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Summer School and Miniconference on
Dynamical Mean-Field Theory for Correlated Electrons:
Applications to Real Materials, Extensions and Perspectives
25 July - 3 August, 2005

DMFT with the Numerical Renormalization Group I & II

Ralf Bulla
Institut fur Physik
Universitat Augsburg
Universitatsstrasse 1
86 159 Augsburg
Germany

DMFT with the Numerical Renormalization Group

Ralf Bulla

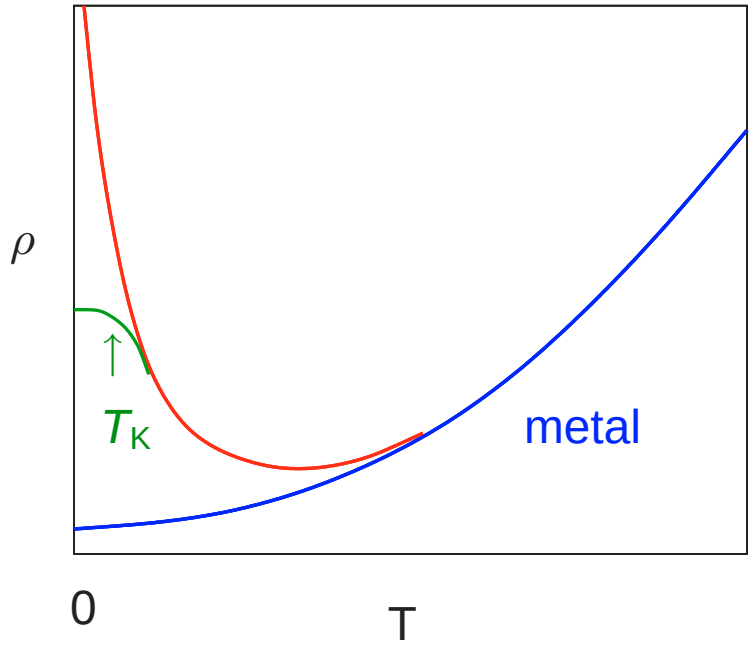
Theoretische Physik III
Institut für Physik
Universität Augsburg

25.-26.07.2005

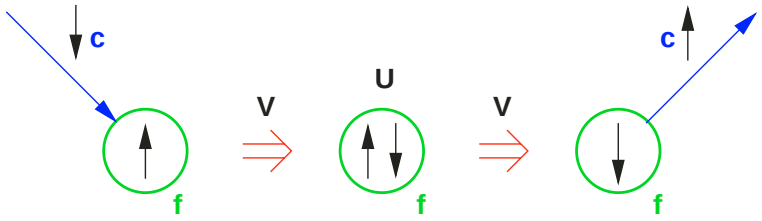
Contents

magnetic impurities in metals

⟶ temperature dependence of resistivity



scattering processes of conduction electrons at magnetic impurities



screening of magnetic moments due to singlet formation

$$\frac{1}{\sqrt{2}}\left(|\uparrow\rangle_f|\downarrow\rangle_c - |\downarrow\rangle_f|\uparrow\rangle_c\right)$$

modelling of magnetic impurities in metals

here: single-impurity Anderson model

[A.C. Hewson, *The Kondo Problem To Heavy Fermions*, CUP 1993]

$$H = \varepsilon_f \sum_\sigma f_\sigma^\dagger f_\sigma + U f_\uparrow^\dagger f_\uparrow f_\downarrow^\dagger f_\downarrow + \sum_{k\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} + V \sum_{k\sigma} \left(f_\sigma^\dagger c_{k\sigma} + c_{k\sigma}^\dagger f_\sigma \right)$$

magnetic impurities in metals

$\longrightarrow$ Kondo effect

[quantum dots, DMFT]

the model describes:

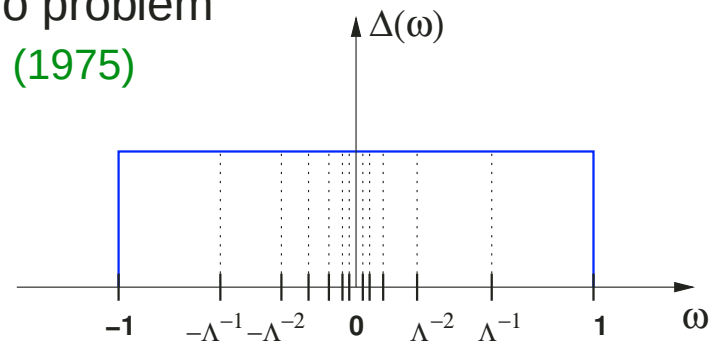
- formation of local moments: $|\uparrow\rangle_f, |\downarrow\rangle_f$
- scattering of conduction electrons
- screening of local moments below temperature scale T_K

Numerical Renormalization Group (NRG)

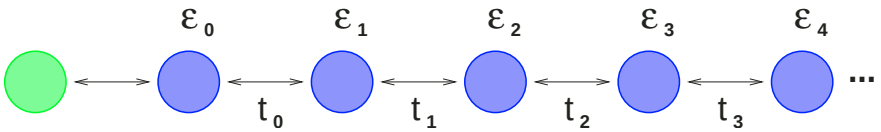
developed by Wilson for the Kondo problem

K.G. Wilson, Rev. Mod. Phys. **47**, 773 (1975)

- logarithmic discretization



- mapping on semi-infinite chain



- iterative diagonalization

1. logarithmic discretization

start with the single-impurity Anderson model in a continuous representation

$$\begin{aligned} H &= \sum_\sigma \varepsilon_f f_\sigma^\dagger f_\sigma + U f_\uparrow^\dagger f_\uparrow f_\downarrow^\dagger f_\downarrow + \sum_\sigma \int_{-1}^{1} \mathrm{d}\varepsilon\, g(\varepsilon) a_{\varepsilon\sigma}^\dagger a_{\varepsilon\sigma} \\ &+ \sum_\sigma \int_{-1}^{1} \mathrm{d}\varepsilon\, h(\varepsilon)\left(f_\sigma^\dagger a_{\varepsilon\sigma} + a_{\varepsilon\sigma}^\dagger f_\sigma\right). \end{aligned} \tag{1}$$

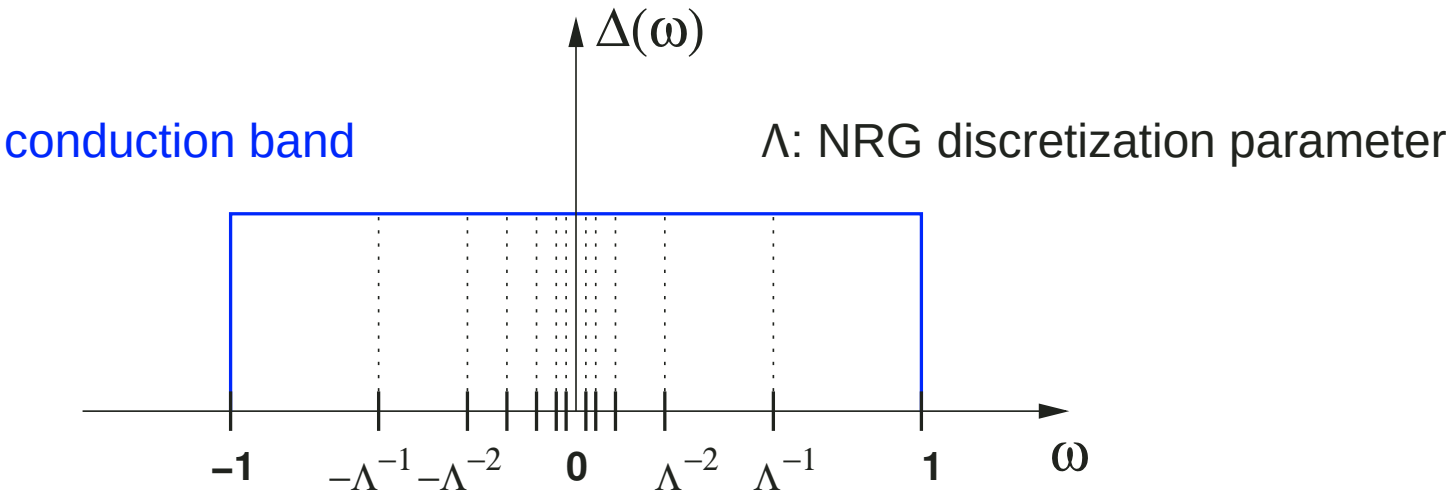
define the hybridization function $\Delta(\omega)$

$$\Delta(\omega) = \pi \sum_k V_k^2 \delta(\omega - \varepsilon_k) \tag{2}$$

here:

$$\Delta(x) = \pi \frac{\mathrm{d}\varepsilon(x)}{\mathrm{d}x} h[\varepsilon(x)]^2 \tag{3}$$

with $\varepsilon(x)$ the inverse function of $g(\varepsilon)$: $g[\varepsilon(x)] = x$



The parameter $\Lambda > 1$ defines a set of intervals with the discretization points

$$x_n = \Lambda^{-n} \tag{4}$$

The width of each interval is

$$d_n = \Lambda^{-n}(1 - \Lambda^{-1}) \tag{5}$$

Within each interval we introduce a complete set of orthonormal functions

$$\psi^{\pm}_{np}(\varepsilon) = \begin{cases} \frac{1}{\sqrt{d_n}} e^{\pm i\omega_n p\varepsilon} & \text{for } x_{n+1} < \pm\varepsilon < x_n \\ 0 & \text{outside this interval} \end{cases} , \tag{6}$$

($p = 0, 1, 2, \ldots$ and $\omega_n = 2\pi/d_n$).
Now: expansion of the operators $a_{\varepsilon\sigma}$ and $a^{\dagger}_{\varepsilon\sigma}$ in this basis

$$a_{\varepsilon\sigma} = \sum_{np} \left[a_{np\sigma}\psi^{+}_{np}(\varepsilon) + b_{np\sigma}\psi^{-}_{np}(\varepsilon) \right] \tag{7}$$

$$\begin{aligned} a_{np\sigma} &= \int_{-1}^{1} \mathrm{d}\varepsilon \left[\psi^{+}_{np}(\varepsilon)\right]^{*} a_{\varepsilon\sigma} , \\ b_{np\sigma} &= \int_{-1}^{1} \mathrm{d}\varepsilon \left[\psi^{-}_{np}(\varepsilon)\right]^{*} a_{\varepsilon\sigma} \end{aligned} \tag{8}$$

The hybridization term transforms as:

$$\int_{-1}^{1} \mathrm{d}\varepsilon\, h(\varepsilon)\left(f_\sigma^\dagger a_{\varepsilon\sigma} + a_{\varepsilon\sigma}^\dagger f_\sigma\right) = \sqrt{\frac{\xi_0}{\pi}}\left(c_{0\sigma}^\dagger f_{-1\sigma} + f_{-1\sigma}^\dagger c_{0\sigma}\right) \tag{9}$$

The conduction electron term transforms as

$$\int_{-1}^{1} \mathrm{d}\varepsilon\, g(\varepsilon) a_{\varepsilon\sigma}^\dagger a_{\varepsilon\sigma} = \sum_{np}\left(\xi_n^+ a_{np\sigma}^\dagger a_{np\sigma} + \xi_n^- b_{np\sigma}^\dagger b_{np\sigma}\right)$$

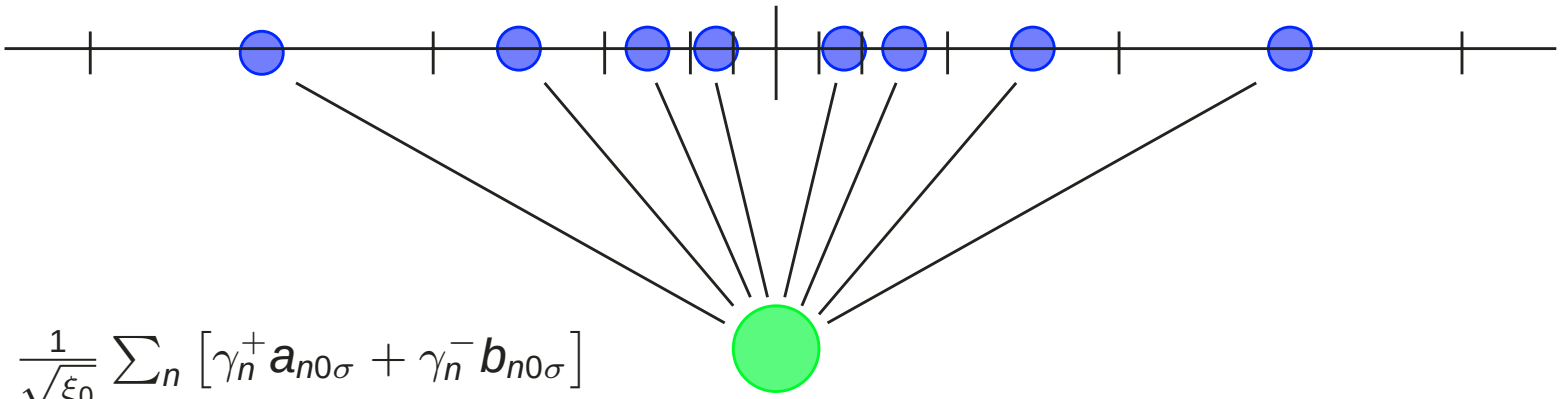
$$+ \frac{1-\Lambda^{-1}}{2\pi i}\sum_{n,p\neq p'} \frac{\Lambda^{-n}}{p'-p}\left(a_{np\sigma}^\dagger a_{np'\sigma} - b_{np\sigma}^\dagger b_{np'\sigma}\right)\exp\left[\frac{2\pi i(p'-p)}{1-\Lambda^{-1}}\right] \tag{10}$$

In the limit $\Lambda \longrightarrow 1$ the term in eq. (10) coupling the states with different p and p' vanishes.
Neglect the $p \neq 0$-states in the following and introduce the notation

$$a_{n\sigma} \equiv a_{n0\sigma}\ ,\ b_{n\sigma} \equiv b_{n0\sigma} \tag{11}$$

The discretized Hamiltonian for the single-impurity Anderson model now takes the form

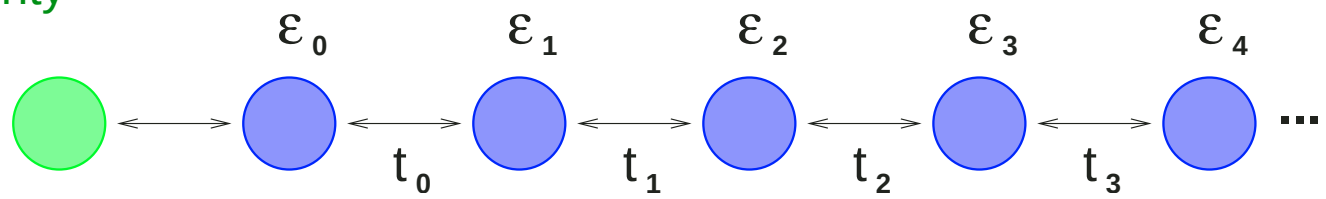
$$\begin{aligned} H &= \sum_{\sigma} \varepsilon_f f_\sigma^\dagger f_\sigma + U f_\uparrow^\dagger f_\uparrow f_\downarrow^\dagger f_\downarrow \\ &+ \sum_{n\sigma} \left[\xi_n^+ a_{n\sigma}^\dagger a_{n\sigma} + \xi_n^- b_{n\sigma}^\dagger b_{n\sigma} \right] \\ &+ \sqrt{\frac{\xi_0}{\pi}} \left[f_\sigma^\dagger c_{0\sigma} + c_{0\sigma}^\dagger f_\sigma \right] . \end{aligned} \tag{12}$$



$$c_{0\sigma} = \frac{1}{\sqrt{\xi_0}} \sum_n \left[\gamma_n^+ a_{n0\sigma} + \gamma_n^- b_{n0\sigma} \right]$$

2. mapping on semi-infinite chain

impurity



$$H = \sum_\sigma \varepsilon_f f_\sigma^\dagger f_\sigma + U f_\uparrow^\dagger f_\uparrow f_\downarrow^\dagger f_\downarrow + \sqrt{\frac{\xi_0}{\pi}} \sum_\sigma \left[f_\sigma^\dagger c_{0\sigma} + c_{0\sigma}^\dagger f_\sigma \right]$$
$$+ \sum_{\sigma n=0}^{\infty} \left[\varepsilon_n c_{n\sigma}^\dagger c_{n\sigma} + t_n \left(c_{n\sigma}^\dagger c_{n+1\sigma} + c_{n+1\sigma}^\dagger c_{n\sigma} \right) \right] . \qquad (13)$$

hopping matrix elements fall off exponentially: $t_N \propto \Lambda^{-N/2}$

3. iterative diagonalization

define a sequence of Hamiltonians H_N so that

$$H = \lim_{N\to\infty} \Lambda^{-(N-1)/2} H_N \tag{14}$$

Two successive Hamiltonians are related by

$$H_{N+1} = \sqrt{\Lambda} H_N + \Lambda^{N/2} \sum_\sigma \varepsilon_{N+1} c^\dagger_{N+1\sigma} c_{N+1\sigma} + \Lambda^{N/2} \sum_\sigma t_N \left(c^\dagger_{N\sigma} c_{N+1\sigma} + c^\dagger_{N+1\sigma} c_{N\sigma} \right) \tag{15}$$

this sequence of hamiltonians is solved by iterative diagonalization:

1st step: • $\longrightarrow E_{m1}, |\psi_m\rangle_1, \langle\psi_m| f_\sigma |\psi_{m'}\rangle_1$

2nd step: •⟷• $\longrightarrow E_{m2}, |\psi_m\rangle_2, \langle\psi_m| f_\sigma |\psi_{m'}\rangle_2$

3rd step: •⟷•⟷• $\longrightarrow E_{m3}, |\psi_m\rangle_3, \langle\psi_m| f_\sigma |\psi_{m'}\rangle_3$

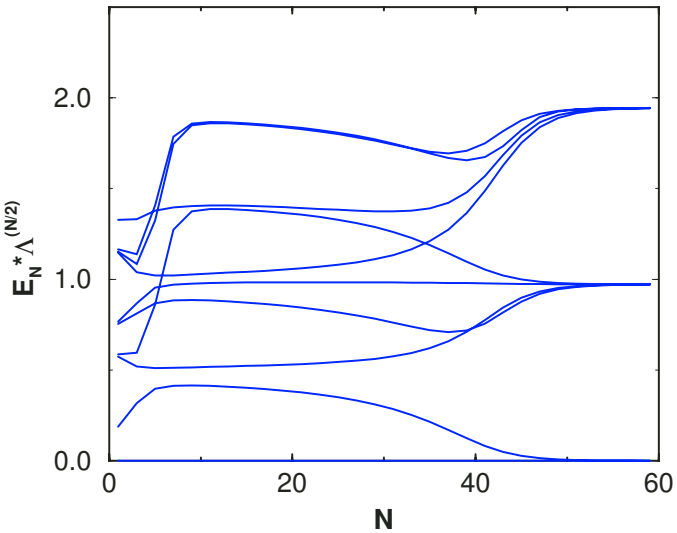
⋮ ⋮ ⋮

number of states grows as 4^N $\longrightarrow$ keep max $\sim$ 500 states at each RG step

results from the NRG

- structure of the fixed points
- thermodynamic quantities (entropy, specific heat)
- dynamic quantities (spectral function, dynamic susceptibilities)

example: flow diagram for the many-particle energies of the single-impurity Anderson model



single-particle Green function

$$G_\sigma(z) = \langle\langle f_\sigma, f_\sigma^\dagger \rangle\rangle_z = i \int_0^\infty \mathrm{d}t \; e^{izt} \langle [f_\sigma(t), f_\sigma^\dagger]_+ \rangle \tag{16}$$

with the self-energy $\Sigma(z)$:

$$G(z) = \frac{1}{z - \varepsilon_\mathrm{f} - \Sigma(z)} \tag{17}$$

this self-energy consist of two parts:

$$\Sigma(z) = \Delta(z) + \Sigma^U(z) \quad , \tag{18}$$

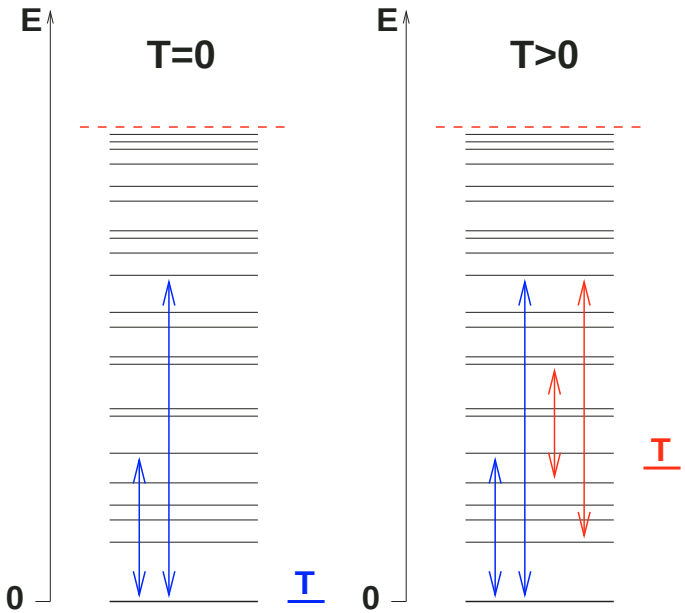
with $\Sigma^U(z)$ the contribution due to the U-term

spectral function:

$$A(\omega) = -\frac{1}{\pi} \mathrm{Im}\; G(\omega + i\delta^+) \; , \tag{19}$$

In each iteration, calculate the spectral function for each cluster of size N via:

$$A_{\sigma N}(\omega) = \frac{1}{Z_N} \sum_{nm} \left| {}_N\left\langle n \left| f_\sigma^\dagger \right| m \right\rangle_N \right|^2 \delta\left(\omega - (E_n^N - E_m^N)\right) \left(e^{-\beta E_m^N} + e^{-\beta E_n^N}\right) \quad (20)$$

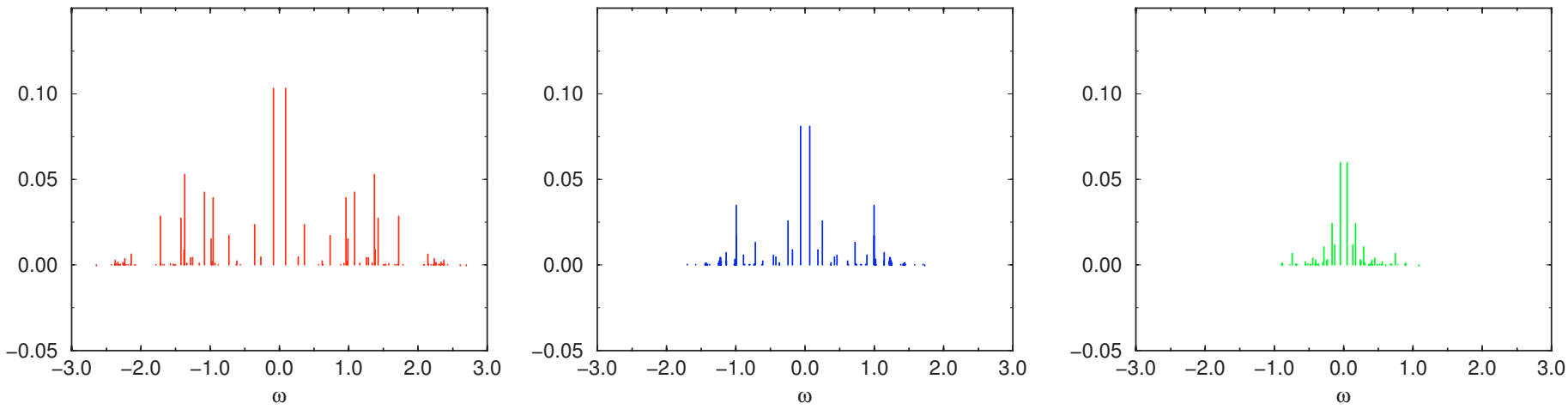


$T = 0$: transitions between ground state and all excited states

$T > 0$: in addition: transitions between excited states

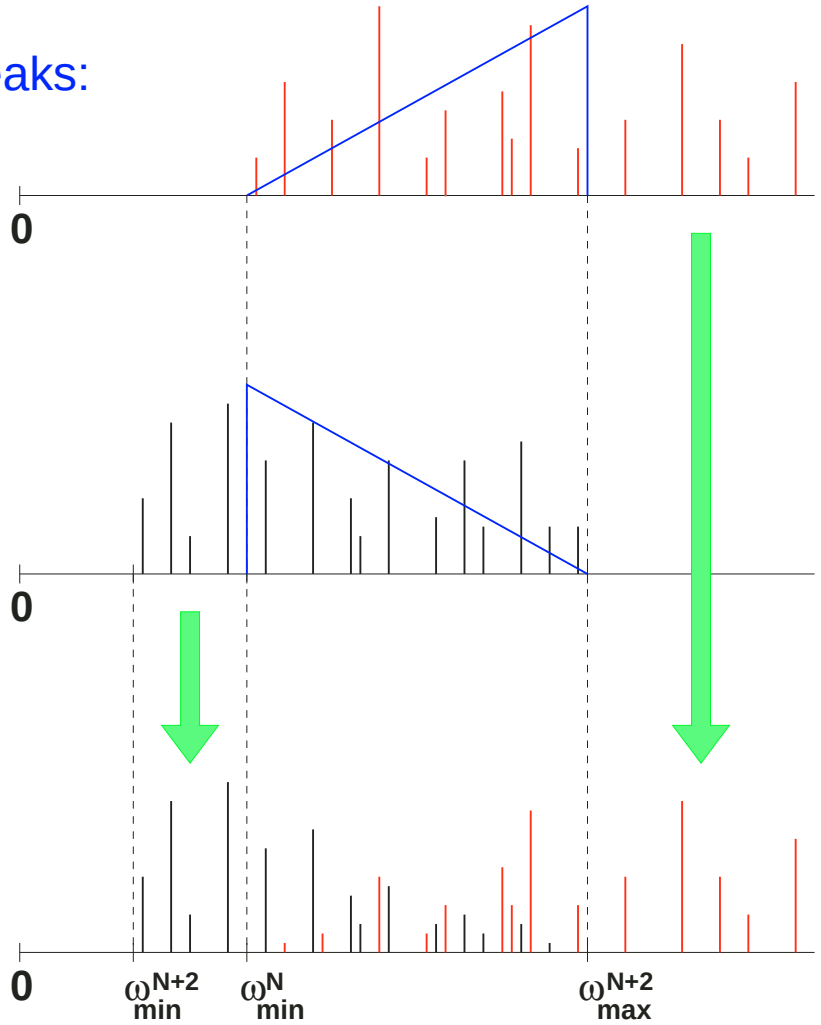
effect of the truncation on the spectral functions of each iteration:

$N = 14$ $N = 16$ $N = 18$



this means:
final spectral function = superposition of the data from all iterations

superposition of δ-Peaks:



up to N

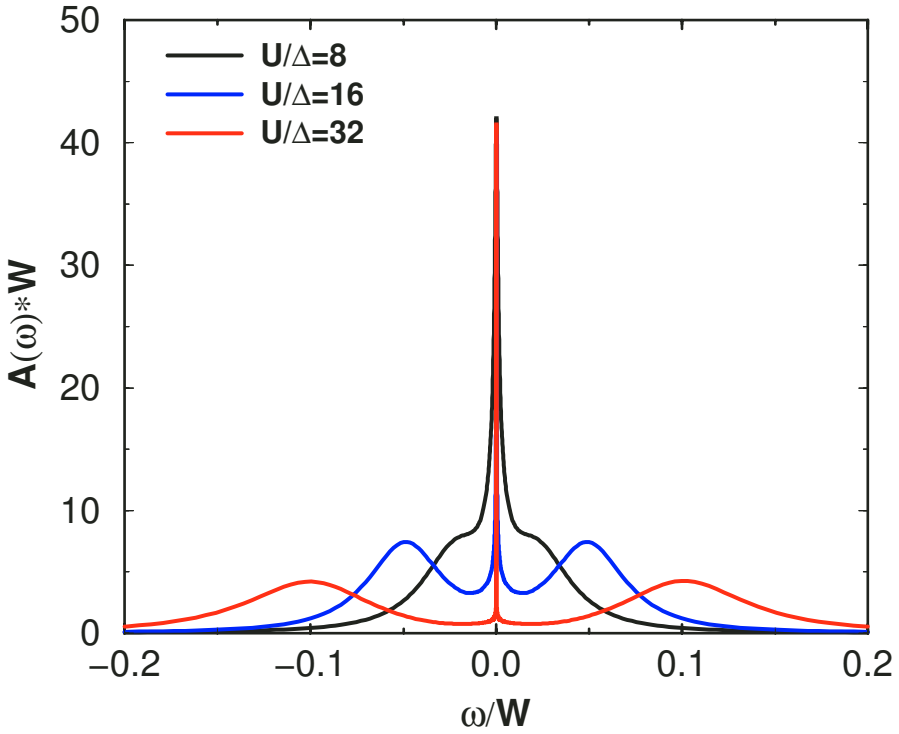
N+2

up to N+2

finally: broadening of the δ-peaks $\longrightarrow$ Gaussian on a logarithmic scale

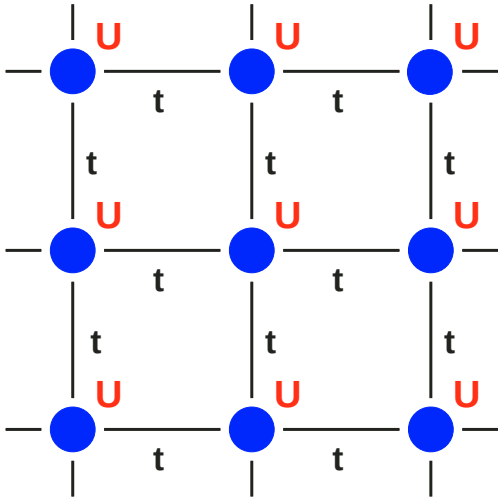
$$\delta(\omega - \omega_n) \longrightarrow \frac{e^{-b^2/4}}{b\,\omega_n\sqrt{\pi}} \exp\left[-\frac{(\ln\omega - \ln\omega_n)^2}{b^2}\right] \tag{21}$$

results for the single-impurity Anderson model:



Hubbard model

$$H = U \sum_i c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow} - t \sum_{<ij>\sigma} c^\dagger_{i\sigma} c_{j\sigma}$$



DMFT: self-consistency

$$\sim\!\!\rightarrow = \frac{1}{\Longrightarrow^{-1} + \Sigma_{HM}}$$

$$\Sigma_{HM} = \Sigma_{AM}[\sim\!\!\rightarrow, U]$$

methods to solve the effective impurity model

method		year	large U	low T	systematic	energy resolution	max # of orbitals	comp. effort
QMC	quantum Monte Carlo	'92	~	~	+	?	~10	$$$
IPT	iterated perturbation theory	'92	–	+	+	+	?	$
NCA	non–crossing approximation	'93	+	~	?	+	~10	$
ED	exact diagonalization	'93	+	~	+	–	2	$$
NRG	numerical renormalization group	'96	+	+	+	log mesh	2	$$
LMA	local moment approach	'99	+	+	?	+	?	$
DMRG	density matrix renormalization group	'03	+	+	+	lin mesh	?	$$$
PQMC	projective quantum Monte Carlo	'04	~	+	?	?	?	$$$

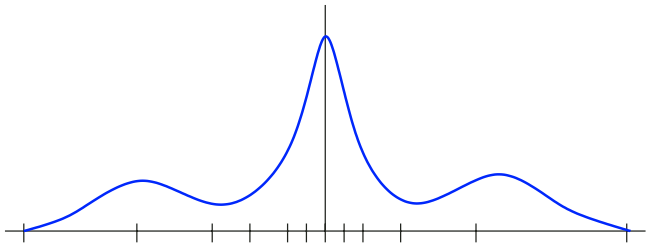
now: use NRG for the calculation of Σ_{AM} within the DMFT selfconsistency

what is different to the NRG for the standard SIAM?

- input $\Delta(z)$ defined via

$$\rightsquigarrow = \frac{1}{z - \varepsilon_f - \Delta(z)}$$

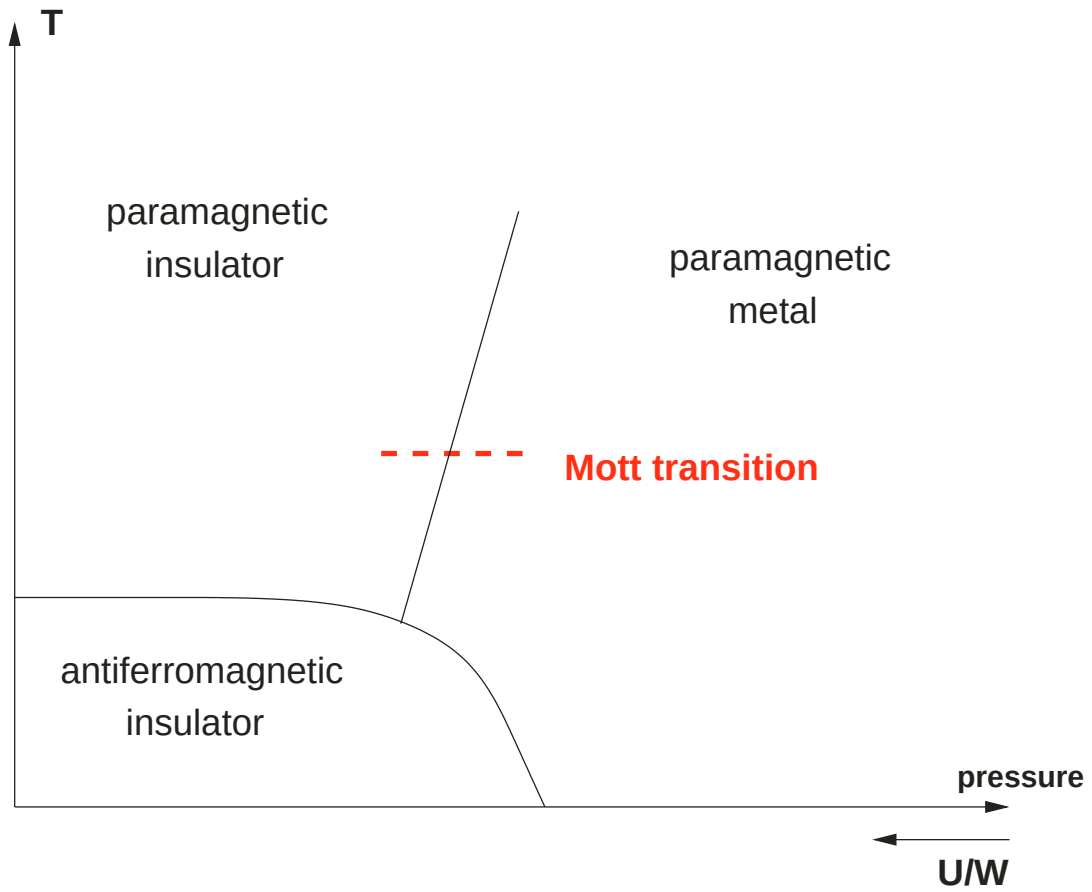
corresponding to an energy dependent density of states of the free conduction band



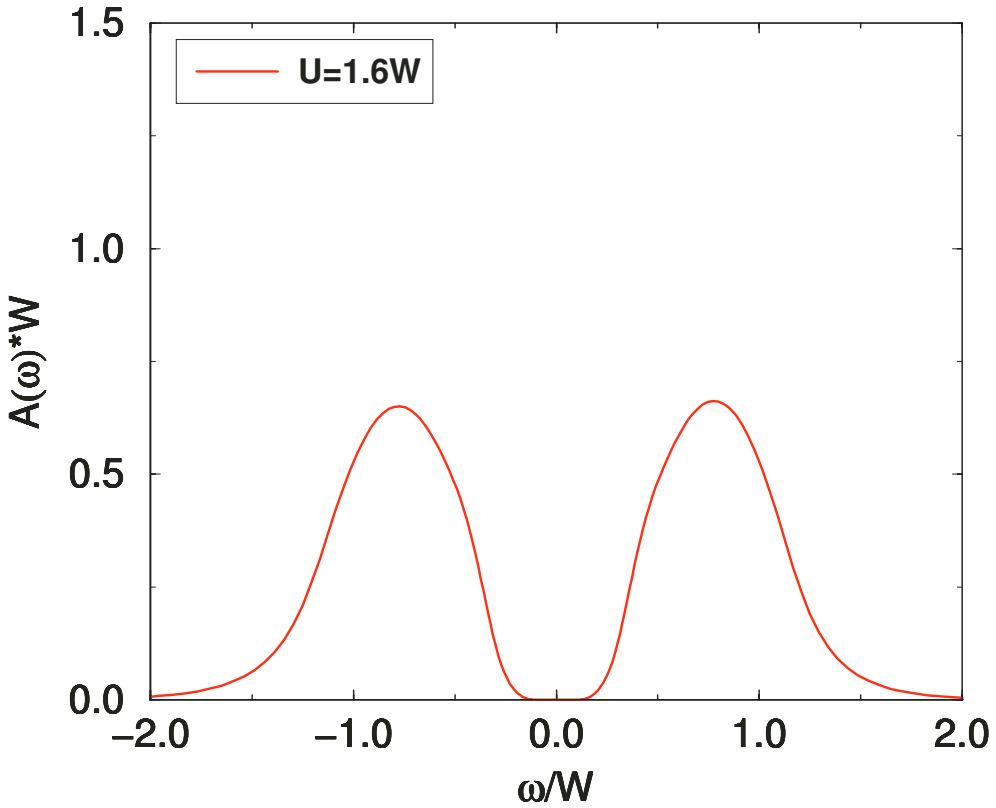
- output $\rightarrow \Sigma_{\mathrm{AM}} = U \langle\langle f_\sigma f_{\bar{\sigma}}^\dagger f_{\bar{\sigma}}, f_\sigma^\dagger \rangle\rangle_z / \langle\langle f_\sigma, f_\sigma^\dagger \rangle\rangle_z$

R. Bulla, A.C. Hewson, and Th. Pruschke
J. Phys.: Condens. Matter **10**, 8365 (1998)

Phase diagram of V_2O_3



Hubbard model with DMFT/NRG: Spectral functions for $T = 0$



$U < U_c \approx 1.5W$:

metallic solution

separation of quasiparticle peak
from upper and lower Hubbard bands

$U > U_c \approx 1.5W$:

insulating solution

R. Bulla, Phys. Rev. Lett. **83**, 136 (1999)

Spectral function for $T = 0$: Bethe vs. hypercubic lattice

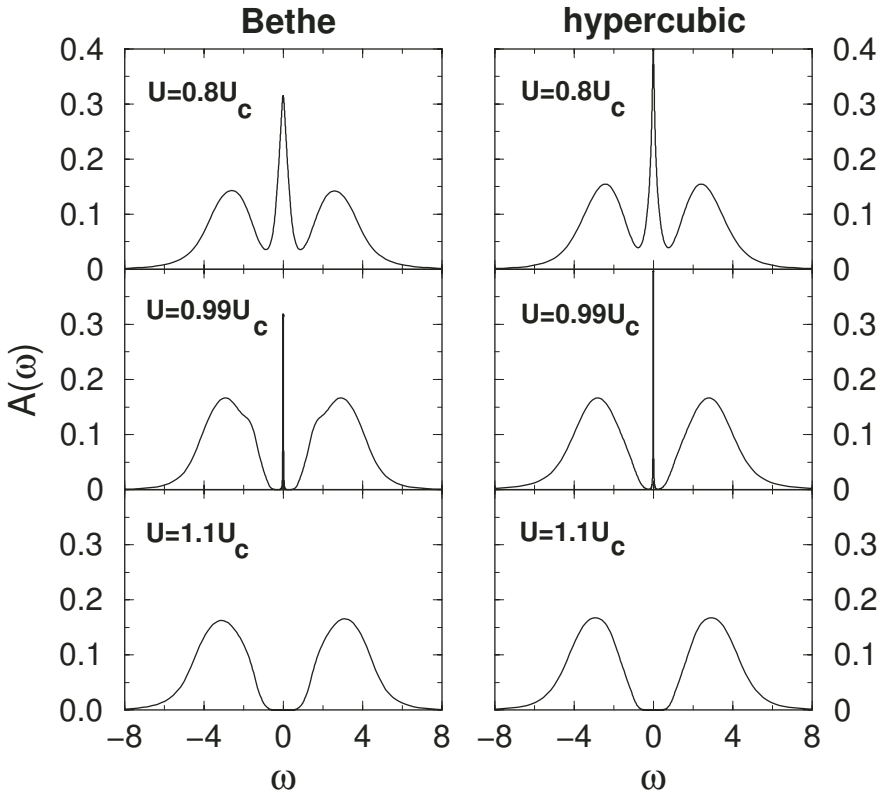
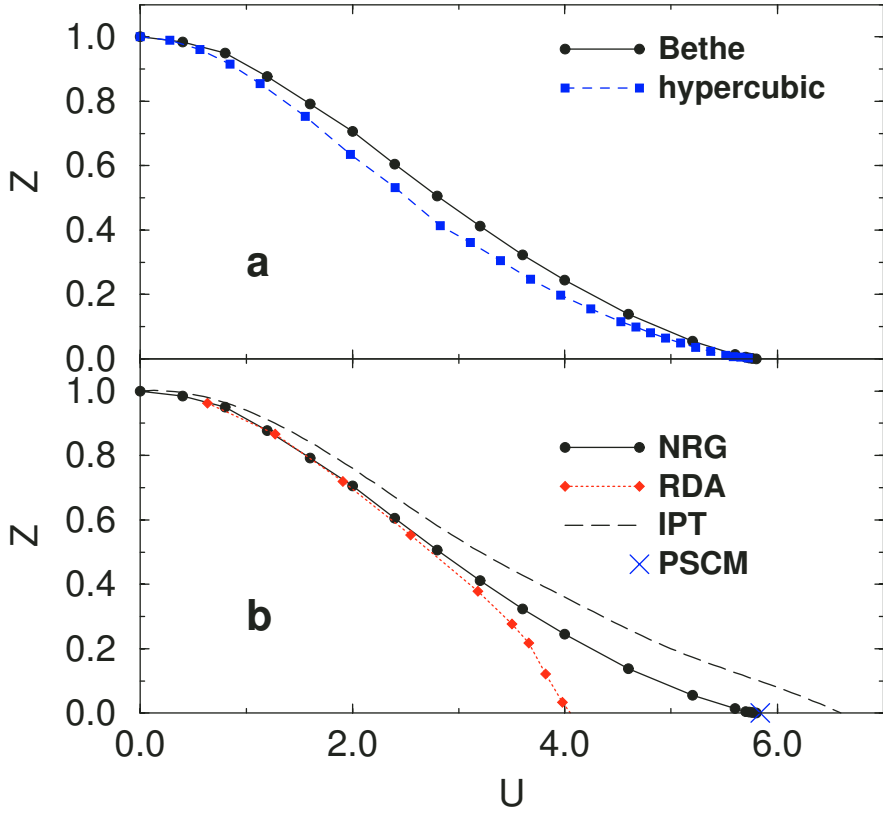


Fig. 2 in

R. Bulla, Phys. Rev. Lett. **83**, 136 (1999)

quasiparticle weight



$$Z = \frac{1}{1 - \frac{\partial Re\Sigma(\omega)}{\partial \omega}|_{\omega=0}}$$

Fig. 1 in

R. Bulla, Phys. Rev. Lett. **83**, 136 (1999)

self-energy

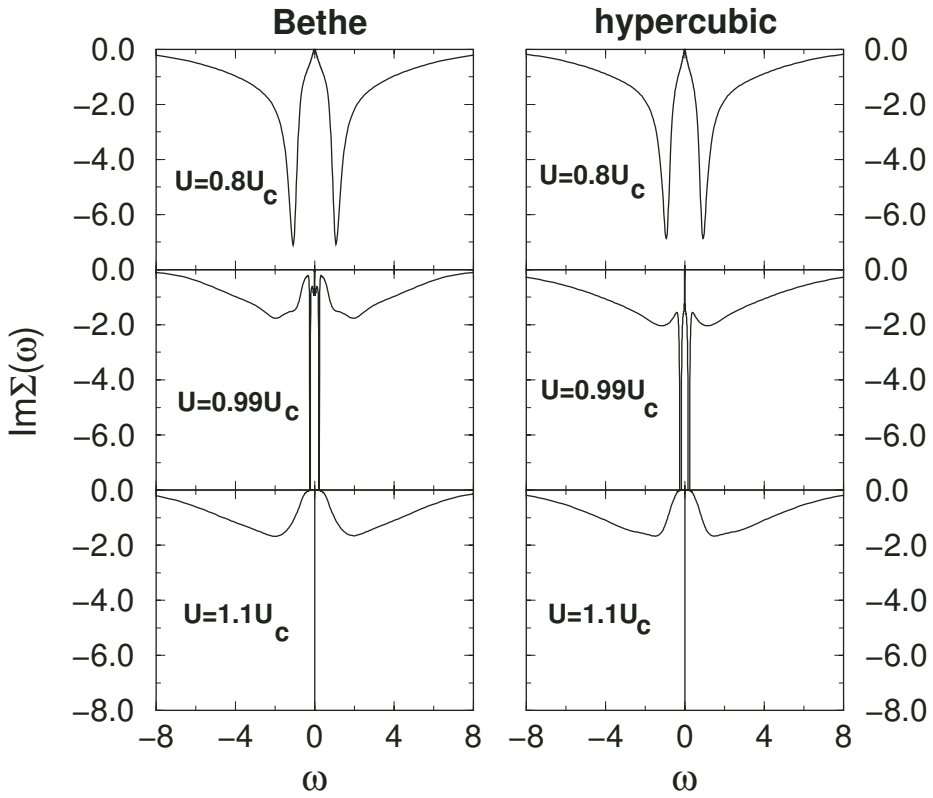
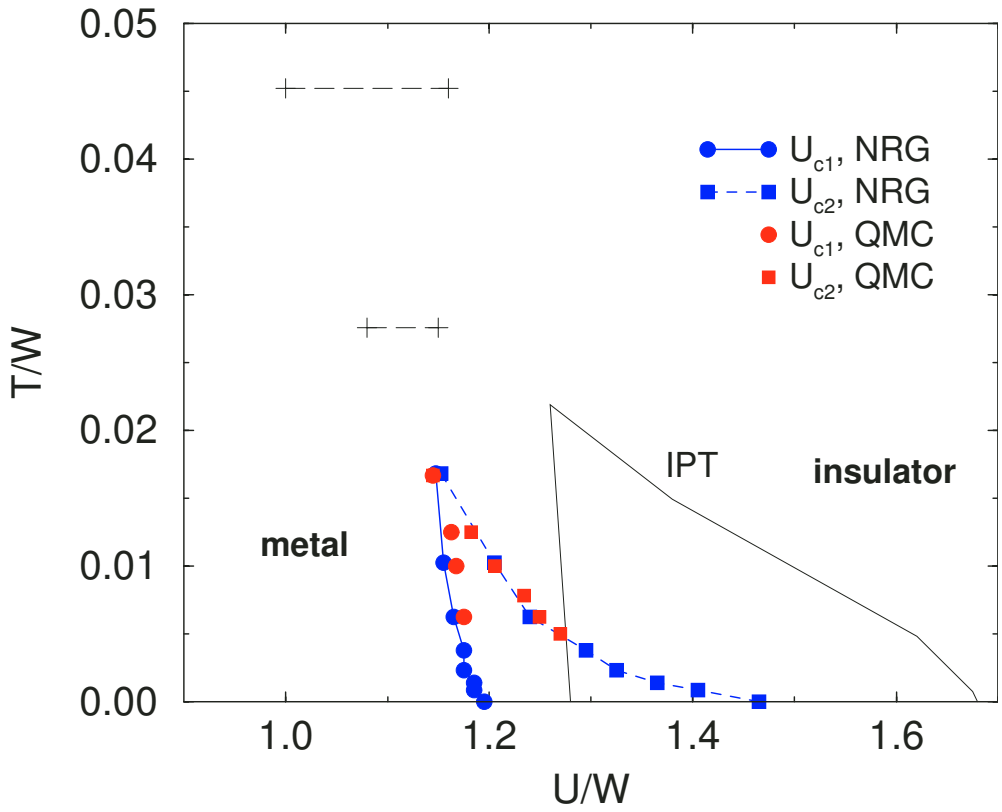


Fig. 3 in

R. Bulla, Phys. Rev. Lett. **83**, 136 (1999)

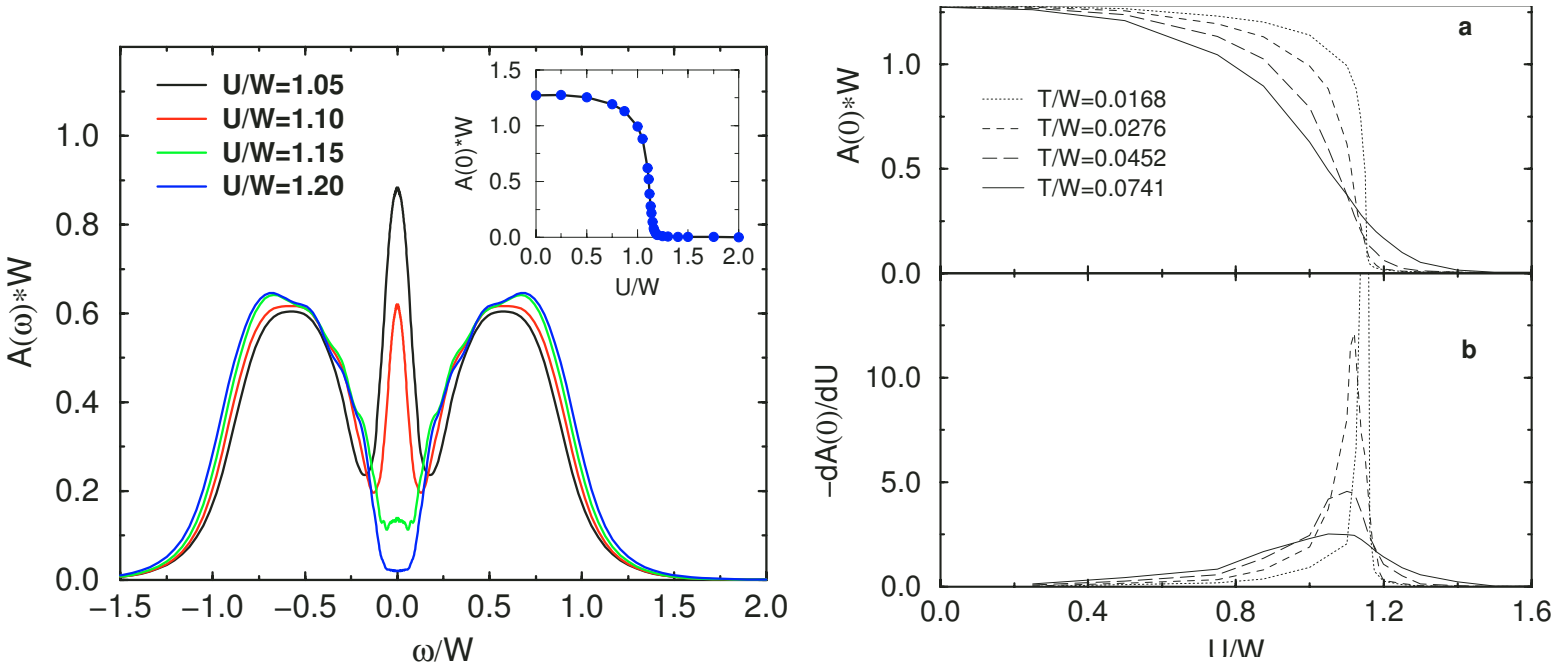
phase diagram of the Hubbard model at half filling



R. Bulla, T.A. Costi, and D. Vollhardt

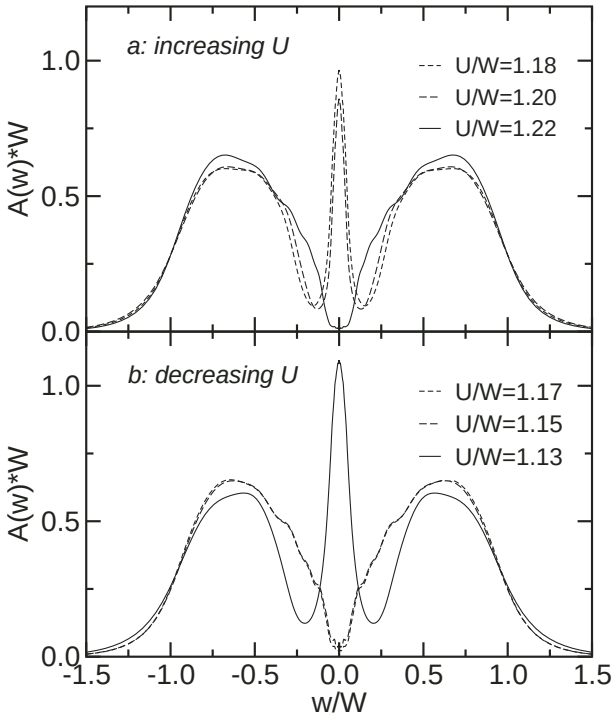
Phys. Rev. B **64**, 045103 (2001)

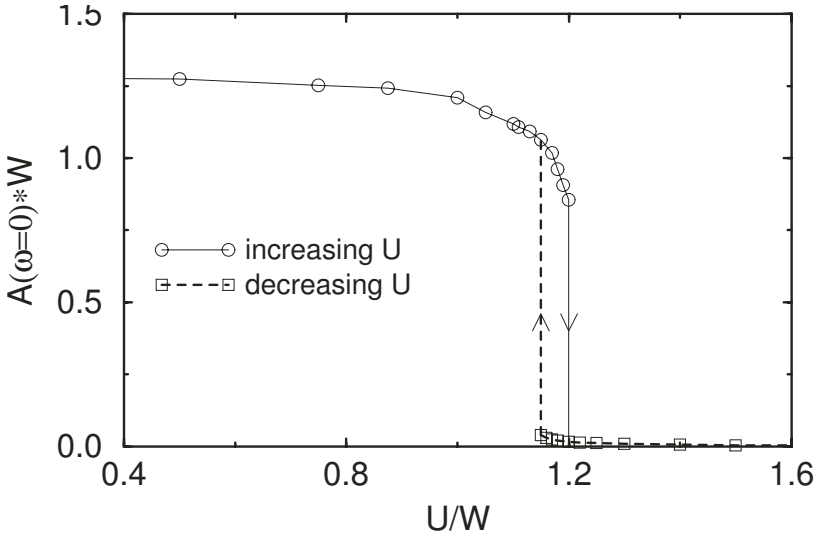
spectral function for finite temperatures ($T > T^*$)



smooth crossover from metallic-like to insulating-like solution

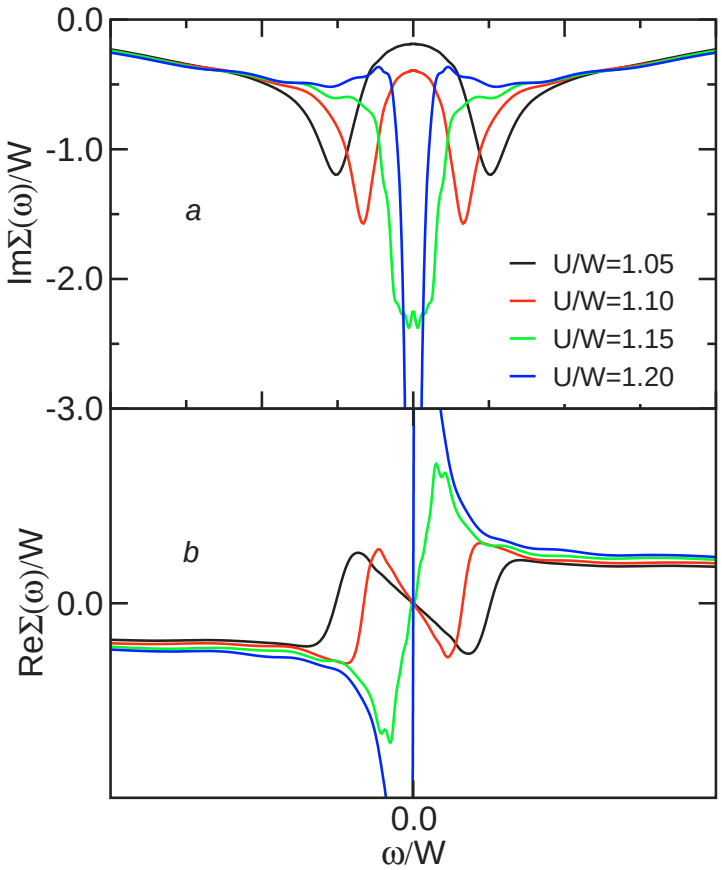
spectral function for finite temperatures ($T < T^*$)





hysteresis!

self-energy (finite temperatures)



summary

the numerical renormalization group for

- quantum impurity systems
  - Kondo effect
  - single-impurity Anderson model
- lattice models within DMFT
  - Hubbard model
  - Mott transition

further reading

- R. Bulla, *The Numerical Renormalization Group Method for correlated electrons*, Adv. Solid State Phys. 40, 169 (2000)
- R. Bulla, *Dynamical Mean-Field Theory - from Quantum Impurity Physics to Lattice Problems*, cond-mat/0412314 (Phil. Mag. 2005)

other applications of DMFT/NRG

- magnetic phases of the Hubbard model
  R. Zitzler *et al.*, Phys. Rev. Lett. **93**, 016406 (2004)
- multiband Hubbard models
  Th. Pruschke, conference: 01.08, 10:00
- lattice models with coupling to phonons
  R. Bulla, conference: 02.08, 16:50
- Hubbard model with disorder
  K. Byczuk, conference: 02.08, 15:45
- periodic Anderson model
  Th. Pruschke, R. Bulla, and M. Jarrell, Phys. Rev. B 61, 12799 (2000)
- Kondo lattice model
  T.A. Costi and N. Manini, J. Low. Temp. Phys. **126**, 835