ARPES spectral function generated by the Continued Fraction Method : « CFM »

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10.4.-11.5.2007 MPIPKS Dresden

Abstract of talk on April 10 2007, opening the seminar period:

1) **Brief tutorial on ARPES and retrospective on corpes05**
Available in extended version under URL
http://www-crismat.ensicaen.fr/ecoleneem/ARPES.pdf

2) **Brief introduction to the Continued Fraction Method: « CFM »**
Available in extended version under URL
http://www.mpipks-dresden.mpg.de/~corpes05/index.html

3) **Generics of « Kinks and waterfalls »:**
Momentum dispersion of ARPES features, interference of coherent and incoherent propagators, dynamical weight transfer.
An extended version is presented in the following 30 panels, taking numerous discussions during the entire corpes07 event into account,

On the generics of « kinks » and « waterfalls » in ARPES

Outline:

- Intrinsic photocurrent (Hedin-Lundquist)
- Green function for the photo hole and Fermi liquid fixed point
- Intrinsic background function $G_b(k,\omega)$ and « incoherent » part
- Covergence radius of the FL expansion in terms of $G_b(k,\omega)$
- Role of « active » low energy spectral weight Q>Z, construction of a generic scenario: Parameter Z*=Z/Q
- Extrema in the energy distribution curve(EDC): General eqs.
- Evolution of extrema within the generic scenario: Role of Z*
- Microscopic backup: How to estimate Q
- Microscopic backup: Details on Hubbard models, solved with the continued fraction method. Comparison w/ other methods
- Outlook on possible collaborations and conclusion

ARPES theory and Green function formalism

Intrinsic, angle resolved photo current in the sudden approximation

"A short reminder"
(3 panels)

For a derivation of Hedin's sudden approximation, see e.g.:
O. Gunnarson, K. Schönhammer, in: K.A. Gschneidner Jr., L. Eyring, S. Hüfner (Eds.), Handbook on the Physics and Chemistry of Rare Earths 10 (103) (1987).

The spectrum of outgoing photoelectrons in plane wave states |f> depends on the conserved component of momentum k and the binding energy ε. The orbital |f> is correlated, via the matrix element $M_{f\lambda}$, with a photohole in the orbital |λ>. The fermionic removal spectrum $A^{<}_{\lambda\lambda}$ is obtained from a diagonal Green function $G_{\lambda\lambda}(k,\omega)$. The "one-step" formula…

$$\langle f|I(k,\varepsilon)|f\rangle = M_{f\lambda} A^{<}_{\lambda\lambda}(k,\varepsilon) M_{\lambda f}$$

…reflects quantum coherence among photohole and photoelectron.
Matrixelement and removal spectrum both depend on the photon field.

After decomposing the annihilation operator for the photohole in any convenient basis {i}: $c_\lambda = \Sigma\, u_{\lambda i} c_i$, a more familiar form of the one-step theory is obtained:

$$\langle f|I(k,\varepsilon)|f\rangle = \sum_{ij} M_{fi} A^{<}_{ij}(k,\varepsilon) M_{jf}$$

Intrinsic removal spectra $A^{<}_{ij}$. Off-diagonal terms, causing interference.
Dependence on the photon field transferred to the matrix elements $M_{fi} = M_{f\lambda} u_{\lambda i}$.

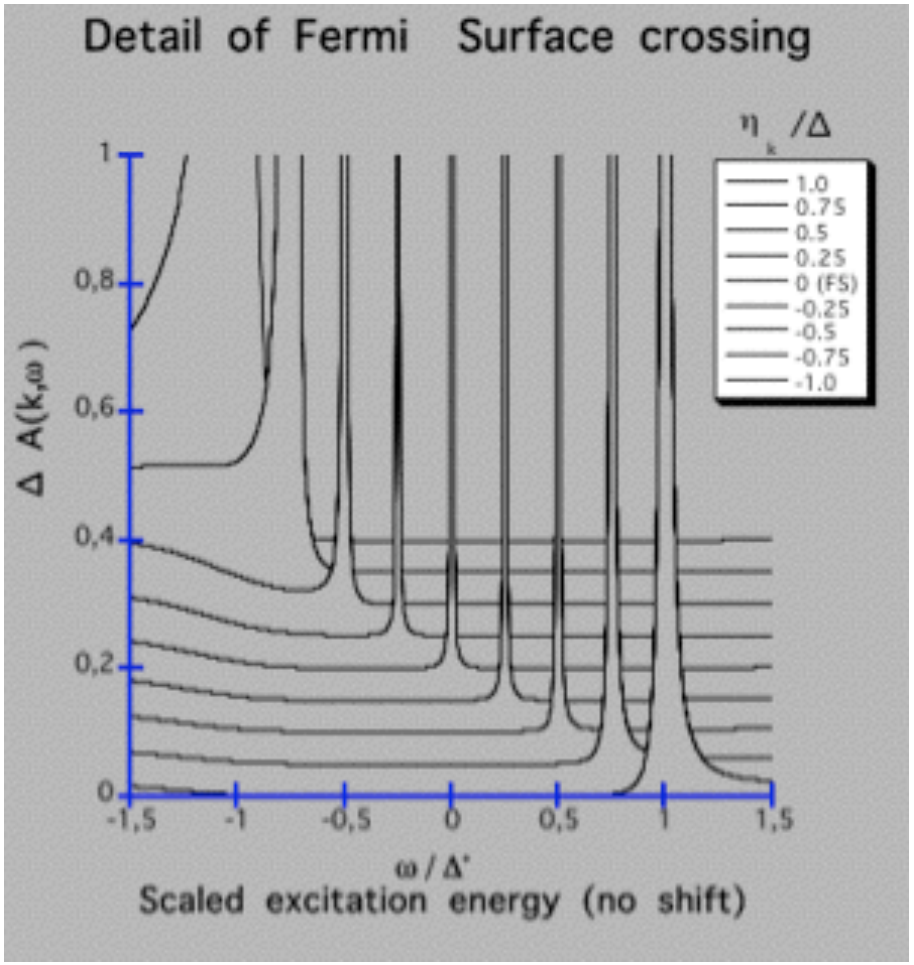
Does the limit of the Fermi Liquid manifest itself in the dispersion of ARPES features ? To answer this question, we analyse the extrema of $A^{<}_{\lambda\lambda}(k,\varepsilon)$

Quasiparticle (QP) resonances in a single band

Momentum k on a FS crossing path parametrised by $\eta \sim k-k_F$

Intrinsic spectrum $A_{ii}(\eta,\varepsilon)$ stripped of all perturbations: Ballistic limit, T=0, no phonons, no defects

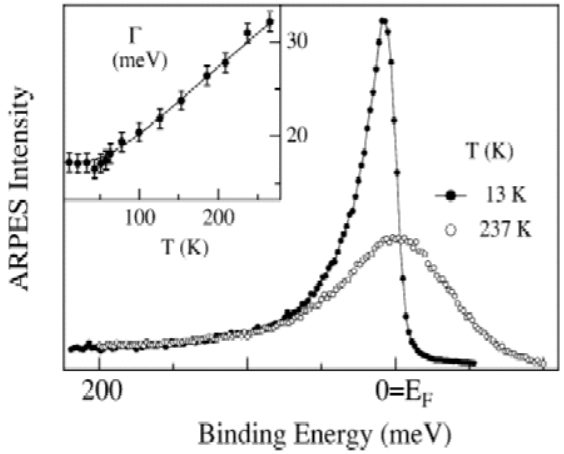
* A stack of idealised Energy Distribution Curves (EDC's). The evolution of lineshapes signals an asymmetric background. This example is characteristic for a hole doped Hubbard model [1,3-5]
* As η increases, the limit of the Fermi Liquid (FL) regime is reached more quickly for $\eta<0$ than for $\eta>0$
* The immediate Fermi Surface (FS) crossing of the QP is nevertheless particle-hole symmetric
* We calculate analytically the trajectory of various intensity minima and maxima in the plane (η,ε), inside the FL regime and beyond.



QP resonances in a real material: $TiTe_2$

Difficulty to extract information on the QP from EDC- or MDC- lineshapes

Perfetti et al.
PRB 64, 115102 (2001)

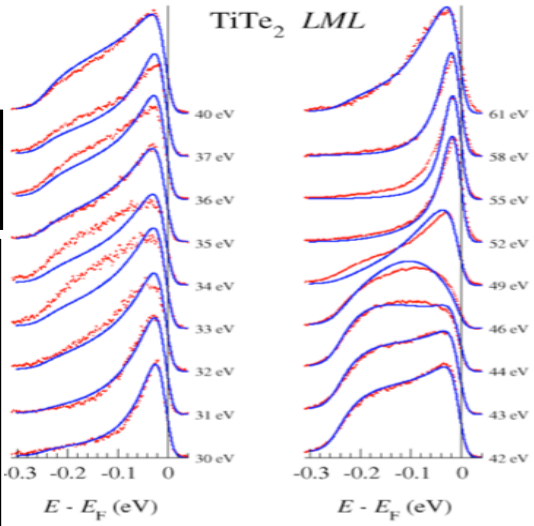


* **Lamellar material with well develpoed QP resonances**
* **Used as "benchmark" for testing ARPES beamlines**
* **Damping coefficient ß [2] in the intrinsic FL spectrum: Lack of agreement on its value over many years.**
  <---- Example: Phonons + defects + convolution with various resolution functions; all not enough to explain the T=0 "offset" in the width Γ at k_F

Latest update of a long quest:
"One-step formula + sudden aproximation achieves quantitative job"

E.Krasovskii corpes07 seminar talk
(see also PRL 98, 217604)

* **Ab initio calculation of matrix elements explains «offset» in Γ as well as variation of lineshape with the photon field ---->**
* **Importance of broadening by non-conserved component of k**



Comment: Various setbacks all along this challenging TiTe2 quest were not in vain.
They helped sharpening the tools for a more quantitative analysis (Conclusion of [4])

« FL fixed point »
(3 panels)

FL fixed point (1)

Gapless excitations and Fermi surface

The FL, wether *weakly correlated* or
strongly correlated,
is characterized by coherent
gapless excitations that live on a FS
and disperse with momentum $k\text{-}k_F$. The propagator for
particle addition or particle removal

$$G_c(k,\omega) = Z_k/(\omega - \varepsilon^*(k))$$

is defined in terms of the QP weight Z_k
and QP energy $\varepsilon^*(k)$
The FS in k-space is defined by all points
where: $\varepsilon^*(k)=0$

FL fixed point (2)

Difference between weakly and strongly correlated FL

Weakly correlated:

$Z_k \approx 1$ **Pauli sumrule for fermions nearly exhausted by QP weight alone**

$\varepsilon^*(k) \approx Z_k(E_k - E_{kF}) = Z_k \varepsilon_k$ **QP energy weakly renormalized, relative to an uncorrelated excitation in a Bloch band**

Strongly correlated:

$Z_k << 1$ **QP weight far from exhausting Pauli sumrule**

$\varepsilon^*(k) = Z_k \eta_k \quad \eta_k = (E_k - E_{kF} + \Sigma(k, \omega=0))$

QP energy affected by a « selfenergy shift »

Simple connection to a Bloch band is lost

Correlated FS (locus of $\varepsilon^*(k) = 0$)

can differ from uncorrelated FS (locus of $E_k = E_{kF}$)

FL fixed point (3)

QP picture and microscopic Green function of the photo hole

$$G_{\lambda\lambda}^{-1}(k,\omega) = \omega - \varepsilon_k - \Sigma(k,\omega)$$

Expand $\Sigma(k,\omega) = \Sigma(k,0) + \alpha_k\omega + \delta\Sigma(k,\omega)$

All terms beyond first order are summed up in $\delta\Sigma(k,\omega)$.

Neglect these to obtain the "coherent part" :

$$G_c^{-1}(k,\omega) = (\omega / Z_k) - \eta_k$$

* **QP-weight:** $Z_k=(1-\alpha_k)^{-1}$ **QP-energy:** $\varepsilon^*(k)= Z_k\eta_k$
* **In the diffusive regime,** $\eta_k= \varepsilon_k + \Sigma(k, 0)$ **is complex**

  In the presence of defects, Im $\Sigma(k,0)$ does not vanish even at T=0 (Taken in account as "offset" in some of the following results). Then, the coherent spectral peak has a residual Lorentzian width and the FS-crossing is not sharply defined (no discontinuity in n(k) at $\mathrm{Re}\eta_k=0$).
* **A real** $\Sigma(k,0)$ **is only possible in the ballistic regime:**

  Temperature T=0, absence of residual defect scattering
* **"The FL fixed point is hard to approach experimentally!"**

« Beyond the FL fixed point » (4 panels)

Beyond the FL fixed point (1)

Reconsider the full Green function, describing also the decay of the QP by many body effects

$$G_{\lambda\lambda}^{-1}(k,\omega) = G_c^{-1}(k,\omega) - \delta\Sigma(k,\omega)$$

* **The coefficient of the leading term: $\delta\Sigma(k,\omega)\approx(i\beta_k\omega^2)$, scales the strength of QP damping $\Gamma_k = ß'(Z_k Re\eta_k)^2$, $ß' = (Z_k Re\beta_k)$**
  Terms such as $\omega^2 ln(\omega)$ in 2d can fragilise, but not destroy the FL.
* **To recover the missing weight 1- Z_k and fully "dress" the damped QP, $\delta\Sigma(k,\omega)$ has to be determined up to the limit of large ω.**

The continued fraction method (CFM) enables to obtain $\delta\Sigma(k,\omega)$ for a given $G_c(k,\omega)$ via a high energy expansion of $G_{\lambda\lambda}(k,\omega)$. First presented at the SNS meeting in Stanford (1995) [1] and applied to Ti Te_2 [2], it has since been developed into a useful link between microscopic theory and phenomenology [3-5].

* **We focus our attention on $\delta\Sigma(k,\omega)$ in the interval around $\omega=0$.**

Our objective: Determine the immediate limit of the FL regime.

Beyond the FL fixed point (2)

A central role in our analysis is played by the

background function

Consider the Laurent expansion of

$$1/(\omega - \alpha_k\omega - \delta\Sigma(k,\omega)) = Z_k/\omega + G_b(k, \omega)$$

The « background function » $G_b(k,\omega)$ is the normal part, after the pole singularity has been isolated. $G_b(k,\omega)$ itself can be expanded in a Taylor series

The physical origin of intrinsic background is the coupling of the propagating fermion to collective (« bosonic ») modes. These modes can originate in the electronic subsystem itself (examples: spin and charge fluctuations in the Hubbard model, plasmons in the case of long range Coulomb interaction) or in the coupled electron-lattice system.

Beyond the FL fixed point (3)

Rigorous definition of the « incoherent » propagator $G_{inc}(k,\omega)$, in agreement with causality

The shift $\eta_k \neq 0$ in the denominator causes a distance from the FL fixed point. Near a FS crossing, one has: $Re\eta_k \sim k-k_F$. This is the generic cause for momentum dispersion of spectral features, irrespective of additional k-dependence in $G_b(k,\omega)$. The shift affects both parts of the Laurent expansion. Therefore, the incoherent propagator:

$$G_{inc}^{-1}(k,\omega) = G_b^{-1}(k,\omega) - \eta_k,$$

is defined in exact analogy to the coherent one:

$$G_c^{-1}(k,\omega) = (\omega / Z_k) - \eta_k.$$

Both are advanced (or retarded) functions with Herglotz property. In this work, the advanced propagators are used.

$G_{inc}(k,\omega)$ disperses with $k-k_F$ even if $G_b(\omega)$ is independent of k

Beyond the FL fixed point (4)

$G_c(k,\omega)$ and $G_{inc}(k,\omega)$ both disperse and they are not additive

The coherent and incoherent propagators combine like in a Fano interference formula:

$$G_{\lambda\lambda}(k,\omega) = \frac{G_c(k,\omega)+G_{inc}(k,\omega)+2\eta_k G_c(k,\omega)G_{inc}(k,\omega)}{1-\eta_k^2 G_c(k,\omega)G_{inc}(k,\omega)}$$

Note: Additivity of «coherent» and «incoherent» spectrum holds only when both $Re\eta_k = Im\,\eta_k = 0$. The strongest possible interference occurs when $Im\eta_k = 0$ (ballistic regime), but $Re\eta_k \neq 0$ (away from the FS):

==> Vanishing spectral intensity at $\omega = 0$.

Mathematical limit of the FL regime in terms of G_b

$$\delta\Sigma(\omega)=(\omega/Z)^2/(G_b^{-1}(\omega)+\omega/Z)$$

Convergence radius of an expansion in powers of ω set by the lowest lying pole in the selfenergy

* **Poles in $\delta\Sigma(\omega)$ obey** $G_b^{-1}(\Omega^*)+\Omega^*/Z=0.$

The solution Ω^* nearest to $\omega=0$ sets the convergence radius.

* **The coefficient of the leading term $\delta\Sigma \approx i\beta\omega^2$ is**

$$i\beta = G_b(0)/Z^2$$

A factor i has been pulled out, to make ß purely real in a particle-hole symmetric scenario [2]. Otherwise, ß is complex and the QP damping is scaled by Reß or $\mathrm{Im}G_b(0)$.

Im $G_b(0)\neq 0$ is necessary and sufficient for QP damping to exist.

One can conclude:

A background spectrum, straddling $\omega=0$, is a generic feature of the FL

* **The QP's are underdamped in the coherence interval - $\Delta^* < \varepsilon < \Delta^*$,**

$$\Delta^* \, \mathrm{Im}G_b(0) = Z$$

These statements hold for the general case. Momentum label k is dropped for simplicity only. However, in the following analysis of generic effects, dispersion other than through η_k will be neglected.

Electronic structure with gaps

« Active » low energy weight and generic background model

* The convergence radius Ω^* of the FL expansion is given by the solution $\Omega^* = -Z/G_b(\Omega^*)$ that is closest to the origin.
  In the limit $Z \ll 1$, Ω^* becomes part of the low energy scenario.

* In the presence of gaps, the spectral sector that straddles the Fermi edge dominates the solution. We therefore define the "active" weight Q as the integrated spectral weight in the low energy sector, including Z: $Z < Q \leq 1$. The case without gaps is represented by the limit Q=1.

Note: Weakly correlated systems with screened Coulomb interaction already have Q considerably below 1, due to plasmon satellites. (GW approximation of Hedin).

* For a generic model, we assume that the active background has no finestructure and can be modeled by a single pole Ω. The solution for Ω^* is then unique. Given Z and Q, Ω^* and Ω can both be expresssed by $G_b(0)$ (i.e. by the complex coefficient β), with between them the relation

$$Q\Omega^* = Z\Omega.$$

We shall discuss the case of competing solutions in the concluding remarks

Generic scenario for « active » background [2] yields

$Z\delta\Sigma(\omega) = (1 - Z^*)\omega^2 /(\omega - Z^*\Omega)$ $\quad Z< Z^*=Z/Q <1$

* Background approximated by a complex pole $\omega=\Omega$, weight Q-Z.
* $G_b^{-1}(\omega) + \omega/Z=0$ yields solution $\Omega^*=Z^*\Omega$ for the selfenergy pole.
* Figure from ref. [2]. Particle-hole symmetric case, $\Omega=i\Delta$:

  (a) spectrum at k_F, (b) trajectories of the 2 poles in $G(k,\omega)$, for $\eta_k \leq 0$, ballistic regime, $\beta' = Z\beta = 1/\Delta^*$.

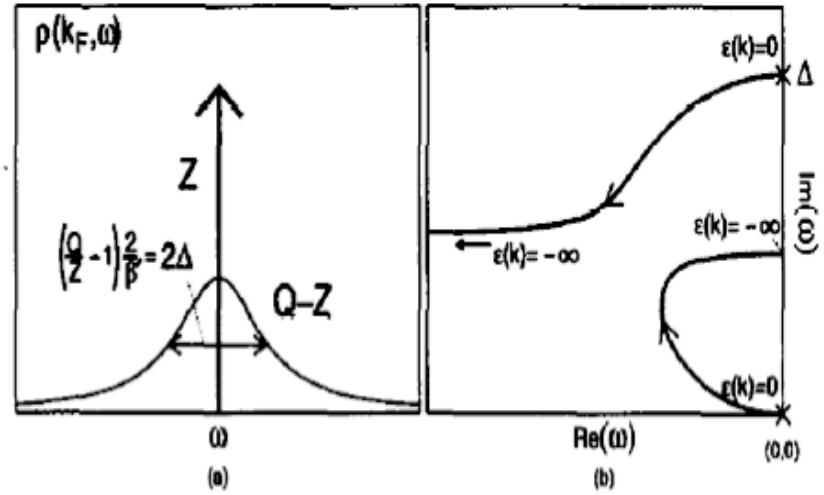


Fig. 1. (a) Spectral function for the Green's function of eq. (2). (b) The trajectories of the two poles derived from eq. (2) and k-independent Σ, shown here for $Q/Z = 2.1$. The X's show the poles for $\mathbf{k}=\mathbf{k}_F$.

$Z^*=Z/Q$ controlls the dispersion changes at the limit of the FL :

<u>1/2≤Z*<1:</u> Mild crossover in EDC or MDC peak dispersions. $Z^*\approx 1/2$ applies to the Hubbard model at n=1. (Recent DMFT study: Byczuk et al., Nature Phys.3, 168(2007))

<u>1/4≤Z*<1/2:</u> Crossover sharpens into « kink ». The low energy QP pole no longer participates in the dispersion. It « bends back » (as shown in the figure).

<u>Range Z*<1/4:</u> Peak-dip-peak feature or «waterfall», a discontinuity in the EDC.

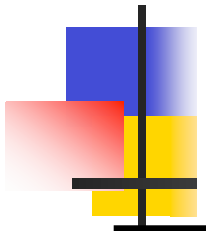
We proceed with a detailed discussion of these phenomena

Extrema in the spectral function of the photohole

$$A_{\lambda\lambda}(k,\varepsilon)=\pi^{-1}\mathrm{Im}\, G_{\lambda\lambda}\,(k,\omega=\varepsilon-i0_+)$$

$$G_{\lambda\lambda}^{-1}(k,\omega=\varepsilon-i0_+)=X(\varepsilon)-iY(\varepsilon),\quad X'(\varepsilon)=dX/d\varepsilon$$

and $Y'(\varepsilon)=dY/d\varepsilon$



Extrema in $A(k,\varepsilon)$ as function of ε obey the condition

$$Y'(X^2-Y^2)-2X'XY=0.$$

Since this equation is quadratic in X, it can be explicitly solved for $\mathrm{Re}\eta_k$, as function of binding energy ε. The plot has one or several vertical asymptotes, depending on the richness of the spectrum. Its inverse indicates all possible branches of extrema or inflexion points at a given $\mathrm{Re}\eta_k$. Provided the relation $\mathrm{Re}\eta_k=F(k)$ can be inverted along a FS crossing path and other k-dependences are negligeable, the extremal lines over the plane $(\mathrm{Re}\eta_k,\varepsilon\leq 0)$ become a plot for the dispersion of peaks or dips in a sequence of EDC's at T=0. Inclusion of the Fermi function, for an evaluation of extrema in $A^<(k,\varepsilon)$ at finite T is straightforward.

Evolution of features along a « path » in k-space

ARPES data are most often represented in a two-dimensional plot over the plane (emission angle, binding energy)

Near a FS crossing, dominant k-dependence is caused by $Re\eta \sim (k-k_F)$.

To take advantage of this fact, I have proposed the following fitting procedure :

* **Evaluate Z_k and $\delta\Sigma(k,\omega)$ « on the FS » i.e.: They may depend on the crossing point k_F, but not on the direction « perpendicular » to the FS. This allows to overcome, at least partly, the limitation of the « infinite dimensional » solutions (e.g.: DMFT), which have identical Z and $\delta\Sigma(\omega)$ everywhere in the Brillouin zone.**

* **Linearise $Re\eta \approx v(k_F)(k-k_F)$, where $v(k_F)=v_0(1+\gamma(k_F))$ allows for the « k-mass-renormalisation » (originating from $\Sigma(k,0)$]) of the bandstructure velocity v_0. The overall effective Fermi velocity (slope of the observed QP dispersion) is $v^*=v_0(1+\gamma)/(1-\alpha) = v_0(1+\gamma)Z$. In infinite dimension, only the factor Z from the « ω-mass-renormalisation » survives. By this ansatz, we avoid another, even more constraining limitation of DMFT [3].**

* **For our generic scenario of $\delta\Sigma(\omega)$, the functions X,X',Y,Y' are easily found analytically. Representative examples are shown in the following 3 panels. The key parameter, controlling the changes in dispersion at the limit of the FL regime, is the ratio $Z^*=Z/Q$. The energy scale is Ω^*, the pole in $\delta\Sigma(\omega)$.**

From crossover to “kink” and “waterfall” (1)

ARPES sector, particle-hole symmetric case, T=0, Imη=0 (No “offset”)

Plotted functions : Maxima and minima of A(η,ε) as function of ε (« EDC »).
For comparison: Maximum of A(η,ε) as function of η (« MDC »).

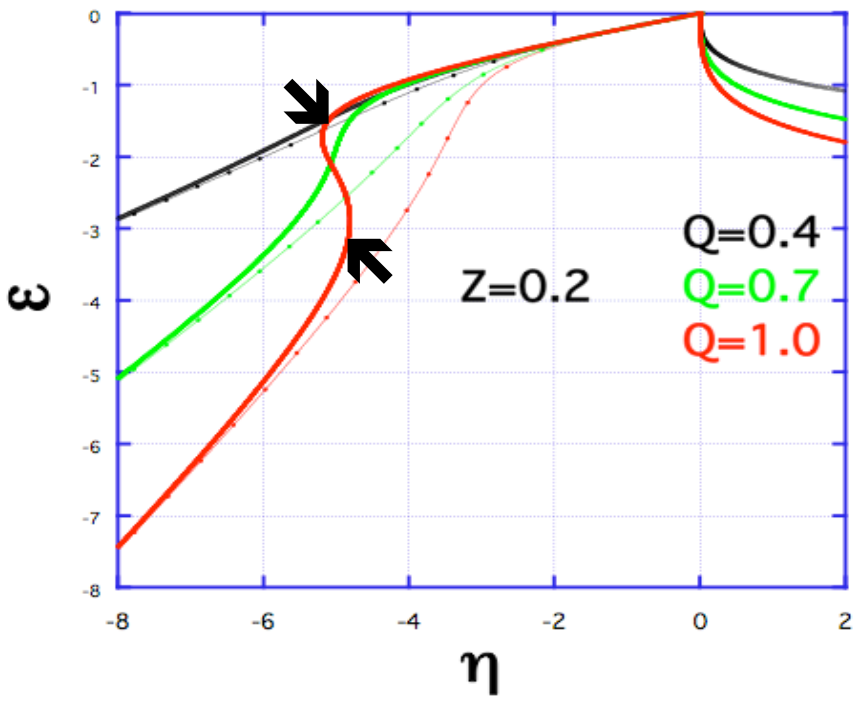
η<0: « occupied » part of Brillouin zone

* **As Z* is lowered, the crossover sharpens, discrepancy between EDC- and MDC- peak increases.**
* **For Z*<1/4, the multivalued portion (arrows) signals a peak-dip-peak sequence of extrema, possibly related to the «waterfall» phenomenon in ARPES**

η>0: « unoccupied » part of BZ

* **Background, straddling the Fermi edge, is observable as a separate dip-peak structure in the EDC («spectral transfer»).**
* **The dip (locus ε=0) signals vanishing intensity by total interference.**

Near the FS crossing: η~k-k_F.



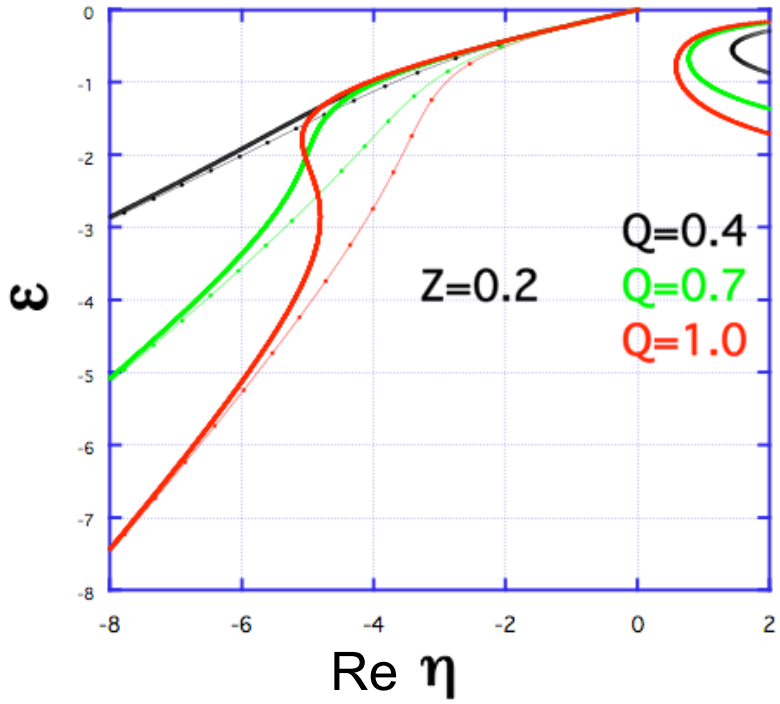
Thick lines: Peaks and dips of the EDC
Thin lines with dots: Peak of the MDC
Energy unit: Distance of nearest selfenergy pole from ω=0.

From crossover to “kink” and “waterfall” (2)

ARPES sector, particle-hole symmetric background.

Influence of a small, finite “offset” $\mathrm{Im}\Sigma(k,0)\neq 0$, e.g. defects at T=0

* $\eta<0$: The main spectral features are not strongly changed by the « offset »
* $\eta>0$: The features of the «spectral transfer» are strongly influenced by the « offset »
* Near k_F ($\mathrm{Re}\eta=0$), spectral transfer no longer observable as a distinct dip-peak
* For sufficiently small « offset », transferred dip-peak reappears at finite $\mathrm{Re}\eta$, (For a discussion, see Ref. [4], below eq.(25))



Thick lines: Peaks and dips of the EDC. Thin lines: Peak of the MDC. Energy scale: Distance from $\omega=0$ of nearest pole in the selfenergy

From crossover to “kink” and “waterfall” (3)

ReΩ<0 (Still T=0, no “offset”):
Particle-hole symmetry is lifted by shifting the maximum of background intensity into the ARPES sector.

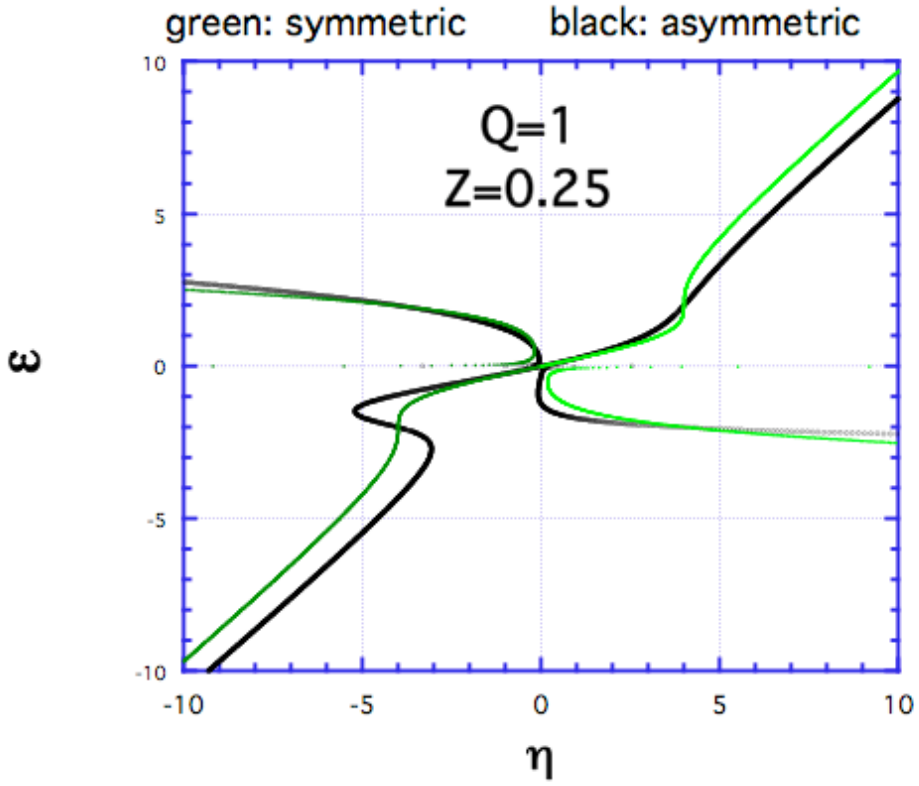
* With particle-hole-symmetry, ReΩ=0, the critical value for a discontinuity in the peak dispersion is Z*=1/4. Here, the « kink » is most pronounced

* Keeping Z*=1/4, what is the effect of a shift ReΩ<0 in the background pole ?

  * ARPES sector: Enhanced background favours discontinuity

  * ARIPES sector: Depleted background leads to a softening of the « kink »

Now plotted: EDC extrema in the ARPES as well as ARIPES sector



Energy scale: Distance of selfenergy pole from ω=0.

Microscopic backup (7 panels)

Low energy weight Q: General statements

Mixed valence: The concept of «configurational crossover» (L.L.Hirst, PRB 15, 1 (1977)) allows to estimate Q in a local (atomic- or cluster-) limit: $Q \approx Q_{at} = Q^{>} + Q^{<}$

* **Both weights, $Q^{>}$ (particle-like) and $Q^{<}$ (hole-like), are generally non-zero, confirming that the spectrum of weight Q straddles the Fermi level.**
* **The partial weights $Q^{>}$ and $Q^{<}$ scale differently as function of the valence mixing than the QP weight Z (Not realizing this, Hirst interpreted Q as QP weight).**
* **In the presence of translational kinetic energy (hopping), Q increases: $\delta Q = Q - Q_{at}$ is called « dynamical weight transfer » (Sawatzky) M.Meinders et al. PRB 48, 3916 (1993).**

Integer valence: Absence of configurational crossover: $Q_{at}=0$.

* **The local estimate for the low energy weight vanishes. In this case, Q is entirely due to « dynamical weight transfer »**
* **Example: Hubbard model at half-filling. As the « bandwidth controlled Mott transition » is approached, both Q and Z vanish together, but Q>Z still holds.**

« Dynamical weight transfer » can only be calculated non-perturbatively. It is crucial for the quantitative description of the FL regime in a strongly correlated metal.

Hubbard model:

Background function $G_b(\omega)$ calculated with the continued fraction method (CFM) [1,3-5]

$$G(k,\omega) = \cfrac{1}{\omega - \omega_1 - \cfrac{s_2^2}{\omega - \omega_3 - s_4^2 G_2(\omega)}}$$

Beginning of the continued fraction (high energy) expansion: Spectral moments up to M_4. Sumrules.

$$\Omega(\omega) = \cfrac{\bar{s}_4^2}{\omega - \bar{\omega}_5 - \cfrac{\bar{s}_6^2}{\omega - \bar{\omega}_7}}$$

Truncation by a terminator allows to make the low energy FL expansion, keeping all the sumrules intact.

The algorithm for a FL terminator $\Omega(\omega)$ distinguishes our CFM from approximations that are based on high energy expansion alone. More generally, the algorithm can be applied after an arbitrary number of stages in the continued fraction, conserving higher spectral moments [4] (e.g. as generated by the Lanczos method).

How is dynamical weight transfer taken into account in determining Q ?

Away from half-filling (doping): Key quantity is a hopping contribution to the « skewness »: $(\omega_3 - \omega_1)/s_2$ [5].

At half filling: Since $\omega_3 = 0$, key quantity is $(s_4)^2$, linked to « excess kurtosis ».

Hubbard models

approaching the Mott transition

Known facts about quasiparticles in the DOS (integrated density)

Half-filled case: DOS from DMFT+NRG at T=0, R. Bulla et al., Physica B 259-61, 721 (1999).

Z-->0
Q-->0
Z*≈1/2

Hole doping: DOS from CFM at T=0. Reference [5].

Z-->0
Q-->1/2
Z*-->0

In both regimes, the damping coefficient Reβ scales like Z^{-2} (see inset above for 1/2-filled case). Concerning the symmetry of the background and the range of our control parameter Z*=Z/Q, the two regimes show essential differences (following panels).

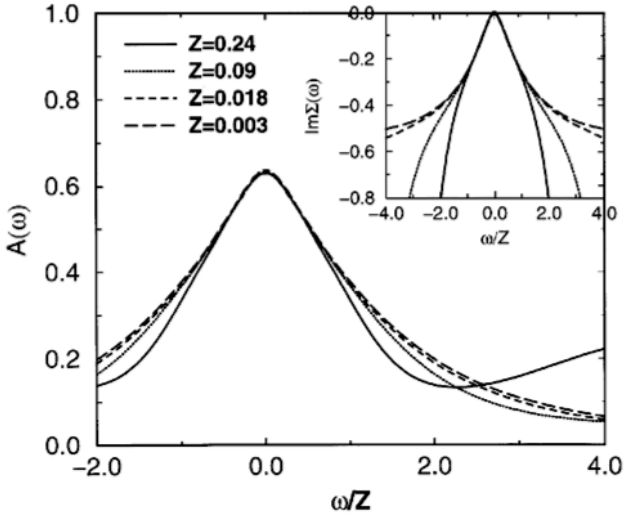


Fig. 1. Scaling behaviour of the local spectral function $A(\omega)$. The inset shows the corresponding scaling behaviour of the imaginary part of the self-energy.

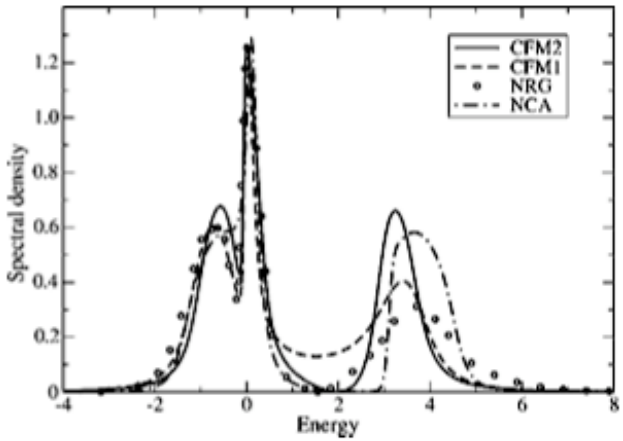
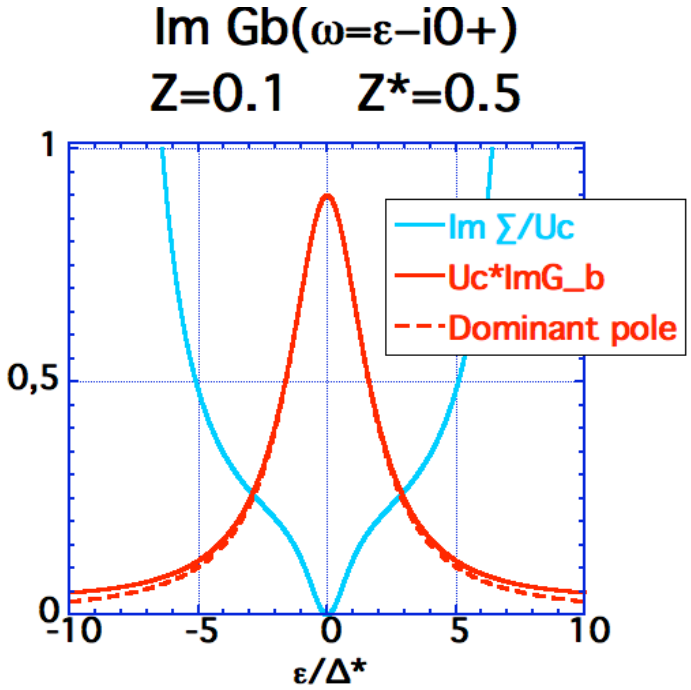


FIG. 5. Spectral density. Comparison of the continued fraction method using the one- and two-pole terminating functions (CFM1 and CFM2) with NCA and NRG (data taken from Ref. 18).

Background and Z* in the half-filled Hubbard model

Sumrule of the kurtosis: $\kappa = M_4/(M_2)^2 = \{(s_2)^2 + (s_4)^2\} / (s_2)^2$

- Weight of low energy central peak
  $Q = (\kappa - 1)/\kappa$ « 3-level system »
  Insulator: $\kappa \dashrightarrow 1$ « 2-level system »
  Condition of validity: Central peak well separated from Hubbard peaks
- Within DMFT + NRG, one finds two invariants as Z-->0 (See Bulla et al., preceding panel) :
  a) $Z/Q = Z^*$, with $Z^* \approx 1/2$
  b) $Z^2\beta = Z/\Delta^* = -iG_b(-i0_+) \approx 2/U_c$,
  with U_c the critical Hubbard U.



Given Z and the two scaling invariants, the terminator $\Omega(\omega)$ of the CFM can be calculated [4]. The central part of the background is well approximated by a dominant pole on the imaginary axis (see figure), confirming the scenario in reference [2]. For $Z^* \approx 1/2$, the crossover in the dispersion at the limit of the FL is quite gentle (see panel 18). Since Q and Z are both small, there is still a strong mass enhancement outside the FL regime. This case was recently studied numerically by Byczuk et al., Nature Phys. 3, 168 (2007).

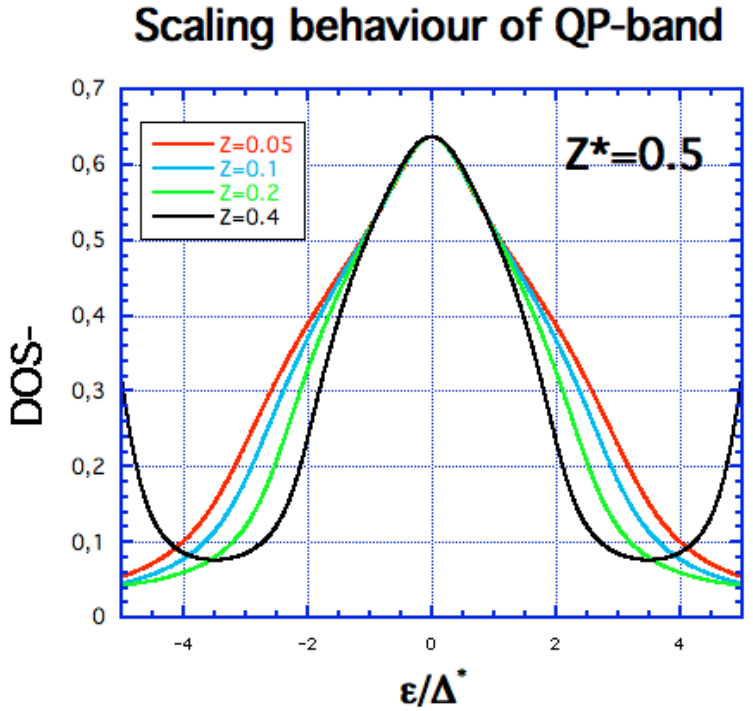
Midgap DOS in the half-filled Hubbard model

A T=0 (ballistic) scenario for $0 \le Z <\approx 1/2$
(Specific U=0 input in the plot: Semi-elliptic DOS)

- **The excess kurtosis**
  $\gamma = \kappa - 1 = (s_4)^2/(s_2)^2$ and the slope
  $\alpha = d\Sigma/d\omega = -(1-Z)/Z$ are nearly inversely proportional:
- **With α , γ and Z*=Z/Q, one can form a « super »-invariant**

$$Q + \alpha\gamma Z = 0$$

- **Exact for small Z, this relation holds qualitatively all the way to Z=1. Correction factors of order 1 depend on the detailed hopping Hamiltonian**



Inserting this invariant in the CFM equation [4], one obtains a canonical solution for the central spectrum in the half-filled Hubbard model, valid up to Z≈1/2. The coherence energy $\Delta^*=(Z\beta)^{-1}$ scales like Z/(1-Z). The dips, at $\varepsilon=\pm s_4$, scale like $Z^{1/2}$. Breakdown of this approximation for Z>1/2 is signaled by the fact that dips and side bands fail to coalesce.

Background and Z* in the doped Hubbard model

CFM solutions at T=0 [5] for hole doping 0<X<1 (Filling n=1-X<1)

* The atomic limit $Q_{at}=(1+X)/2$ yields a lower bound for the « active » spectral weight Q. The dynamical weight transfer $\delta Q(X)>0$ vanishes linearly for X-->0 and also vanishes identically for $U>>U_c$.

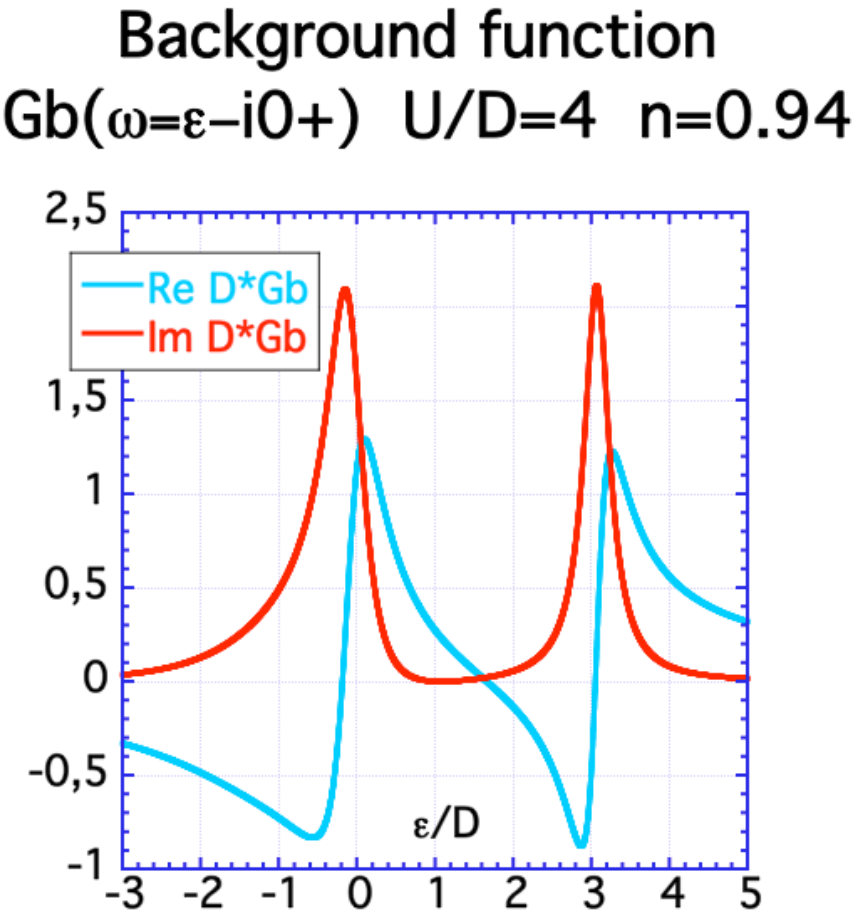
$$Q=Q_{at}+\delta Q(X)>(1+X)/2$$

* The Gutzwiller-Brinkmann-Rice approximation $Z_{GW}=2X/(1+X)$ yields an upper bound for the QP weight Z. The correction $\delta Z<0$ vanishes linearly with X but does not vanish identically for $U>>U_c$.

$$Z=Z_{GW}+\delta Z(X)<2X/(1+X)$$

* Q_{at} and Z_{GW} yield an upper bound for Z* that vanishes linearly with X:

$$Z^*=Z/Q<Z_{GW}/Q_{at}=4X/(1+X)^2$$

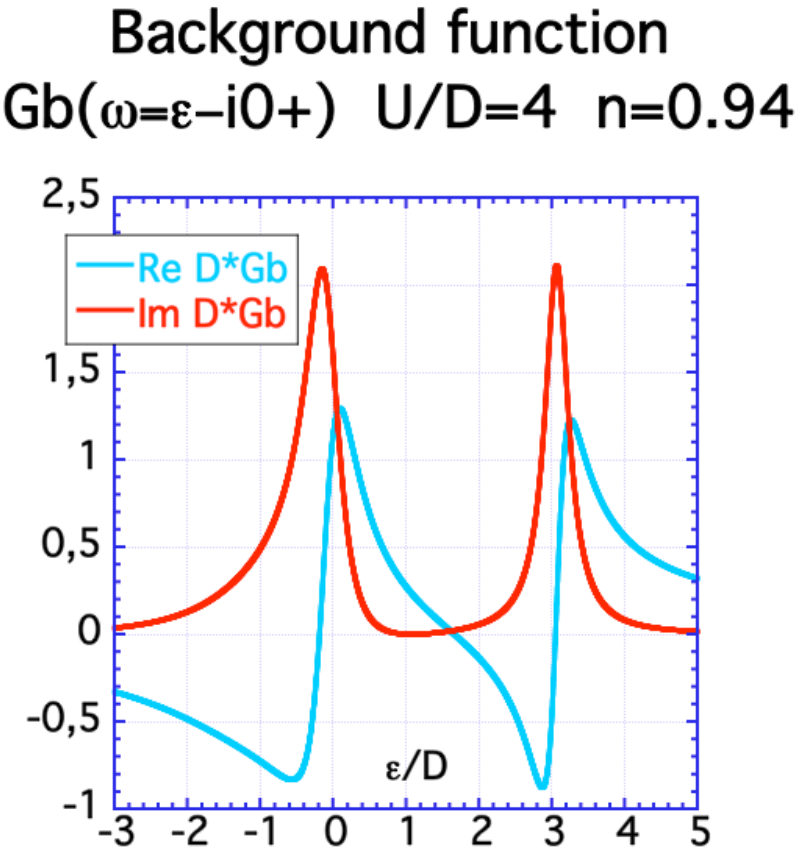


The CFM results for δZ are comparable to DMFT+NRG, those for δQ are even superior, because moment sumrules are obeyed rigorously [5].

Doping controlled Mott transition: As Z*-->0, the FL regime becomes "precarious"!

Background weight in the low energy sector largely exceeds QP weight.
The structureless $G_b(\omega)$ can be mapped onto the generic scenario.
Absence of particle-hole symmetry taken in account by $Re\Omega \neq 0$.

The low energy part of $G_b(\omega)$ in the doped Hubbard model is again well approximated by a dominant pole [1,2] : In the example plotted here [5], $ReG_b(-i0_+) \approx ImG_b(-i0_+) > 0$. Then, a high energy pole Ω (background) and a low energy pole $\Omega^*=Z^*\Omega << \Omega$ (selfenergy) both lie on the diagonal in the upper left quadrant of the complex ω-plane.
As Z*-->0, this mapping onto the generic scenario predicts pronounced discontinuities in the EDC dispersion (see panel 20), which should also be checked by DMFT+NRG.



Outlook:

$G_b(k,\omega)$ beyond the FL regime

* Strategy followed to reveal the generic behaviour: Retain only the pole Ω^* in $\delta\Sigma(k,\omega)$ that is closest to $\omega=0$. After the crossover that marks the limit of the FL regime, the main spectral peak then has an apparent « asymptotic » dispersion

$$\varepsilon \approx Q\eta$$

Wether this law is obeyed in some transition interval, depends on the fine structure of $G_b(k,\omega)$ and on the gaps. Obviously, unless Q=1, this cannot be the real asymptotics!

* In the infinite-dimensional Hubbard model, our chosen microscopic example, the bosonic modes are local spin fluctuations, the scale Ω^* is the binding energy of the Kondo effect. The absence of other, competing modes explains that the low energy background has negligeable finestructure. (Nevertheless, at half-filling, DMFT+NRG data seem to indicate a small splitting into two particle-hole symmetric poles).

* In Hubbard models at finite dimension, even more so in Hubbard-Holstein type models (adding electron-phonon coupling) competing bosonic modes can cause several, momentum dependent selfenergy poles to « invade » the low energy sector. Theory and experiment on strongly correlated materials have to cope with this situation.

The CFM offers a hands-on procedure to parametrise the non-universal behaviour beyond the FL and thus interprete complex ARPES spectra. The connection to moment sumrules gives access to microscopic interpretations in terms of static correlation functions, dictated by (i.e.: also bound to change with…) the choice of a Hamiltonian.

Comments for experimentalists who wish to model ARPES peaks with

$$G_{\lambda\lambda}(k,\omega) \approx Z/\{\omega - Z\eta_k - Z\delta\Sigma(k_F,\omega)\}$$

* Keeping Z and $\delta\Sigma(k_F,\omega)$ k-independant on a given FS-crossing path, but allowing them to depend on the choice of the crossing point k_F, is a well founded approximation. The data analysis can thus be carried beyond DMFT, e.g. to low dimensional systems. Using the CFM, it can also be carried beyond the FL regime and the generic one-pole background scenario that marks the crossover to higher binding energy. Caveat: as binding energy increases, extrinsic secondaries not included here, also grow.
* It is an experimental fact of ARPES that peak positions depend on the photon field. This seems to exclude that the spectrum is "intrinsic". In fact, it is readily explained by relative changes in the strength of matrix elements, when the photoelectron is coupled to more than one intrinsic orbital (see panels 3 and 5).

I have given examples of multi orbital Dyson equations, for which Z, η_k and $\delta\Sigma(\omega)$ of the photohole can be evaluated within the CFM for any set of the dipolar matrix elements [4]. Data taken with varying photon energy and polarisation can thus be analysed consistently.

This conclusion was extracted from reference [4]

Conclusion

The formula of Hedin and Lundquist is over thirty years old. For a long time, poor ARPES resolution did not warrant the effort to exploit all its possibilities. Now, there is an exciting perspective of using it to study and understand new fundamental concepts in strong fermionic correlations. By showing how the manybody dressing of the photohole can be carried out, we provide only one of the necessary new tools. Great rigour in its handling and appreciation of all uncertainties is still required. The other tools, having to do with the photoelectron diffraction and inverse LEED calculation of matrixelements, need to be sharpened simultaneously, in order to fully implement the one step formula. An in depth discussion of this topic, involving all players, is now required. We hope to have conveyed the idea, that the project of extracting generic information from ARPES is not unrealistic. It probably has a great future, both for fundamental and material science.

References

The cited work spreads over a considerable period

([4] and [5] give relevant references to a long line of work from other authors, to whom the CFM ows some input)

- [1] Photoemission: Low energy and high energy scales
  J. Phys. Chem. Sol. 56, 1735 (1995)
- [2] Fermi liquids and non-Fermi liquids - The view from photoemission (with J. Allen, G.-H. Gweon and R. Claessen)
  J. Phys. Chem. Sol. 56, 1735 (1995)
- [3] Study of strongly correlated electrons with valence band photoemission, Molecular Physics Reports 17, 141 (1997)
- [4] ARPES spectral function near a Mott transition
  J. of Electr. Spectr. & Rel. Phenom. 117-118, 13 (2001)
- [5] Spectral density of the Hubbard model by the continued fraction method (with R. Hayn and P. Lombardo)
  PR B 74, 205124 (2006)