Dynamical mean-field theory and the NRG as the impurity solver

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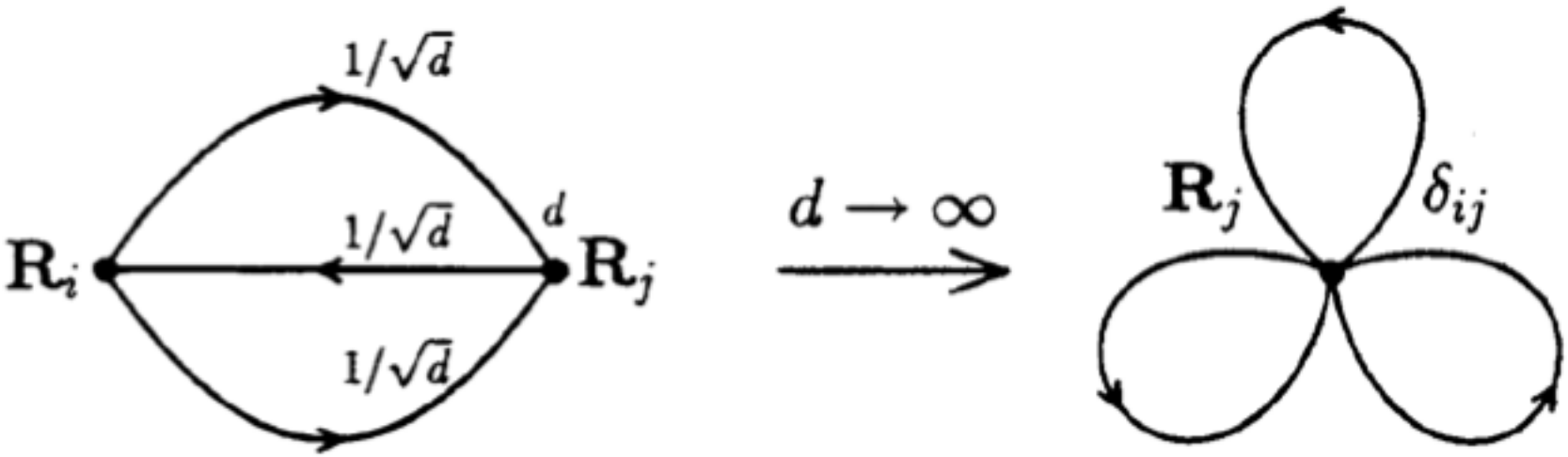
DMFT

- Goal: study and explain lattice systems of strongly correlated electron systems.
- Approximation: local self-energy Σ
- Dynamical: on-site quantum fluctuations treated exactly
- Pro: tractable (reduction to an effective quantum impurity problem subject to self-consistency condition)
- Con: non-local correlations treated at the static mean-field level

Infinite-D limit

$$t \to \frac{t^*}{\sqrt{d}},\ t^* = \text{const.} \longrightarrow G^0_{ij,\sigma} \sim \mathcal{O}\left(1/d^{\|\boldsymbol{R}_i - \boldsymbol{R}_j\|/2}\right)$$



See, for example, D. Vollhardt **in The LDA+DMFT approach to strongly correlated materials**, Eva Pavarini, Erik Koch, Dieter Vollhardt, and Alexander Lichtenstein (Eds.), 2011

Infinite-D limit

$$\Sigma(\omega, \mathbf{k}) \to \Sigma(\omega)$$

Derivation of the DMFT equations by cavity method:

- write the partition function as an integral over Grassman variables
- integrate out all fermions except those at the chosen single site
- split the effective action
- take the D to infinity limit to simplify the expression
- result: self-consistency equation

Georges et al., RMP 1996

Hubbard ⇒ SIAM

$$H_{\mathrm{Hubbard}} = \sum_{\mathbf{k}\sigma} (\epsilon_{\mathbf{k}} - \mu) c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

$$H_{\mathrm{SIAM}} = \sum_{k\sigma} (\varepsilon_k - \mu) f^{\dagger}_{k\sigma} f_{k\sigma} - \mu n + U n_{\uparrow} n_{\downarrow} + \sum_{k\sigma} V_k \left(f^{\dagger}_{k\sigma} d_{\sigma} + \mathrm{H.c.} \right)$$

$\Gamma(\omega)$=-Im[$\Delta(\omega+i\delta)$]

$$\Delta(z) = \sum_{k} \frac{|V_k|^2}{z - \varepsilon_k}$$

hybridization plays the role of the Weiss field

$$\Delta_{\sigma}(z) = z + \mu - \left(G^{-1}_{\mathrm{loc},\sigma}(z) + \Sigma_{\sigma}(z) \right)$$

$$\Sigma_\sigma(z) = \frac{\langle\langle [d_\sigma, H_{\rm int}]; d_\sigma^\dagger \rangle\rangle_z}{\langle\langle d_\sigma; d_\sigma^\dagger \rangle\rangle_z}$$

$$G_{\mathbf{k}\sigma}(z) = \langle\langle c_{\mathbf{k}\sigma}; c_{\mathbf{k}\sigma}^\dagger \rangle\rangle_z$$

$$A_{\mathbf{k}\sigma}(\omega) = -\frac{1}{\pi} \mathrm{Im} G_{\mathbf{k}\sigma}(\omega + i\delta)$$

$$G_{\mathbf{k}\sigma}(z) = \frac{1}{z + \mu - \epsilon_{\mathbf{k}} - \Sigma_\sigma(z)}$$

$$G_{\mathrm{loc},\sigma}(z) = \frac{1}{N}\sum_{\mathbf{k}} \frac{1}{z+\mu-\epsilon_{\mathbf{k}}-\Sigma_\sigma(z)}$$

$$= \int \frac{\rho_0(\epsilon)\mathrm{d}\epsilon}{[z+\mu-\Sigma_\sigma(z)]-\epsilon}$$

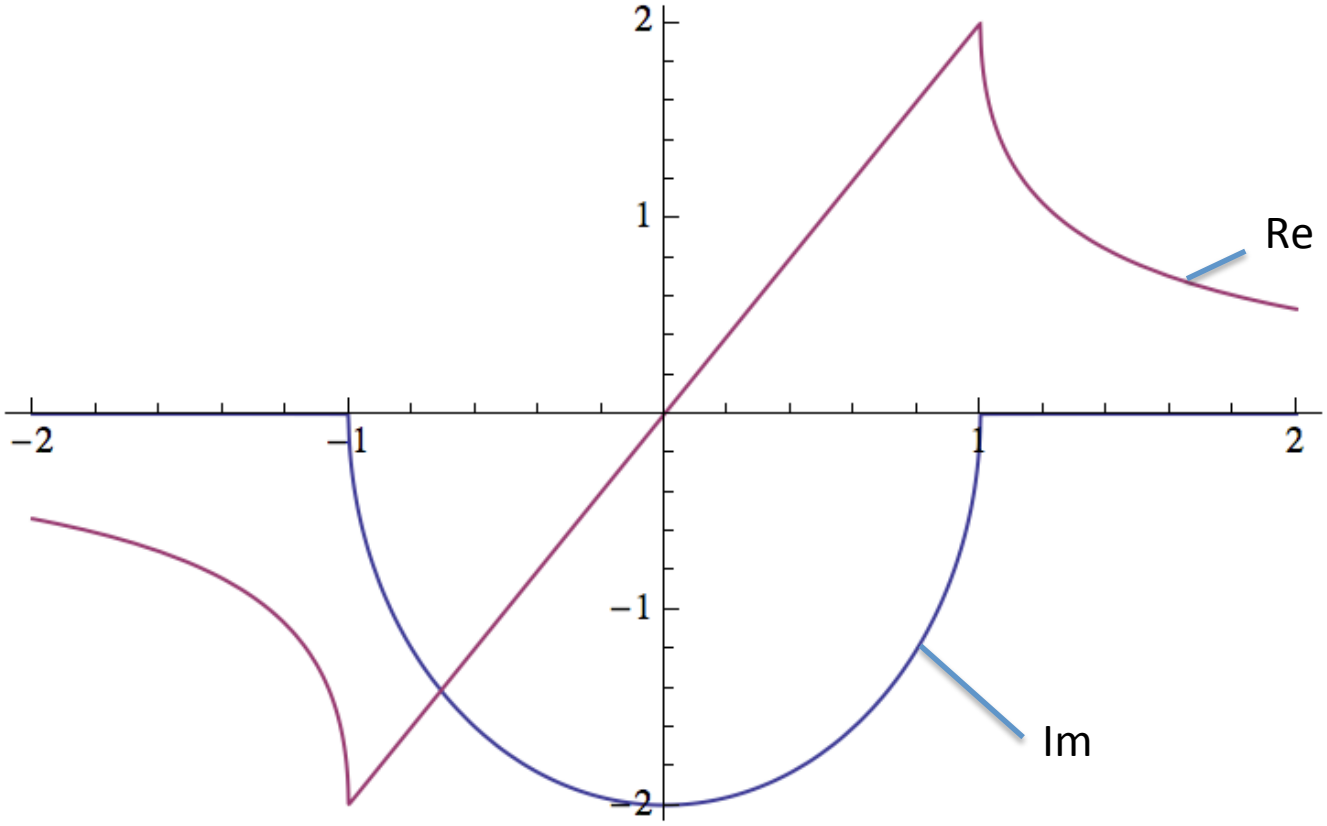
$$= G_0[z+\mu-\Sigma_\sigma(z)].$$

$$\rho_0(\epsilon) = \frac{1}{N}\sum_{\mathbf{k}} \delta(\epsilon-\epsilon_{\mathbf{k}})$$

$$G_0(z) = \int_{-\infty}^{\infty} \frac{\rho_0(\epsilon)\mathrm{d}\epsilon}{z-\epsilon}$$

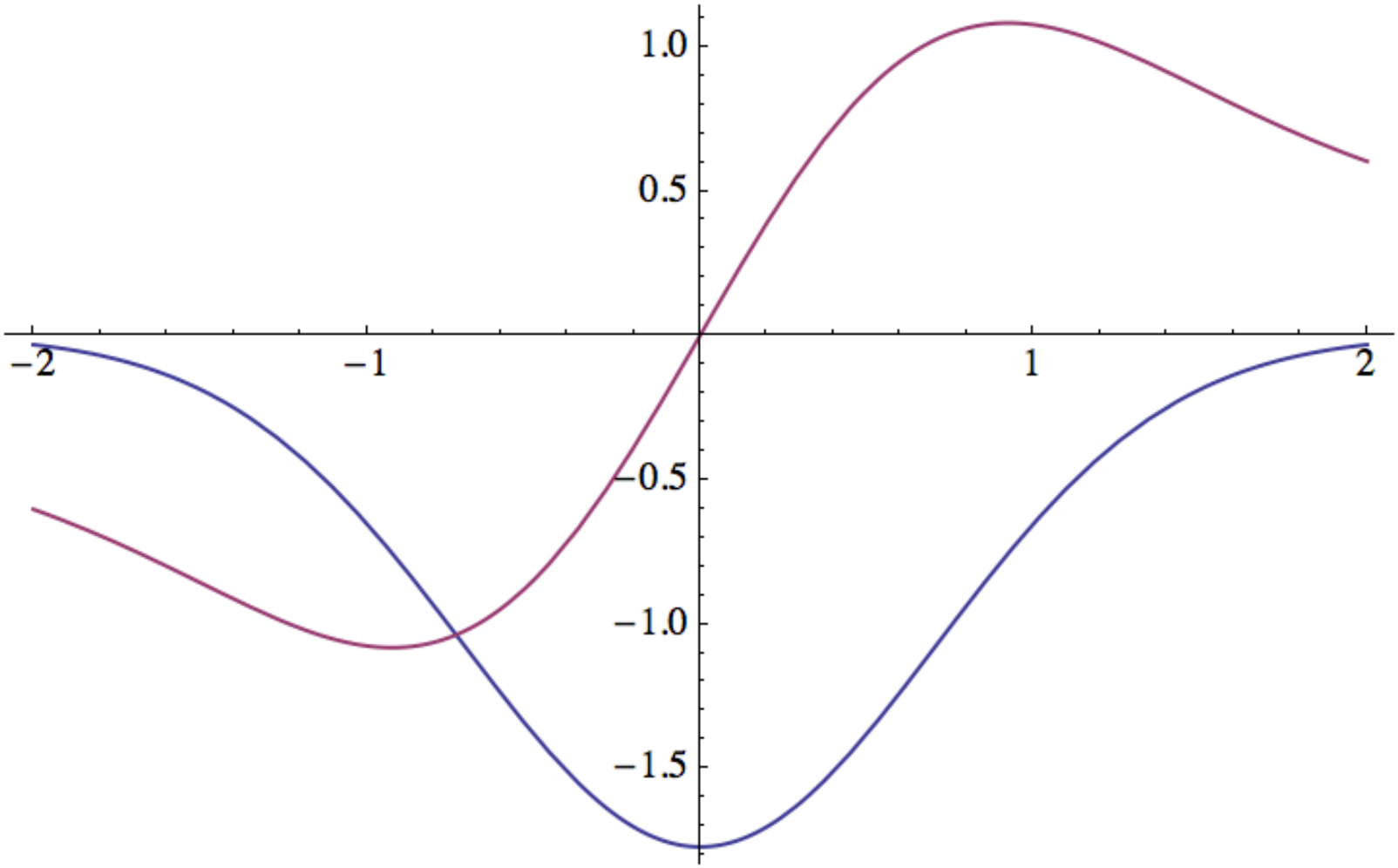
Bethe lattice

$$2\left(z - i\sqrt{1 - z^2}\ \mathrm{Sign}[\mathrm{Im}[z]]\right)$$



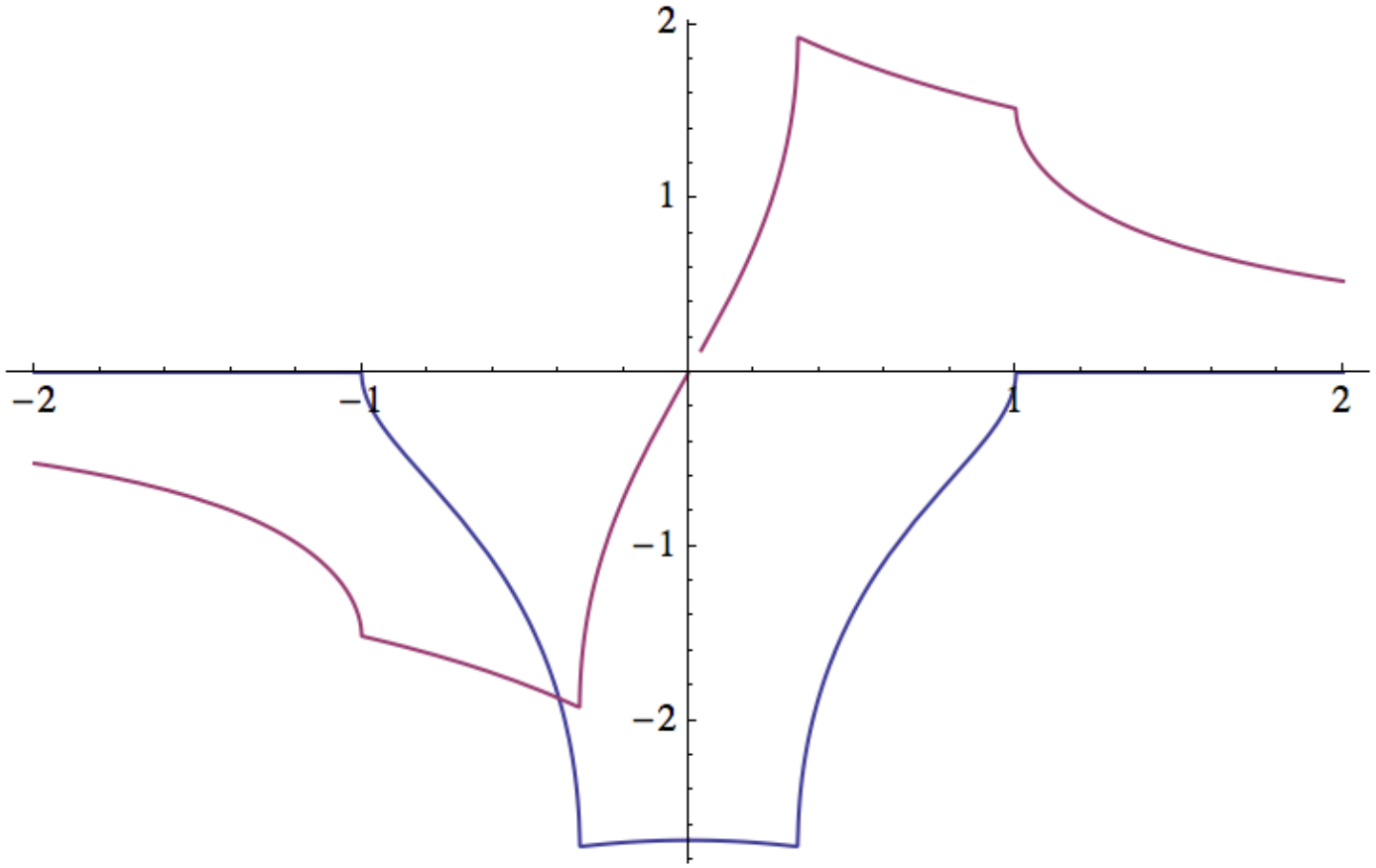
Hypercubic lattice

$$-i\, e^{-z^2} \sqrt{\pi}\, \mathrm{Erfc}[-i\, z\, \mathrm{Sign}[\mathrm{Im}[z]]]\, \mathrm{Sign}[\mathrm{Im}[z]]$$



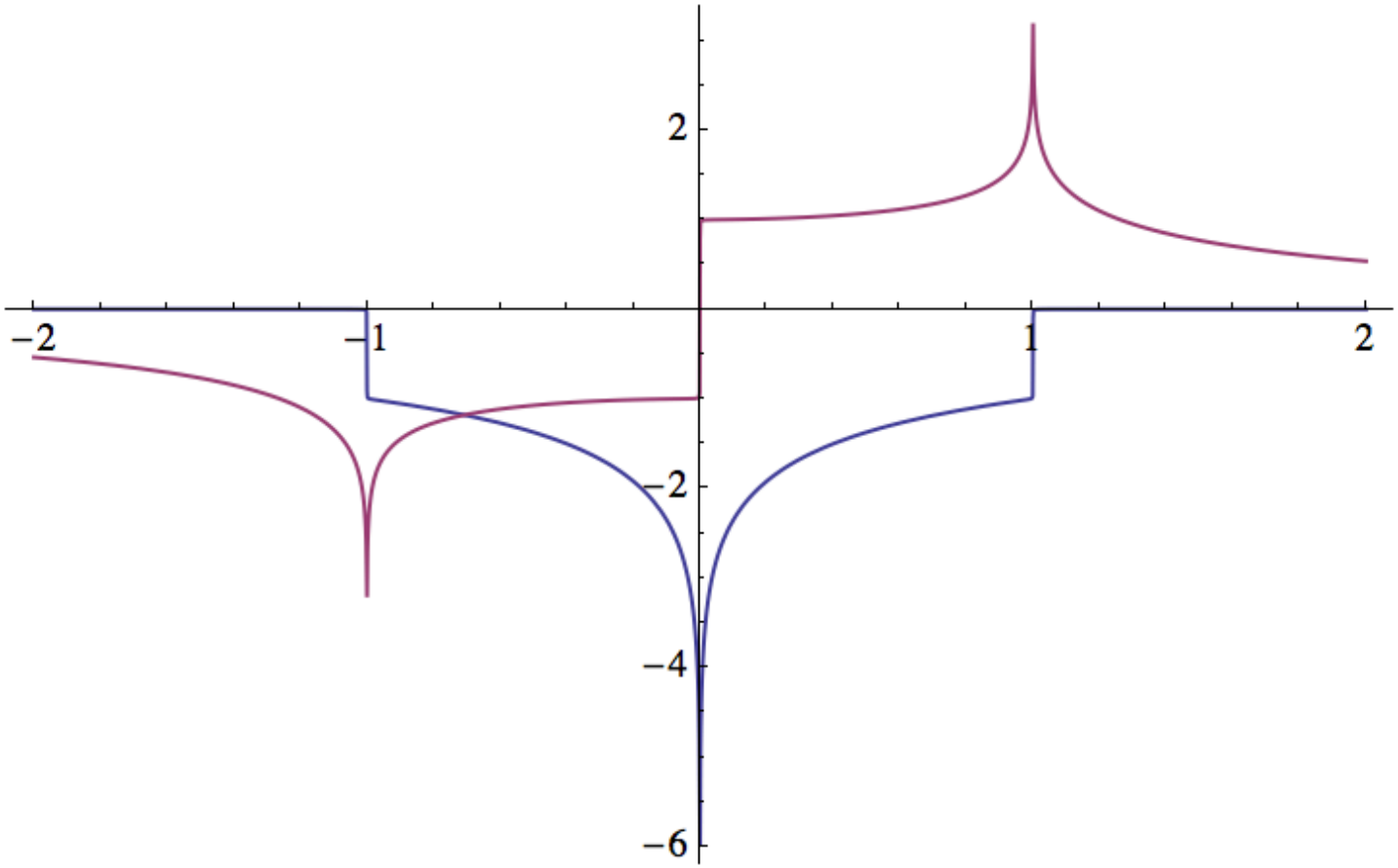
3D cubic lattice

```
x1 = 1 / 2 + (1 / 2) (3 / (3 z) ^ 2) - (1 / 2) Sqrt[1 - 9 / (3 z) ^ 2] Sqrt[1 - 1 / (3 z) ^ 2]
x2 = x1 / (x1 - 1)
kp2 = 1 / 2 + (1 / 4) x2 Sqrt[4 - x2] - (1 / 4) (2 - x2) Sqrt[1 - x2]
km2 = 1 / 2 - (1 / 4) x2 Sqrt[4 - x2] - (1 / 4) (2 - x2) Sqrt[1 - x2]
(1 / z) (Sqrt[1 - (3 / 4) x1] / (1 - x1) ((2 / Pi) EllipticK[kp2]) ((2 / Pi) EllipticK[km2]))
```



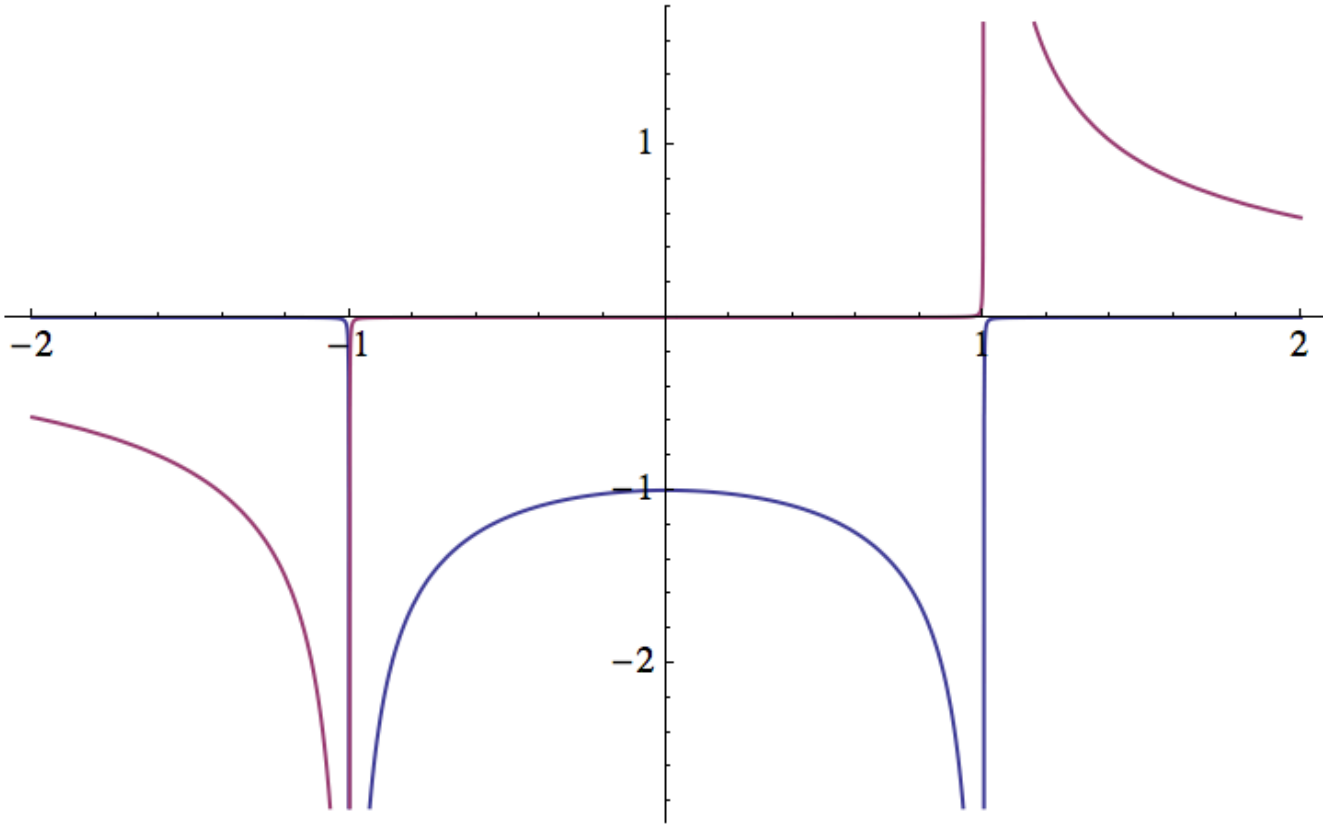
2D cubic lattice

$$\frac{2\,\text{EllipticK}\left[\frac{1}{z^2}\right]}{\pi\, z}$$



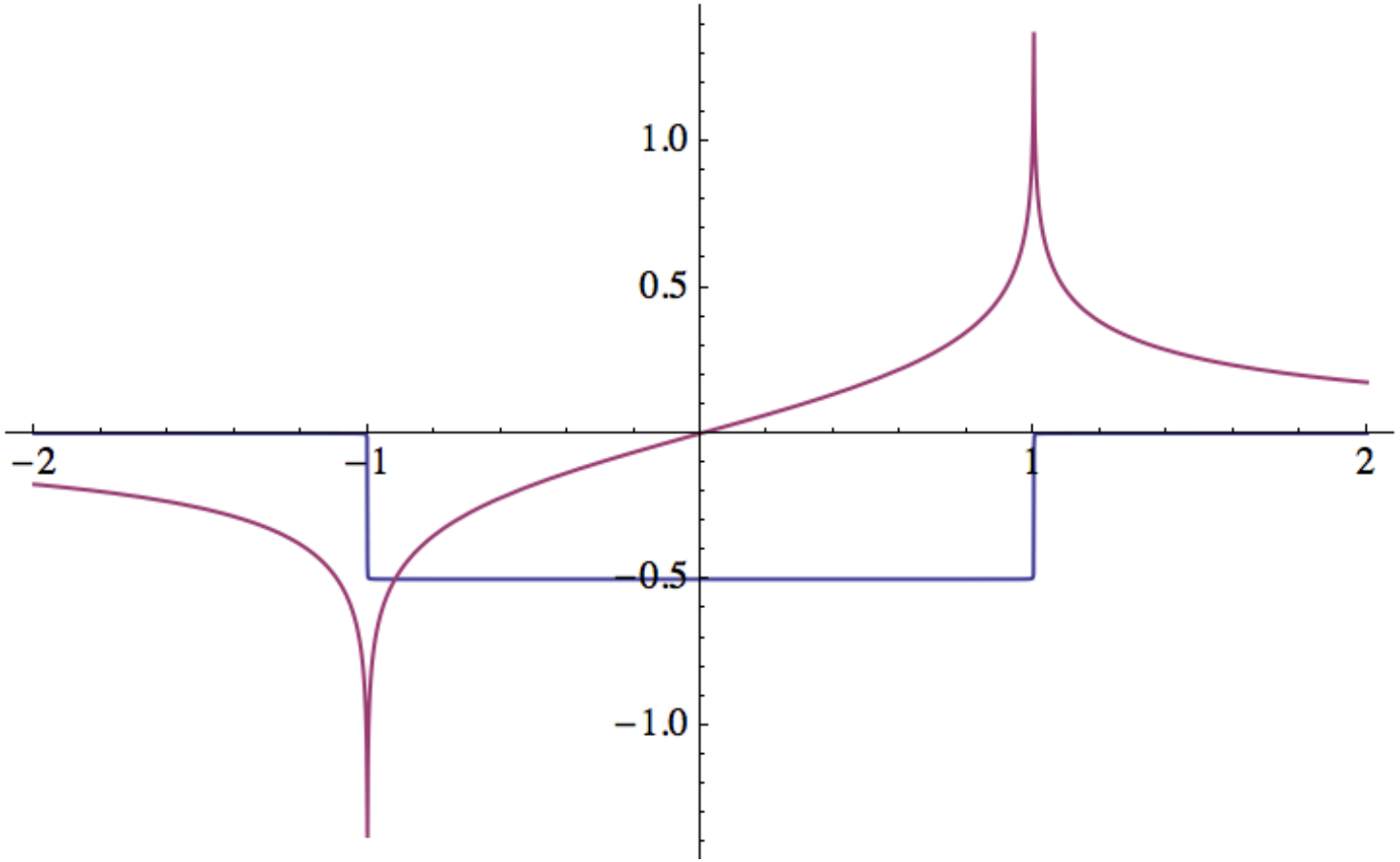
1D cubic lattice (i.e., chain)

$$\frac{1}{\sqrt{1 - \frac{1}{z^2}\ z}}$$



Flat band

$$-\frac{\mathrm{Log}\left[\frac{-1+z}{1+z}\right]}{2\pi}$$



Achieving convergence: self-consistency constraint viewed as a system of equations

DMFT step:

$$\Gamma_\sigma^{\mathrm{new}} = \Gamma_\sigma^{\mathrm{new}} \left\{ \Gamma^{\mathrm{old}}(\omega) \right\}$$

$$F(\Gamma_\sigma) = \Gamma_\sigma^{\mathrm{new}} \left\{ \Gamma_\sigma \right\} - \Gamma_\sigma$$

Self-consistency:

$$\Gamma_\sigma^{\mathrm{new}} \left\{ \Gamma_\sigma^{\mathrm{old}}(\omega) \right\} = \Gamma_\sigma^{\mathrm{old}}$$

$$F(\Gamma_\sigma) = 0$$

Linear mixing (parameter α in [0:1]):

$$\Gamma^{\mathrm{input},(m)} = \alpha \Gamma^{\mathrm{new},(\mathrm{m})} + (1-\alpha)\Gamma^{\mathrm{input},(\mathrm{m}-1)}$$

Broyden method

$\mathbf{F}^{(m)}=\mathbf{F}[\,\mathbf{V}^{(m)}\,]$

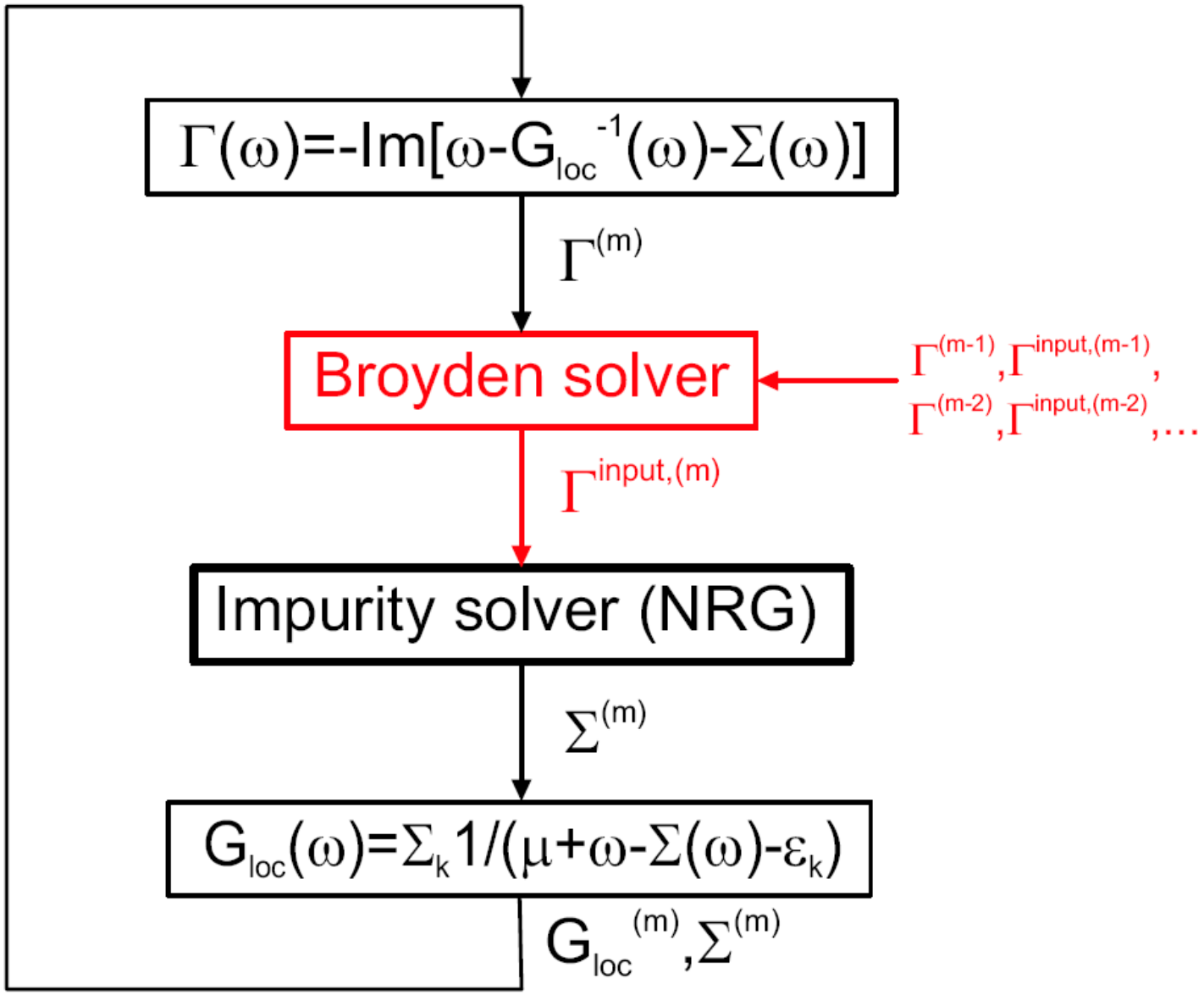
Newton-Raphson method: $$\mathbf{V}^{(m+1)} = \mathbf{V}^{(m)} - \left[J^{(m)}\right]^{-1}\mathbf{F}^{(m)}$$

Broyden update: $$B^{(m)} = -\left[J^{(m)}\right]^{-1}$$

$$B^{(m+1)} = B^{(m)} + \left(\Delta\mathbf{V}^{(m)} - B^{(m)}\Delta\mathbf{F}^{(m)}\right) \otimes \Delta\mathbf{F}^{(m)}$$

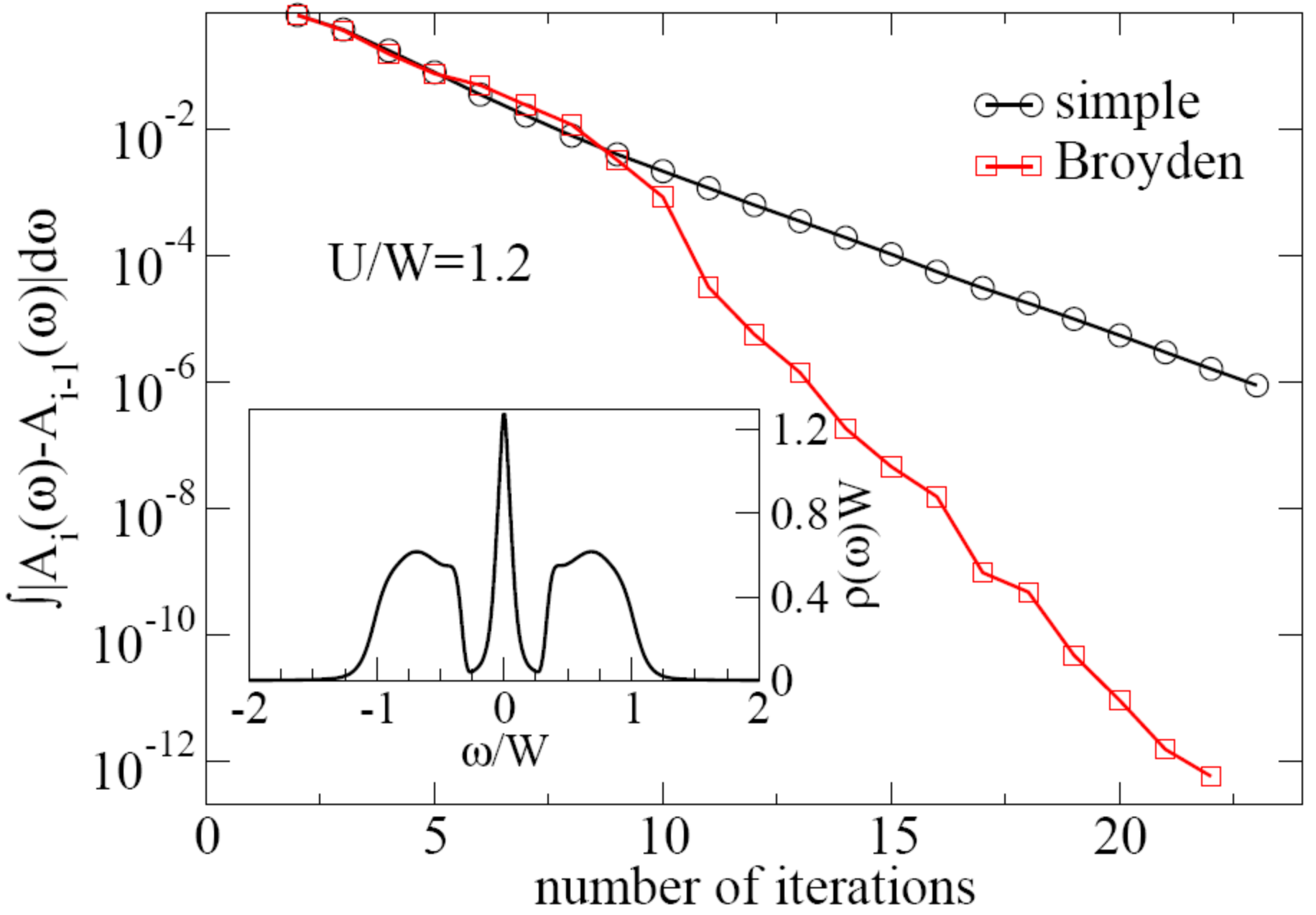
$$\Delta\mathbf{V}^{(m)} = \frac{\mathbf{V}^{(m+1)} - \mathbf{V}^{(m)}}{\left|\mathbf{F}^{(m+1)} - \mathbf{F}^{(m)}\right|}$$

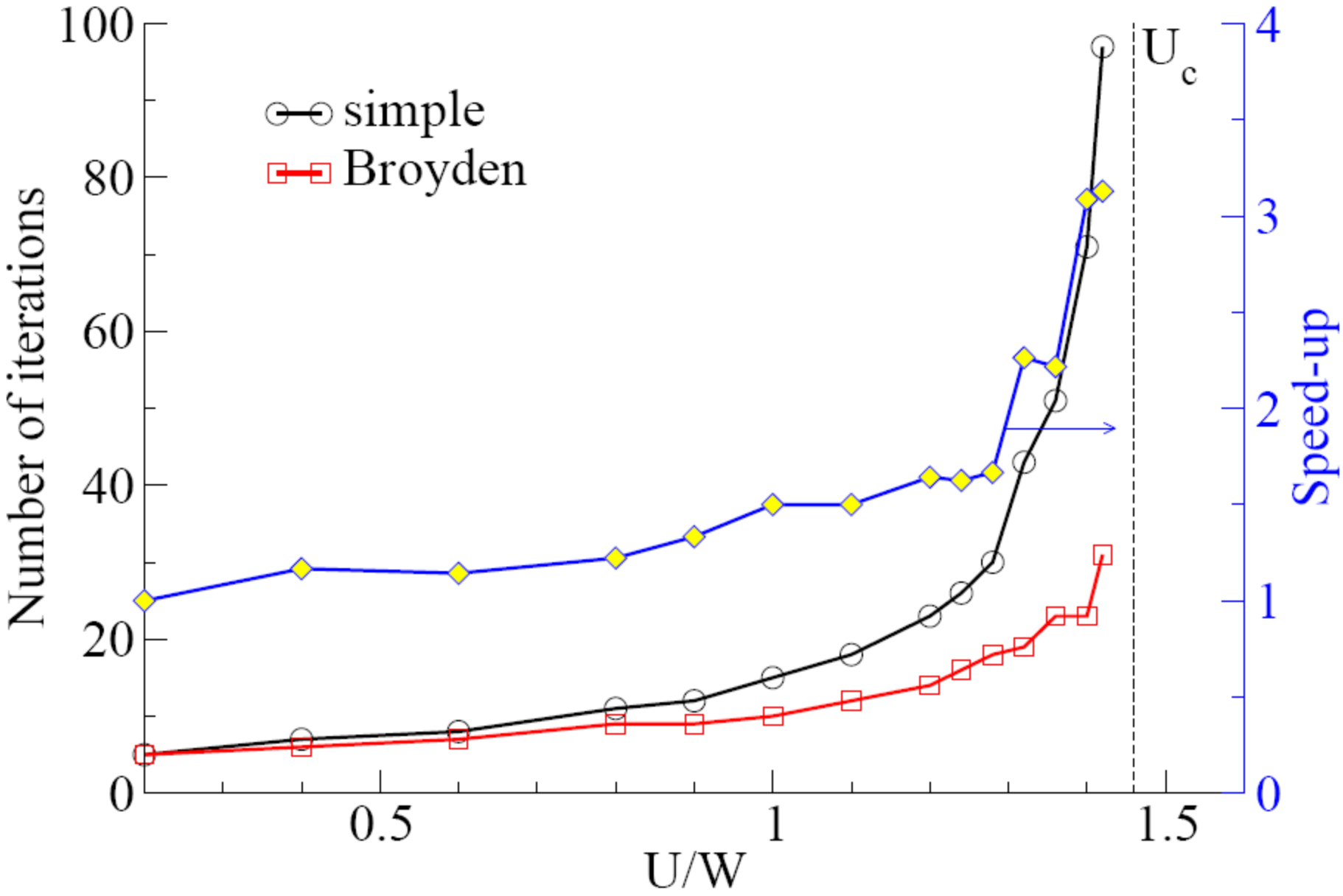
$$\Delta\mathbf{F}^{(m)} = \frac{\mathbf{F}^{(m+1)} - \mathbf{F}^{(m)}}{\left|\mathbf{F}^{(m+1)} - \mathbf{F}^{(m)}\right|}$$



Note: can also be used to control the chemical potential in fixed occupancy calculations.

R. Žitko, PRB **80**, 125125 (2009).


simple
Broyden
U/W=1.2
$\int |A_i(\omega)-A_{i-1}(\omega)|d\omega$
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
0
5
10
15
20
number of iterations
1.2
0.8
0.4
0
$\rho(\omega)W$
-2
-1
0
1
2
ω/W


100
80
60
40
20
0
Number of iterations
simple
Broyden
U_c
4
3
2
1
0
Speed-up
0.5
1
1.5
U/W

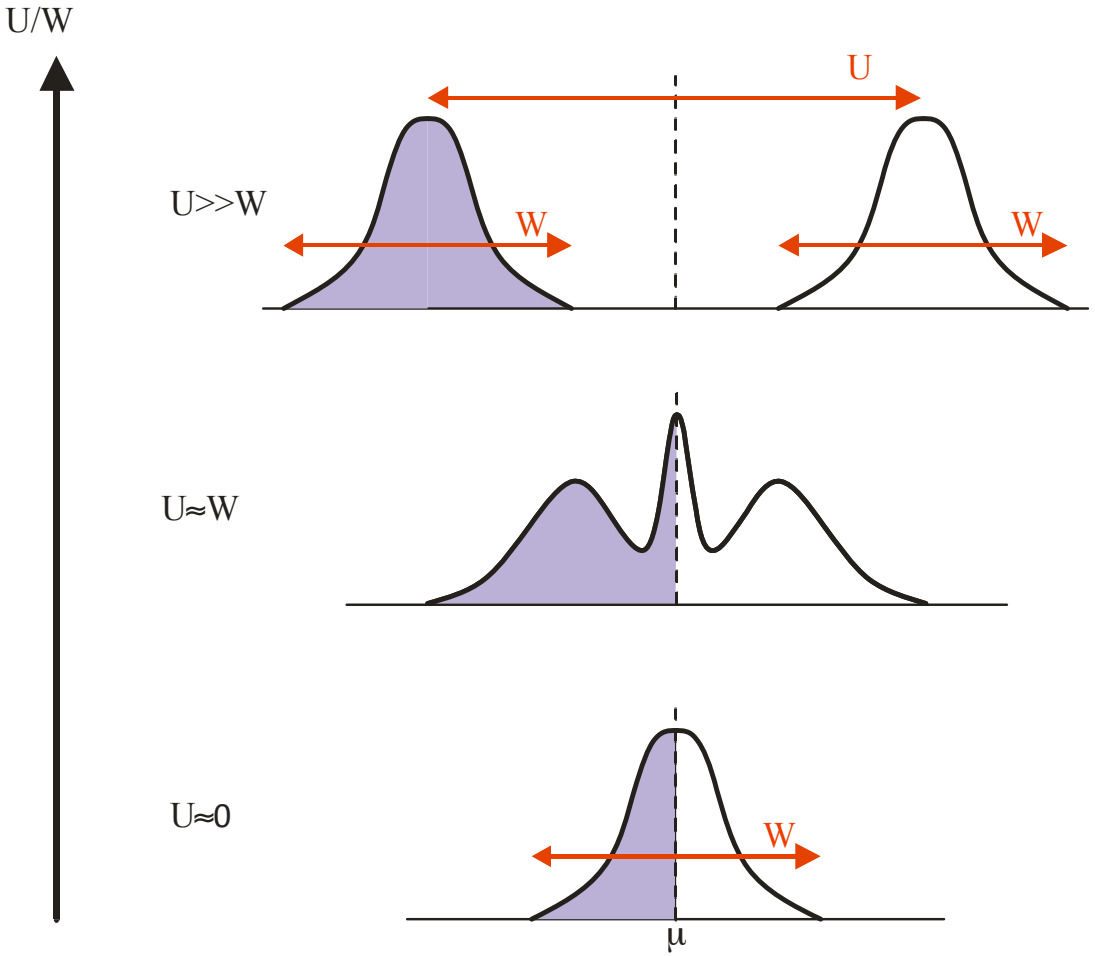
Recent improvements in NRG

- DM-NRG, CFS, FDM algorithms ⇒ more reliable spectral functions, even at finite T
- discretization scheme with reduced artifacts ⇒ possibility for improved energy resolution

NRG vs. CT-QMC

- NRG: extremely fast for single-impurity problems
- NRG: access to arbitrarily low temperature scales, but decent results even at high T (despite claims to the contrary!)
- NRG: spectral functions directly on the real-frequency axis, no analytic continuation necessary
- NRG: any local Hamiltonian can be used, no minus sign problem
- NRG: efficient use of symmetries
- CT-QMC: (numerically) exact
- CT-QMC: can handle multi-orbital problems (even 7-orbital f-level electrons)

Mott-Hubbard phase transition

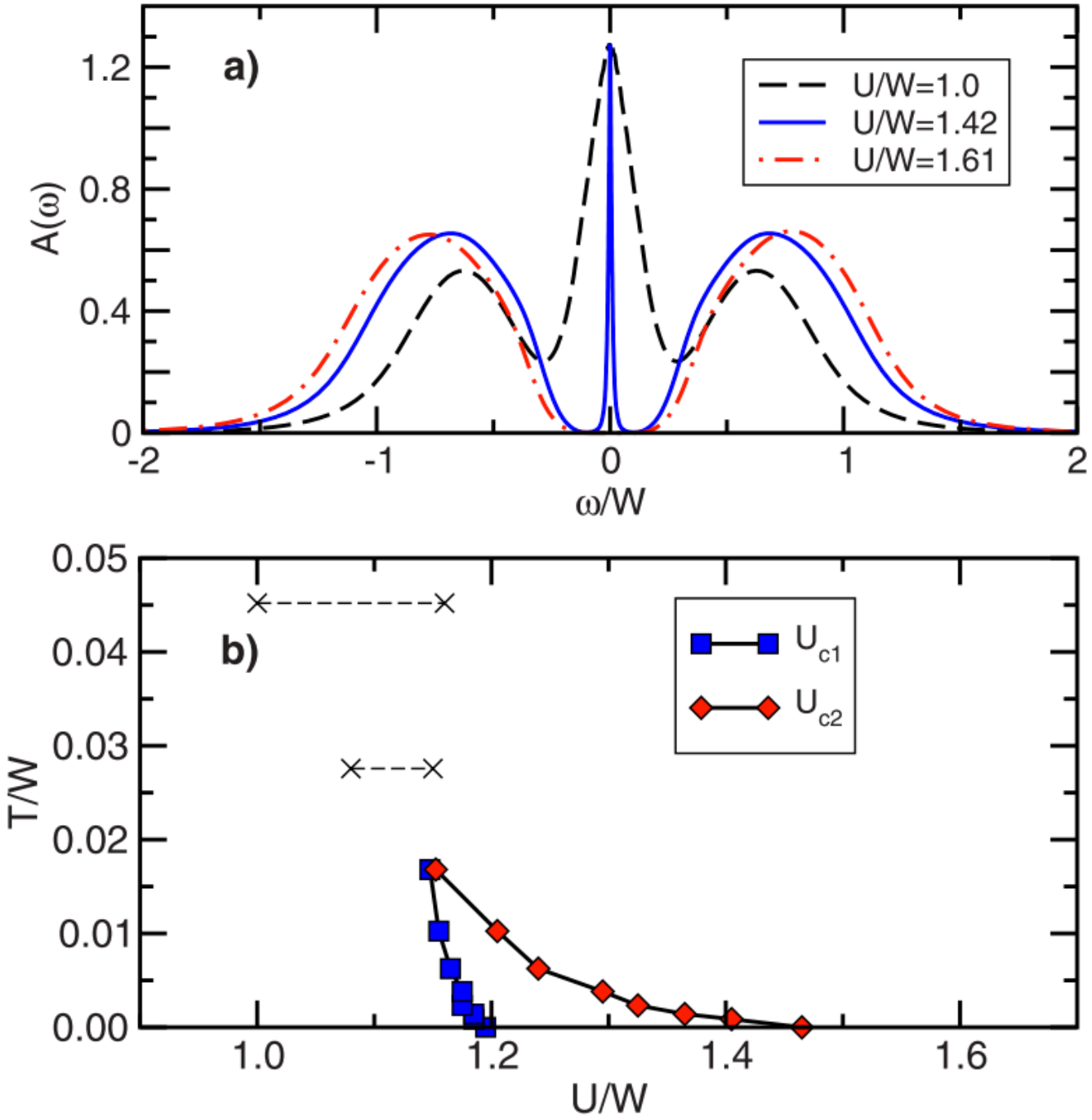


Mott insulator

← DMFT prediction

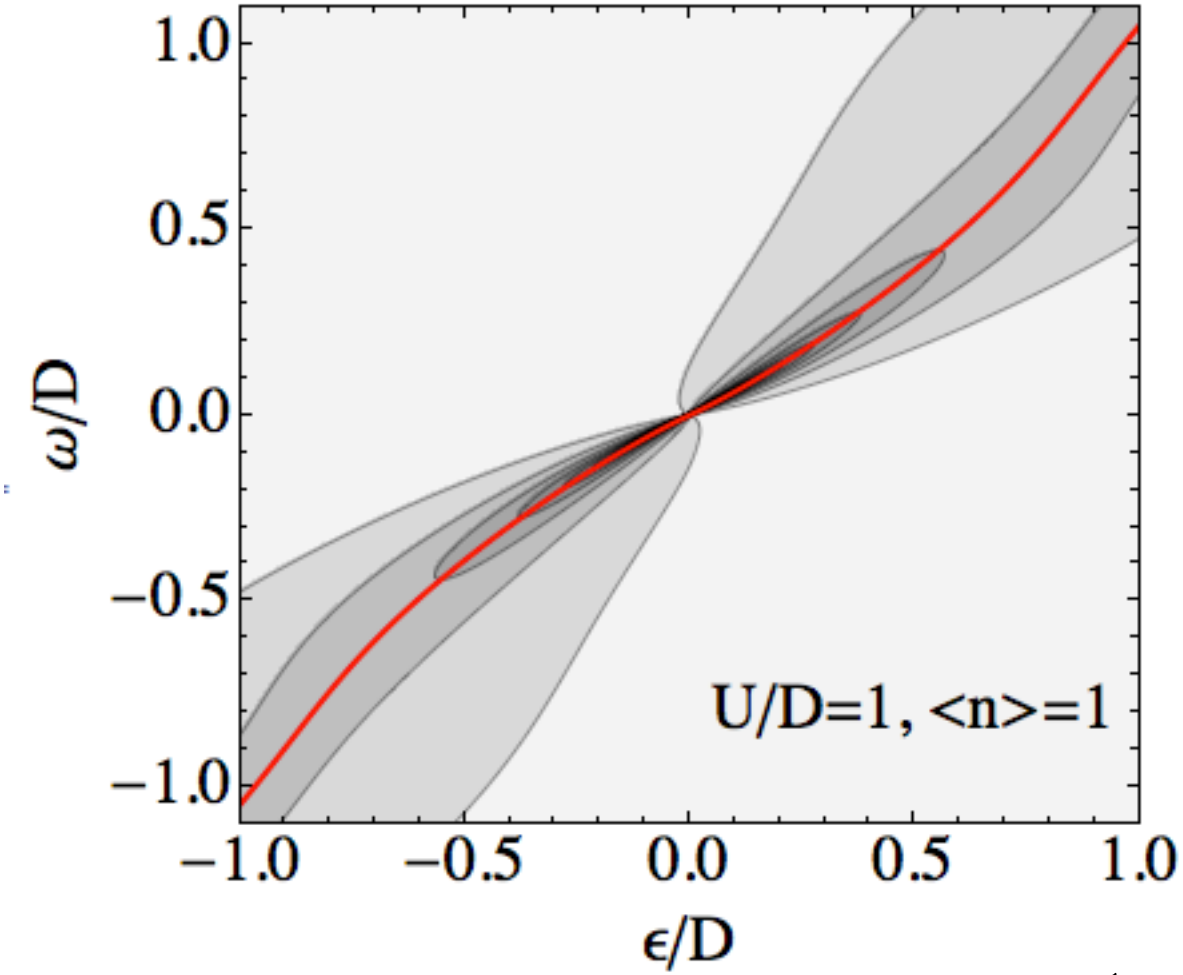
non-correlated metal

Kotliar, Vollhardt

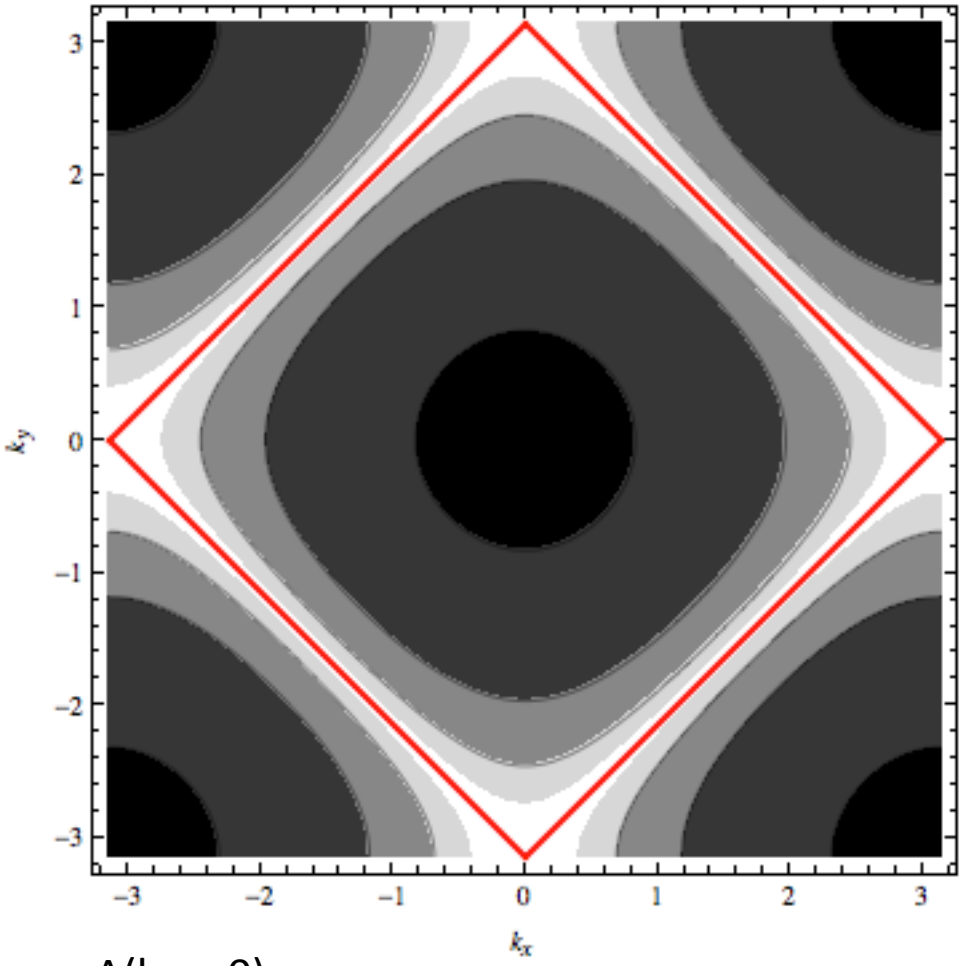


Bulla, 1999, Bulla et al. 2001.

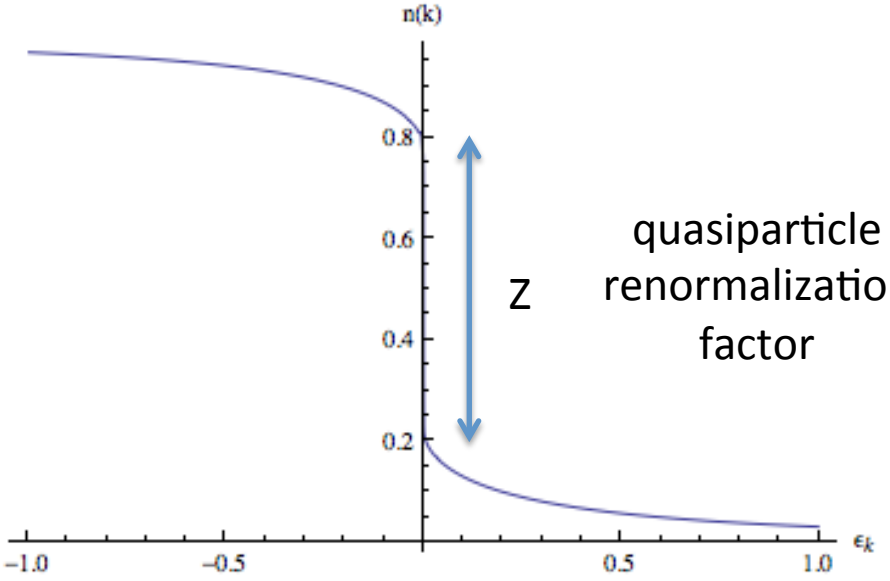
k-resolved spectral functions



$$A(k,\omega) = -\frac{1}{\pi}\mathrm{Im}\frac{1}{\omega - \epsilon_k - \Sigma(\omega)}$$



A(k,ω=0)

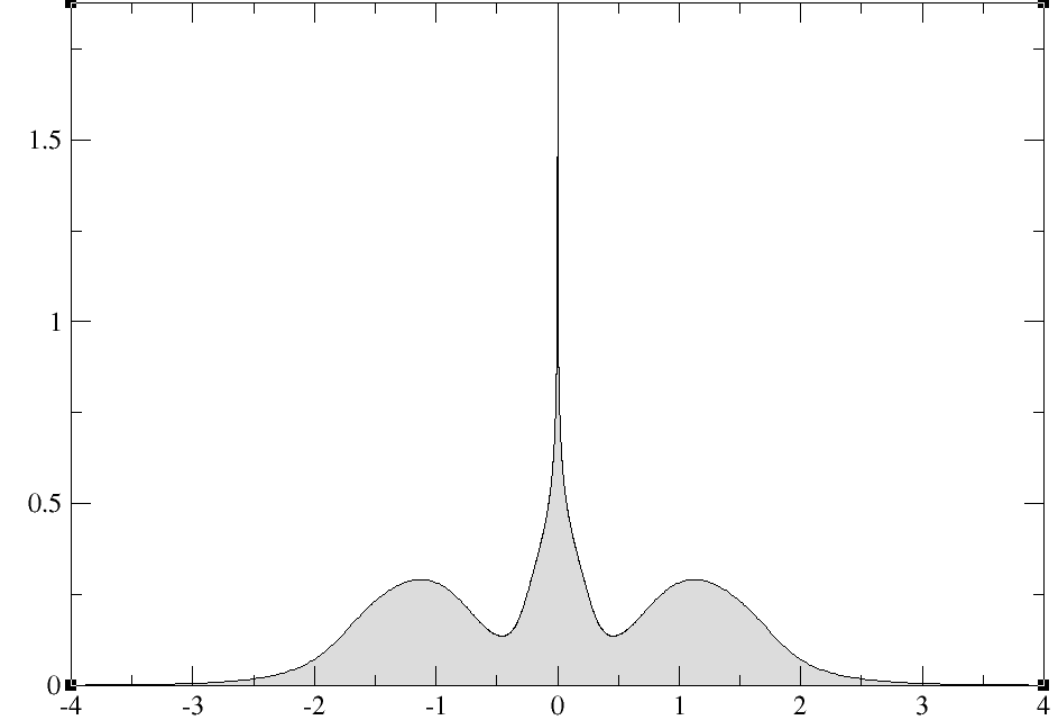


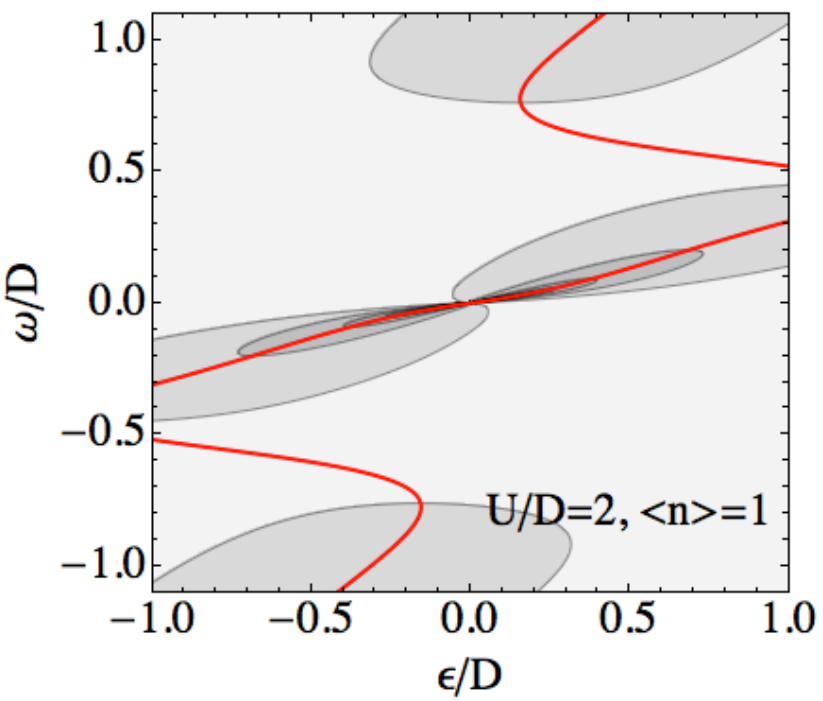
quasiparticle renormalization factor

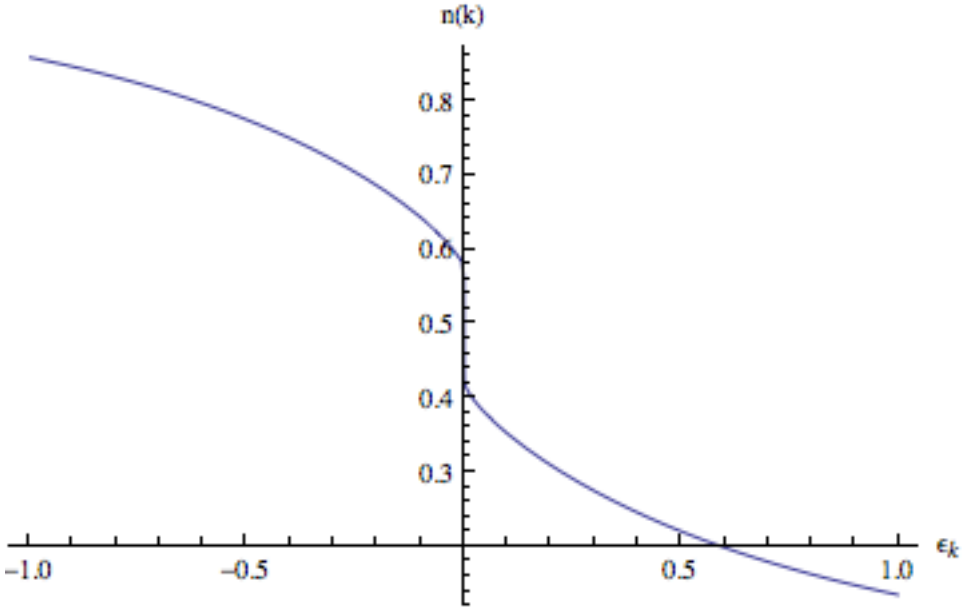
Momentum distribution function

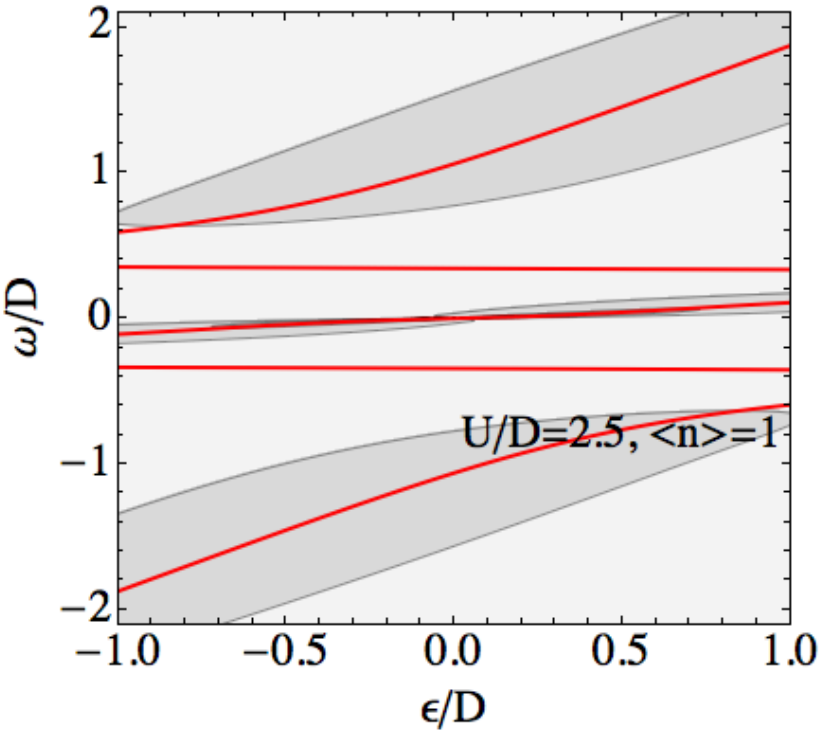
2D cubic lattice DOS: $\epsilon_k = \frac{D}{2}\left(\cos k_x + \cos k_y\right)$

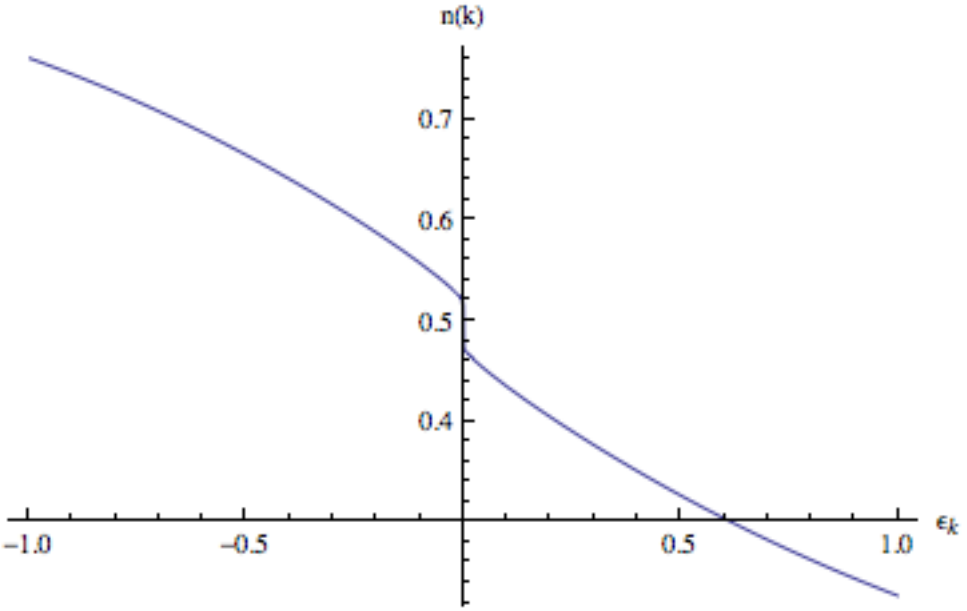
Caveat: obviously, DMFT is not a good approximation for 2D problems.
But 2D cubic lattice is nice for plotting...


1.5
1
0.5
0
-4
-3
-2
-1
0
1
2
3
4


1.0
0.5
0.0
−0.5
−1.0
ω/D
−1.0
−0.5
0.0
0.5
1.0
ϵ/D
U/D=2, <n>=1


n(k)
0.8
0.7
0.6
0.5
0.4
0.3
−1.0
−0.5
0.5
1.0
ϵk

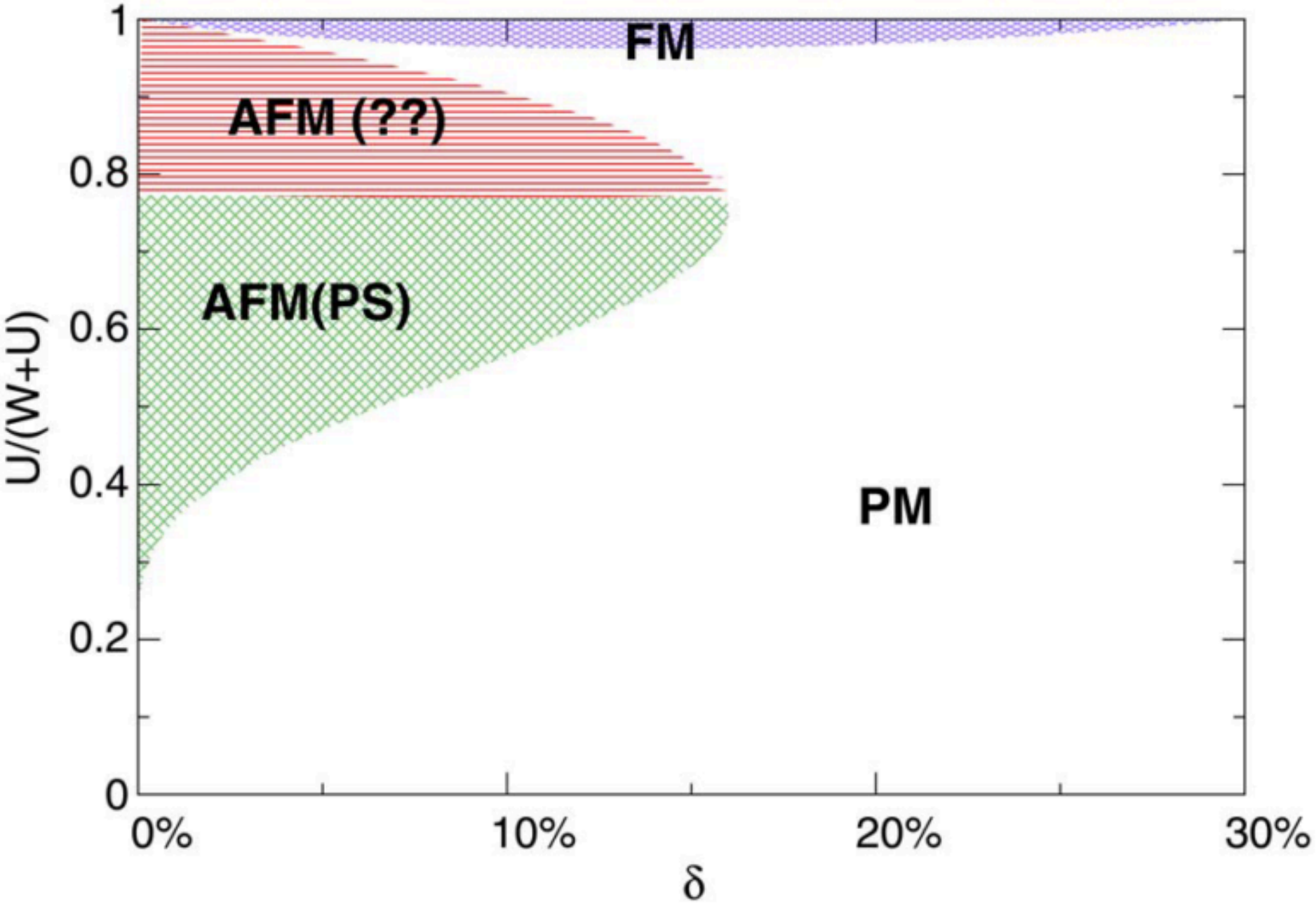

2
1
0
−1
−2
ω/D
U/D=2.5, <n>=1
−1.0
−0.5
0.0
0.5
1.0
ϵ/D


n(k)
0.7
0.6
0.5
0.4
−1.0
−0.5
0.5
1.0
ϵk

Ordered phases

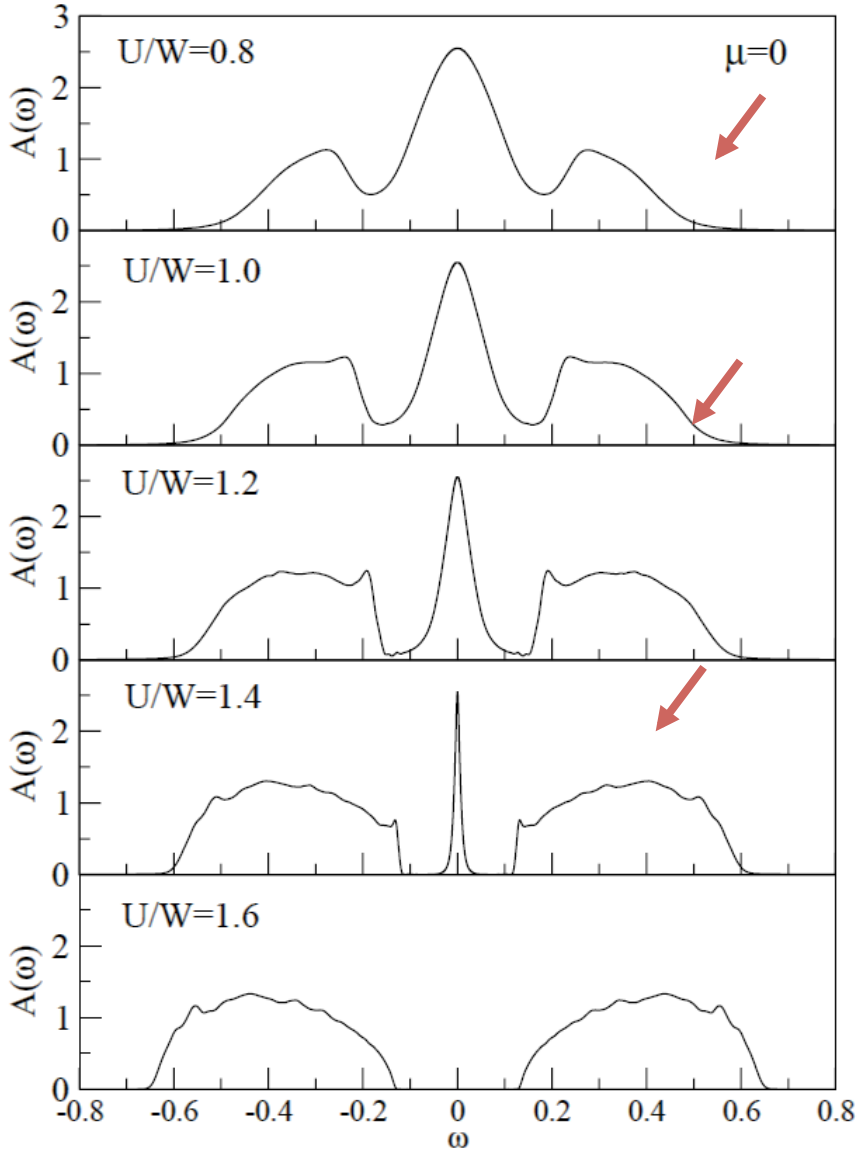
- **Ferromagnetism**: break spin symmetry (i.e., add spin index σ, use QSZ symmetry type)
- **Superconductivity**: introduce Nambu structure, compute both standard G and anomalous G (use SPSU2 symmetry type)
- **Antiferromagnetism**: introduce AB sublattice structure, do double impurity calculation (one for A type, one for B type)

Hubbard model: phase diagram



Zitzler et al.

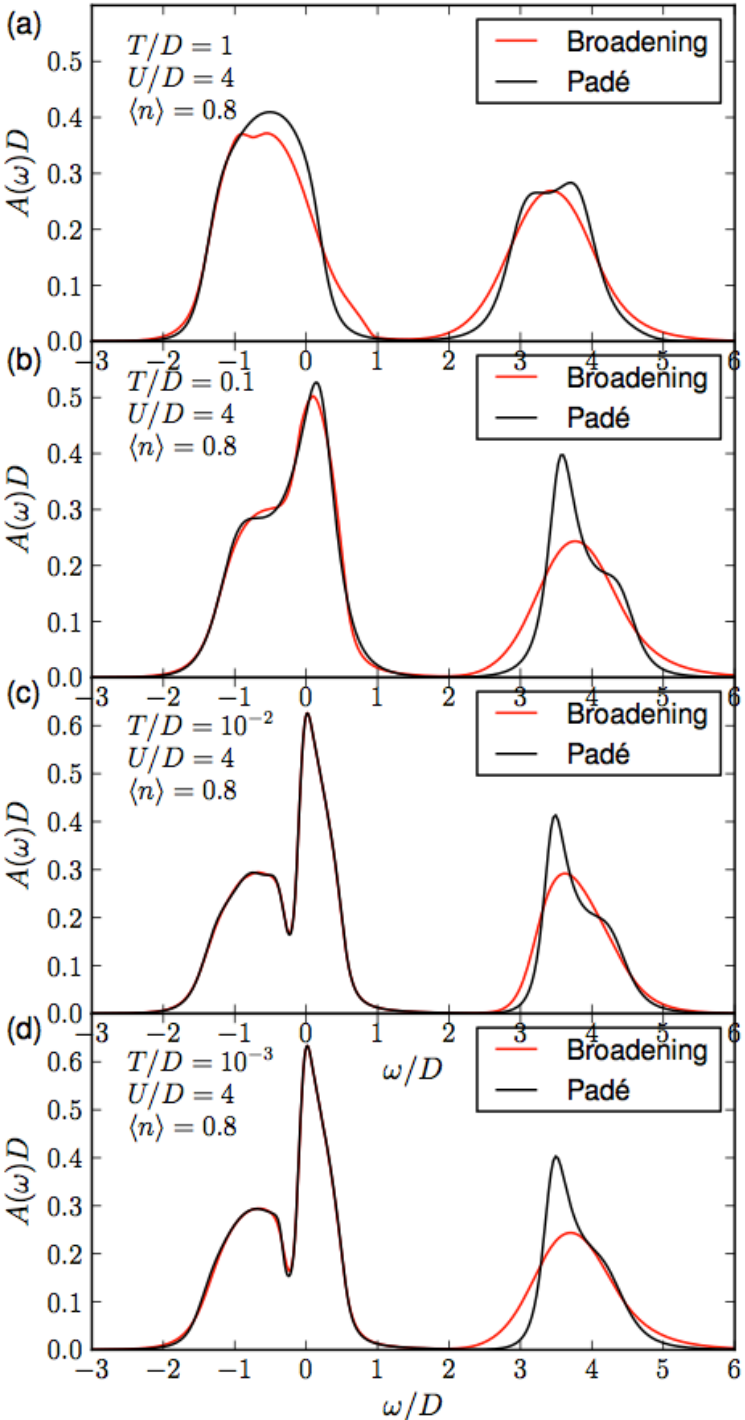
High-resolution spectral functions?



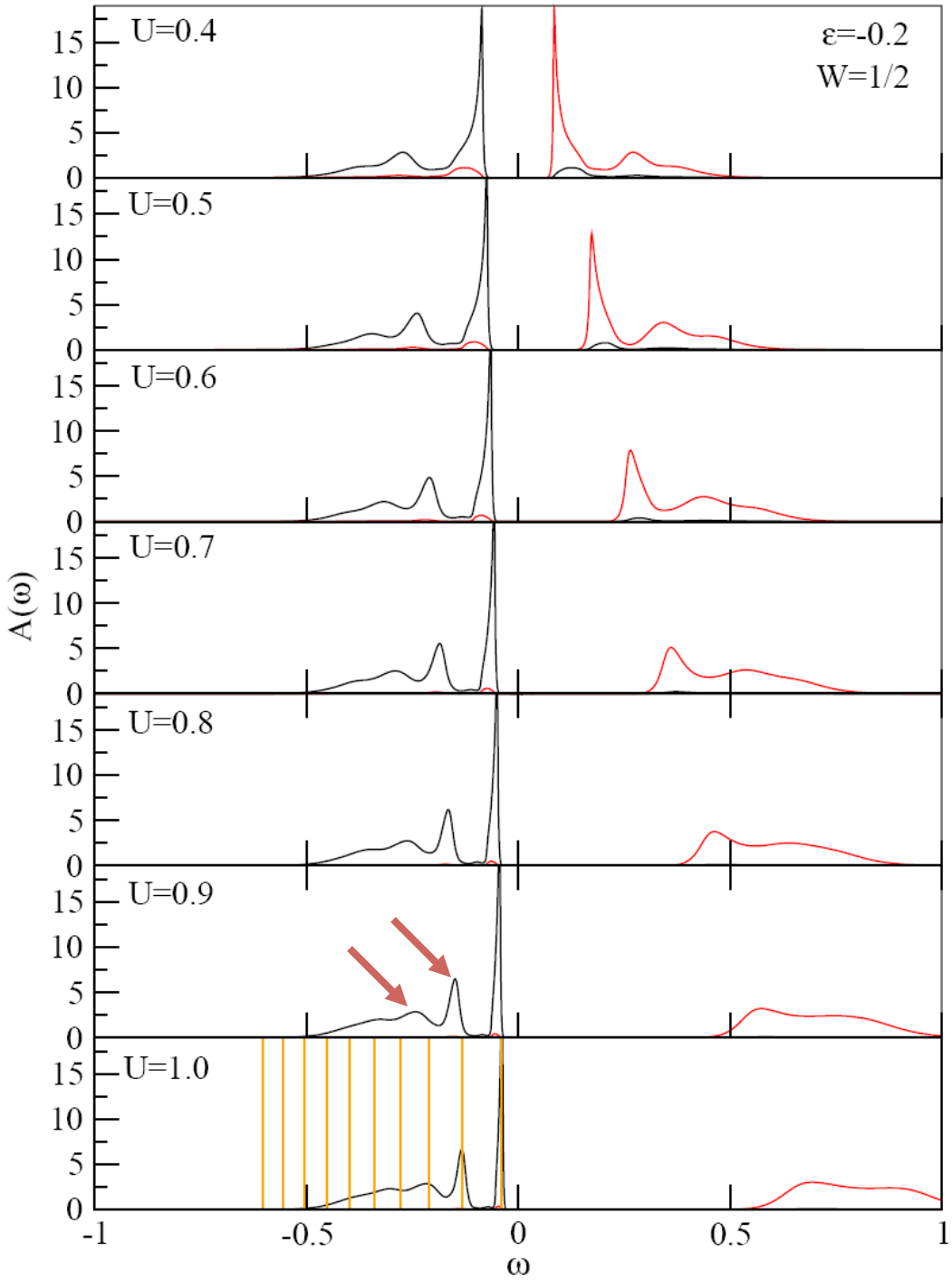
Hubbard model on the Bethe lattice, PM phase

inner band-edge features

See also DMRG study, Karski, Raas, Uhrig, PRB **72**, 113110 (2005).

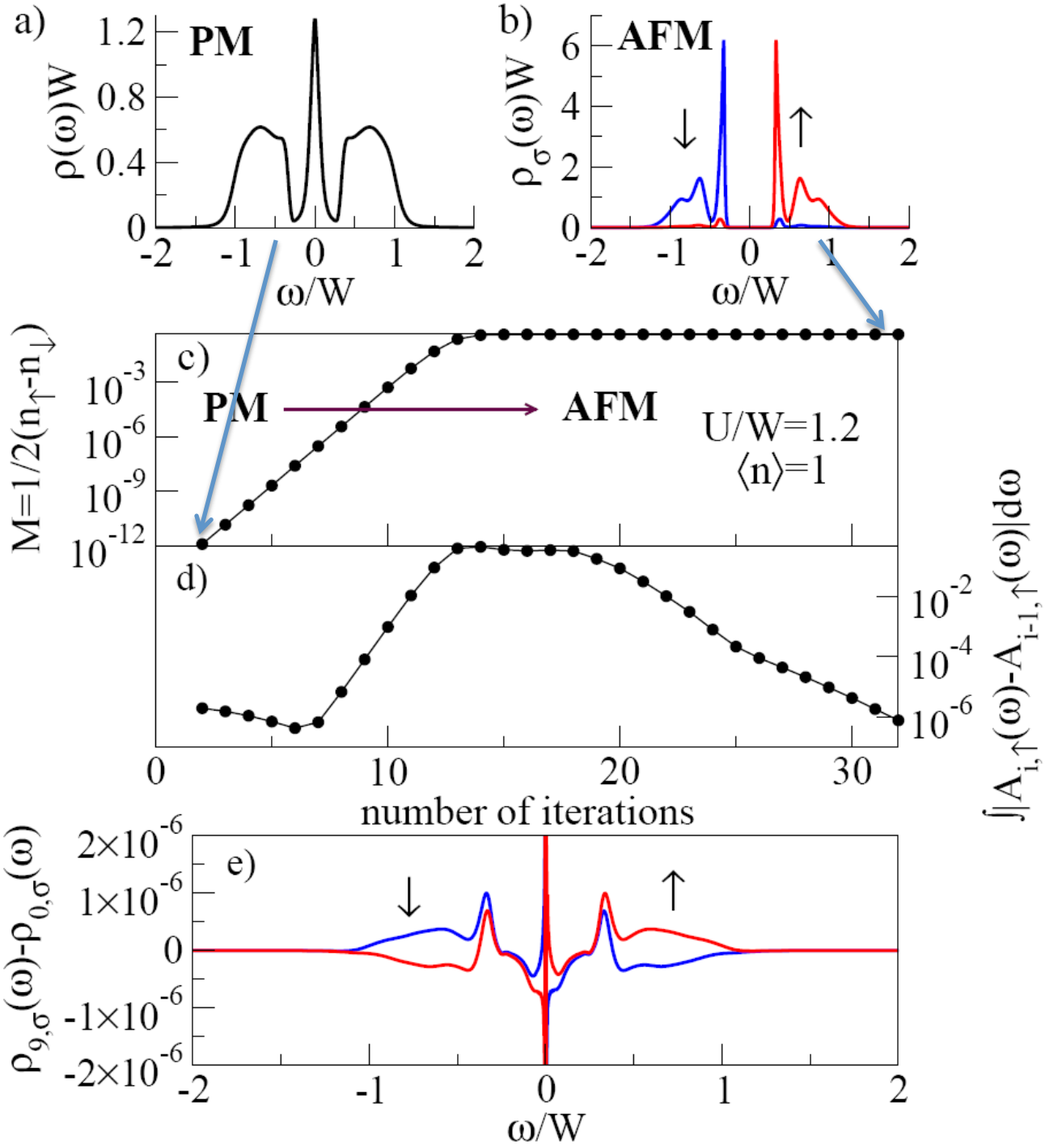


Z. Osolin, RZ, 2013



Hubbard model on the Bethe lattice, AFM phase

spin-polaron structure ("string-states")


a)
PM
ρ(ω)W
ω/W
b)
AFM
ρσ(ω)W
ω/W
c)
PM
AFM
U/W=1.2
⟨n⟩=1
M=1/2(n↑-n↓)
d)
number of iterations
∫|Ai,↑(ω)-Ai-1,↑(ω)|dω
e)
ρ9,σ(ω)-ρ0,σ(ω)
ω/W

Thermodynamics

$$E_{\rm kin} = \sum_k \epsilon_k \langle n_k \rangle \qquad E_{\rm pot} = U \sum_i \langle n_i \rangle$$

$$\langle n_k \rangle = G(k, \tau = 0^-) = \frac{1}{\beta} \sum_n G(k\sigma, i\omega_n) \exp(i\omega_n 0^+) = {\rm Tr}[G(k)]$$

Note: $G(k) = G(\epsilon_k)$

$$E_{\rm kin} = \int {\rm d}\epsilon \, \rho(\epsilon) \, {\rm Tr}[G(\epsilon)]$$

Bethe lattice:

$$E_{\rm kin} = \frac{D^2}{4} T \sum_n [G(i\omega_n)]^2$$

$$S(T_2) - S(T_1) = \int_{T_1}^{T_2} {\rm d}S = \int_{T_1}^{T_2} \frac{{\rm d}E}{T} = \frac{E(T_2)}{T_2} - \frac{E(T_1)}{T_1} + \int_{T_1}^{T_2} \frac{E(T)}{T^2} {\rm d}T$$

Transport in DMFT

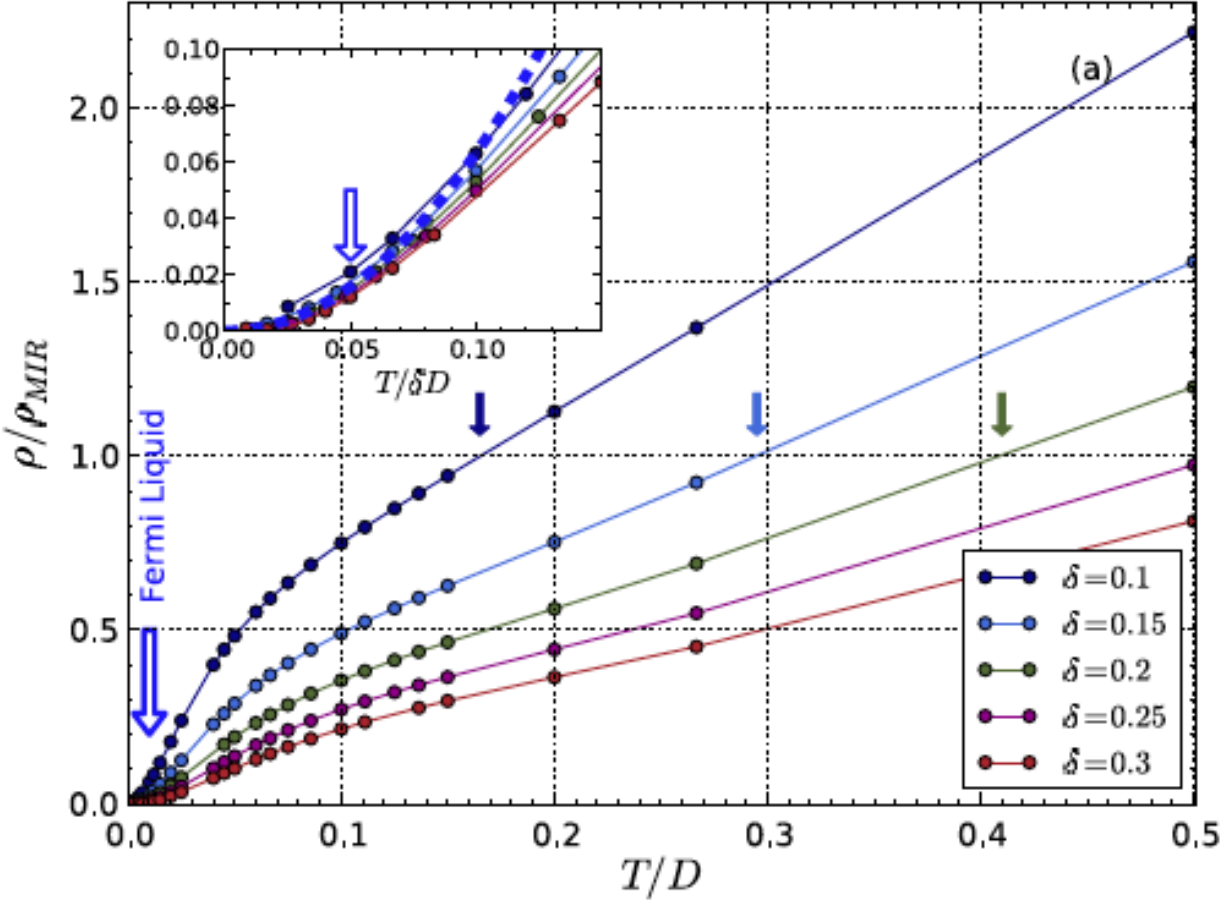
Vertex corrections drop out, because Σ is local, and $\mathbf{v}_k$ and ε_k have different parity.

$$\sigma(\omega) = \frac{2\pi e^2}{\hbar} \int \mathrm{d}\omega' F_{\omega,\omega'} \int \mathrm{d}\epsilon\, \Phi(\epsilon) A_{\mathbf{k}}(\omega') A_{\mathbf{k}}(\omega'+\omega)$$

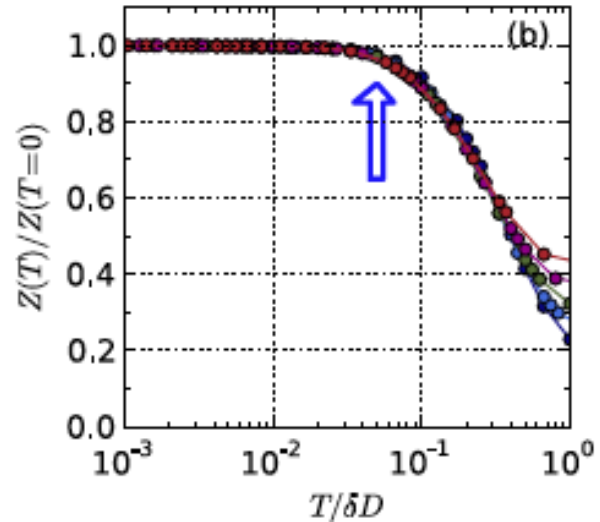
$$F_{\omega,\omega'} = [f(\omega') - f(\omega+\omega')]/\omega$$

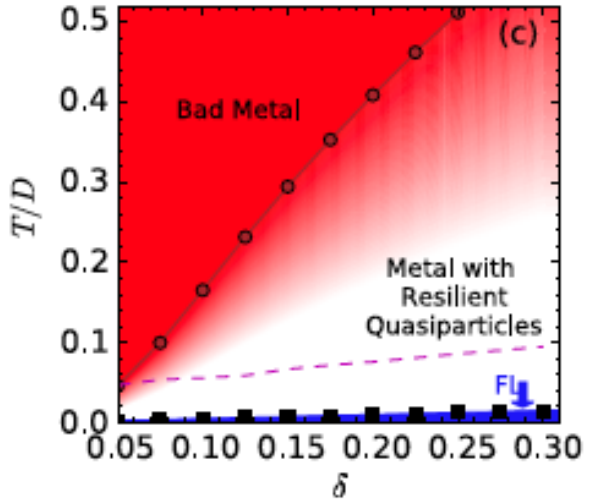
$$A_{\mathbf{k}}(\omega) = -\frac{1}{\pi}\mathrm{Im}[\omega + \mu - \epsilon_{\mathbf{k}} - \Sigma(\omega)]^{-1}$$

$$\Phi(\epsilon) = \frac{1}{V}\sum_{\mathbf{k}} \left(\frac{\partial \epsilon_{\mathbf{k}}}{\partial \mathbf{k}_x}\right)^2 \delta(\epsilon - \epsilon_{\mathbf{k}})$$

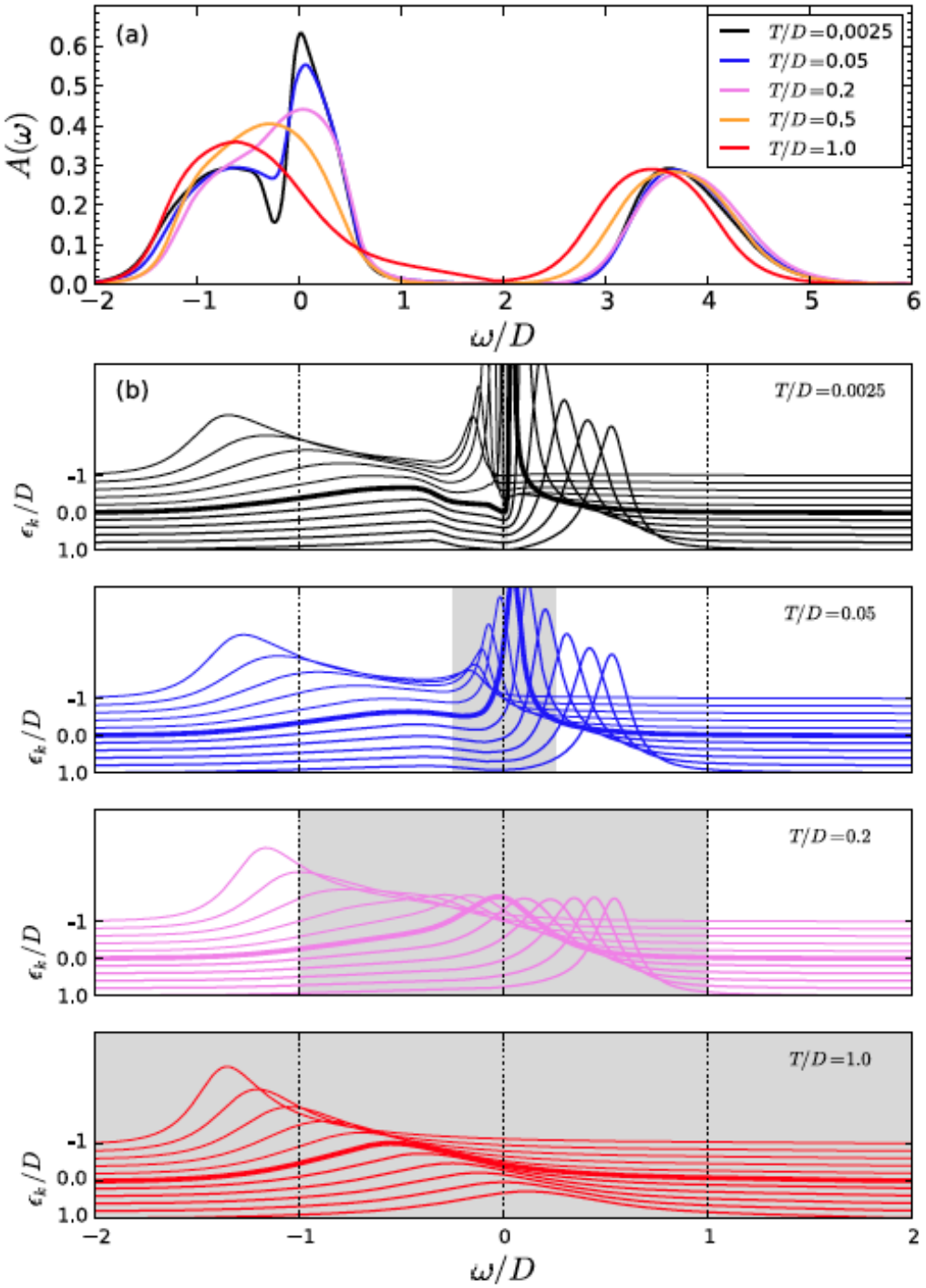


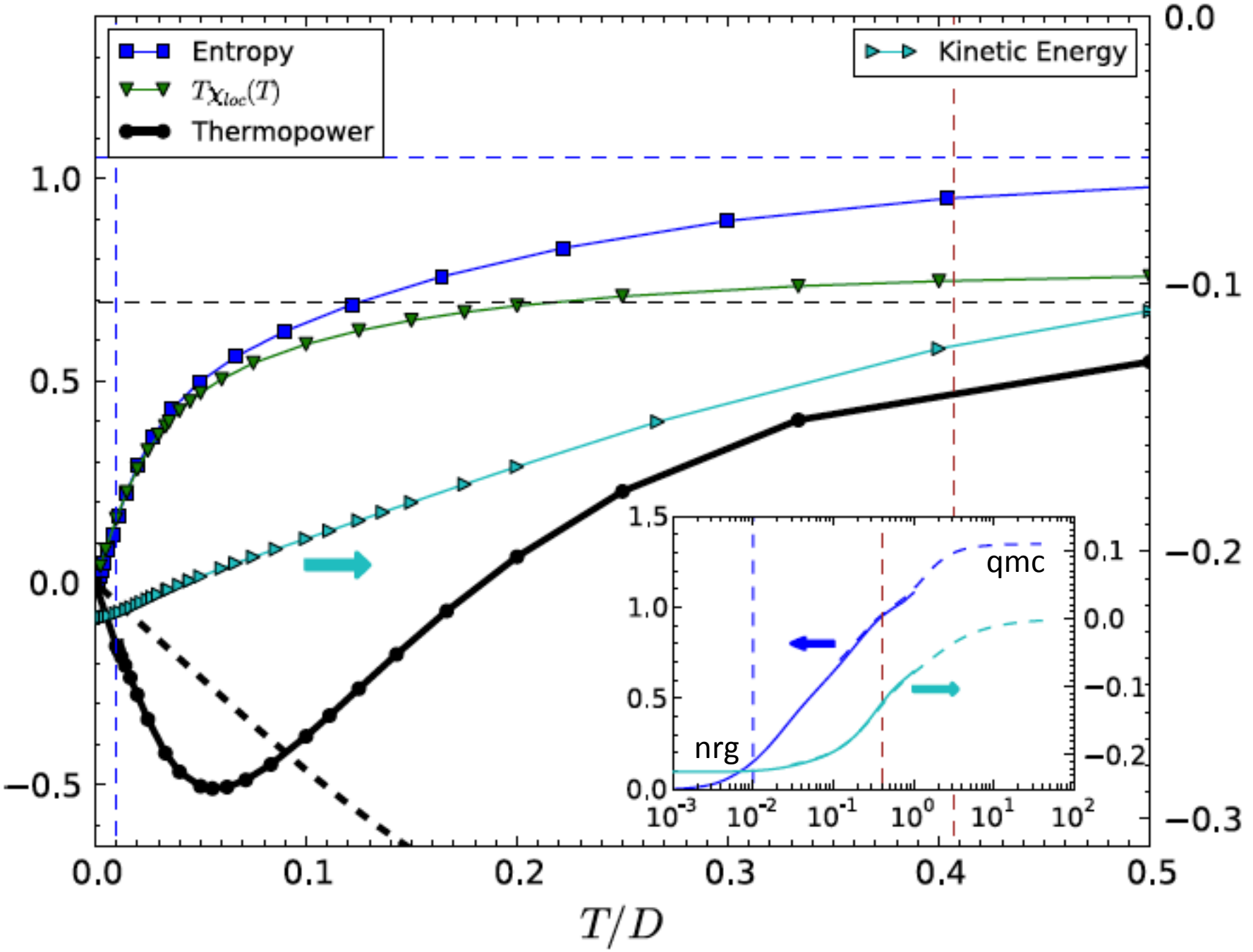
$$\rho_{\mathrm{MIR}} = \hbar D/e^2\Phi(0)$$





X. Deng, J. Mravlje, R. Zitko,
M. Ferrero, G. Kotliar,
A. Georges, PRL 2013.


(a)
T/D=0,0025
T/D=0.05
T/D=0.2
T/D=0,5
T/D=1.0
$A(\omega)$
ω/D
(b)
T/D=0.0025
T/D=0.05
T/D=0.2
T/D=1.0
ϵ_k/D
ω/D


Entropy
$T\chi_{loc}(T)$
Thermopower
Kinetic Energy
1.0
0.5
0.0
−0.5
0.0
−0.1
−0.2
−0.3
0.0
0.1
0.2
0.3
0.4
0.5
T/D
1.5
1.0
0.5
0.0
0.1
0.0
−0.1
−0.2
qmc
nrg
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}

Other applications

- Hubbard (SC, CO)
- two-orbital Hubbard model
- Hubbard-Holstein model (near half-filling)
- Kondo lattice model (PM, FM, AFM, SC phases)
- Periodic Anderson model (PAM), correlated PAM