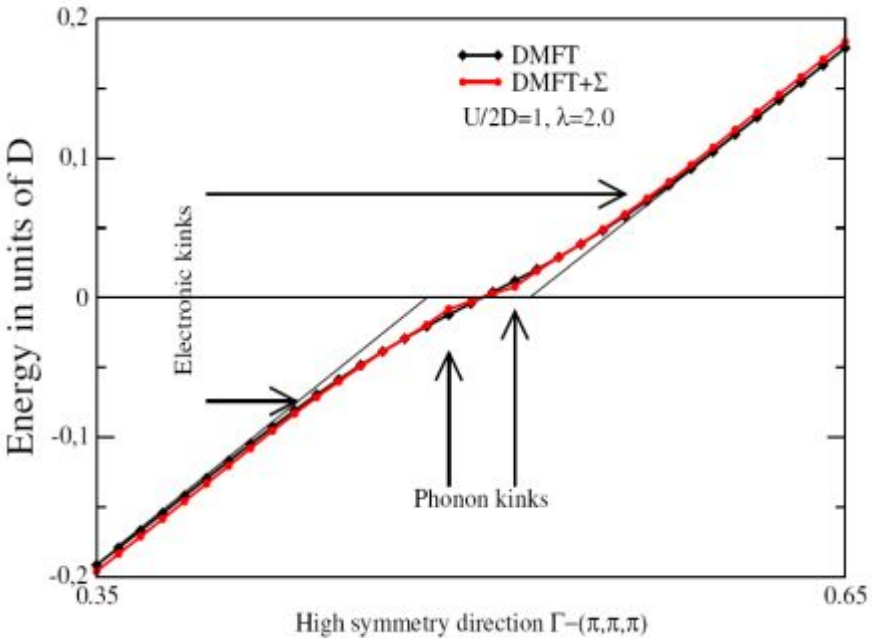
$$\lambda = g^2 N_0(\varepsilon_F)\frac{\omega_D^2}{4\omega_c^2}$$

Different “geometries” of “kinks” due to electron-phohon interaction and correlations

DMFT+Σ: Self-energy and Dispersion

M.V.Sadovskii, I.A.Nekrasov,E.Z.Kuchinskii (2009)



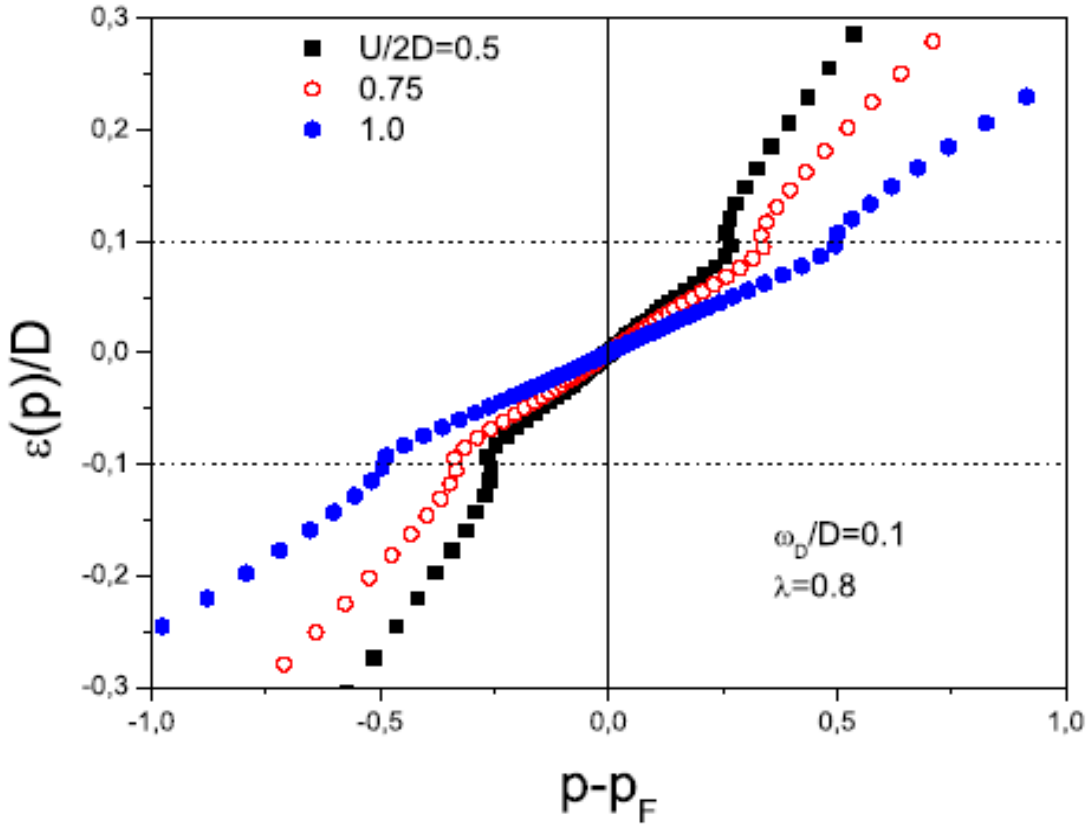


"Kinks" coexist if: $\omega_D \ll \omega^*$

Now we can choose parameters of our model to make both kinks simultaneously visible. First of all one should take care that $\omega_D \ll \omega^*$. For $U/2D=1$ with $U=3.5$ eV we get $\omega^* \sim 0.1$ D and a reasonable value of Debye frequency is $\omega_D \sim 0.01$ D. To make phonon kink pronounced at such relatively low Debye frequency [cf. Eq. (10)] we have to increase EPI constant. So we take $\lambda=2.0$.

Dependence of electron – phonon “kink” on U

M.V.Sadovskii, I.A.Nekrasov,E.Z.Kuchinskii (2006)



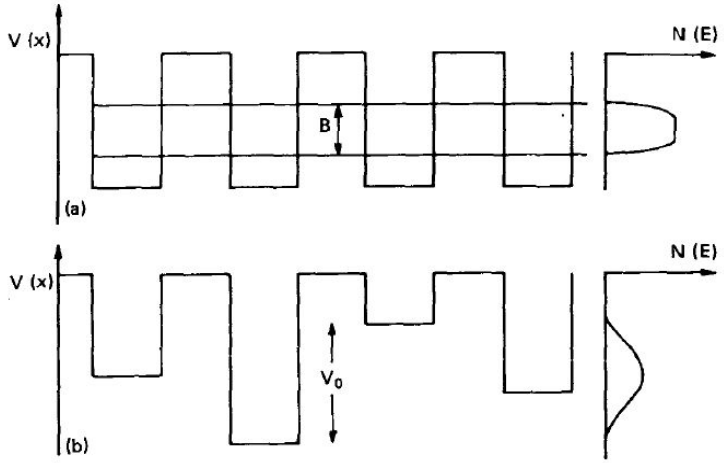
Quasiparticle dispersions around Fermi level with phonon kinks obtained from DMFT+● calculations for different interaction strengths: U/2D= 0.5, 0.75, 1.0; ● = 0.8; ◆$_D$=0.1D.

Disorder Induced Metal-Insulator Transition

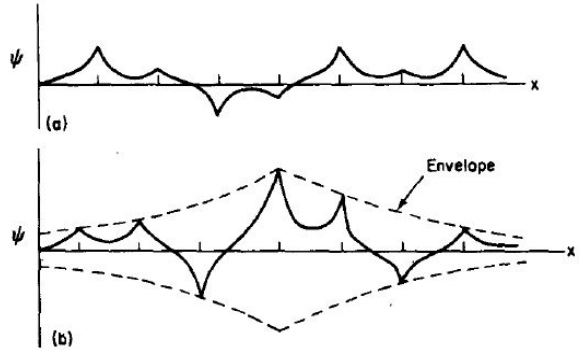
Anderson model

P.W.Anderson (1958)

$$H = -t \sum_{\langle ij \rangle \sigma} a^{\dagger}_{i\sigma} a_{j\sigma} + \sum_{i\sigma} \epsilon_i n_{i\sigma}$$



1.17 Potential energy used by Anderson (1958): (a) without a random potential and (b) with such a potential. The density of states is also shown.



1.18 Wave function ψ of an electron when $l \sim a$: (a) extended states; (b) weakly localized states.

At small disorder dc conductivity of a metal at $T = 0$ is determined by Drude expression:

$$\sigma_0 = \frac{ne^2}{m}\tau = \frac{ne^2}{p_F}l \qquad (2.2)$$

where τ — is the mean free time, n — is electron density and e — its charge. Usual kinetic theory can be applied if

$$\frac{p_F l}{\hbar} \gg 1 \text{ or } \frac{E_F \tau}{\hbar} \gg 1 \qquad (2.3)$$

which is a condition of weak scattering (disorder). From Eq. (2.2) and Eq. (2.3), taking into account $n = p_F^3/(3\pi^2\hbar^3)$, we can estimate the lower limit of conductivity for which Drude approximation is still valid:

$$\sigma_0 = \frac{e^2 p_F}{3\pi^2\hbar^2}\left(\frac{p_F l}{\hbar}\right) \gg \frac{e^2 p_F}{3\pi^2\hbar^2} \qquad (2.4)$$

The conductivity value:

$$\sigma_c \approx \frac{e^2 p_F}{3\pi^2\hbar^2} \qquad (2.5)$$

is usually called the "minimal metallic conductivity" [Mott N.F. (1974)

Anderson - Hubbard Model

Our aim is to consider non–magnetic disordered Anderson–Hubbard model (mainly) at half–filling for arbitrary interaction and disorder strengths. Mott–Hubbard and Anderson MITs will be investigated on an equal footing. The Hamiltonian of the model under study is written as:

$$H = -t \sum_{\langle ij \rangle \sigma} a^{\dagger}_{i\sigma} a_{j\sigma} + \sum_{i\sigma} \epsilon_i n_{i\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}, \qquad (1)$$

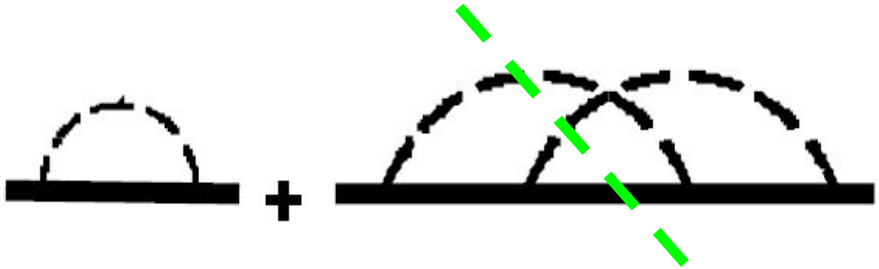
where $t > 0$ is the amplitude for hopping between nearest neighbors, U is the on–site repulsion, $n_{i\sigma} = a^{\dagger}_{i\sigma} a_{i\sigma}$ is the local electron number operator, $a_{i\sigma}$ ($a^{\dagger}_{i\sigma}$) is the annihilation (creation) operator of an electron with spin σ, and the local ionic energies ϵ_i at different lattice sites are considered to be independent random variables. To simplify diagrammatics in following we assume Gaussian probability distribution for ϵ_i:

$$\mathcal{P}(\epsilon_i) = \frac{1}{\sqrt{2\pi}\Delta} \exp\left(-\frac{\epsilon_i^2}{2\Delta^2}\right) \qquad (2)$$

Here the parameter Δ is just a measure of disorder strength, and Gaussian ("white" noise) random field of energy level ϵ_i at lattice cites produces "impurity" scattering, leading to the standard diagram technique for calculation on the averaged Green's functions[19].

Σ for impurity scattering

Self-consistent Born approximation



$$\Sigma_{\mathbf{p}}(i\varepsilon) = \Delta^2 \sum_{\mathbf{p}} G(i\varepsilon, \mathbf{p}) \equiv \Sigma_{imp}(i\varepsilon)$$

$$\Sigma^{R,A}_{imp}(\varepsilon) = \Delta^2 \sum_{\mathbf{p}} G^{R,A}(\varepsilon, \mathbf{p}) = \mathrm{Re}\Sigma_{imp}(\varepsilon) \pm i\gamma(\varepsilon)$$

$$\gamma(\varepsilon) = \pi \Delta^2 N(\varepsilon)$$

Semi - elliptic DOS:

$$N(\varepsilon) = \frac{2}{\pi D^2}\sqrt{D^2 - \varepsilon^2} \qquad W = 2D \Rightarrow W_{eff} = W\sqrt{1 + 16\frac{\Delta^2}{W^2}}$$

Dynamic conductivity in DMFT+Σ

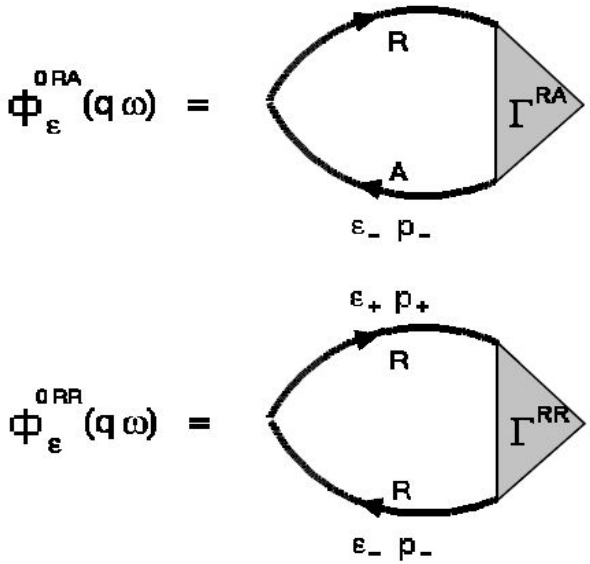
M.V.Sadovskii, I.A.Nekrasov, E.Z.Kuchinskii (2006)

A. Basic expressions for optical conductivity

To calculate dynamic conductivity we use the general expression relating it to retarded density – density correlation function $\chi^R(\omega, \mathbf{q})$

$$\sigma(\omega) = -\lim_{q\to 0} \frac{ie^2\omega}{q^2}\chi^R(\omega, \mathbf{q})$$

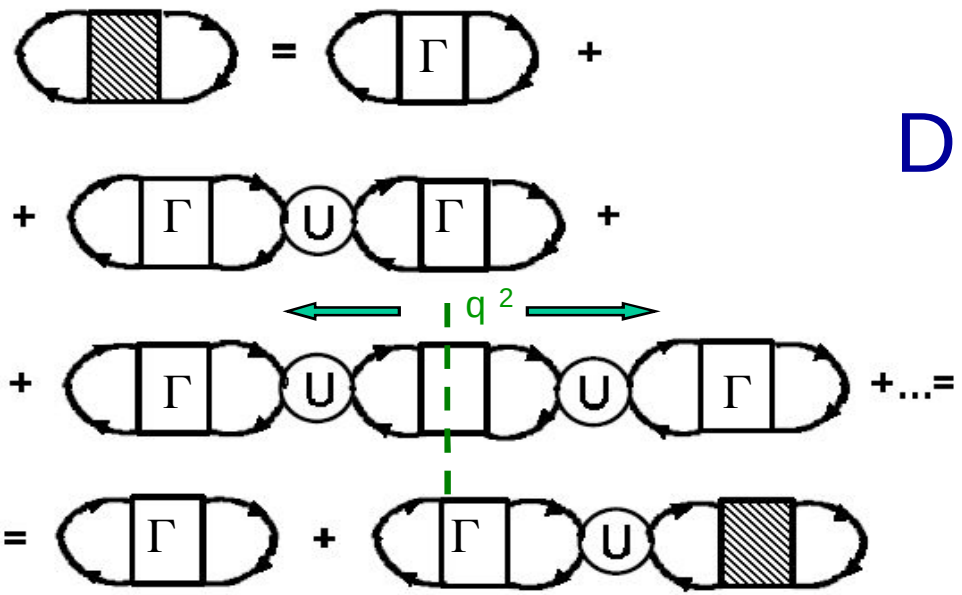
where e is electronic charge.



$$\chi^R(\omega, \mathbf{q}) = \int_{-\infty}^{\infty} \frac{d\varepsilon}{2\pi i} \left\{ [f(\varepsilon_+) - f(\varepsilon_-)]\, \Phi_\varepsilon^{RA}(\mathbf{q}, \omega) + f(\varepsilon_-)\Phi_\varepsilon^{RR}(\mathbf{q}, \omega) - f(\varepsilon_+)\Phi_\varepsilon^{AA}(\mathbf{q}, \omega) \right\}$$

Dynamic (optical) conductivity

$$\sigma(\omega) = \lim_{q\to 0}\left(-\frac{e^2\omega}{2\pi q^2}\right)\int_{-\infty}^{\infty} d\varepsilon \left\{\left[f(\varepsilon_+) - f(\varepsilon_-)\right]\left[\Phi_\varepsilon^{RA}(\mathbf{q},\omega) - \Phi_\varepsilon^{RA}(0,\omega)\right] + \right.$$
$$\left. + f(\varepsilon_-)\left[\Phi_\varepsilon^{RR}(\mathbf{q},\omega) - \Phi_\varepsilon^{RR}(0,\omega)\right] - f(\varepsilon_+)\left[\Phi_\varepsilon^{AA}(\mathbf{q},\omega) - \Phi_\varepsilon^{AA}(0,\omega)\right]\right\}$$



DMFT+Σ!

$$\Phi_{i\varepsilon i\varepsilon'}(i\omega\mathbf{q}) = \Phi^0_{i\varepsilon}(i\omega\mathbf{q})\delta_{\varepsilon\varepsilon'} + \Phi^0_{i\varepsilon}(i\omega\mathbf{q})\sum_{\varepsilon''} U_{i\varepsilon i\varepsilon''}(i\omega)\Phi_{i\varepsilon'' i\varepsilon'}(i\omega,\mathbf{q})$$

General expression for dynamic conductivity in DMFT+Σ:

$$Re\sigma(\omega) = \frac{e^2\omega}{2\pi}\int_{-\infty}^{\infty} d\varepsilon\,[f(\varepsilon_-) - f(\varepsilon_+)]\,Re\left\{\phi_\varepsilon^{0RA}(\omega)\left[1 - \frac{\Sigma^R(\varepsilon_+) - \Sigma^A(\varepsilon_-)}{\omega}\right]^2 - \right.$$
$$\left. -\phi_\varepsilon^{0RR}(\omega)\left[1 - \frac{\Sigma^R(\varepsilon_+) - \Sigma^R(\varepsilon_-)}{\omega}\right]^2\right\}$$

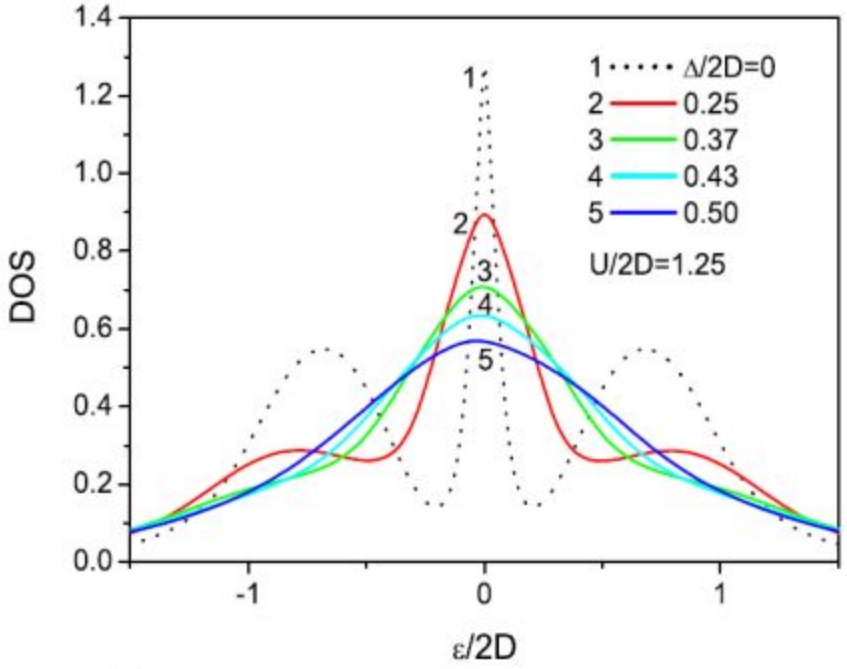
No Hubbard U in vertices here!

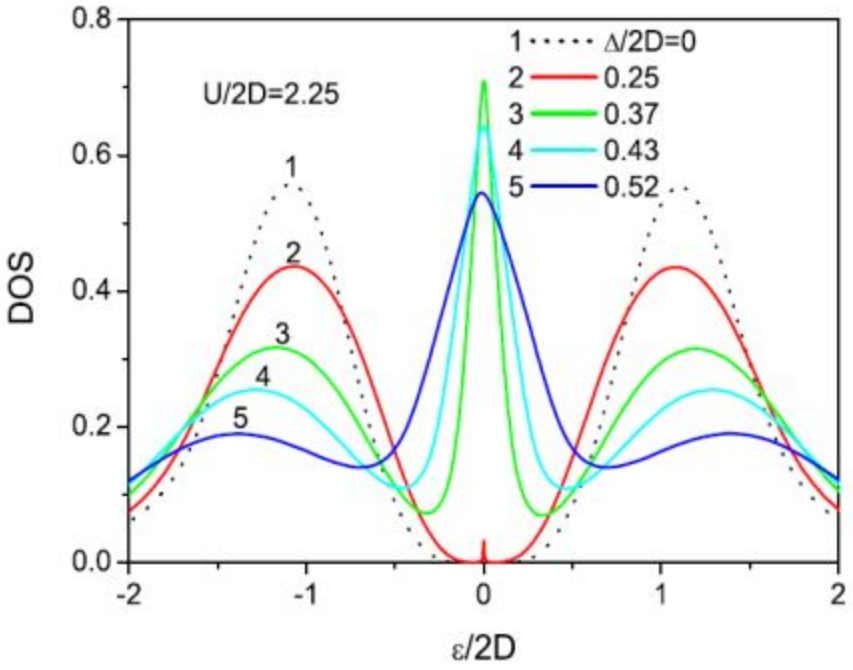
$$\phi_\varepsilon^{0RA}(\omega) = \lim_{q\to 0}\frac{\Phi_\varepsilon^{0RA}(\omega,\mathbf{q}) - \Phi_\varepsilon^{0RA}(\omega,0)}{q^2}$$

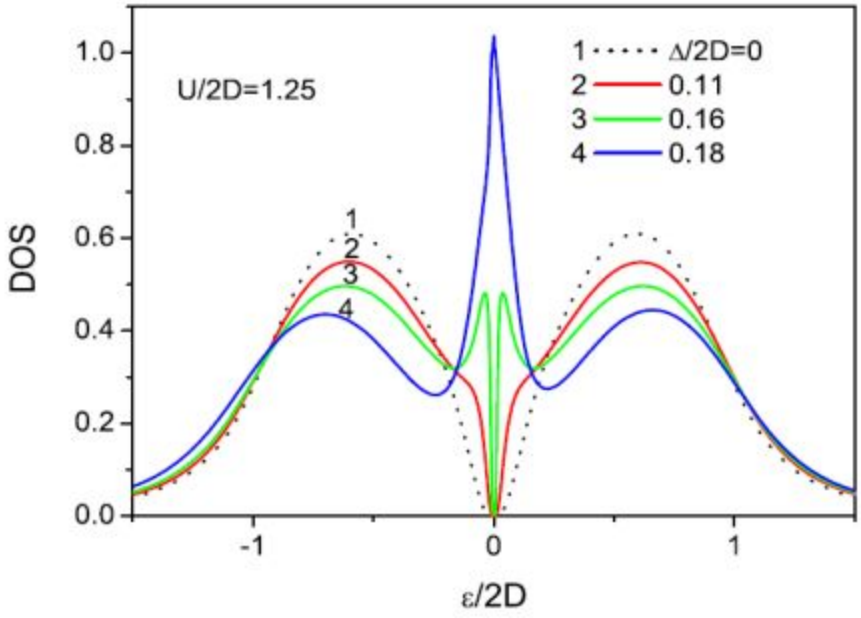
$$\phi_\varepsilon^{0RR}(\omega) = \lim_{q\to 0}\frac{\Phi_{i\varepsilon}^{0RR}(\omega,\mathbf{q}) - \Phi_{i\varepsilon}^{0RR}(\omega,0)}{q^2}$$

M.V.Sadovskii, I.A.Nekrasov,E.Z.Kuchinskii (2006)

Density of States (d=3)



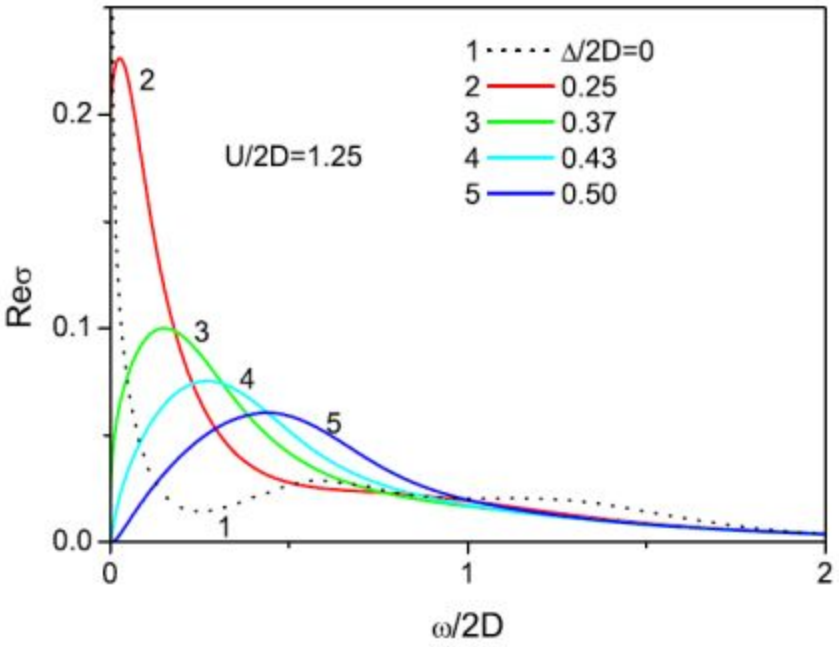


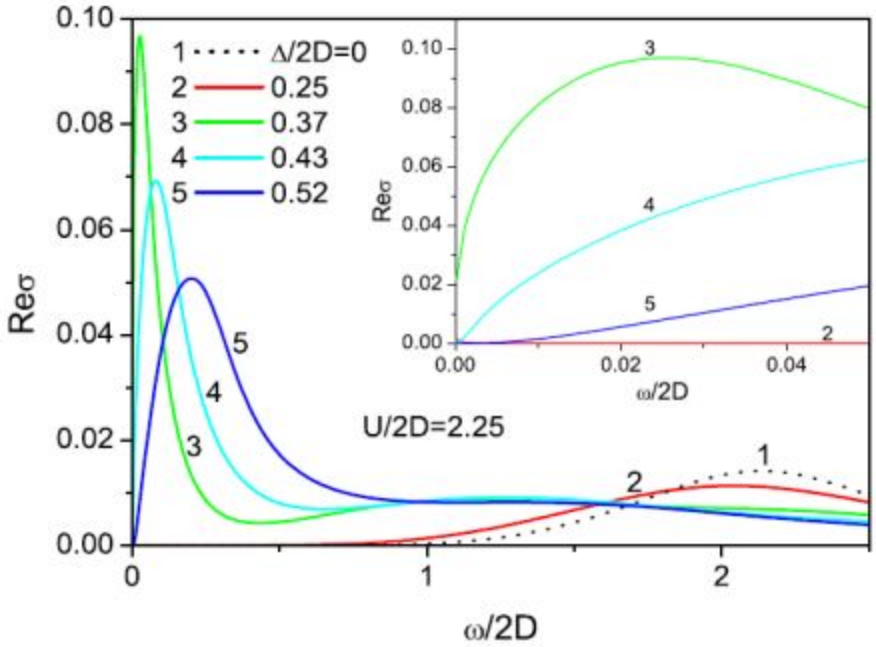


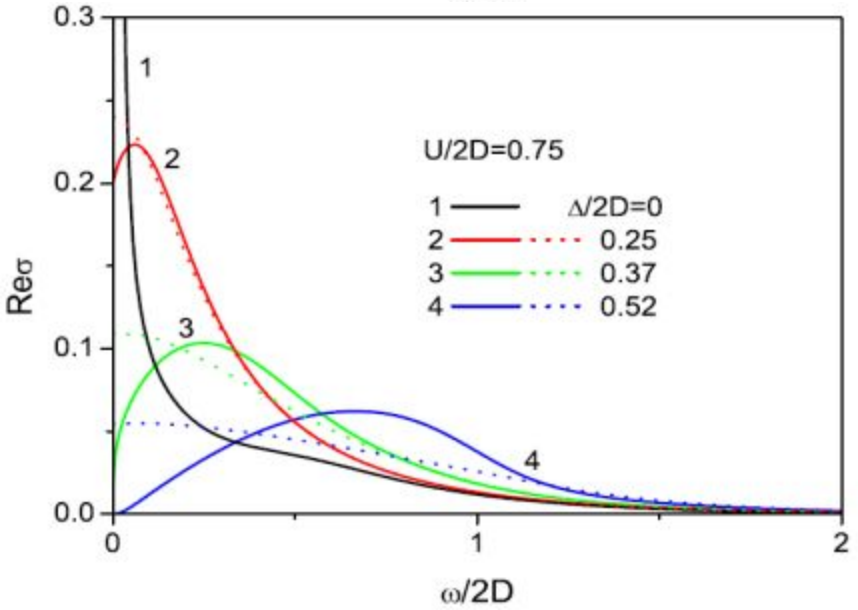
$$\frac{U_{c1,c2}(\Delta)}{W_{eff}} = \frac{U_{c1,c2}}{W}$$

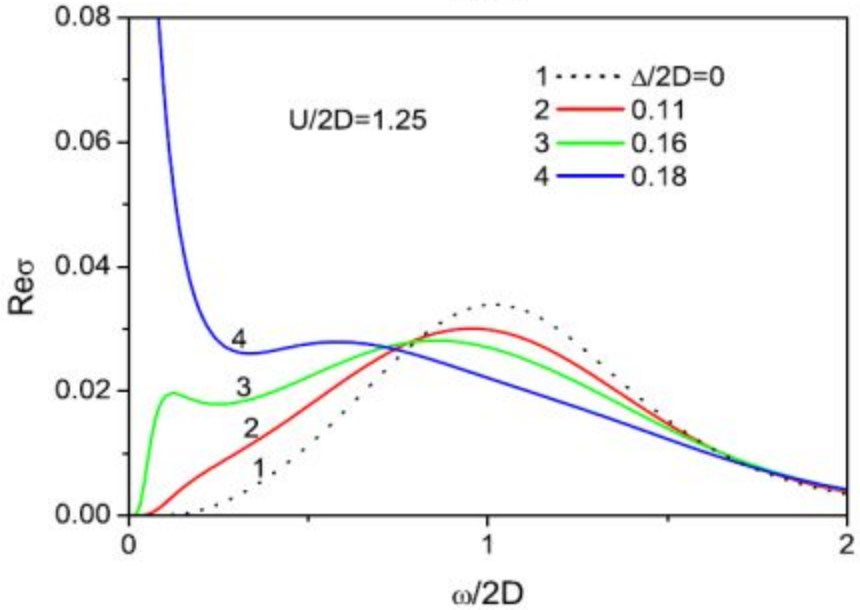
$$W_{eff} = W\sqrt{1+16\frac{\Delta^2}{W^2}}$$

Conductivity and Metal-Insulator Transition (d=3)





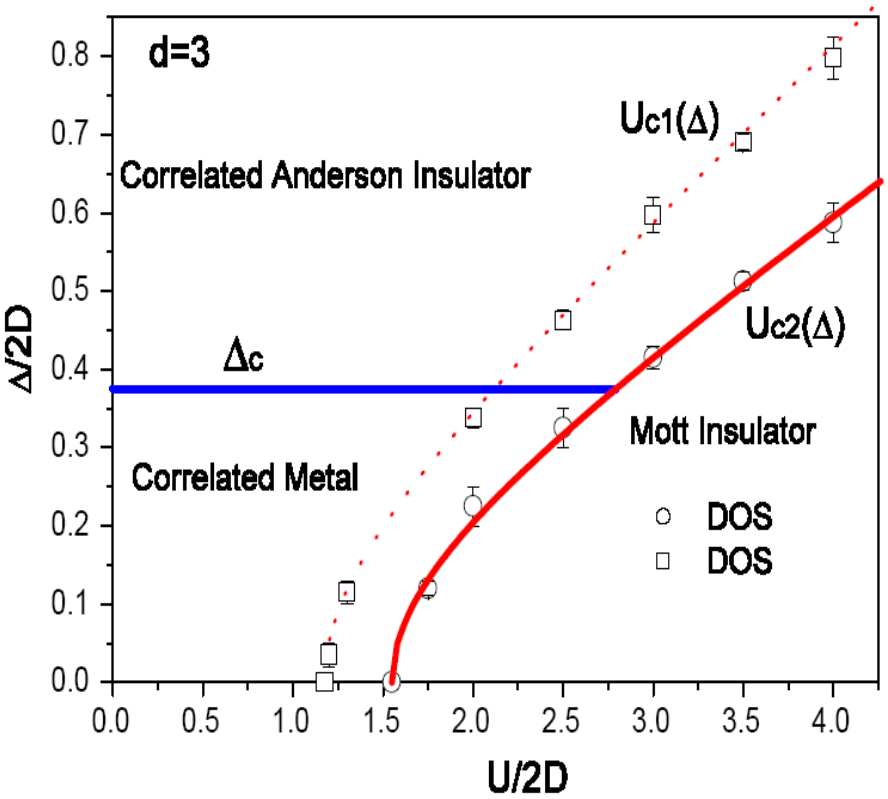


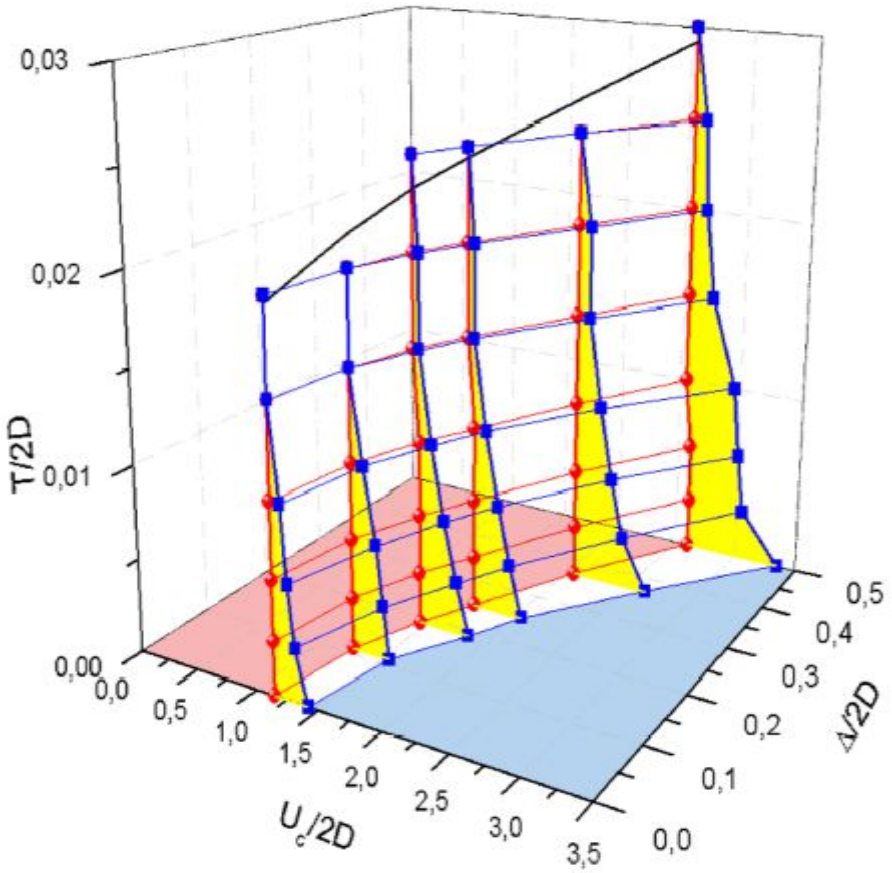


Phase Diagram (d=3)

M.V.Sadovskii, I.A.Nekrasov,E.Z.Kuchinskii (2006 - 2012)

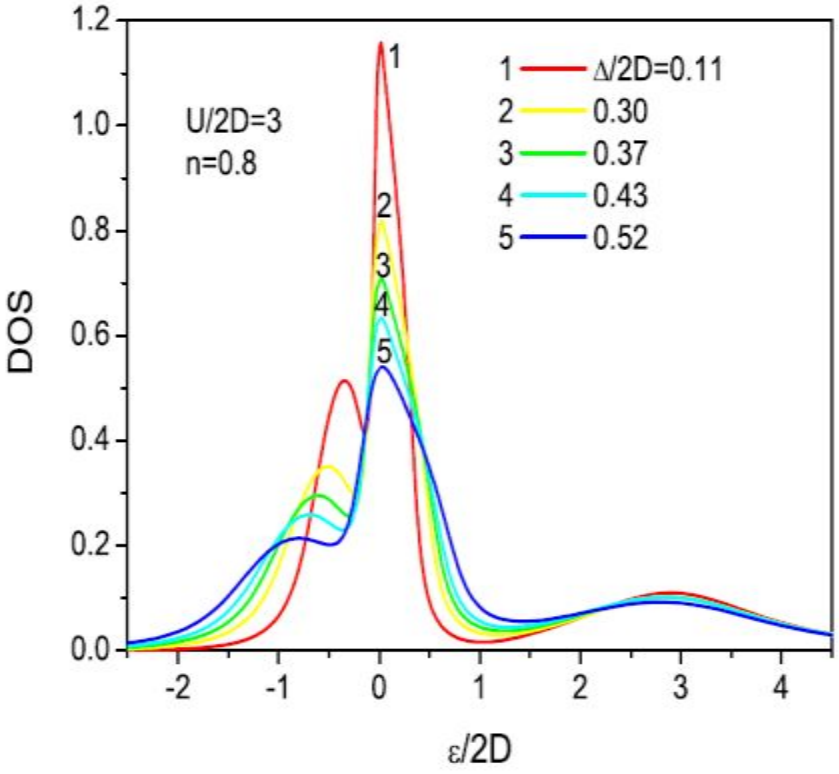
Calculated in DMFT+Σ

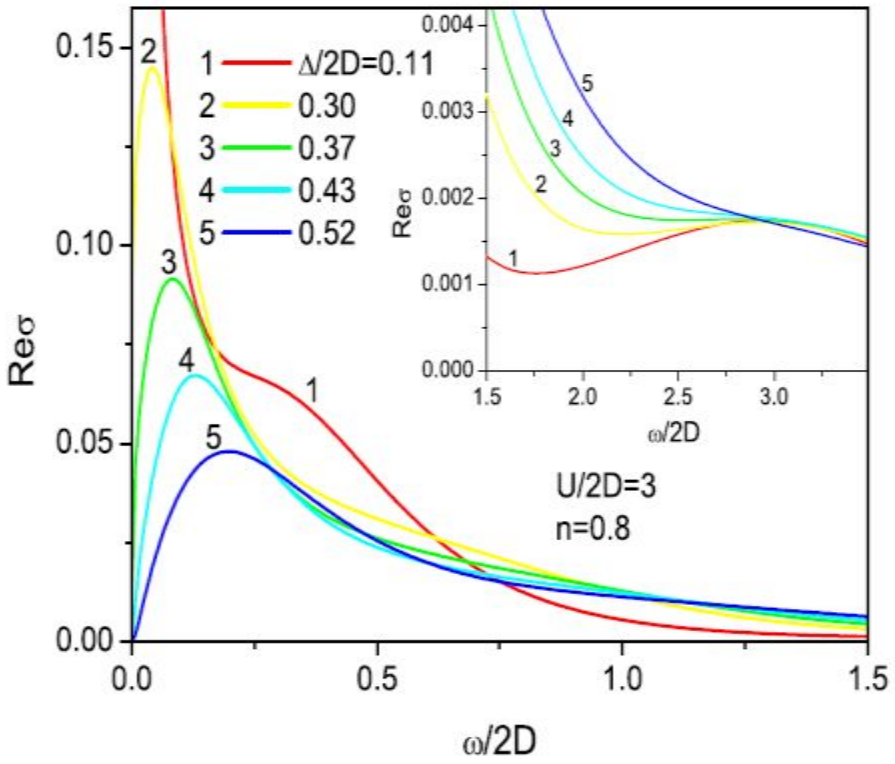




As a rule of thumb Gaussian value of Δ_c should be multiplied by $\sqrt{12}$ to obtain the critical disorder value for rectangular distribution. This gives $\Delta_c \approx 1.28$ in rather good agreement with $\Delta_c(U=0) \approx 1.35W$ value of K. Byczuk, W. Hofstetter, D. Vollhardt.

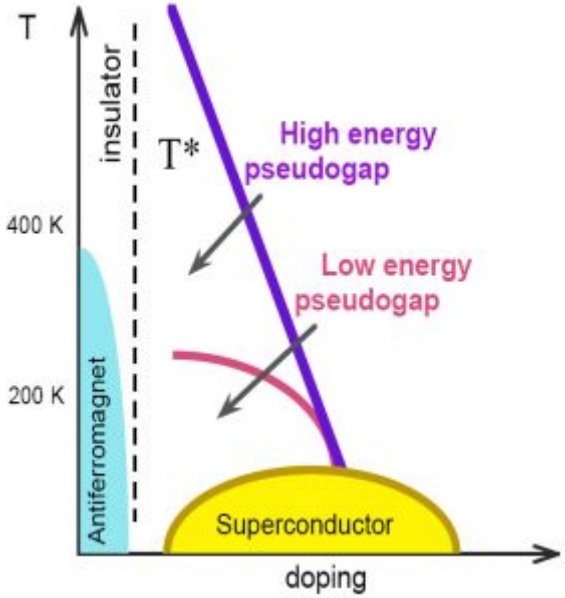
Doped Mott insulator (T=0, d=3)

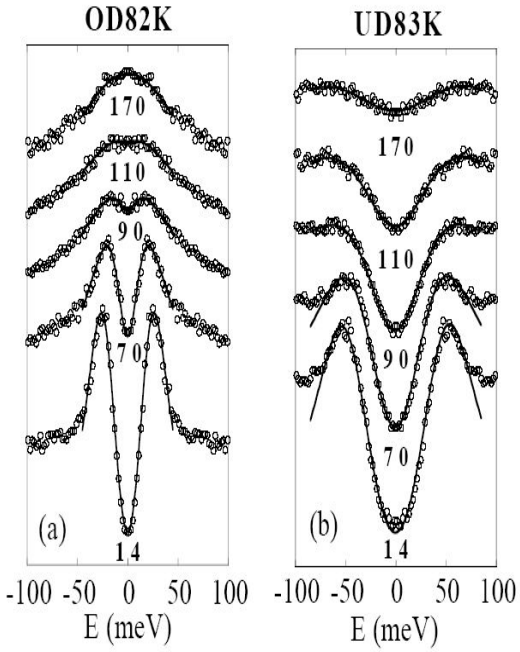




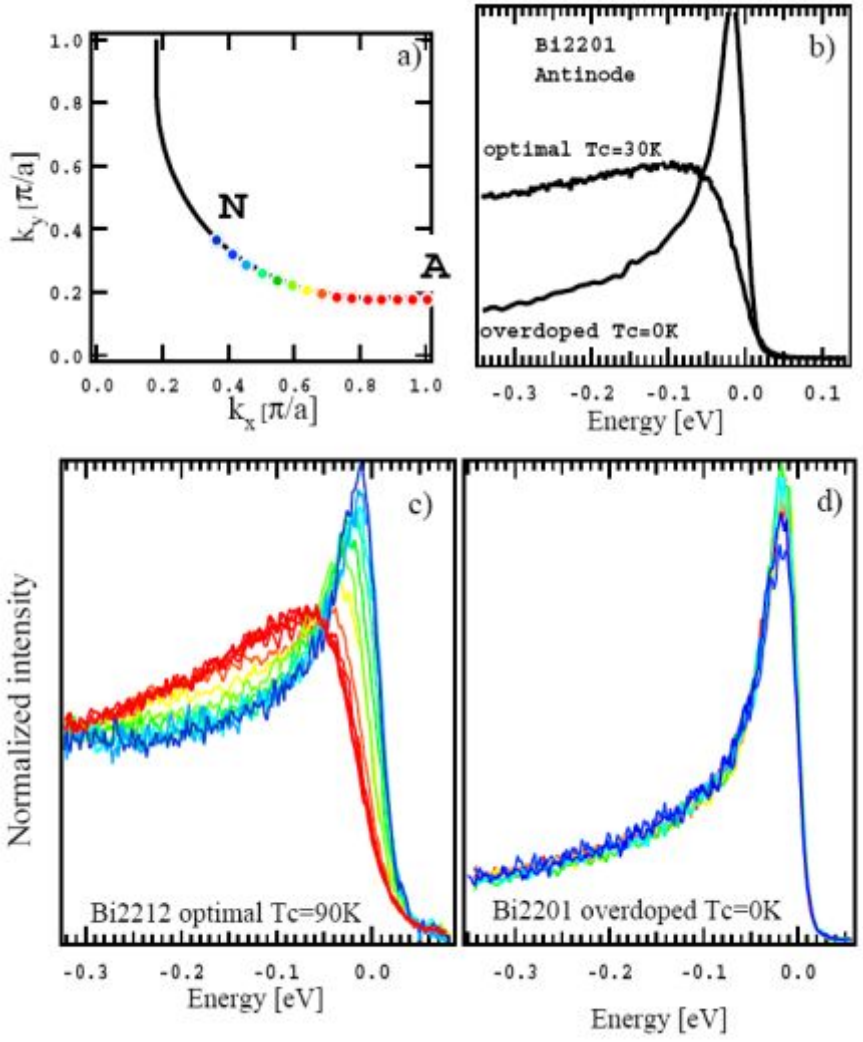
No Mott-Hubbard Insulator! Correlated Metal and Anderson Insulator!

Pseudogap in Cuprates





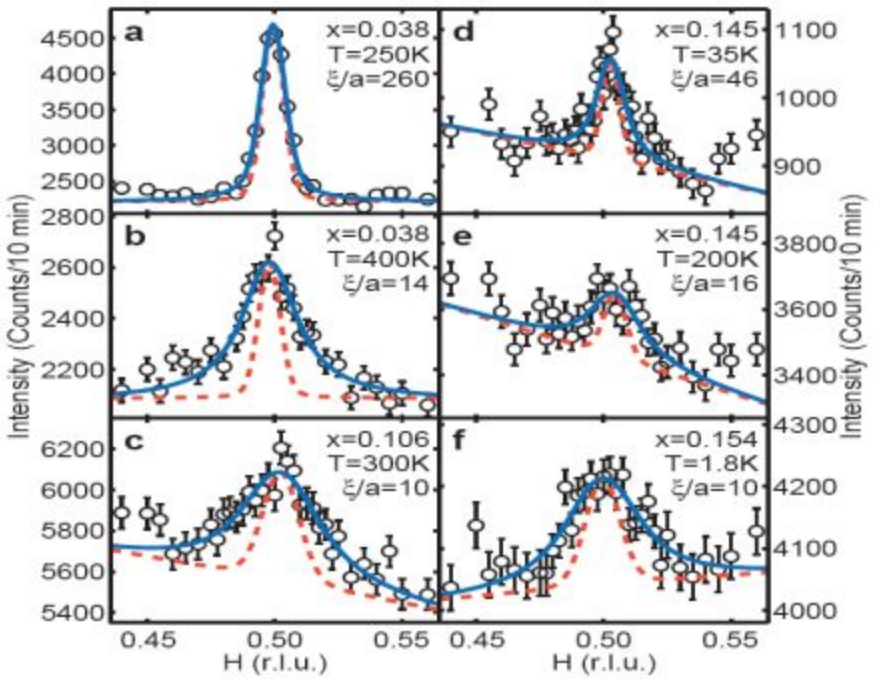
M.Norman et al. (1998)

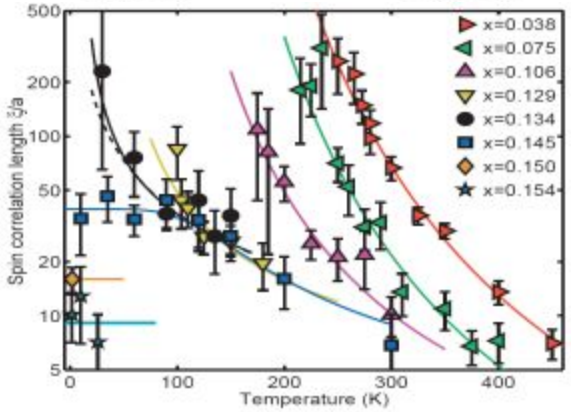


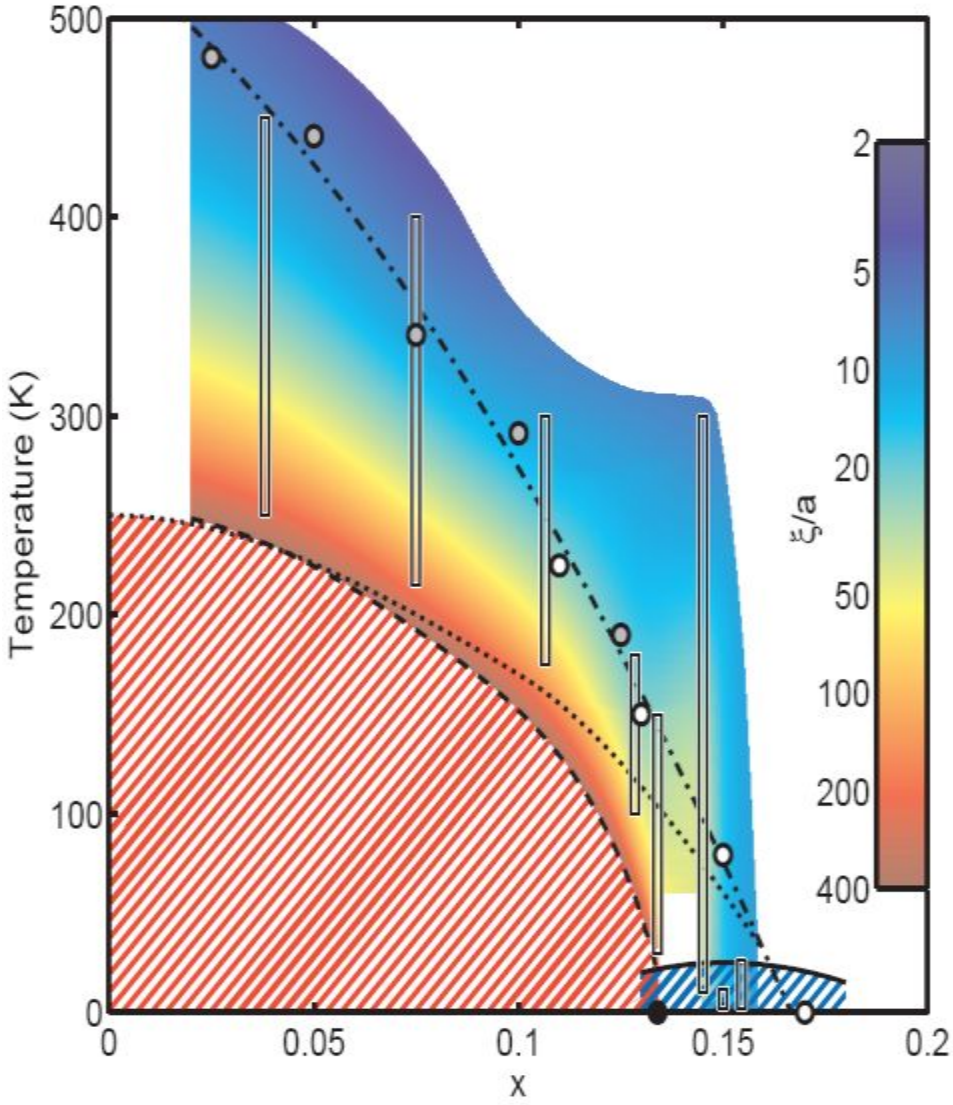
J.Campuzano et al. (2004)

Spin correlations of the electron-doped high transition-temperature superconductor $Nd_{2-x}Ce_xCuO_{4\pm\delta}$

E.M. Motoyama[1], G. Yu[1], I.M. Vishik[1], O.P. Vajk[2], P.K. Mang[3] & M. Greven[3,4]



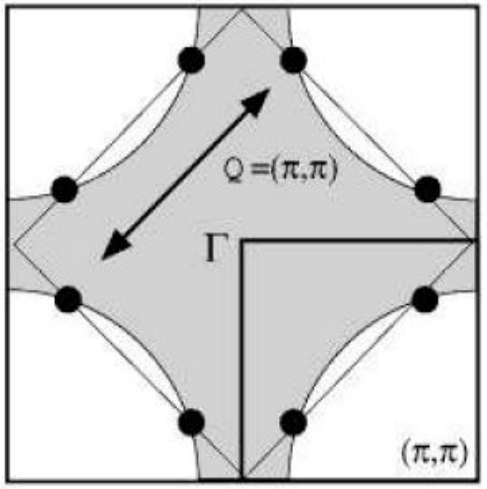




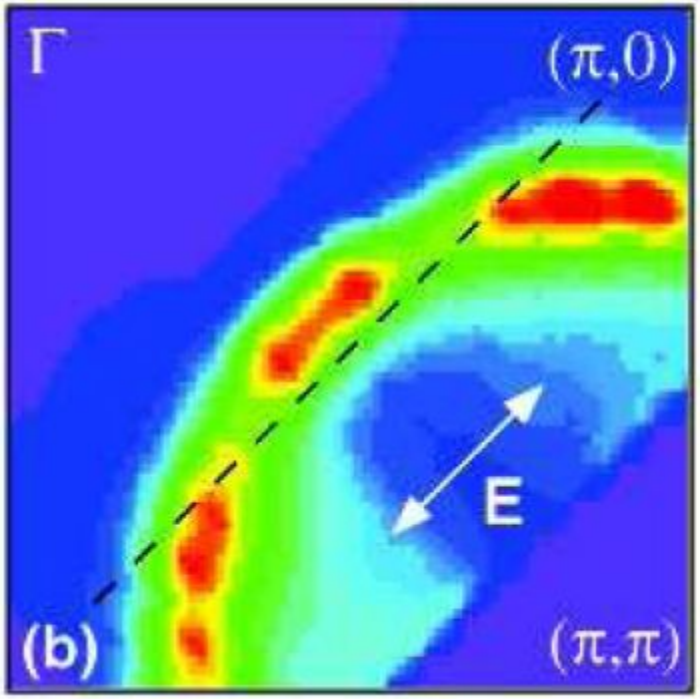
Pseudogaps and “Hot - Spots” model

$$V_{eff}(\mathbf{q},\omega) = g^2\chi_{\mathbf{q}}(\omega) \approx \frac{g^2\xi^2}{1+\xi^2(\mathbf{q}-\mathbf{Q})^2 - i\frac{\omega}{\omega_{sf}}}$$

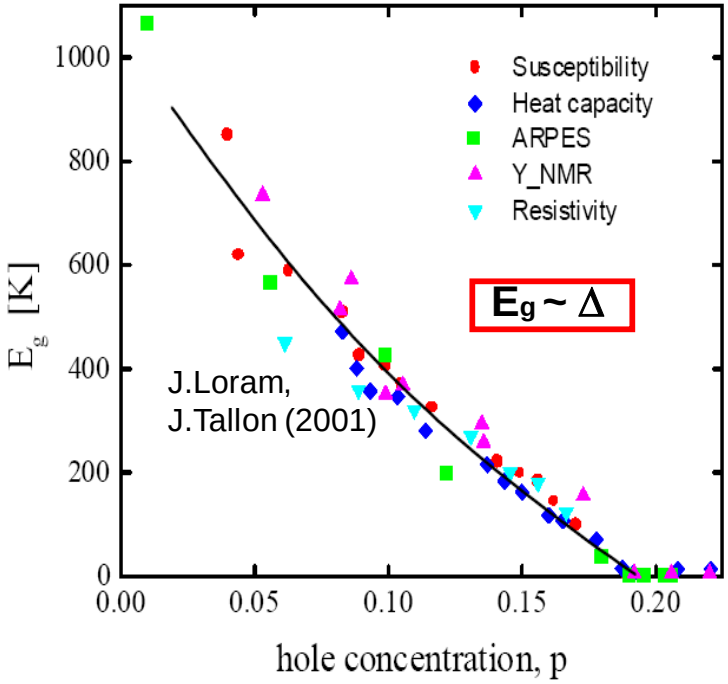
ξ - correlation length ω_{sf} - frequency of fluctuations



D.Pines et al.
SF-model
(1990 - 1999)



NdCeCuO - N.Armitage et al. (2001)



Σ_k for AFM (CDW) fluctuations

Spin - Fermion (SF) or CDW model

We take into account ALL(!) diagrams for quenched (Gaussian) AFM (CDW) fluctuations

Valid for $T>>\omega_{sf}$!

$\Sigma_k(i\omega)$

M.V.Sadovskii, 1979
E.Z.Kuchinskii, M.V.Sadovskii, 1999
D.Pines, J.Schmalian, B.Stoikovic,1999

$$\Sigma_{\mathbf{k}}(i\omega) = \Sigma_{n=1}(i\omega\mathbf{k})$$

with

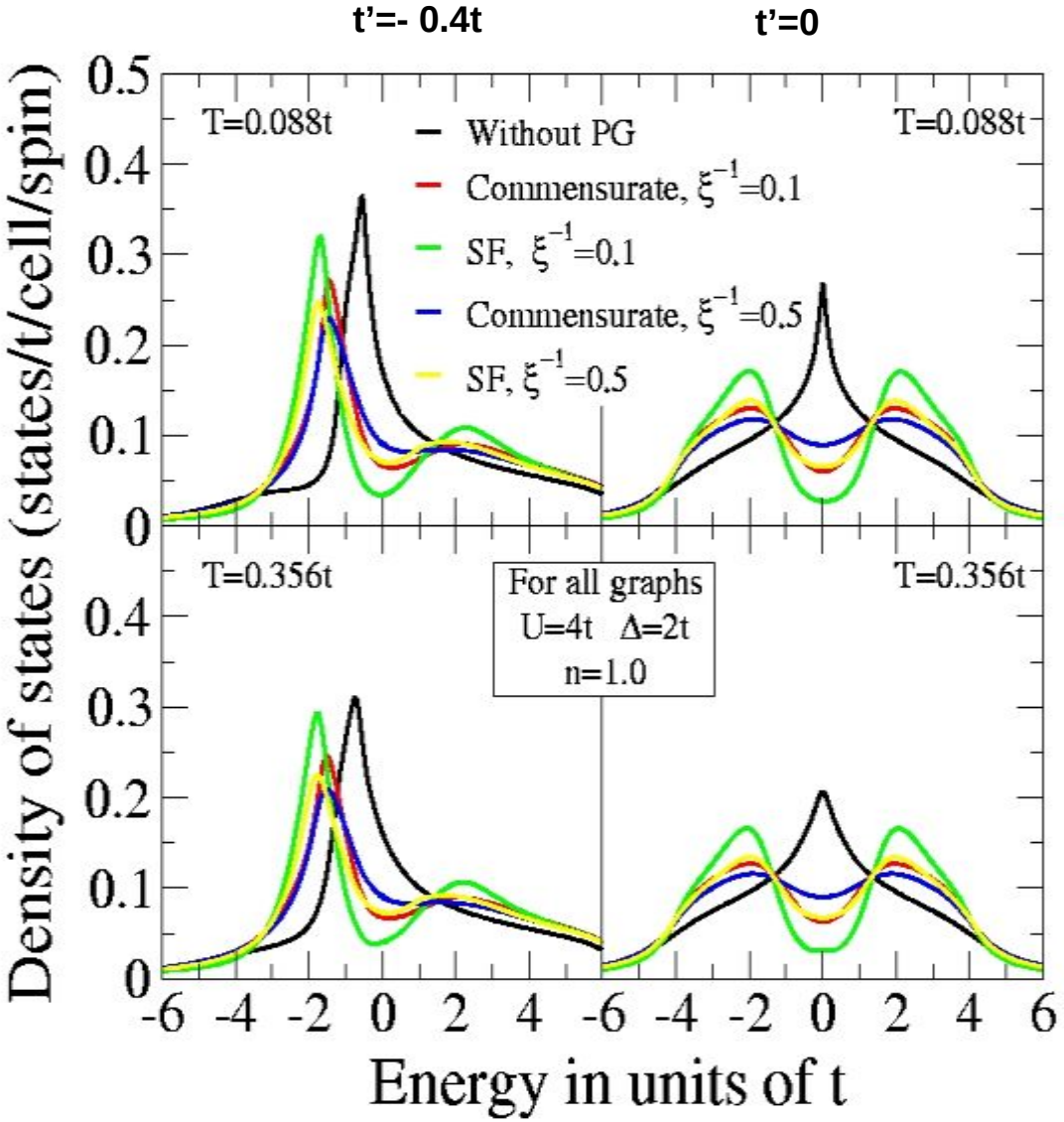
$$\Sigma_n(\omega\mathbf{k}) = \Delta^2 \frac{s(n)}{i\omega + \mu - \Sigma(i\omega) - \varepsilon_n(\mathbf{k}) + inv_n\kappa - \Sigma_{n+1}(i\omega\mathbf{k})}$$

where Δ characterizes the energy scale and $\kappa = \xi^{-1}$ is the inverse correlation length of SDW (CDW) fluctuations, $\varepsilon_n(\mathbf{k}) = \varepsilon(\mathbf{k}+\mathbf{Q})$ and $v_n = |v^x_{\mathbf{k}+\mathbf{Q}}| + |v^y_{\mathbf{k}+\mathbf{Q}}|$ for odd n while $\varepsilon_n(\mathbf{p}) = \varepsilon(\mathbf{p})$ and $v_n = |v^x_{\mathbf{k}}| + |v^y_{\mathbf{k}}|$ for even n, with velocity projections $v^x_{\mathbf{k}}$ and $v^y_{\mathbf{k}}$ determined by usual momentum derivatives of the "bare" spectrum which we always take in the standard form:

$$\varepsilon(\mathbf{k}) = -2t(\cos k_x a + \cos k_y a) - 4t' \cos k_x a \cos k_y a$$

S(n) - is defined by diagram combinatorics (AFM(SDW), CDW, commensurate etc.)

Densities of states - correlated metal (U<W)

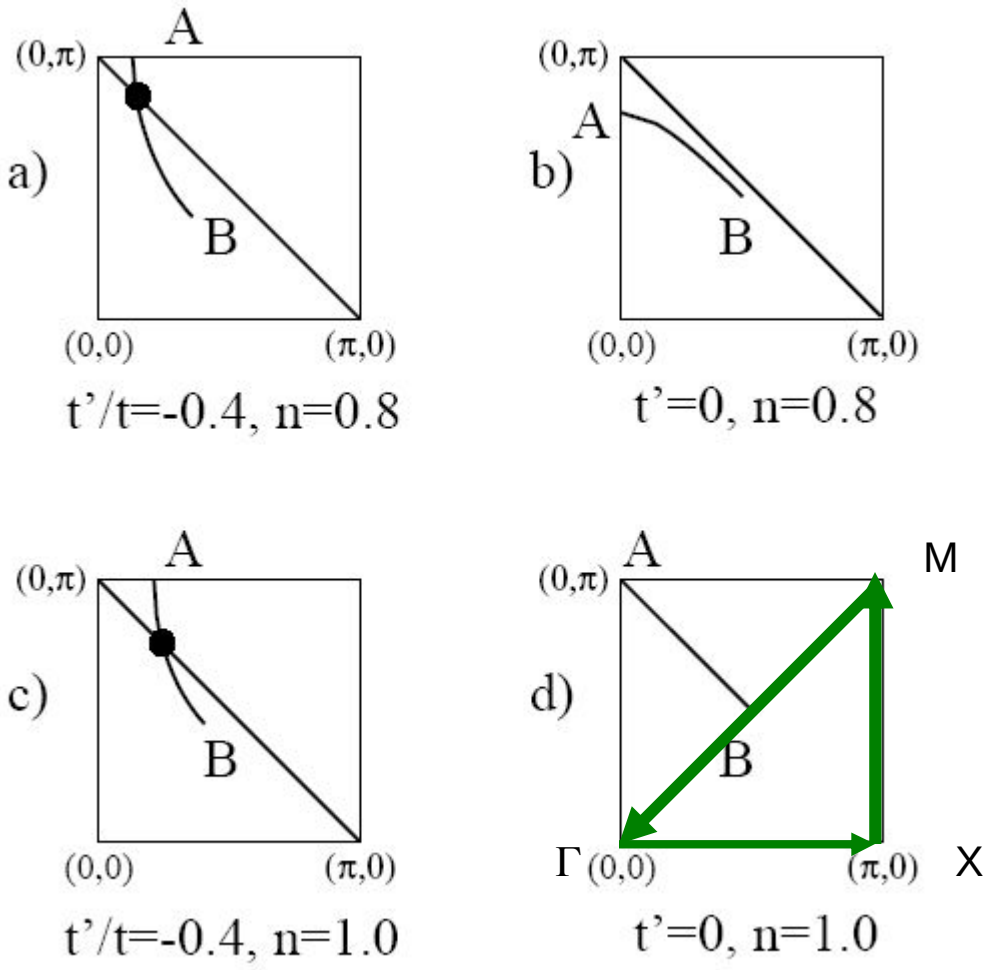


DMFT+Σ_k results

Impuruty solver -NRG

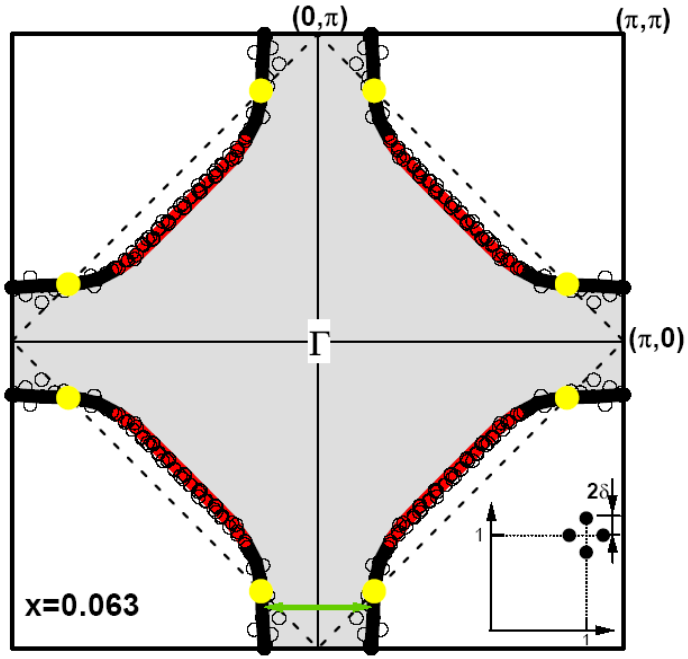
K.G.Wilson, 1975,
R.Bulla, A.C.Hewson,
Th. Pruschke, 1999

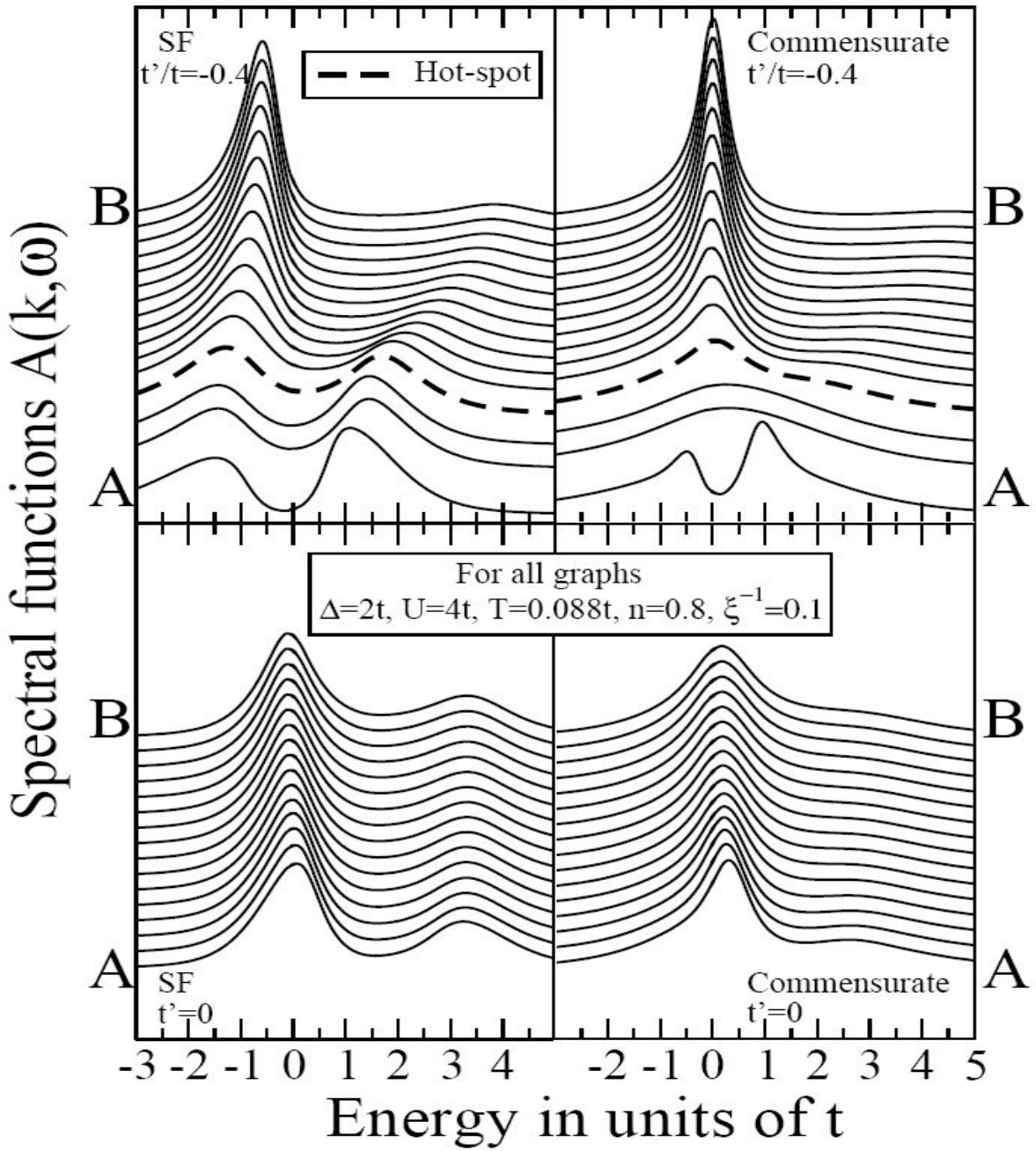
Spectral densities and ARPES

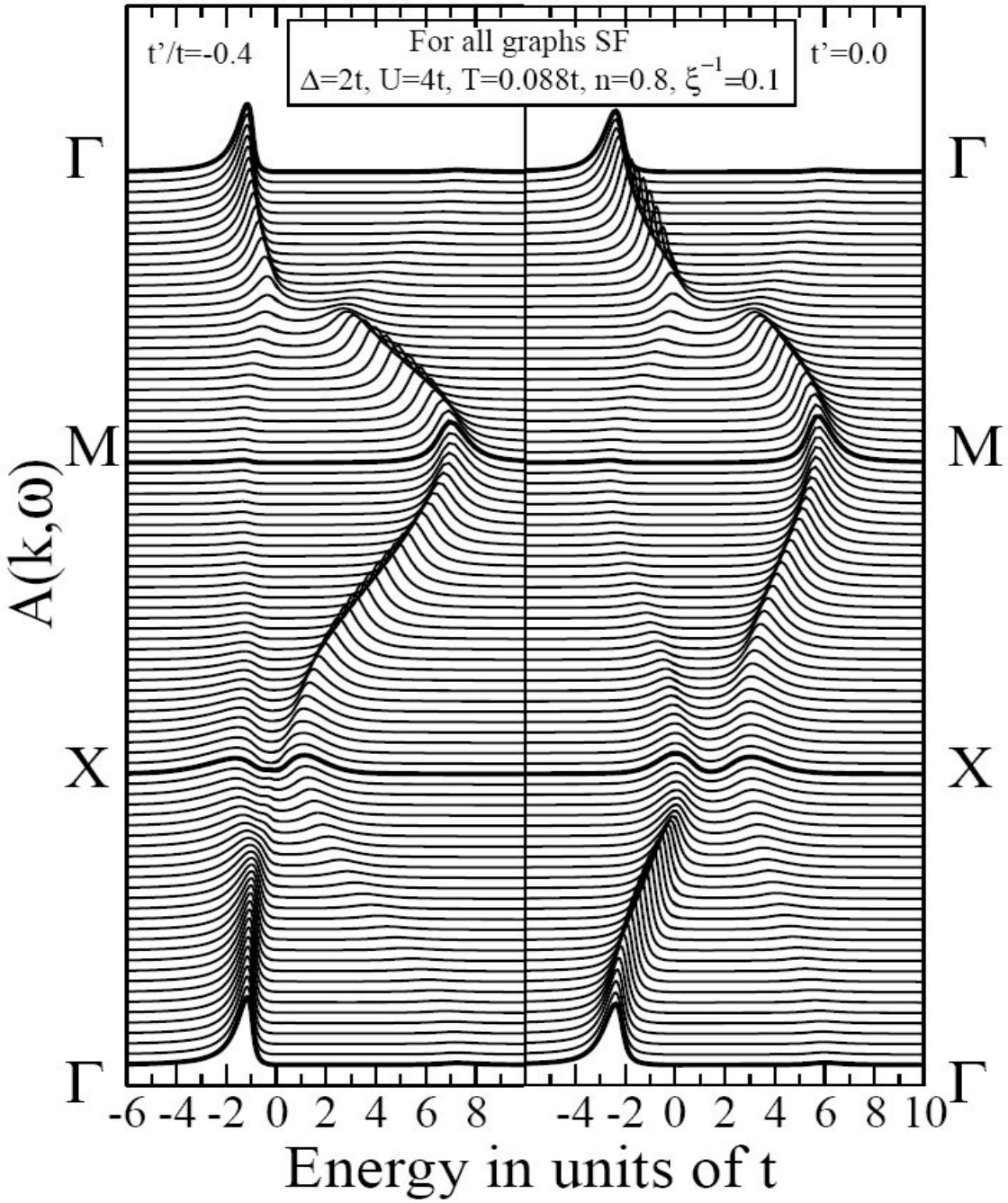


Typical Fermi surface of copper - oxide superconductor ($La_{2-x}Sr_xCuO_4$)

Z.X.Shen et al. (2004)

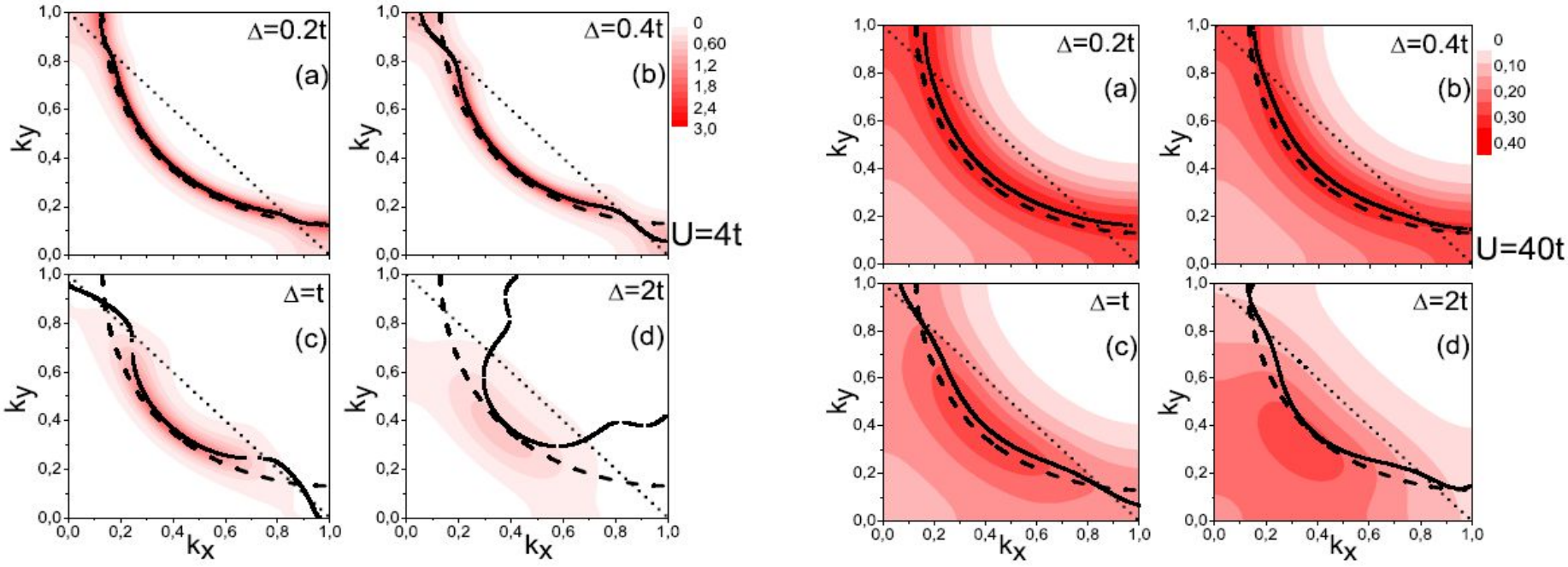



SF
t'/t=-0.4
Hot-spot
Commensurate
t'/t=-0.4
B
A
B
A
For all graphs
Δ=2t, U=4t, T=0.088t, n=0.8, ξ^-1=0.1
B
A
B
A
SF
t'=0
Commensurate
t'=0
-3 -2 -1 0 1 2 3 4
-2 -1 0 1 2 3 4 5
Energy in units of t
Spectral functions A(k,ω)


t'/t=-0.4
For all graphs SF
Δ=2t, U=4t, T=0.088t, n=0.8, ξ^-1=0.1
t'=0.0
Γ
M
X
Γ
Γ
M
X
Γ
A(k,ω)
-6 -4 -2 0 2 4 6 8
-4 -2 0 2 4 6 8 10
Energy in units of t

“Destruction” of the Fermi surface

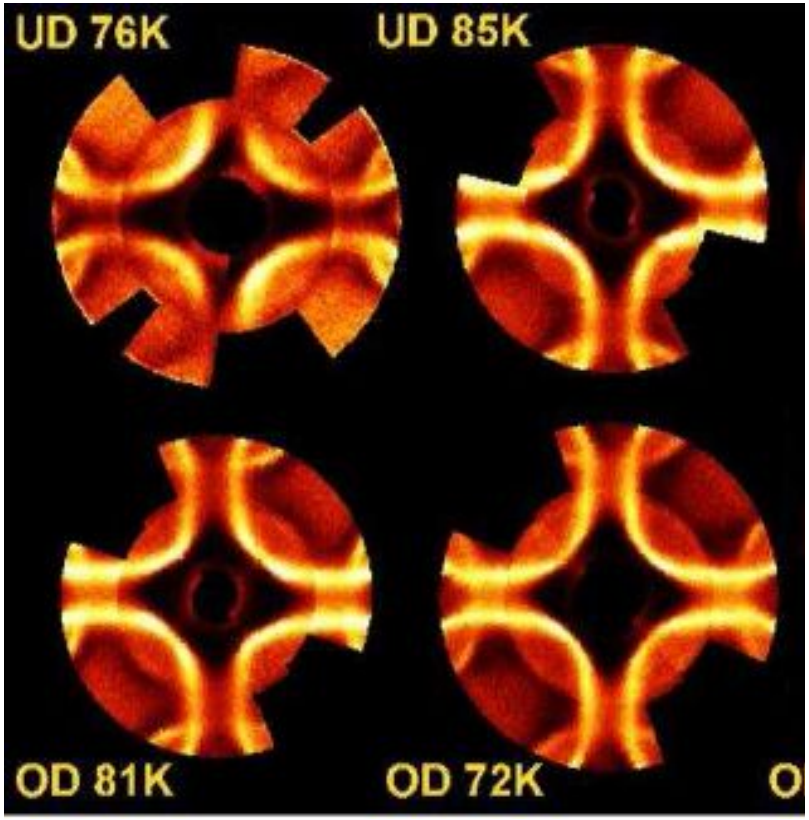
M.V.Sadovskii, I.A.Nekrasov,E.Z.Kuchinskii (2005)

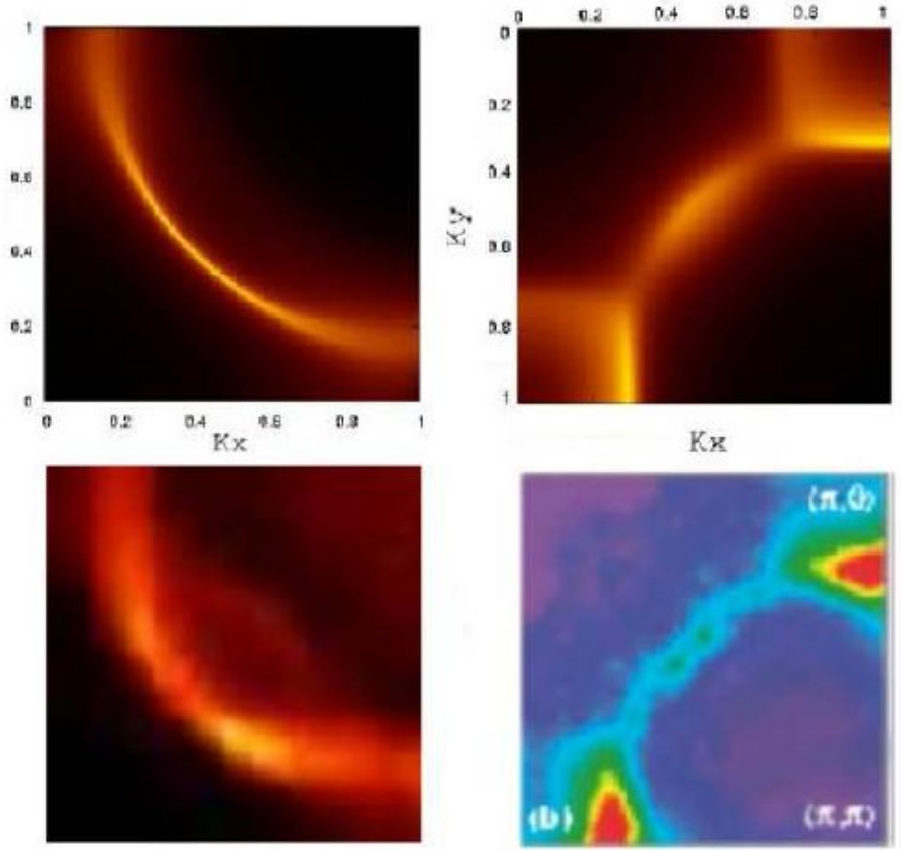


DMFT(NRG)+Σ picture of the Fermi surface “destruction” Ref. [24] On the left – for $U = 4t$. On the right – for $U = 40t$ (a) $\Delta = 0.2t$; (b) $\Delta = 0.4t$; (c) $\Delta = t$; (d) $\Delta = 2t$. Band filling is $n = 0.8$. Dashed line – “bare” Fermi surface. Full lines – solutions of

$$\omega - \varepsilon(\mathbf{k}) + \mu - Re\Sigma(\omega) - Re\Sigma_{\mathbf{k}}(\omega) = 0$$

ARPES Fermi surface - (Bi,Pb)2212, NCCO





A.Kordyuk, S.Borisenko, J.Fink et al. (2002)

FIG. 7: LDA+DMFT+$\Sigma_{\mathbf{k}}$ Fermi surfaces for Bi2212 (upper left panel) and NCCO (upper right panel) 1/4 of BZ (k_x, k_y in units of π/a). Experimental FS for Bi2212 (lower left panel, Ref.[36]) and NCCO (lower right panel, Ref.[33]).

ARPES and LDA+DMFT+Σ:

Electronic structure of $Pr_{2-x}Ce_xCuO_4$ studied via ARPES and LDA+DMFT+Σ_k

I. A. Nekrasov, N. S. Pavlov, E. Z. Kuchinskii, and M. V. Sadovskii
Institute for Electrophysics, Russian Academy of Sciences, Ekaterinburg 620016, Russia

Z. V. Pchelkina
Institute for Metal Physics, Russian Academy of Sciences, Ekaterinburg 620219, Russia

V. B. Zabolotnyy, J. Geck, B. Büchner, and S. V. Borisenko
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D. S. Inosov
Max-Planck-Institute for Solid State Research, Heisenbergstrasse 1, D-70569 Stuttgart, Germany and Institute for Solid State Research, IFW-Dresden, P.O. Box 270116, D-01171 Dresden, Germany

A. A. Kordyuk
Institute for Solid State Research, IFW-Dresden, P.O. Box 270116, D-01171 Dresden, Germany and Institute of Metal Physics of National Academy of Sciences of Ukraine, 03142 Kyiv, Ukraine

M. Lambacher and A. Erb
Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Walther-Meißner Strasse 8, 85748 Garching, Germany

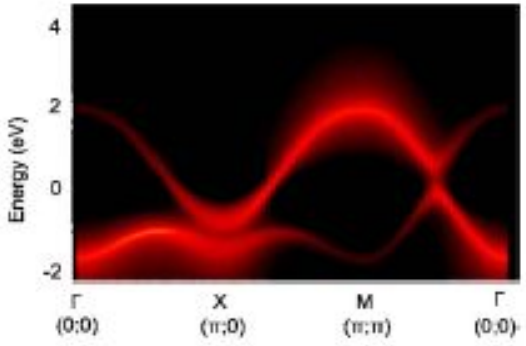


FIG. 2. (Color online) LDA+DMFT+Σ_k quasiparticle energy dispersion of PCCO Cu-$3d(x^2-y^2)$ orbital for high symmetry directions of square Brillouin zone. The Fermi level is zero. Here and below intensity goes down as yellow-red-black.

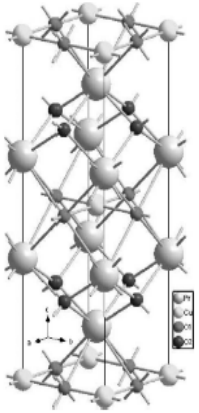


FIG. 1. The crystal structure of Pr_2CuO_4. Medium size gray spheres correspond to the copper atoms, small dark and black spheres are O1 and O2 atoms, respectively, and big gray spheres correspond to praseodymium atoms.

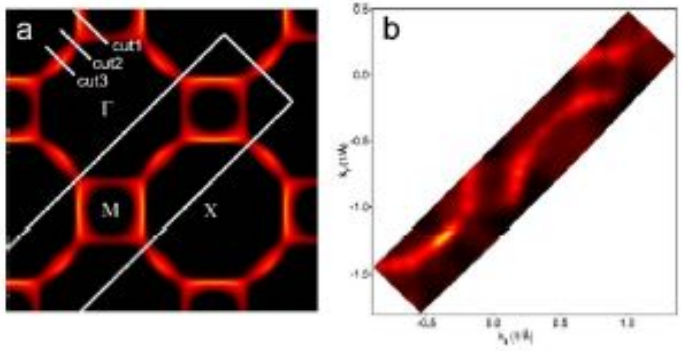


FIG. 3. (Color online) (a) Extended Fermi surfaces for PCCO-LDA+DMFT+Σ_k data. White rectangle in (a) schematically shows the part of reciprocal space measured experimentally (b). Lower left corner is X point $(\pi,0)$.

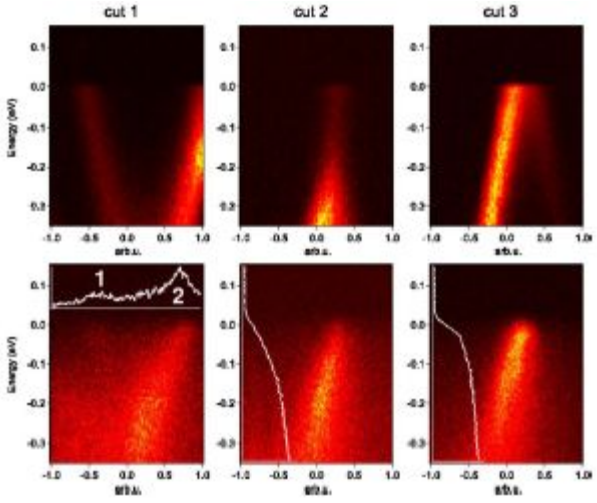
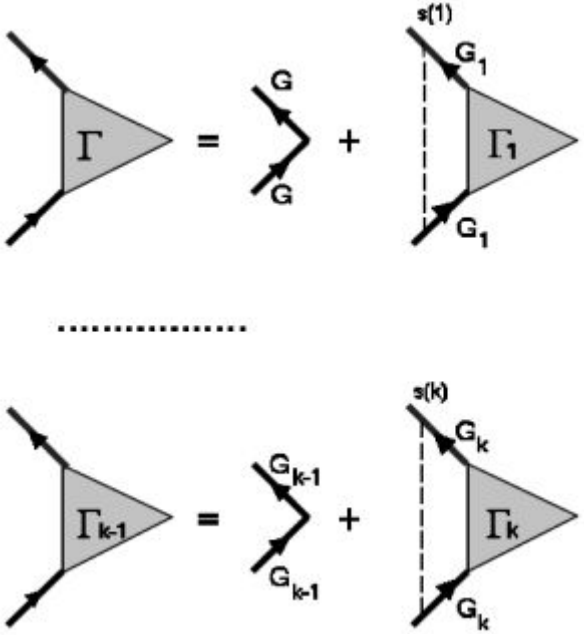


FIG. 4. (Color online) Energy-momentum intensity distributions for the specific cuts drawn in Fig. 3 (upper panels: theoretical data; lower panels: experimental photoemission intensity). To judge about the absolute intensities of the shadow (1) and main band (2), cut 1 contains momentum distribution curves (MDC) integrated in an energy window of 60 meV centered at the FL. Similarly, integral energy distribution curves (EDC) for cut 2 (hot spot) show suppression of the intensity at the FL as compared to cut 3, which is located further away from the hot spot. The FL is zero.

Two-particle properties and Linear Response



Recursion relations for effective vertex - interaction with pseudogap fluctuations.

M.V.Sadovskii, N.A.Strigina (2002)

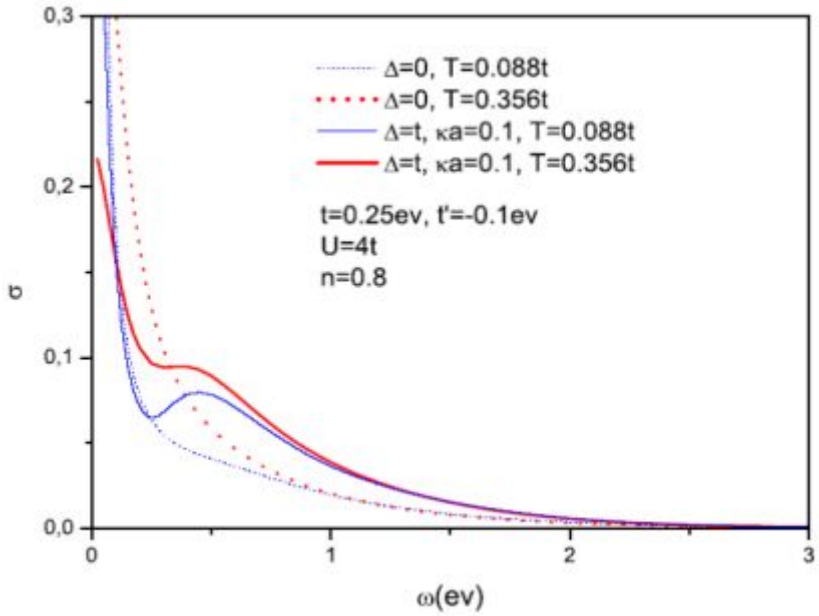
M.V.Sadovskii, I.A.Nekrasov,E.Z.Kuchinskii (2007)

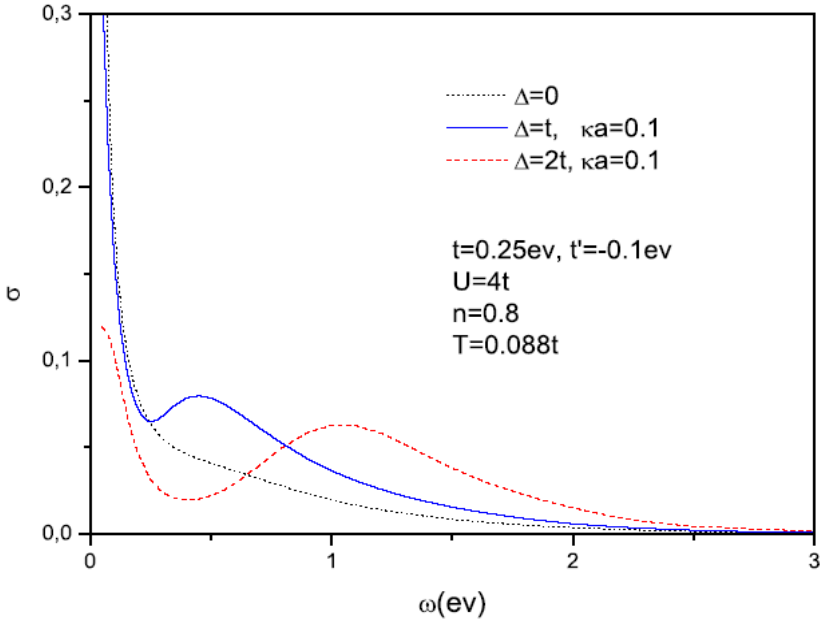
$$\Gamma^{RR}_{k-1}(\varepsilon,\mathrm{p};\varepsilon+\omega,\mathrm{p}+\mathrm{q}) = 1+\Delta^2 s(k) G^R_k(\varepsilon_-,\mathrm{p}_-) G^R_k(\varepsilon_+,\mathrm{p}_+)\Gamma^{RR}_k(\varepsilon,\mathrm{p};\varepsilon+\omega,\mathrm{p}+\mathrm{q})$$

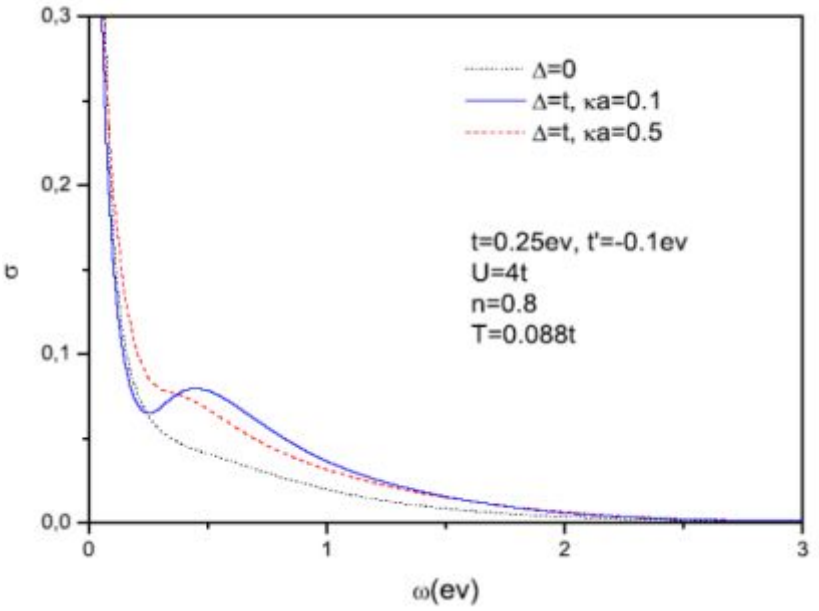
$$\Gamma^{RA}_{k-1}(\varepsilon_-,\mathrm{p}_-;\varepsilon_+,\mathrm{p}_+) = 1+\Delta^2 s(k) G^A_k(\varepsilon_-,\mathrm{p}_-) G^R_k(\varepsilon_+,\mathrm{p}_+)\times$$
$$\times\left\{1+\frac{2iv_k\kappa k}{\omega-\varepsilon_k(\mathrm{p}_+)+\varepsilon_k(\mathrm{p}_-)-\Sigma^R(\varepsilon_+)+\Sigma^A(\varepsilon_-)-\Sigma^R_{k+1}(\varepsilon_+,\mathrm{p}_+)+\Sigma^A_{k+1}(\varepsilon_-,\mathrm{p}_-)}\right\}$$
$$\times\Gamma^{RA}_k(\varepsilon_-,\mathrm{p}_-;\varepsilon_+,\mathrm{p}_+),$$

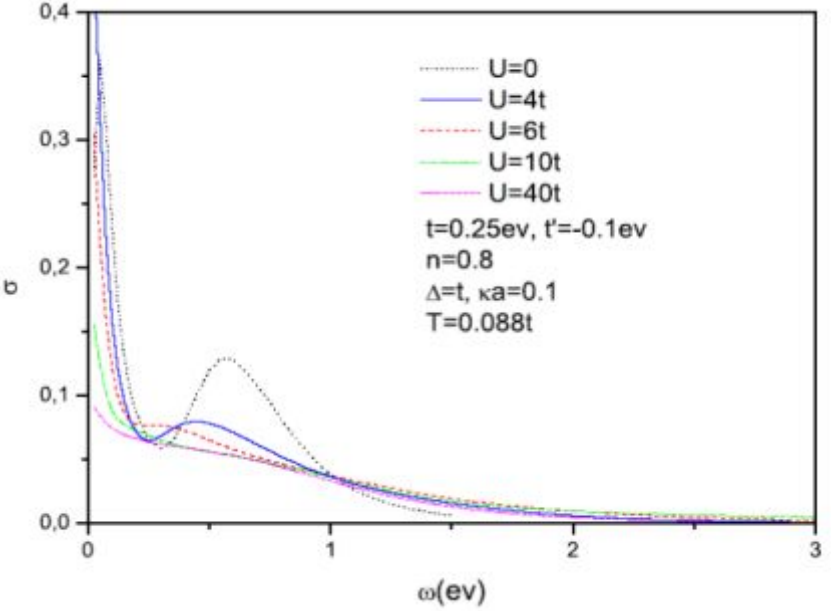
$$G^{R,A}_k(\varepsilon_\pm,\mathrm{p}_\pm) = \frac{1}{\varepsilon_\pm-\varepsilon_k(\mathrm{p}_\pm)\pm ikv_k\kappa-\Sigma^{R,A}(\varepsilon_\pm)-\Sigma^{R,A}_{k+1}(\varepsilon_\pm,\mathrm{p}_\pm)}$$

DMFT+Σ optical conductivity in strongly correlated metal



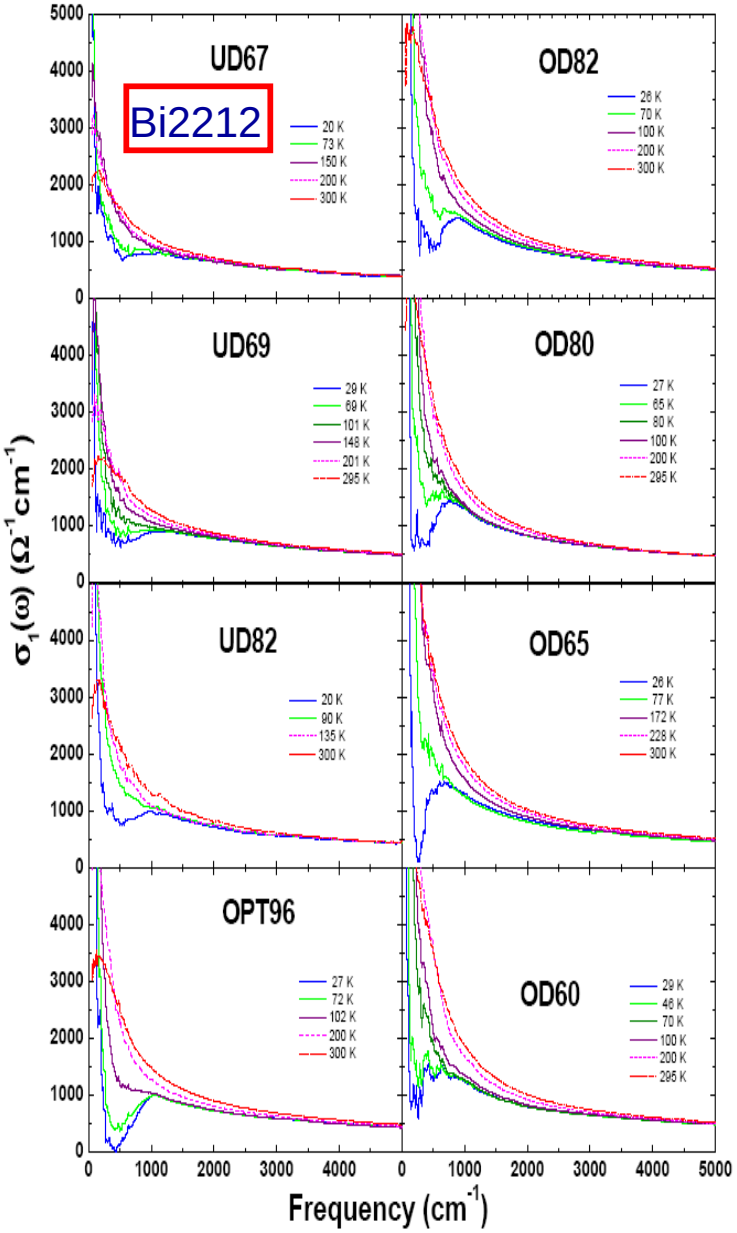




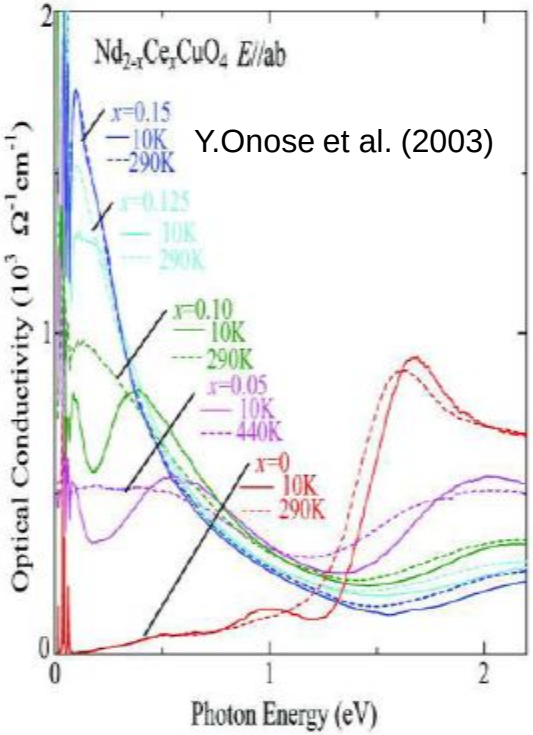


Conductivity in units of $\sigma_0 = \frac{e^2}{\hbar} = 2.5\ 10^{-4}\ \mathrm{Ohm}^{-1}$

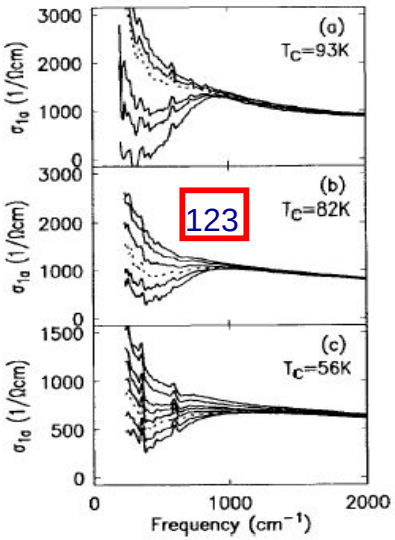
Optical evidence for pseudogaps in oxides

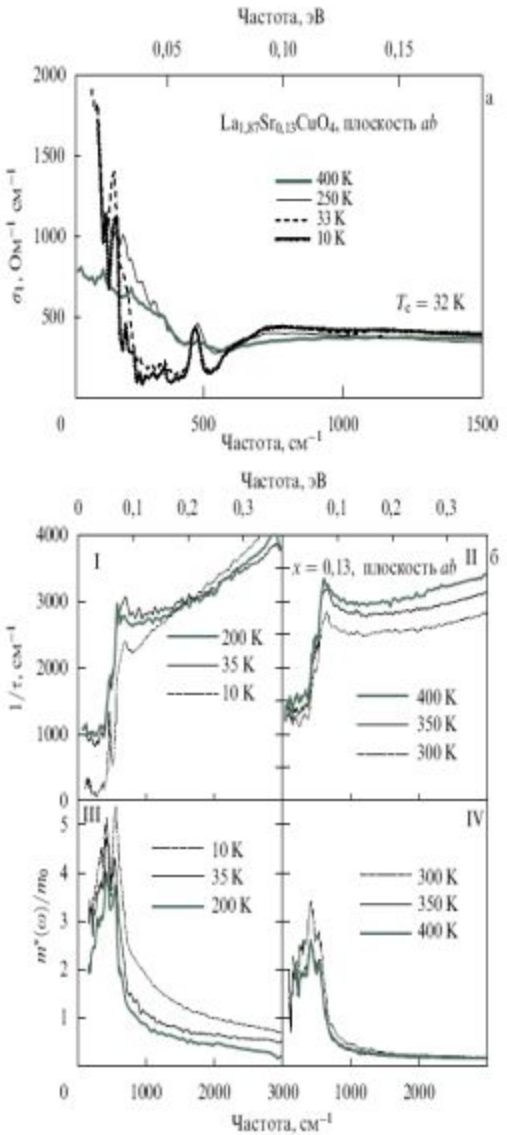


T.Timusk et al. (2006)



Y.Onose et al. (2003)





T.Startseva et al. (1999)

Single band sum rule:

If one considers electrons in a crystal and confines himself to the electrons in a particular band neglecting interband transitions, the sum rule has to be modified to

$$\frac{2}{\pi}\int_0^\infty \mathrm{Re}\,\sigma^s_{\mu\nu}(\omega)\,d\omega = -\lim_{\omega\to\infty}\omega\,\mathrm{Im}\,\sigma^s_{\mu\nu}(\omega) = e^2\,\mathrm{Tr}\{\rho\cdot\partial^2 E(p)/\partial p_\nu \partial p_\mu\}\,. \quad (8.12)$$

This holds if the electron system is described by the Hamiltonian

$$\mathscr{H} = \sum_i E(p_i) + V(r_1, \cdots r_N) \quad (8.13)$$

where $E(p)$ is the energy of an electron with the crystal moments p. Also one has to omit the interband elements of the potential V.

$$\int_{-\infty}^{\infty} d\omega Re\sigma_{xx}(\omega) = \pi e^2 \sum_{\mathbf{p},\sigma} \frac{\partial^2 \varepsilon_p}{\partial p_x^2} n(\varepsilon_p)$$

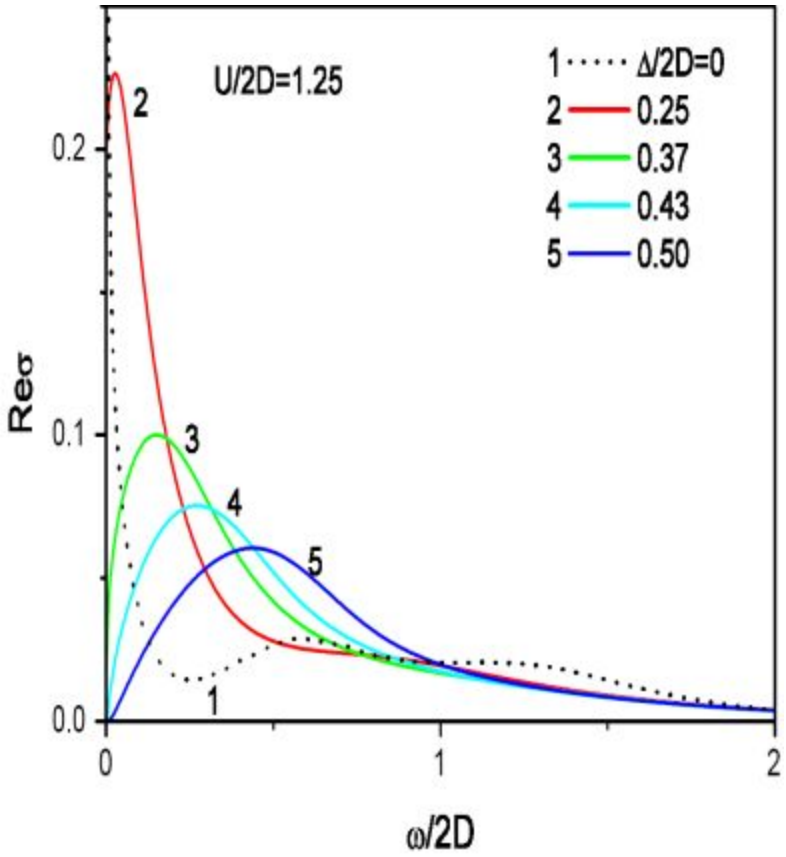
$$n(\varepsilon_p) = -\frac{1}{\pi}\int_{-\infty}^{\infty} d\varepsilon f(\varepsilon) Im G^R(\varepsilon, \mathbf{p})$$

This should be valid in any reasonable model of optical conductivity!

Dependence of the r.h.s. on temperature and any other parameter is sometimes called “sum rule violation”.

Check of the general optical sum rule (d=3):

$$\int_{-\infty}^{\infty} d\omega Re\sigma_{xx}(\omega) = \pi e^2 \sum_{\mathbf{p},\sigma} \frac{\partial^2 \varepsilon_p}{\partial p_x^2} n(\varepsilon_p)$$



$\Delta/2D$	$\pi e^2 \sum_{\mathbf{p},\sigma} \frac{\partial^2 \varepsilon_p}{\partial p_x^2} n(\varepsilon_p)$	$\int_{-\infty}^{\infty} d\omega Re\sigma_{xx}(\omega)$
0	0,063	0,064
0,25	0,068	0.07
0,37	0,06	0.061
0,43	0,056	0.056
0,50	0,049	0.05

Conclusions:

- DMFT+Σ - universal and effective way to include “external” interactions to DMFT
- DMFT+Σ - effective way to take into account nonlocal corrections to DMFT
- DMFT+Σ can be easily generalized for “realistic” calculations (LDA+DMFT+Σ)
- Many applications already demonstrated the effectiveness of DMFT+Σ, more to come

- Review: E.Z.Kuchinskii, I.A.Nekrasov, M.V.Sadovskii. Physics Uspekhi 55, No.4. (2012); ArXiv: 1109.2305; УФН 182, No.4, 345-378 (2012)