Numerical renormalization group
part 4

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- Validation
- Discretization revisited
- Application to DMFT
- Parallelization issues

Validation: are spectral functions correct?

- normalization to 1 (follows directly from the canonical anticommutation relations)
- fluctuation-dissipation theorem
- spectral moments (high-frequency expansion)

Alternative methods (simulations): Quantum Monte Carlo

$$\langle A \rangle = \frac{\mathrm{Tr}\left(Ae^{-\beta H}\right)}{\mathrm{Tr}\left(e^{-\beta H}\right)} \qquad \beta = \frac{1}{k_B T}$$

$$\mathrm{Tr}(e^{-\beta H}) = \mathrm{Tr}\prod_{i=1}^{L} e^{-\Delta\tau H} \qquad \beta = L\Delta\tau$$

imaginary-time discretization

$$e^{-\Delta\tau H} = e^{-\Delta\tau H_1} e^{-\Delta\tau H_2} + \mathcal{O}(\Delta\tau^2)$$

Suzuki-Trotter decomposition

Monte-Carlo sampling over auxiliary variables with Metropolis-Hastings algorithm

Example: Hirsch-Fye QMC algorithm for the Anderson impurity model

Continuous-Time QMC Algorithms

$$H = H_a + H_b$$

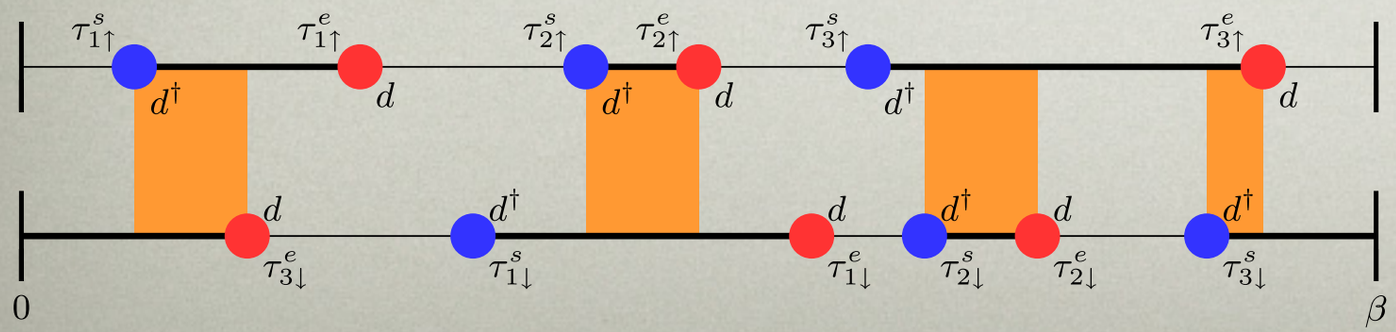
$$\mathrm{Tr}\left(e^{-\beta H}\right) = \mathrm{Tr}\left(T_\tau e^{-\beta H_a} \exp\left[-\int_0^\beta \mathrm{d}\tau\, H_b(\tau)\right]\right)$$

$$= \sum_k \frac{(-1)^k}{k!} \int_0^\beta \mathrm{d}\tau_1 \int_0^\beta \mathrm{d}\tau_2 \cdots \int_0^\beta \mathrm{d}\tau_k \mathrm{Tr}\left(T_\tau e^{-\beta H_a} H_b(\tau_k) H_b(\tau_{k-1}) \cdots H_b(\tau_1)\right)$$

- no time-discretization errors
- no auxiliary-field decomposition

CT-HYB expansion: $H_a = H_{\mathrm{imp}} + H_{\mathrm{band}}$

$H_b = H_{\mathrm{hyb}}$



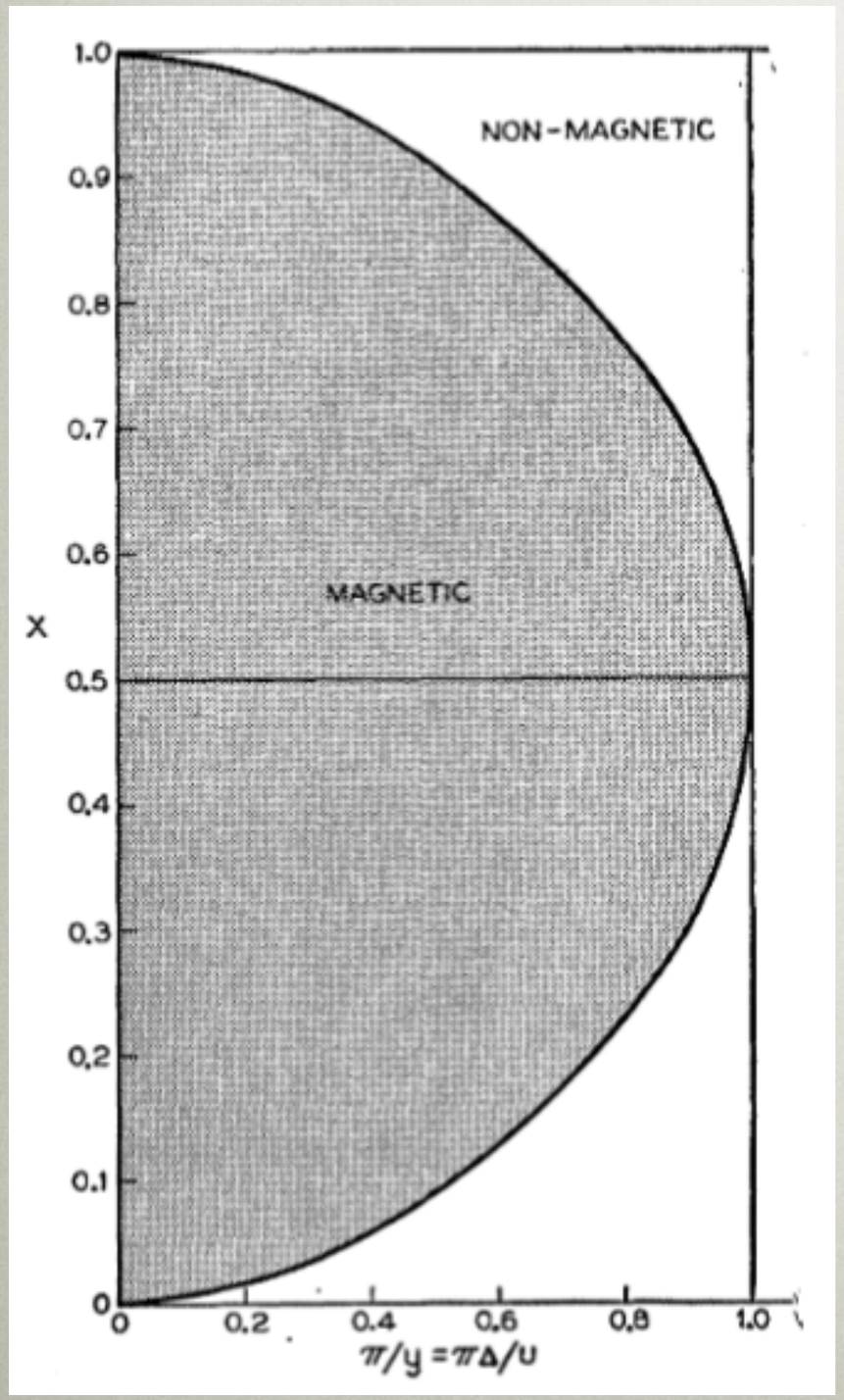
N. V. Prokof'ev et al.,
JETP Lett. **64**, 911 (1996)

P. Werner et al., PRL **97**, 076405 (2006)

K. Haule, PRB **75**, 155113 (2007)

E. Gull et al., RMP **83**, 349 (2011)

Hartree-Fock



$$H = H_0 + H' ,$$

$$H_0 = \sum_{\boldsymbol{k},\sigma} \varepsilon_{\boldsymbol{k}} c^{+}_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma} + \sum_{\sigma} E_{\mathrm{d}} c^{+}_{\mathrm{d}\sigma} c_{\mathrm{d}\sigma} + V \sum_{\boldsymbol{k},\sigma} (c^{+}_{\boldsymbol{k}\sigma} c_{\mathrm{d}\sigma} + c^{+}_{\mathrm{d}\sigma} c_{\boldsymbol{k}\sigma}) - \langle n_{\mathrm{d}} \rangle^2 U ,$$

$$H' = U(c^{+}_{\mathrm{d}\uparrow} c_{\mathrm{d}\uparrow} - \langle n_{\mathrm{d}} \rangle)\,(c^{+}_{\mathrm{d}\downarrow} c_{\mathrm{d}\downarrow} - \langle n_{\mathrm{d}} \rangle) ,$$

$$E_{\mathrm{d}} = \varepsilon_{\mathrm{d}} + \langle n_{\mathrm{d}} \rangle U .$$

requires numerical solution
of a transcendent equation

Anderson 1961
Newns 1969

Perturbation theory (2nd order)

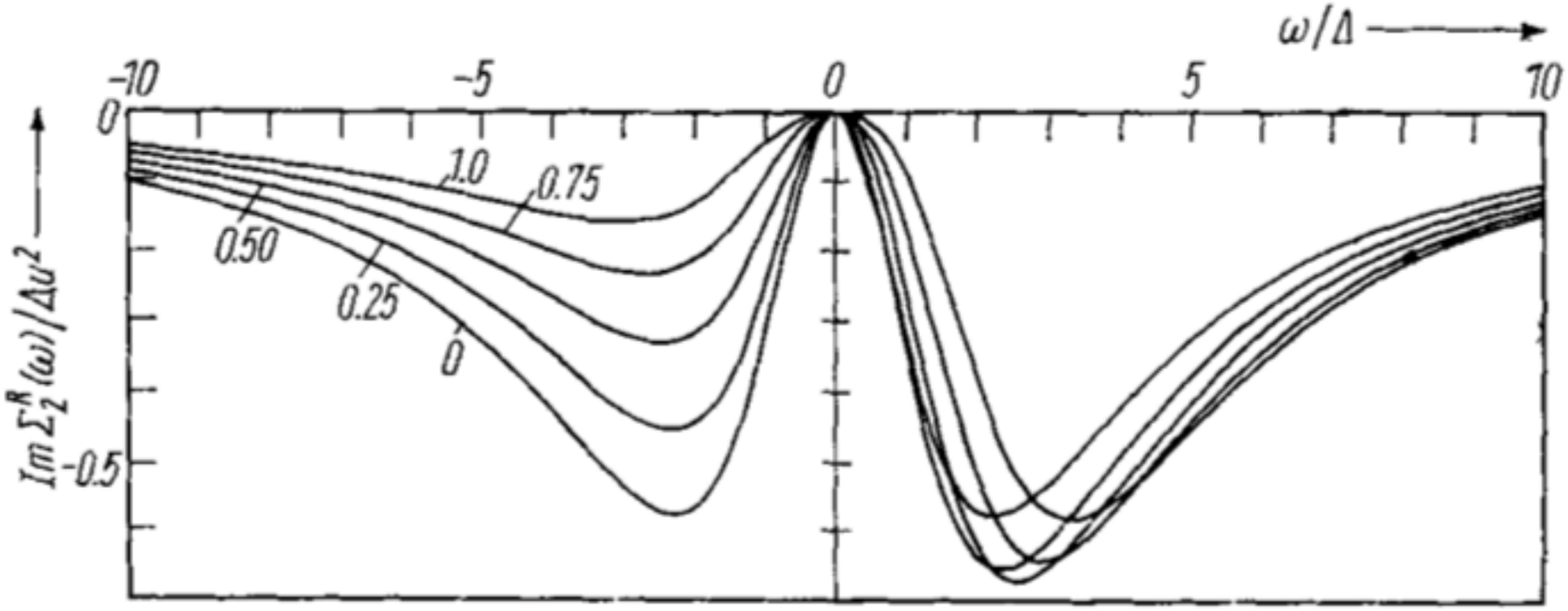
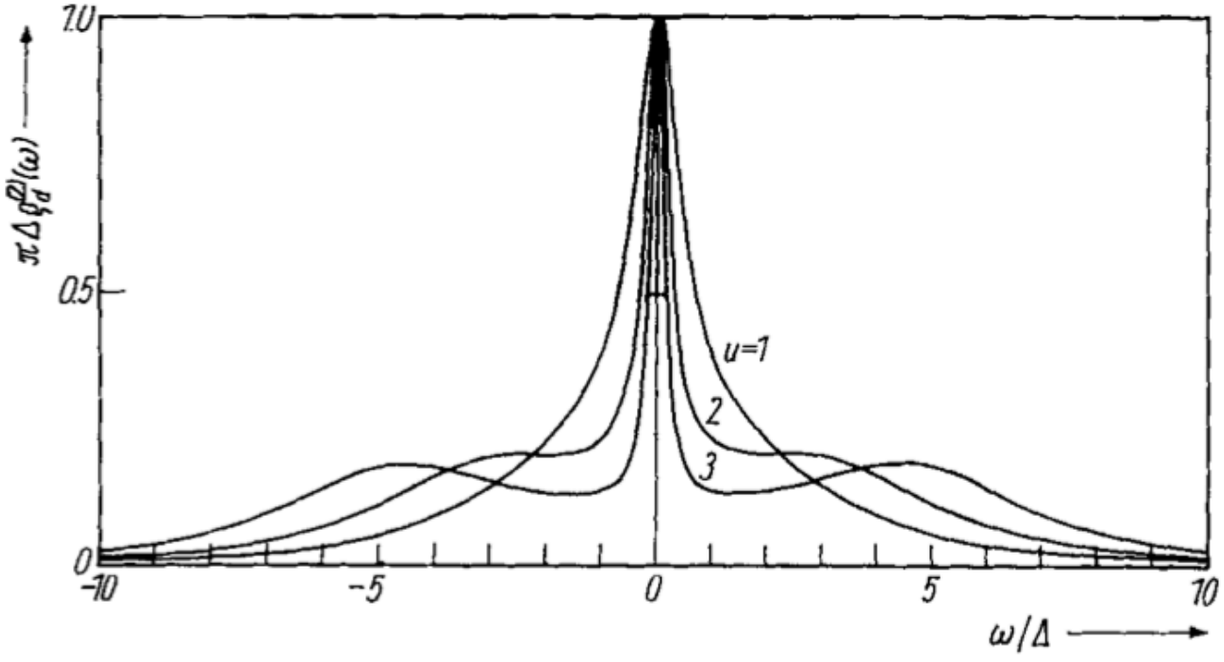


Fig. 2. Imaginary part of $\Sigma_2^{\mathrm{R}}(\omega)$ at $T = 0$ for various values of the asymmetry parameter E_{d}/Δ



Analytical expressions!

Yosida, Yamada

Horvatić, Zlatić, 1980, 1982

Fluctuation-dissipation theorem

$$\langle A(t)B\rangle = -\int_{-\infty}^{\infty} \frac{d\omega}{\pi} e^{-i\omega t} \frac{G''_{AB}(\omega)}{1+\epsilon e^{-\beta\omega}}$$

ε=+1 for fermions

$$\langle AB\rangle = -\int_{0}^{\infty} d\omega \left[-\frac{1}{\pi} G''_{AB}(\omega)\right]$$

at T=0

Caveat: G"(ω) may have a delta peak at ω=0, which NRG will not capture.

Not an issue when calculating with fluctuation parts, A-⟨A⟩.

$$C^{>}_{AB}(t) = \langle A(t)B \rangle$$

$$C^{<}_{AB}(t) = \langle BA(t) \rangle$$

$$C^{>,<}_{AB}(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} C^{>,<}_{AB}(t)$$

$$C^{<}_{AB}(\omega) = e^{-\beta\omega} C^{>}_{AB}(\omega)$$

$$C^{>}_{AB}(\omega) = \sum_{nm} p_n A_{nm} B_{mn} 2\pi\delta(\omega + E_n - E_m)$$

$$C^{<}_{AB}(\omega) = \sum_{nm} p_m B_{mn} A_{nm} 2\pi\delta(\omega + E_n - E_m)$$

$$G''_{AB}(\omega) = -\pi \sum_{nm} p_n A_{nm} B_{mn} \delta(\omega + E_n - E_m)(1 + \epsilon e^{-\beta\omega})$$

$$\langle A(t)B \rangle = -\int_{-\infty}^{\infty} \frac{d\omega}{\pi} e^{-i\omega t} \frac{G''_{AB}(\omega)}{1 + \epsilon e^{-\beta\omega}}$$

Well satisfied in NRG at T=0, at T>0 some issues.

Spectral sum-rules

$$\mu_m = \int_{-\infty}^{\infty} \omega^m A_\sigma(\omega) \mathrm{d}\omega$$

$$\mu_0 = 1 \qquad \mu_m = \left\langle \left\{ [d_\sigma, H]_m , d_\sigma^\dagger \right\} \right\rangle$$

$$[A, B]_1 = [A, B] = AB - BA$$
$$[A, B]_{n+1} = [[A, B]_n, B]$$

"well-known", but first published by S. White, PRB 1991

ALTERNATIVE VERSION

$$\bar{\mu}_m = \int_{-\infty}^{\infty} \omega^m A_\sigma(\omega)/(1+\exp(\beta\omega))\mathrm{d}\omega$$

$$\bar{\mu}_m = \langle d_\sigma^\dagger, [d_\sigma, H] \rangle$$

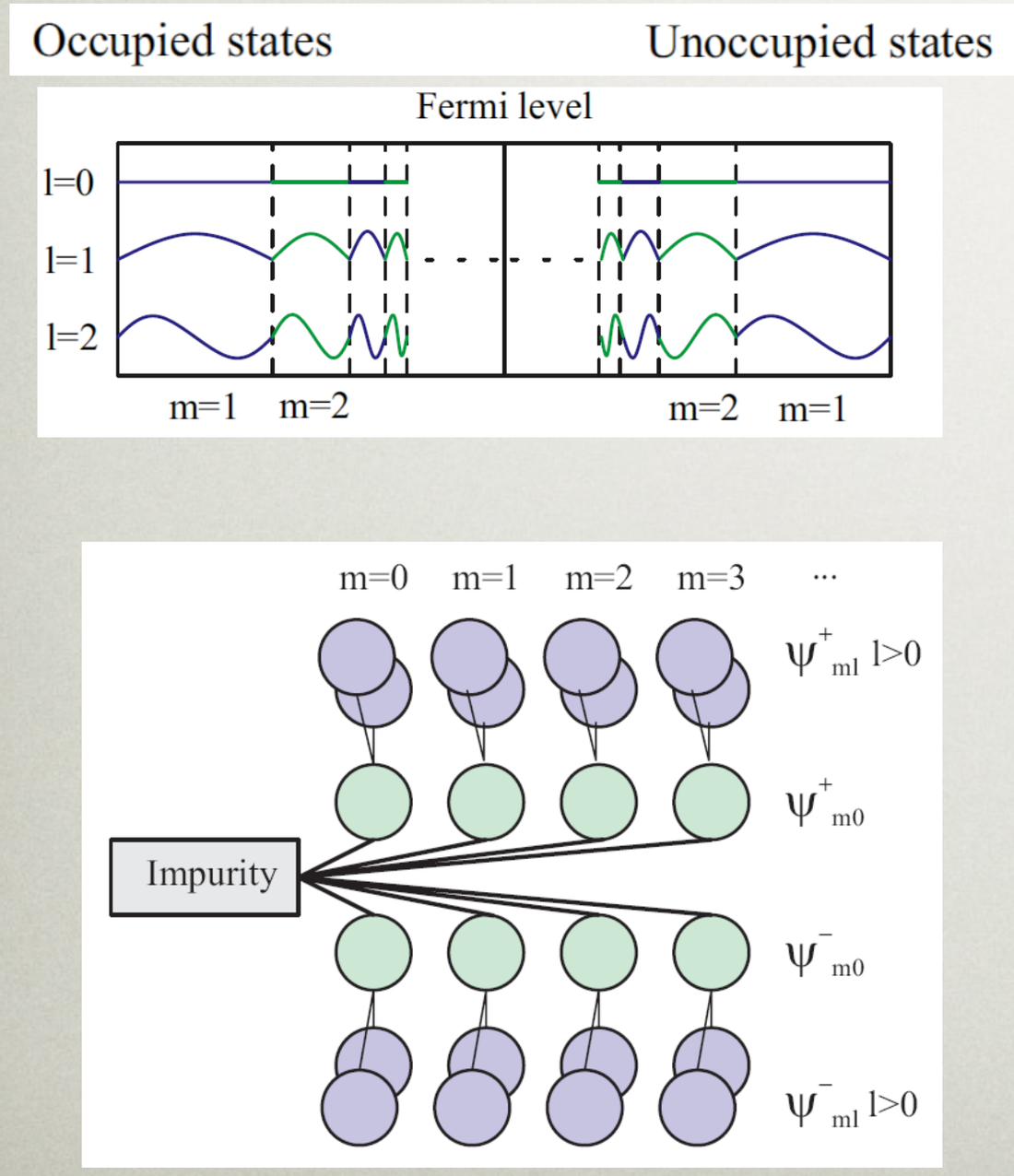
$$\mu_1 = \epsilon + U \langle n_{-\sigma} \rangle$$

$$\mu_2 = V^2 + \epsilon^2 + (U + 2\epsilon)U \langle n_{-\sigma} \rangle$$

$$\begin{aligned}\mu_3 =& \epsilon^3 + 2\epsilon V^2 + U(3\epsilon^2 + 3\epsilon U + U^2 + 4V^2) \langle n_{-\sigma} \rangle \\ & - \frac{UV}{2}\left(4V \langle n_{f,-\sigma} \rangle + (U + 2\epsilon) \left\langle h^{(0)}_{-\sigma} \right\rangle\right) \\ & + t_0 UV \left\langle h^{(1)}_{-\sigma} \right\rangle .\end{aligned}$$

$$\begin{aligned}\mu_4 =& \epsilon^4 + 3\epsilon^2 V^2 + V^4 + U\left(4\epsilon^3 + 6\epsilon^2 U + 4\epsilon U^2 + U^3 + 2(7\epsilon + 4U)V^2\right) \langle n_{-\sigma} \rangle \\ & + \quad UV\left[(U + 2\epsilon)^2 \left\langle h^{(0)}_{-\sigma} \right\rangle + V\left((8\epsilon + 3U) \langle n_{f,-\sigma} \rangle + U \langle g_{-\sigma} \rangle\right)\right] + t_0^2 V^2 + 2t_0 U(U + 2\epsilon) \left\langle h^{(1)}_{-\sigma} \right\rangle\end{aligned}$$

Discretization



We keep only l=0.

These are the “representative states”

First site of the Wilson chain

$$H_{\mathrm{hyb}} = \sum_{k\sigma} \left(V_k c^\dagger_{k\sigma} d_\sigma + \mathrm{h.c.} \right)$$

$$V f^\dagger_{0\sigma} = \sum_{k\sigma} V_k c^\dagger_{k\sigma}$$

$$H_{\mathrm{hyb}} = V f^\dagger_{0\sigma} d_\sigma + \mathrm{H.c.}$$

The f_0 orbital is the “average state” of all “representative states”.

Zero-bandwidth approximation (ZBW)

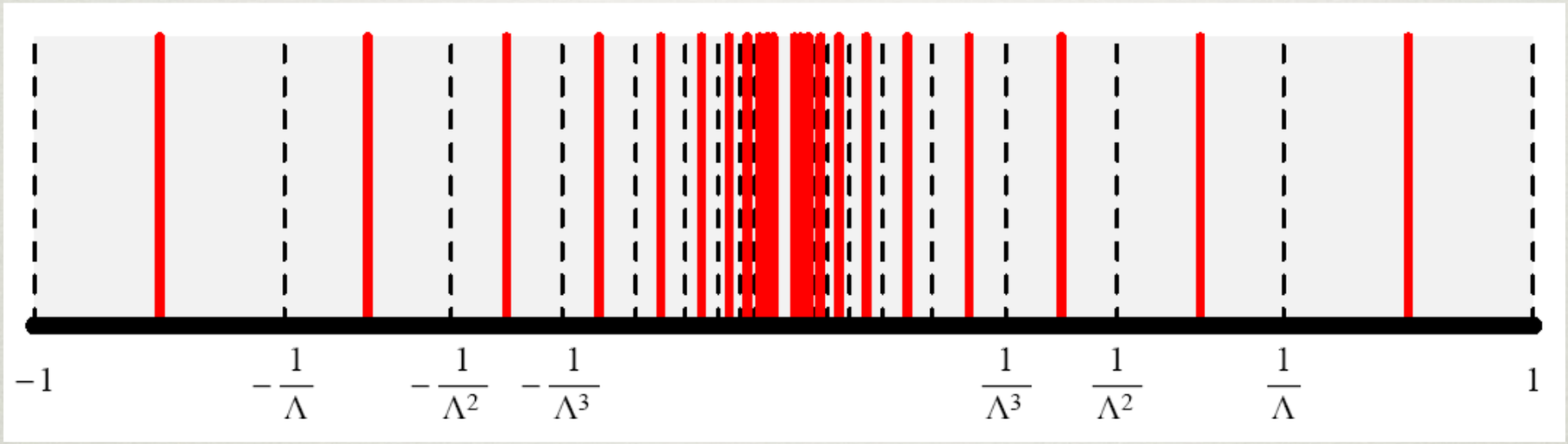
Idea: keep only f_0.

Qualitatively describes the nature of the ground state.

Example: Kondo singlet approximated by an AFM state formed between the impurity orbital and the f_0 orbital.

Exact results for flat band

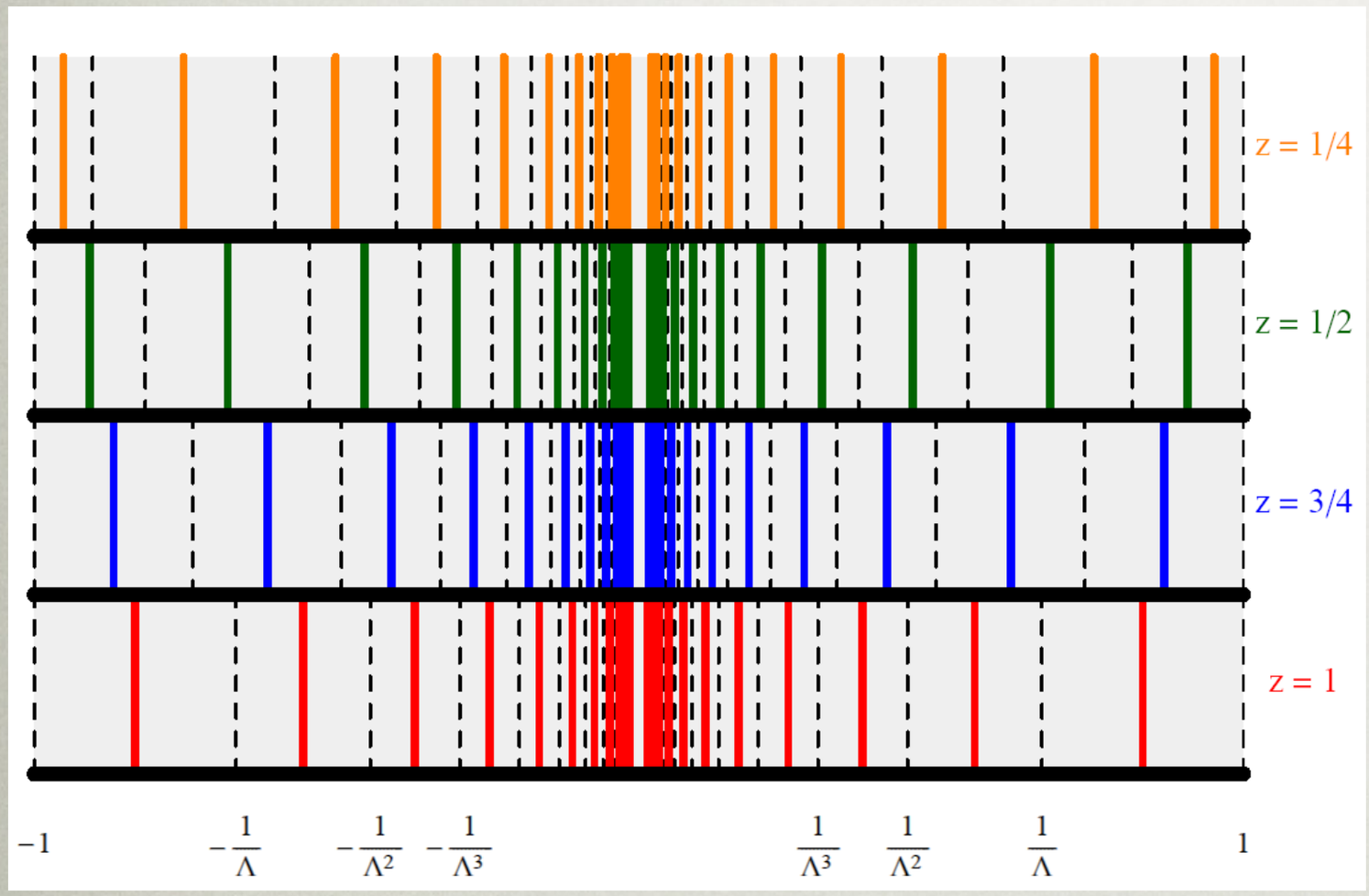
$$\Gamma(\epsilon) = \frac{1}{2D} \quad \text{for} \quad -D < \epsilon < D$$



$$t_i = D\frac{(1+\Lambda^{-1})(1-\Lambda^{-i-1})}{2\sqrt{1-\Lambda^{-2i-1}}\sqrt{1-\Lambda^{-2i-3}}}\Lambda^{-i/2}$$

$$A_\Lambda = \frac{\ln\Lambda}{2}\frac{1+\Lambda^{-1}}{1-\Lambda^{-1}}$$

Z-AVERAGING



$$\epsilon_1^z = D$$

$$\epsilon_j^z = D\Lambda^{2-j-z}$$

$$z \in (0:1]$$

works best for $N_z=2^N$

similar to *twist averaging* over different boundary conditions in finite clusters to reduce the finite-size effects (better k-space sampling)

Frota, Oliveira, PRB 33, 7871 (1986)
Oliveira, Oliveira, PRB 49, 11986 (1994)

Discretization schemes

1) Conventional scheme

$$\mathcal{E}_j^z = \frac{\int_{I_j} \rho(\epsilon)\, \epsilon\, d\epsilon}{\int_{I_j} \rho(\epsilon) d\epsilon}$$

Chen, Jayaprakash, JPCM 7, L491 (1995)
Ingersent, PRB 54, 11936 (1996)
Bulla, Pruschke, Hewson, JPCM 9, 10463 (1997)

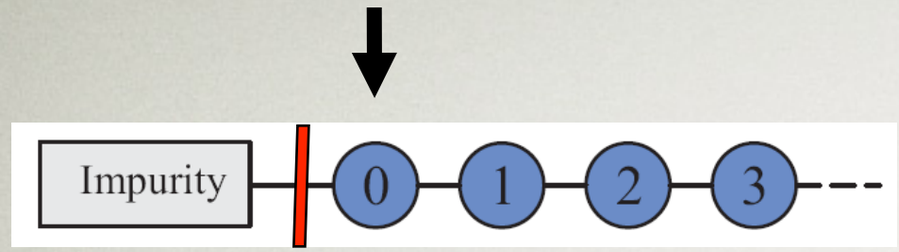
$$A_\Lambda = \frac{1}{2}\frac{1+1/\Lambda}{1-1/\Lambda}\ln\Lambda$$
$$A_\Lambda \approx 1.04 \text{ for } \Lambda = 2$$
$$A_\Lambda \approx 1.16 \text{ for } \Lambda = 4$$

2) Campo-Oliveira scheme

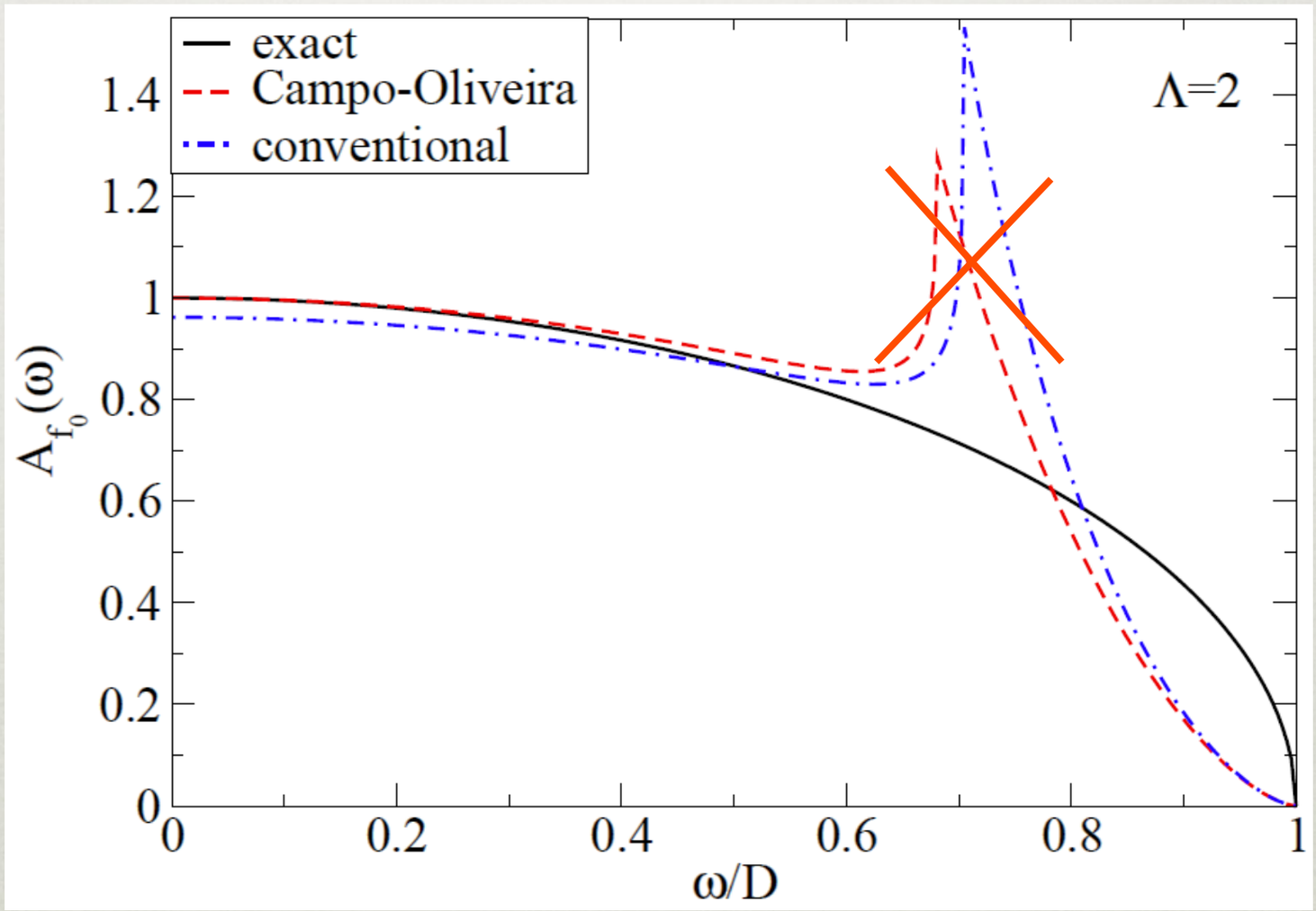
$$\mathcal{E}_j^z = \frac{\int_{I_j} \rho(\epsilon) d\epsilon}{\int_{I_j} \rho(\epsilon)\frac{1}{\epsilon}\, d\epsilon}$$

Campo, Oliveira, PRB 72, 104432 (2005)

$\mathcal{E}_j^z$: representative energy for interval $I_j = [\epsilon_{j+1}^z : \epsilon_j^z]$



$$\rho(\omega) = \rho_0 \sqrt{1 - \left(\frac{\omega}{D}\right)^2}$$



Spectral function of the first site of the Wilson chain

Flat band: $$A_{f_0}(\omega) = \frac{\epsilon_j^z - \epsilon_{j+1}^z}{2D|d\mathcal{E}_j^z/dz|} \qquad \mathcal{E}_j^z = \omega$$

Campo, Oliveira, PRB 72, 104432 (2005)

Generally: $$A_{f_0}(\omega) = \frac{\int_{I_j} \rho(\epsilon)\mathrm{d}\epsilon}{|d\mathcal{E}_j^z/dz|}$$

Can we do better?

Yes! We demand $A_{f_0}(\omega) = \rho(\omega)$

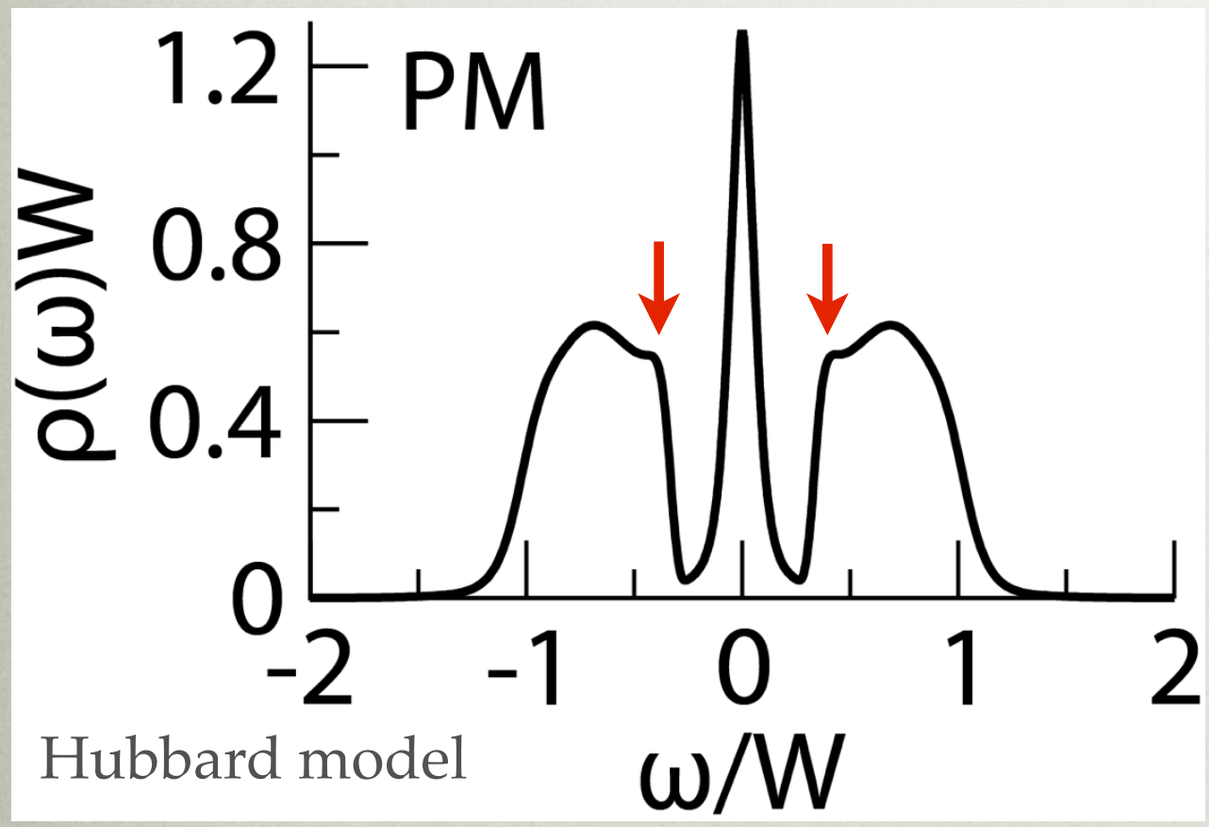
$$\frac{\int_{I_j} \rho(\epsilon) d\epsilon}{|d\mathcal{E}_j^z / dz|} = \rho(\omega)$$

$$x = j + z \qquad\qquad \mathcal{E}(x) = D f(x) \Lambda^{2-x}$$

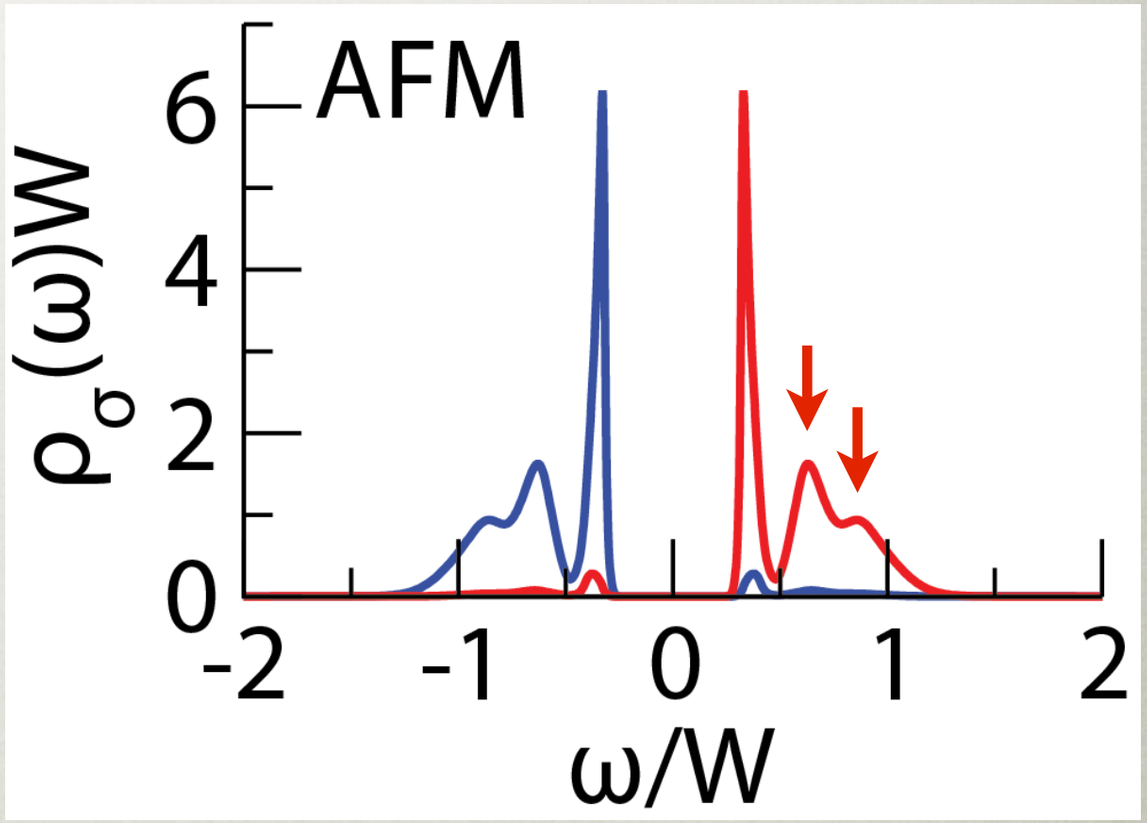
$$\frac{df(x)}{dx} = \ln \Lambda \, f(x) - \frac{\int_{\epsilon(x+1)}^{\epsilon(x)} \rho(\omega) d\omega}{\Lambda^{2-x} \rho[\mathcal{E}(x)]}$$

R. Žitko, Th. Pruschke, PRB 79, 085106 (2009)
R. Žitko, Comput. Phys. Comm. 180, 1271 (2009)

High-resolution spectra



Hubbard model



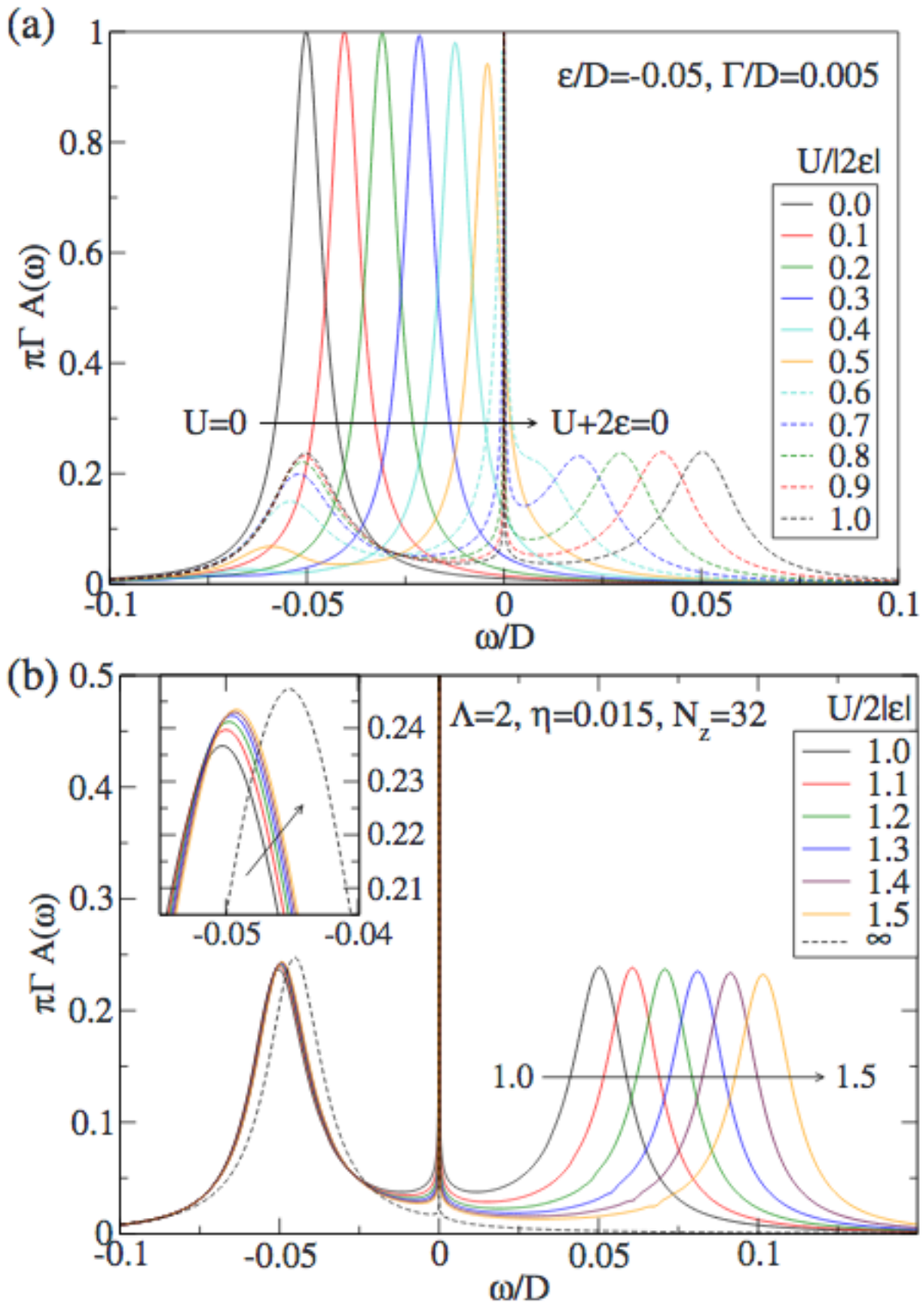


FIG. 14. (Color online) Spectral functions of the Anderson model for increasing U.

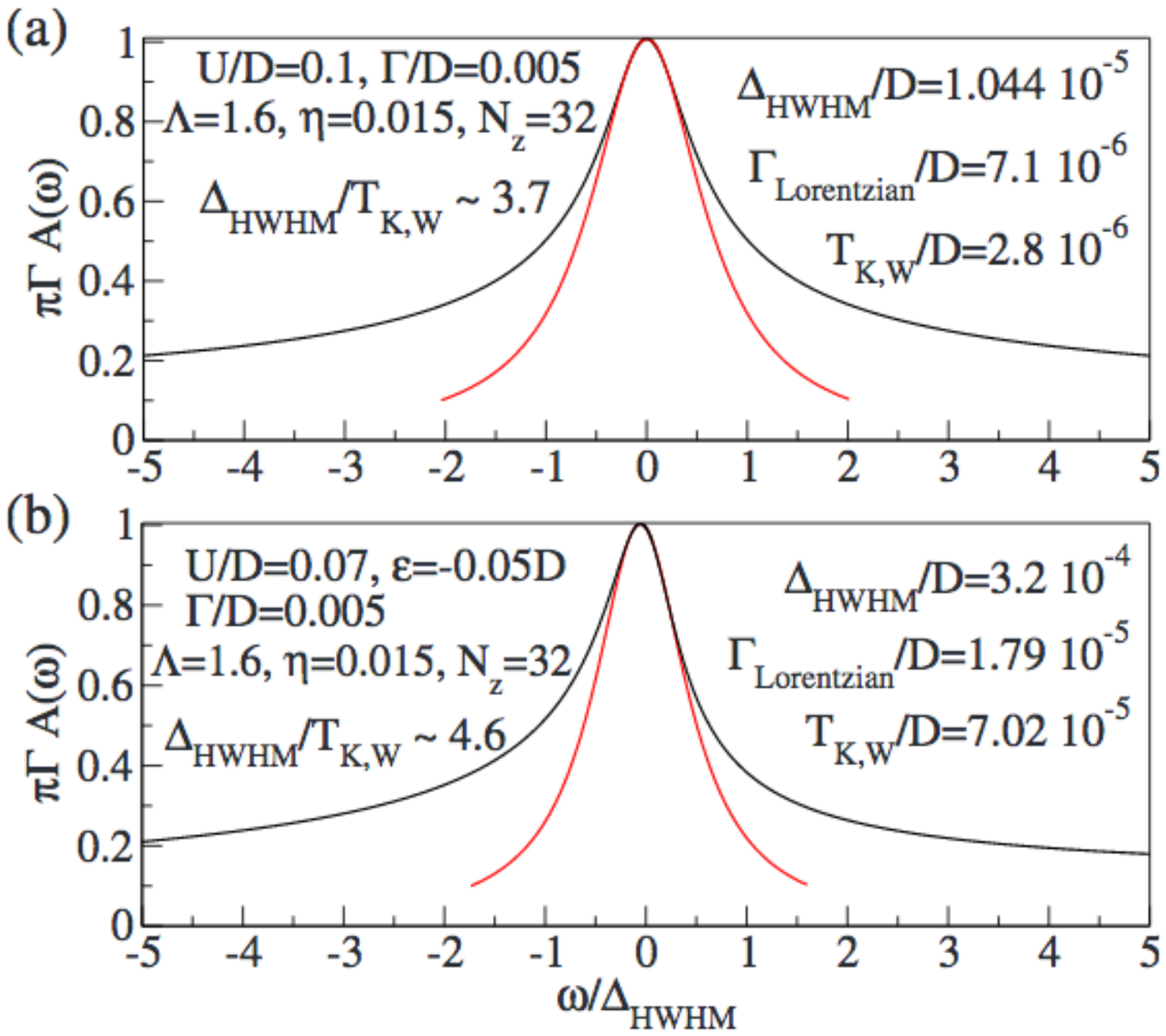
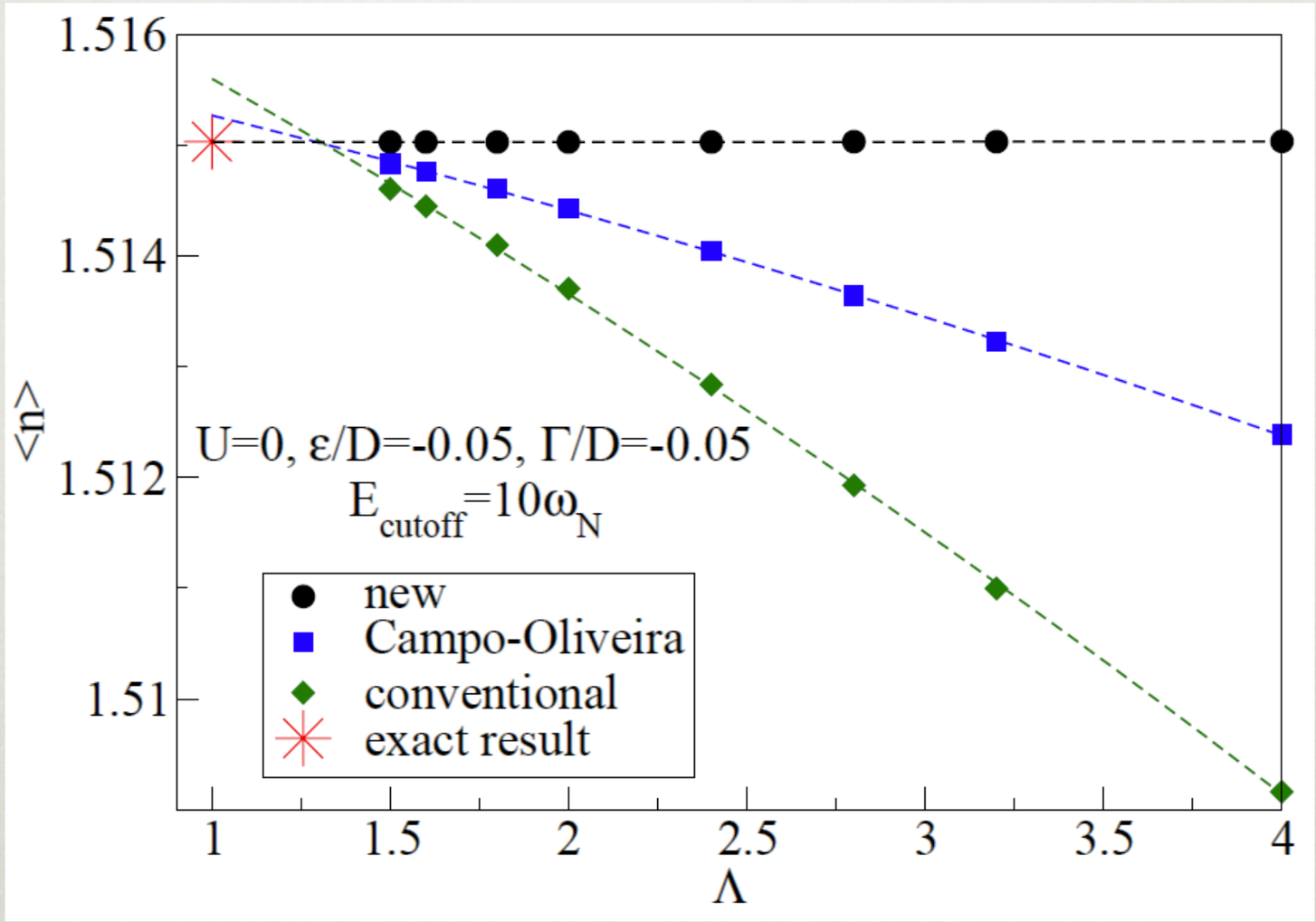
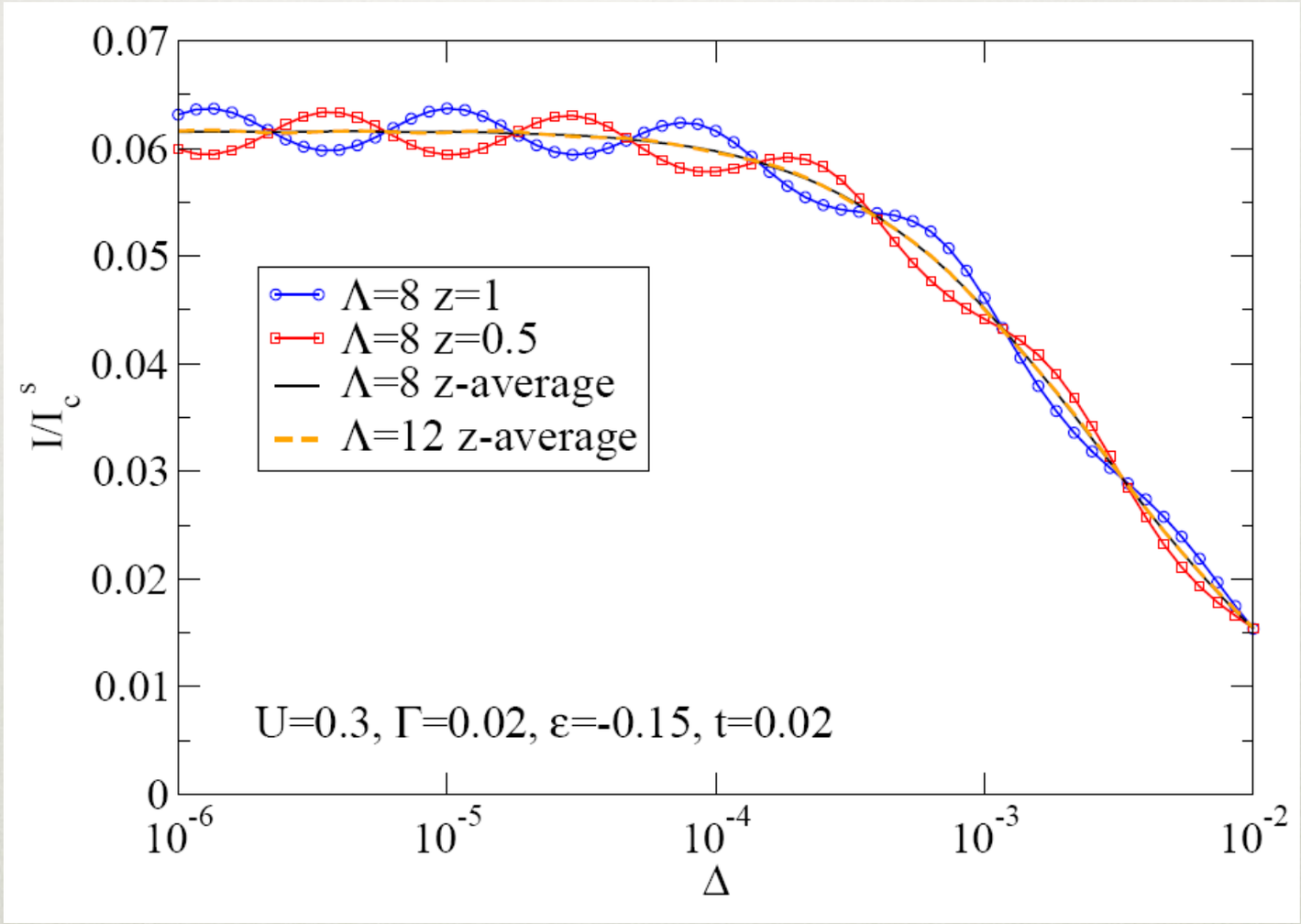
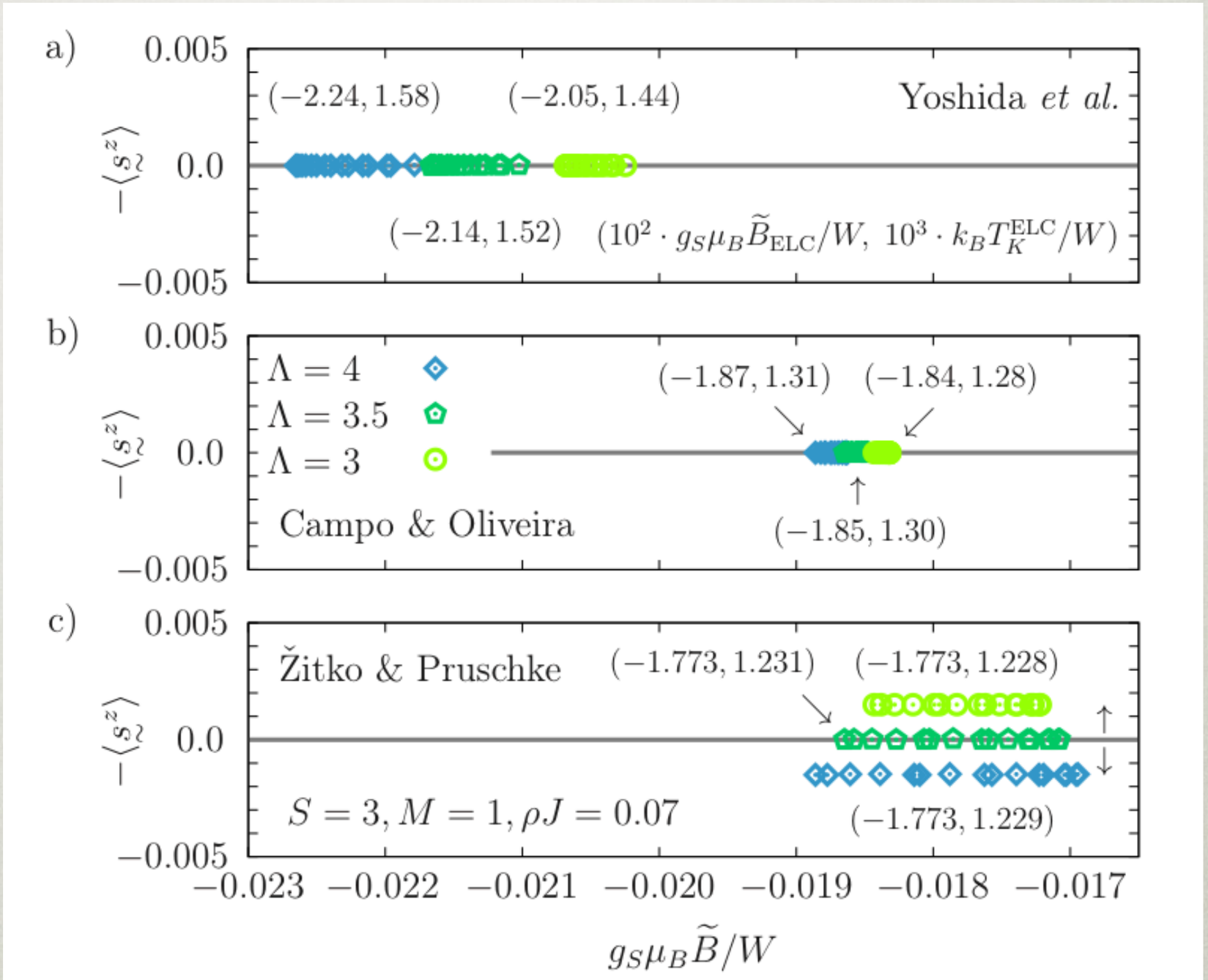


FIG. 15. (Color online) Close-up on the Kondo resonance of (a) symmetric and (b) asymmetric Anderson impurity model and a fit to a Lorentzian (red/gray curve) in the Fermi-liquid regime for $\omega \ll T_K$.


1.516
1.514
1.512
1.51
⟨n⟩
U=0, ε/D=-0.05, Γ/D=-0.05
E_cutoff=10ω_N
new
Campo-Oliveira
conventional
exact result
1
1.5
2
2.5
3
3.5
4
Λ


0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
I/I_c^s
Λ=8 z=1
Λ=8 z=0.5
Λ=8 z-average
Λ=12 z-average
U=0.3, Γ=0.02, ε=-0.15, t=0.02
10^-6
10^-5
10^-4
10^-3
10^-2
Δ



Höck, Schnack, PRB 2013

There are several schemes for logarithmically discretizing the continuum of the bath degrees of freedom:

- `Y` - the scheme proposed in the paper by Yoshida, Whitaker, Oliveira, Phys. Rev. B 41, 9403 (1990).
- `C` - the scheme proposed in the paper by Campo, Oliveira, Phys. Rev. B 72, 104432 (2005). It corrects the systematic underestimation of the bath density of states of scheme `Y`.
- `Z` - the scheme proposed in the paper by Zitko, Pruschke, Phys. Rev. B 79, 085106 (2009). It corrects the systematic error in the first energy interval of scheme `C`.

Recommendation: **`discretization=Z`**

Hubbard model

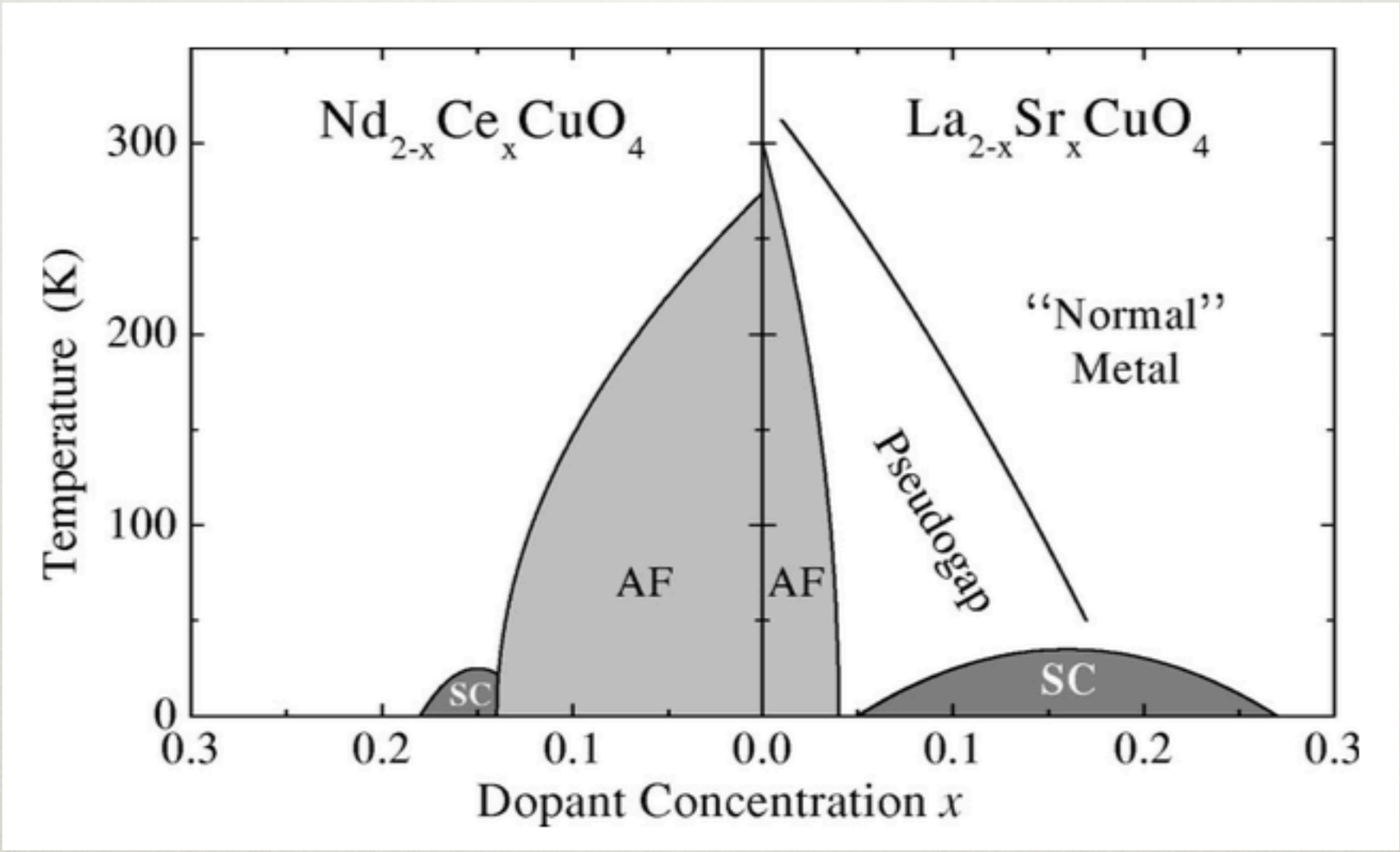
$$H = -t \sum_{\langle i,j \rangle,\sigma} \left(c^{\dagger}_{i\sigma} c_{j\sigma} + \text{H.c.} \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

t-J model:

$$H = -t \sum_{\langle i,j \rangle,\sigma} \left(\tilde{c}^{\dagger}_{i\sigma} \tilde{c}_{j\sigma} + \text{H.c.} \right) + J \sum_{\langle i,j \rangle} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{n_i n_j}{4} \right)$$

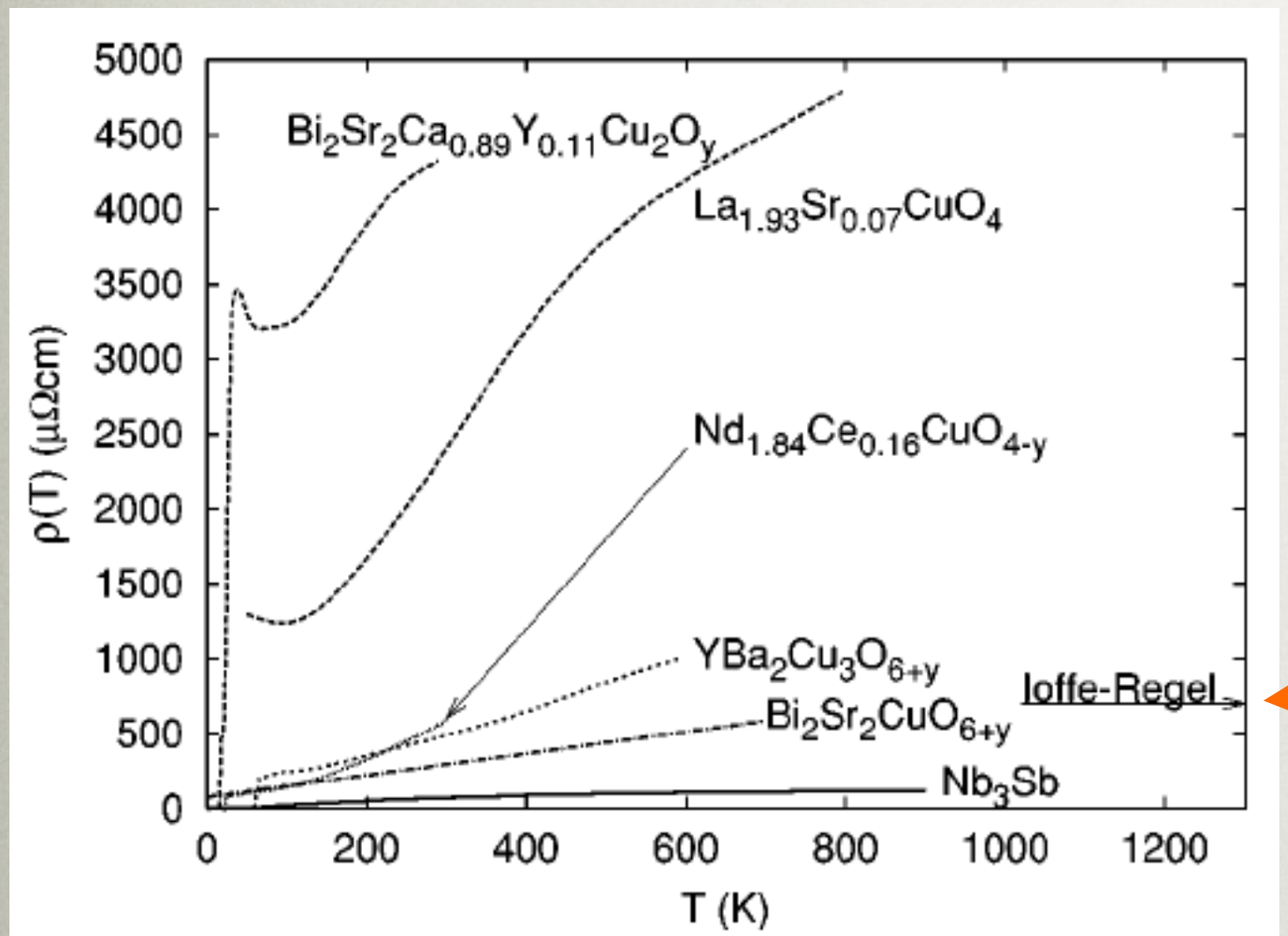
$$\tilde{c}_{i\sigma} = c_{i\sigma}(1 - n_{i\bar{\sigma}}) \qquad J = \frac{4t^2}{U}$$

What are the properties of the "normal" metal?



hole doped case

Cuprates are bad metals



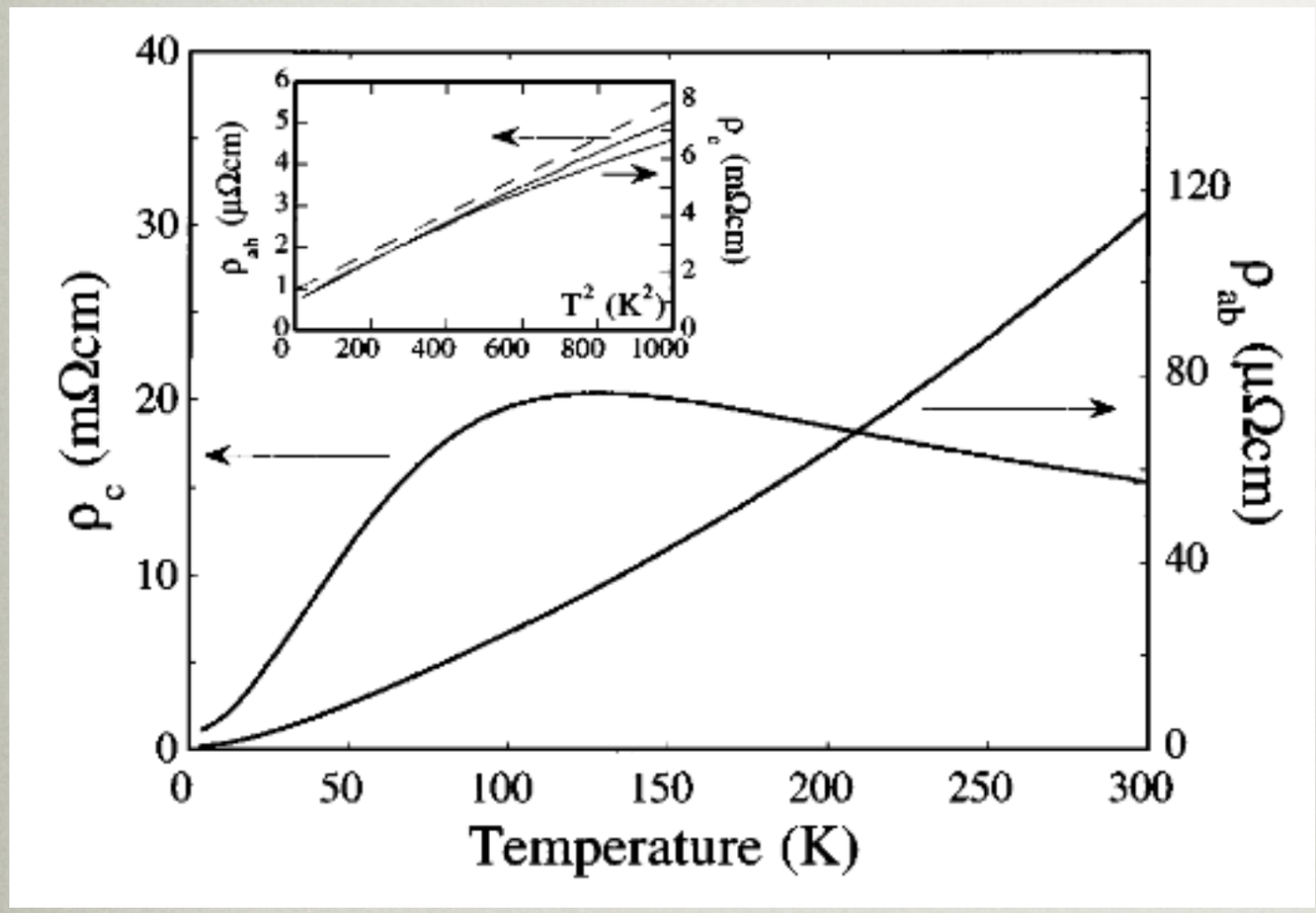
Mott-Ioffe-Regel limit:

mean-free-path shorter than the interatomic distance

BAD METALS: materials where the transport cannot be described using the concept of coherent quasiparticles

other bad metals: ruthenates, organics, alkali doped fullerides

Do bad metals turn good at low temperatures?



Sr_2RuO_4

Hussey et al., Phys. Rev. B (1998)

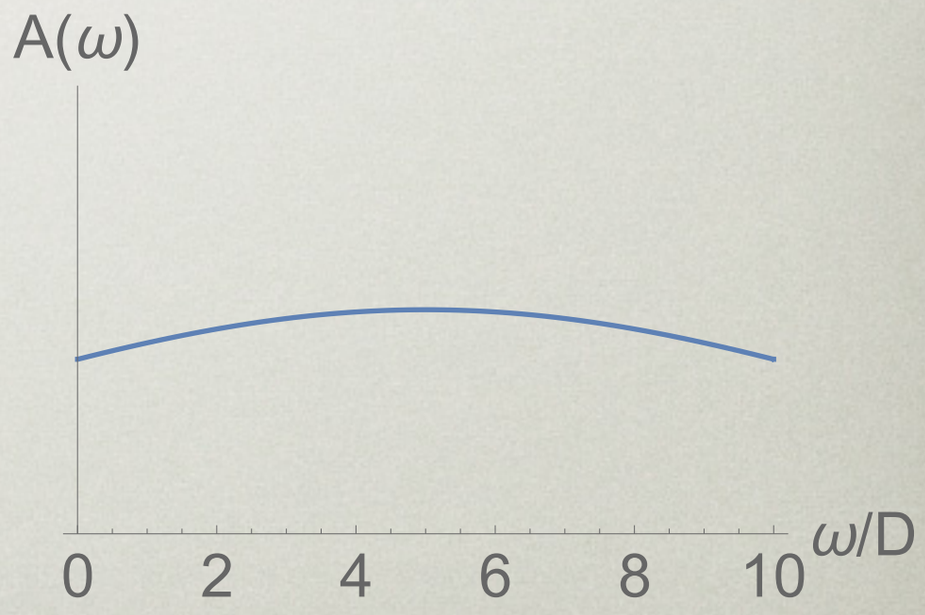
Are there quasiparticles? At what T do they disappear?
What happens after the Drude picture breaks down?

What happens at very high T?

What does the density of states (DOS) look like at infinite temperature?

$$T \to \infty \text{ such that } U \gg T \text{ implying } U = \infty$$

atomic-like?



very diffuse?

Dynamical mean field theory (DMFT)

1) local dynamics: exact calculation!
2) non-local correlations: static mean-field approximation

assumption:

$$\Sigma(k,\omega) \to \Sigma(\omega) \qquad \text{or} \qquad \Sigma_{i,j}(\omega) \to \delta_{ij}\Sigma(\omega)$$

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

$$G_{\rm loc}(z) = \frac{1}{N}\sum_{\mathbf{k}} \frac{1}{z + \mu - \epsilon_{\mathbf{k}} - \Sigma(z)} = \int \frac{\rho_0(\epsilon)\,{\rm d}\epsilon}{[z + \mu - \Sigma(z)] - \epsilon} = G_0[z + \mu - \Sigma(z)]$$

$$\Delta(z) = z + \mu - \left[G_{\rm loc}^{-1}(z) + \Sigma(z)\right]$$

A. Georges et al., Rev. Mod. Phys. (1996)

DMFT:
Conductivity for d=∞

No vertex corrections, just the "zero-th order bubble":

$$\sigma = 2\pi D\sigma_0 \int d\omega \int d\epsilon \left(-\frac{\partial f}{\partial \omega}\right) \phi(\epsilon) A^2(\epsilon,\omega)$$

$\sigma_0 = \frac{e^2}{\hbar}\frac{\Phi(0)}{D}$ Mott-Ioffe-Regel conductivity

$$\Phi(\epsilon) = \sum_{\mathbf{k}} \left(\frac{\mathrm{d}\epsilon_{\mathbf{k}}}{\mathrm{d}k_x}\right)^2 \delta(\epsilon - \epsilon_{\mathbf{k}}) \qquad \phi(\epsilon) = \Phi(\epsilon)/\Phi(0)$$

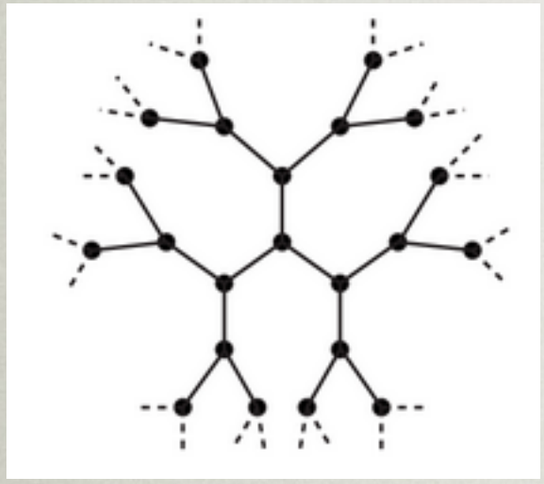
$$A(\epsilon,\omega) = \mathrm{Im}\frac{1}{\omega - \epsilon - \Sigma(\omega)}$$

computed within the dynamical mean-field theory (DMFT) approach

Metzner, Vollhardt, PRL **62**, 324 (1989)
Georges, Kotliar, Krauth, Rozenberg, RMP **68**, 13 (2006)
Khurana, PRL **64**, 1990 (1990)

Case study and tools

single-band Hubbard model, semicircular DOS (Bethe lattice)



$$t \to t^*/\sqrt{2d}$$

$$\rho(\epsilon) = \frac{2}{\pi}\sqrt{1-\epsilon^2}$$ for half-bandwidth D=1

$$\Phi_{xx}(\epsilon) = \frac{1}{3d}(D^2-\epsilon^2)\rho(\epsilon)$$

in typical material D=1eV=11600K

DMFT equations solved with accurate impurity solvers:
- continuous-time quantum Monte Carlo (TRIQS, O. Parcollet, M. Ferrero: http://ipht.cea.fr/triqs), Padé analytical continuation
- numerical renormalization group (NRG Ljubljana, RŽ: http://nrgljubljana.ijs.si/)

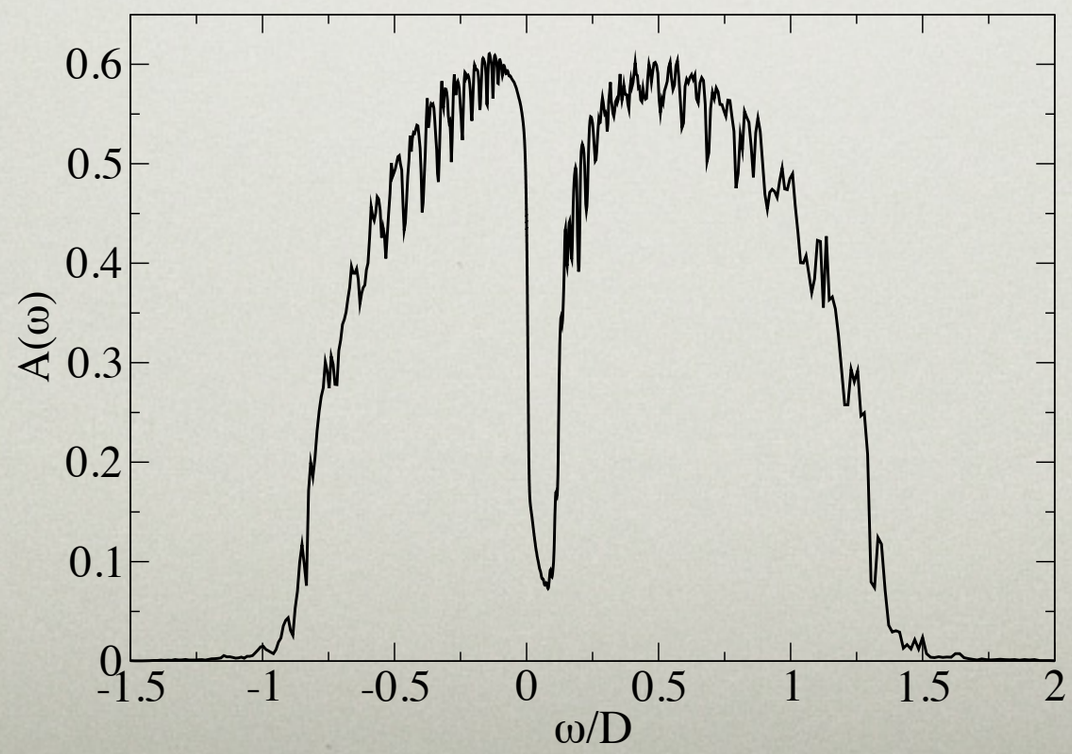
converged and compatible results using both techniques

NRG in the limit of very high temperatures

Turns out, it works!

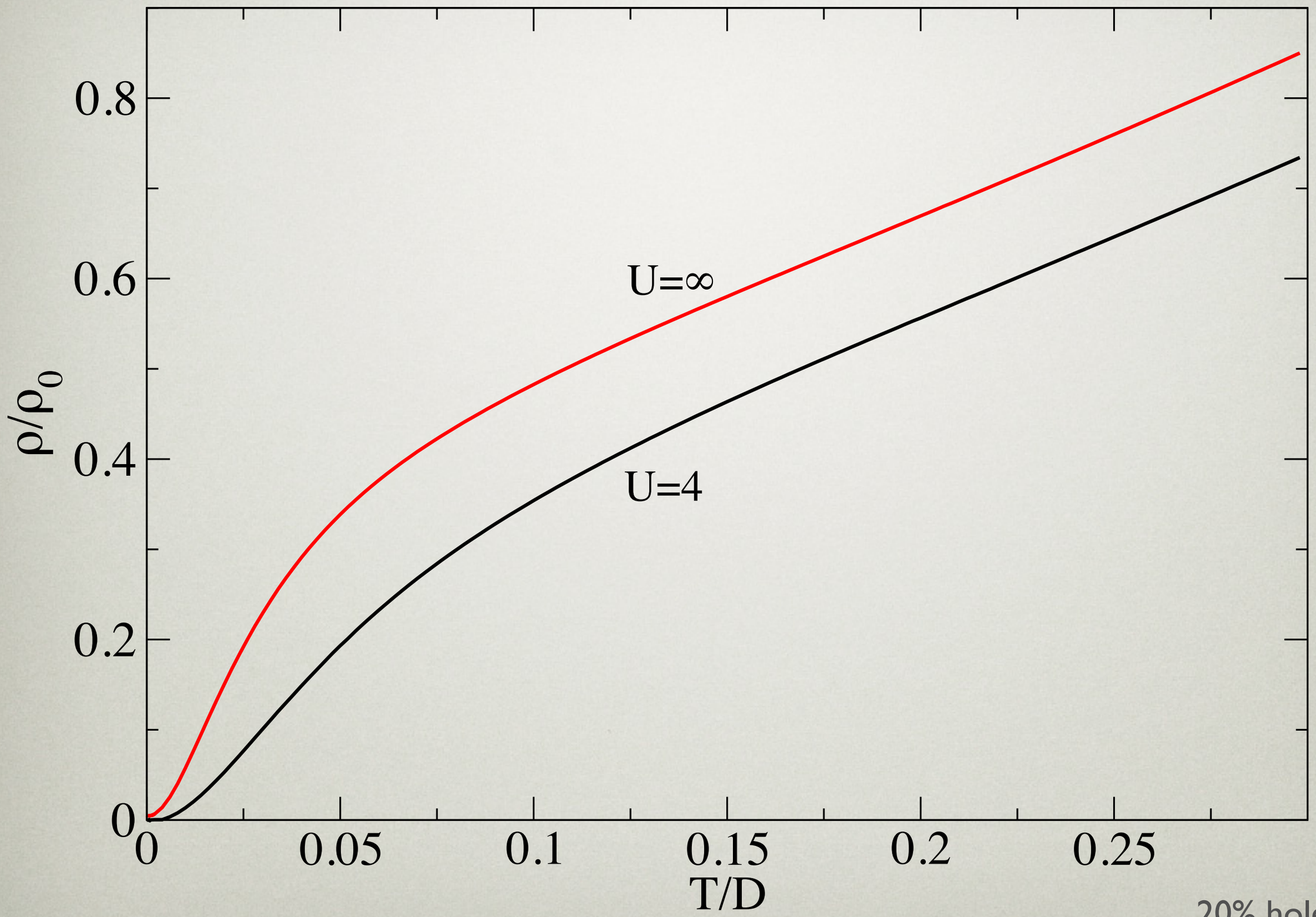
Recipe:

- Gaussian broadening with constant kernel width γ
- reduce γ until integrated quantities are converged (overbroadening → overestimated ρ)



ρ_0 = Mott-Ioffe-Regel resistivity

D = half-bandwidth (also used as the energy unit)

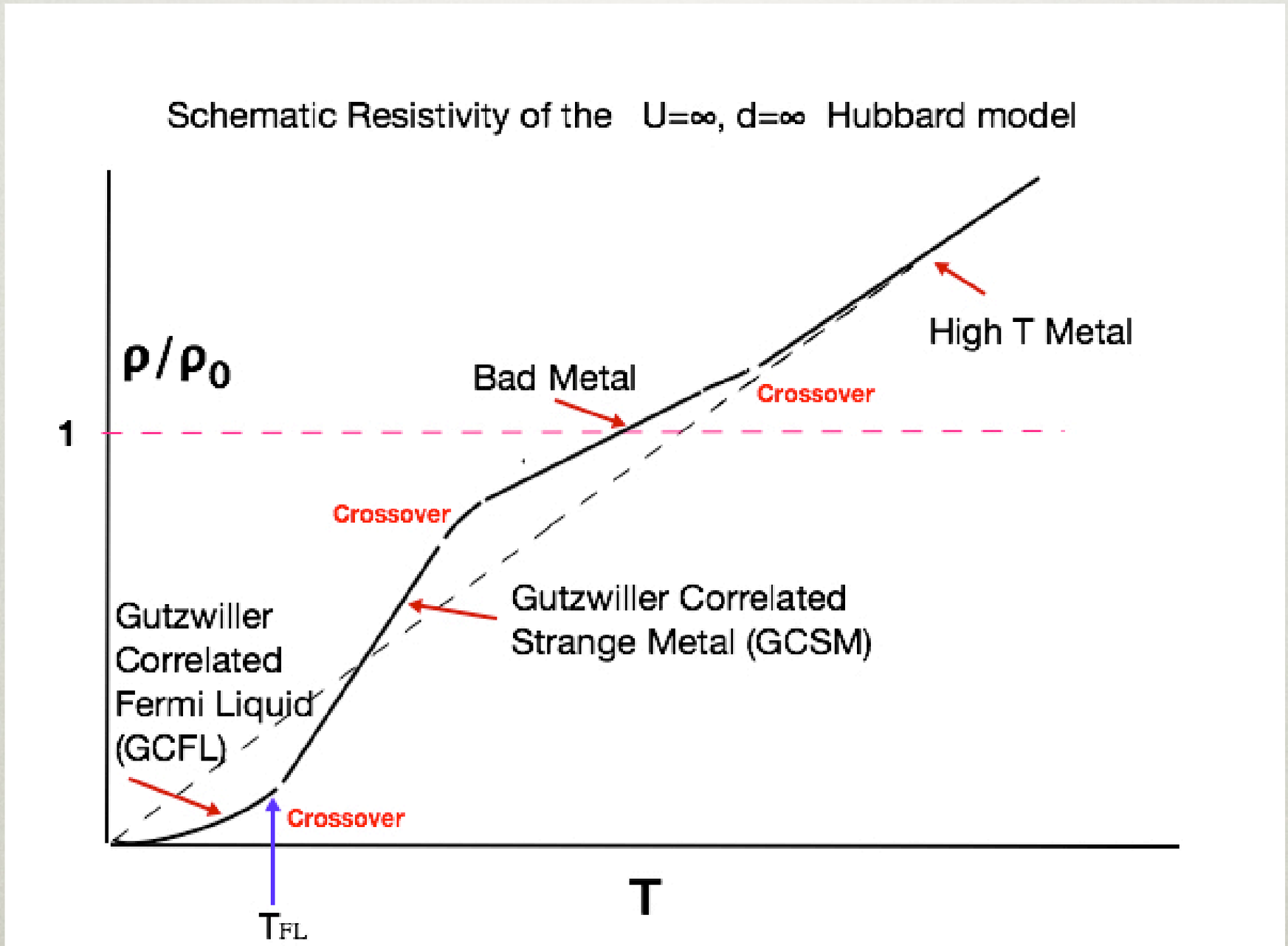


20% hole doping

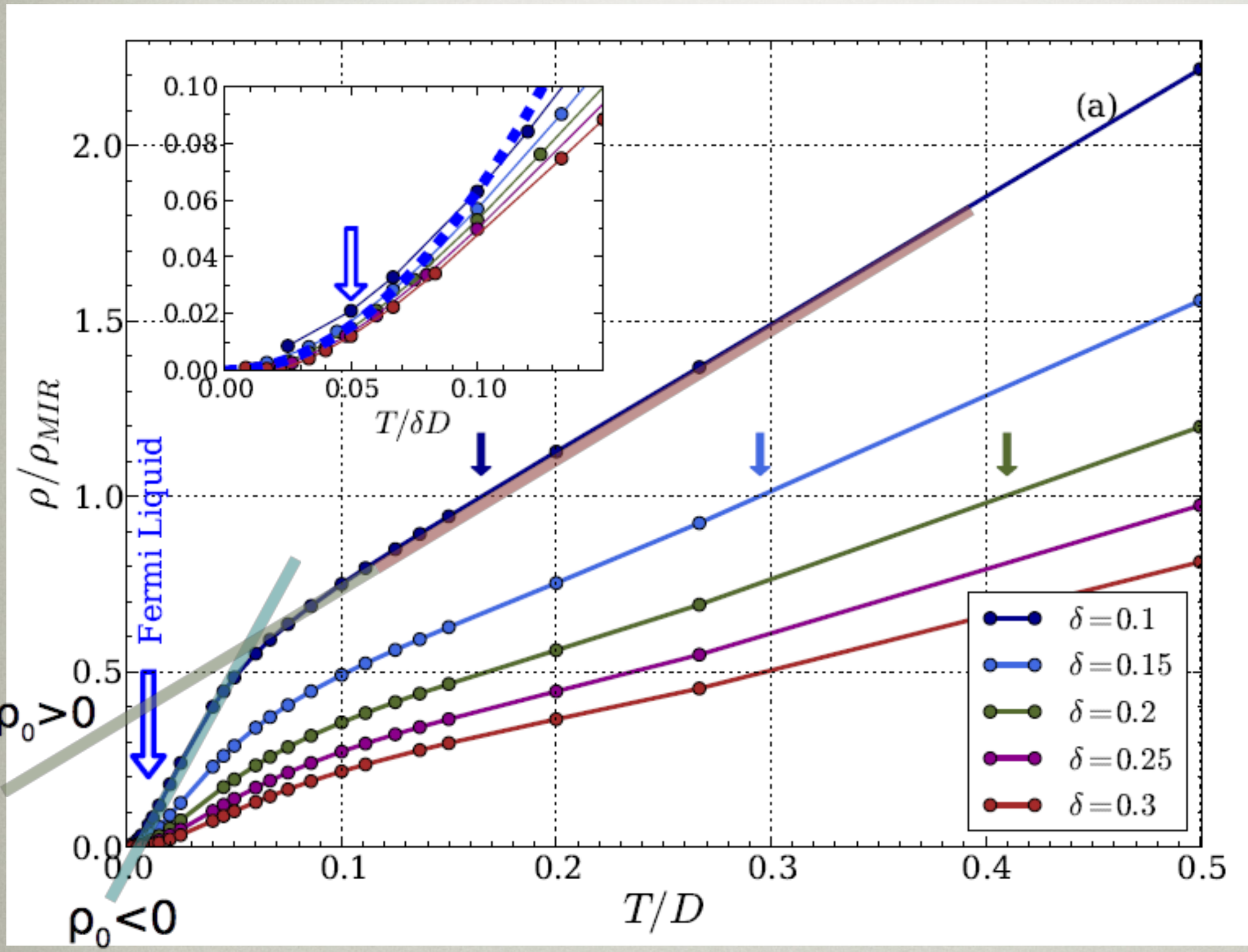
n=0.8

DMFT(NRG) calculation

Overview:
Transport in Hubbard model



$$1/\rho_{\mathrm{MIR}} = \frac{e^2}{\hbar}\frac{\Phi(0)}{D}$$



several regimes:

FL: $\rho \sim T^2, T<T_{FL}$

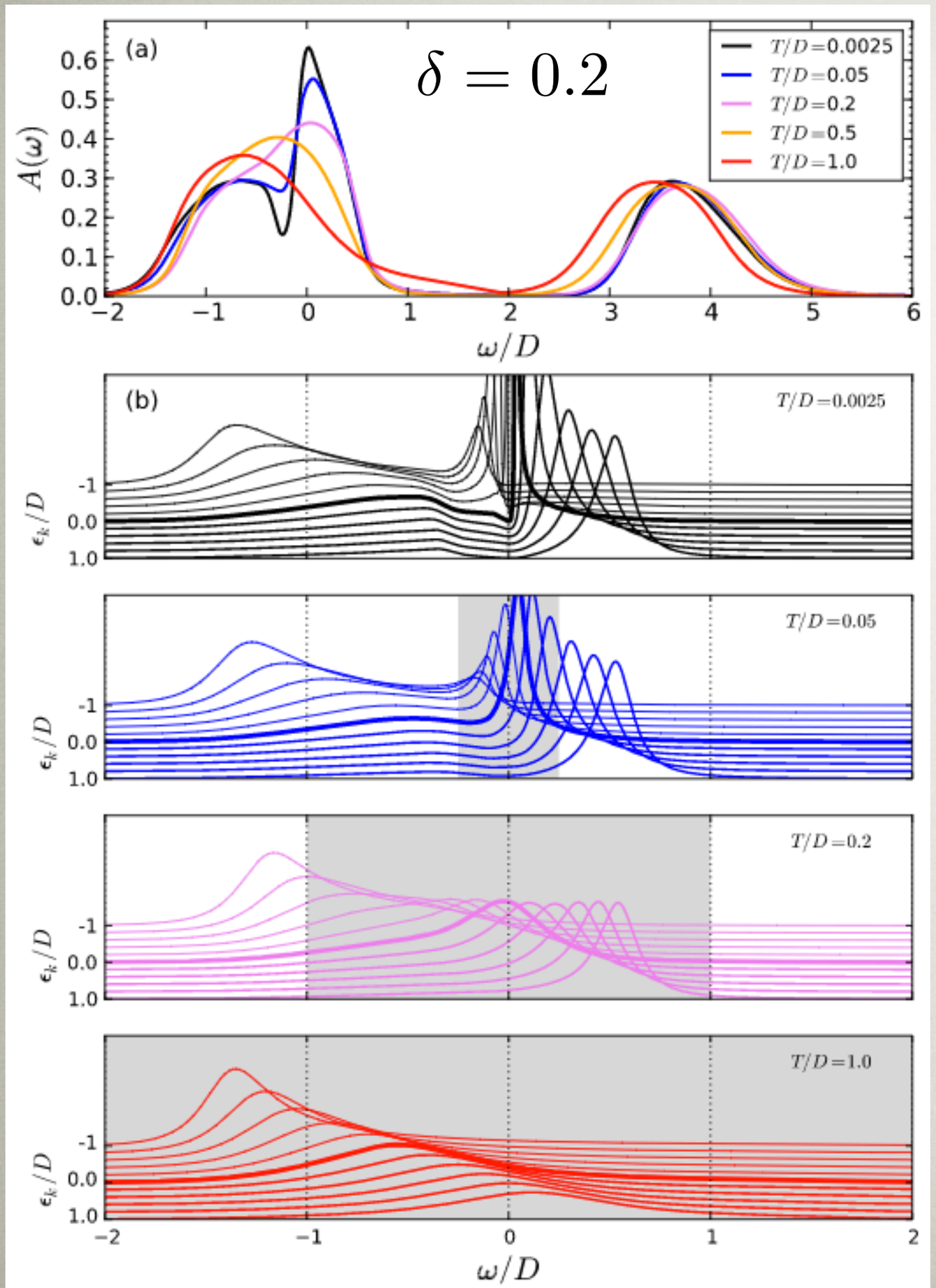
$\rho \sim T$ with $\rho_0<0$

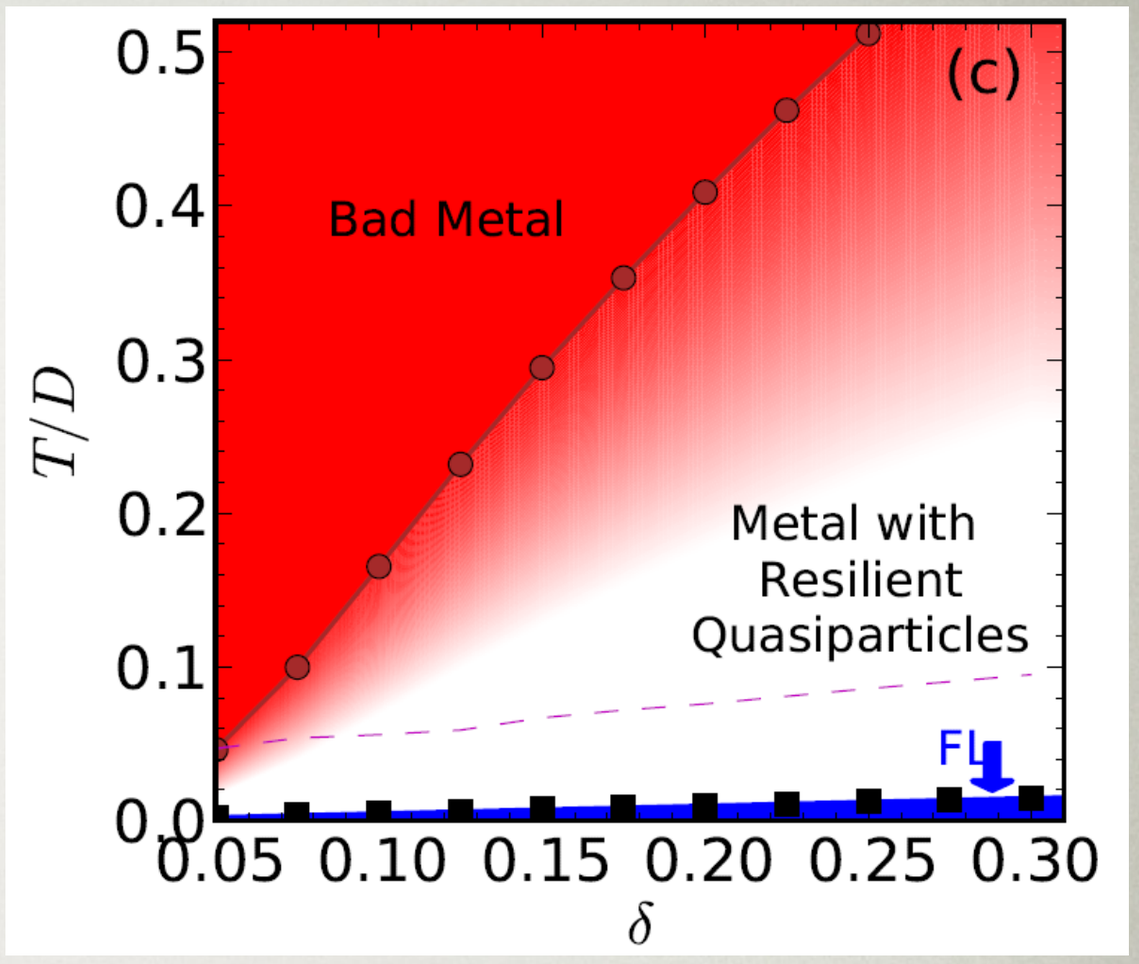
$\rho \sim T$ with $\rho_0>0$

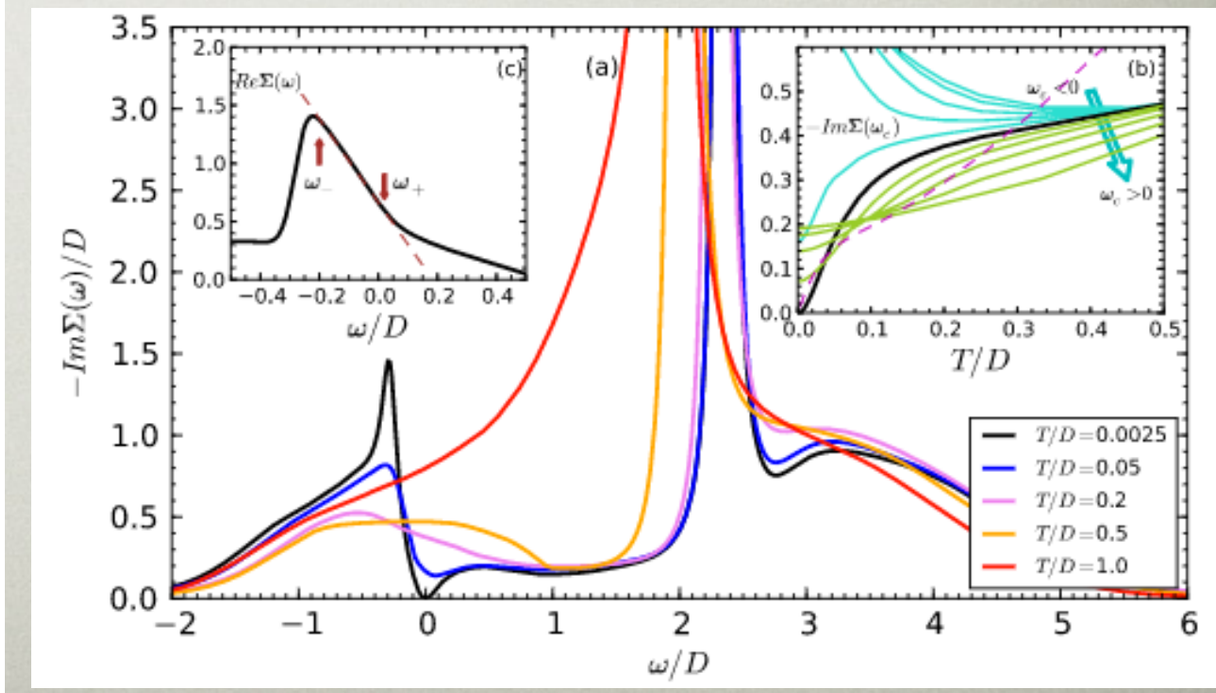
hole doping:

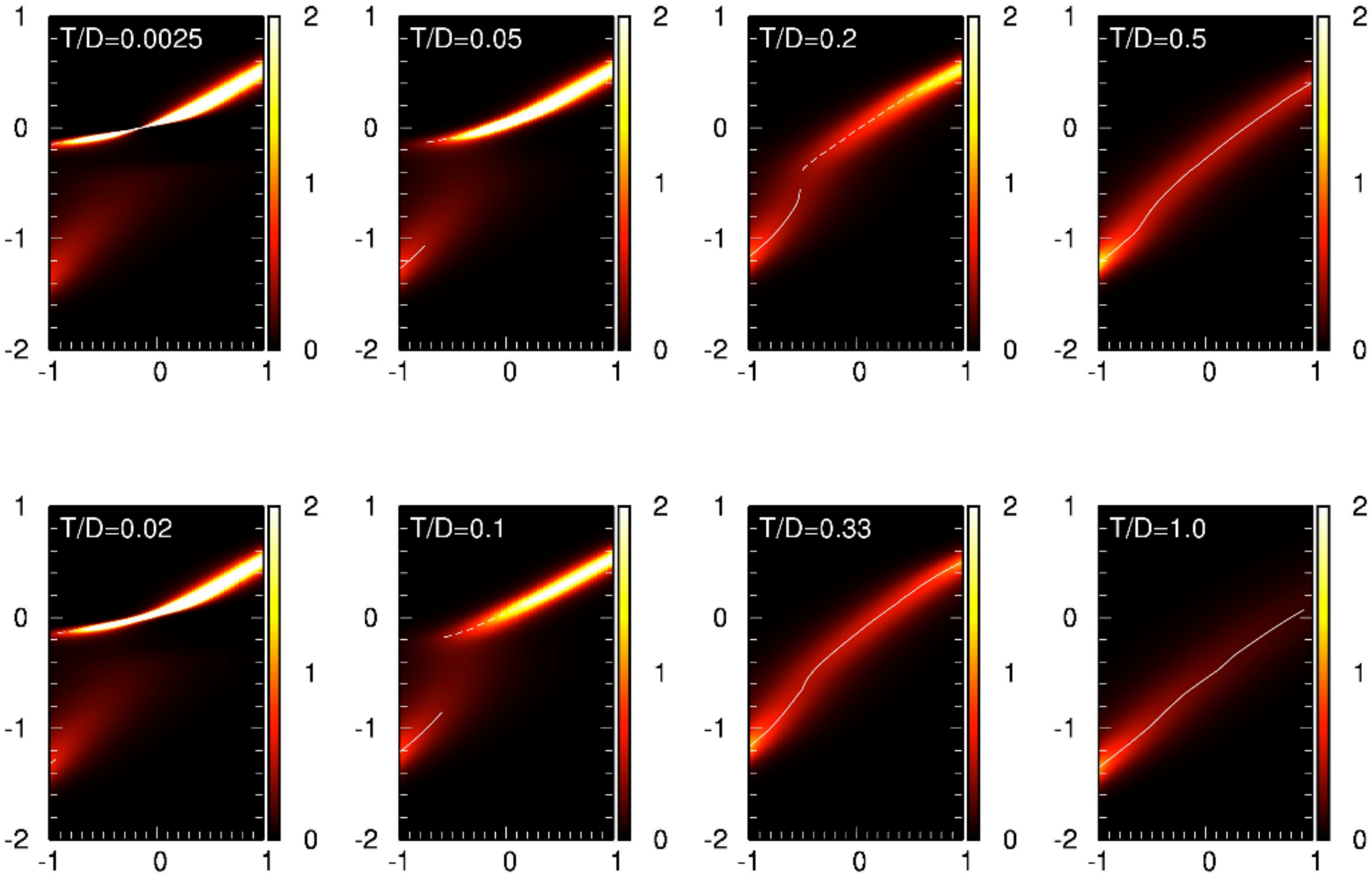
$$\delta = 1 - n$$

$$T_{\mathrm{FL}} \approx 0.05\delta D \qquad T_{\mathrm{MIR}} \sim 2\delta D$$


(a)
$\delta = 0.2$
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


(c)
Bad Metal
Metal with
Resilient
Quasiparticles
FL
T/D
δ


(a)
(b)
(c)
$-Im\Sigma(\omega)/D$
ω/D
$Re\Sigma(\omega)$
ω_-
ω_+
$-Im\Sigma(\omega_c)$
$\omega_c<0$
$\omega_c>0$
T/D
T/D=0.0025
T/D=0.05
T/D=0.2
T/D=0.5
T/D=1.0

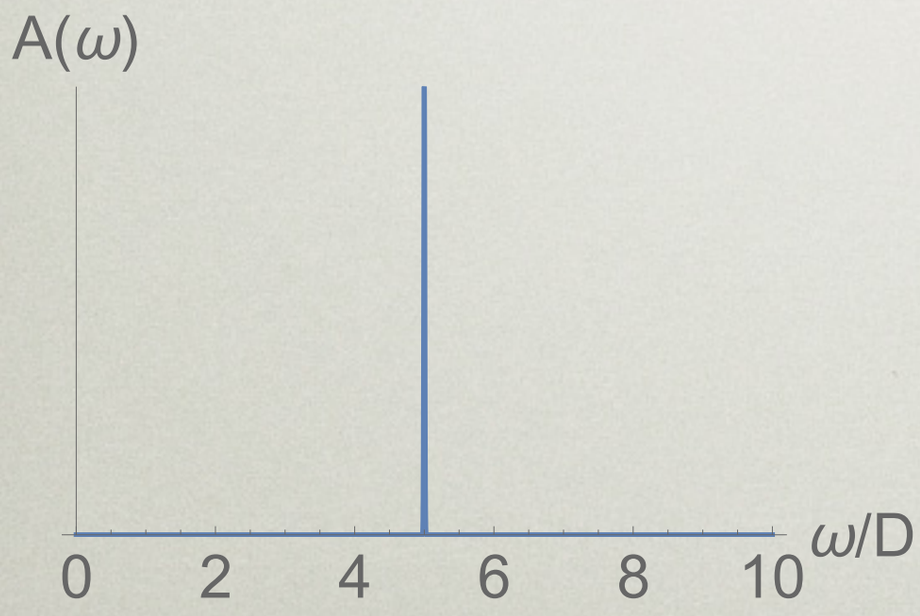


Temperature range $T_{FL}<T<T_{MIR}$ where the concept of quasiparticles is still defined.
Their width $\Gamma>T$, but quasiparticles still discernible.

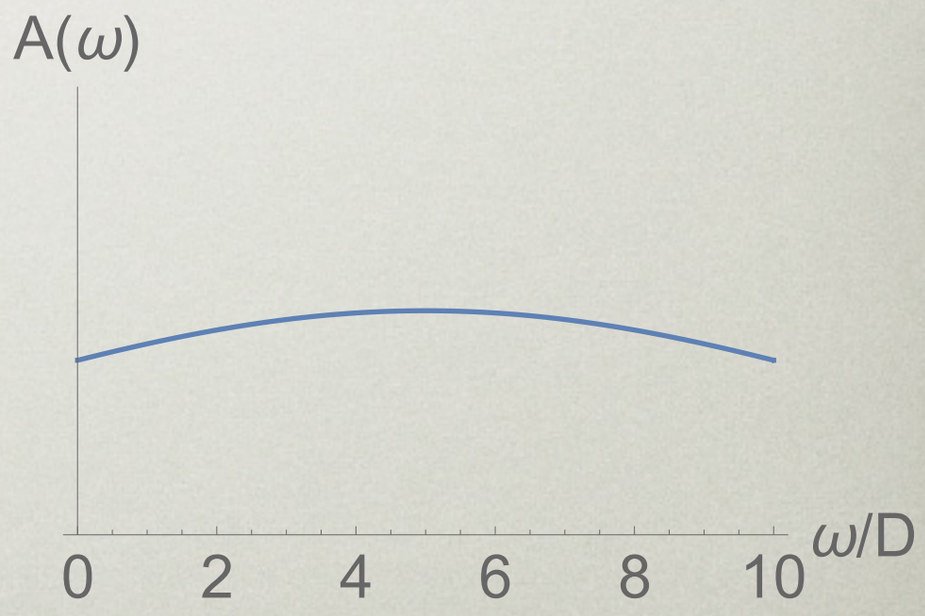
What happens at very high T?

What does the density of state (DOS) look like at infinite temperature?

$$T \to \infty \text{ such that } U \gg T \text{ implying } U = \infty$$

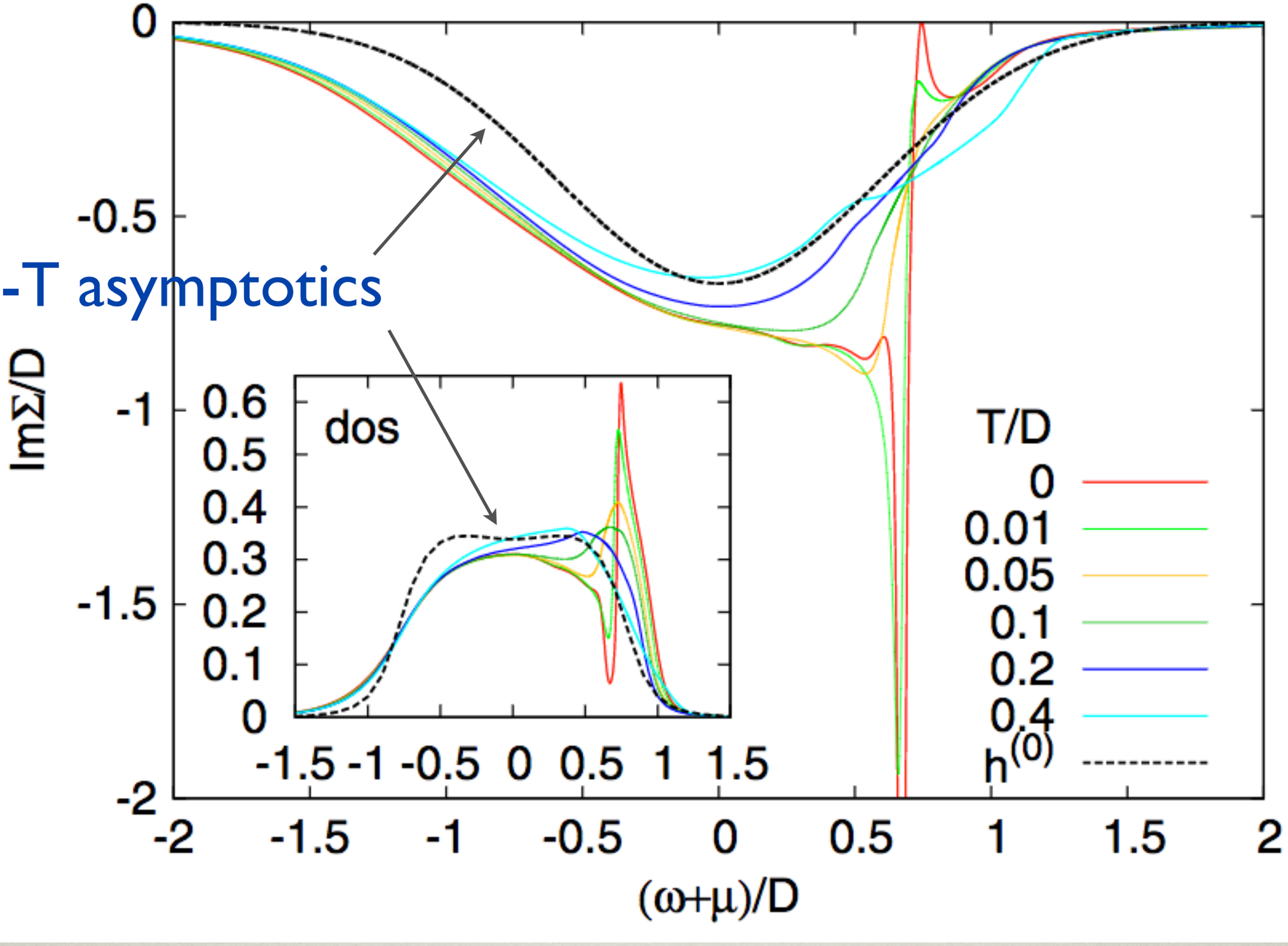


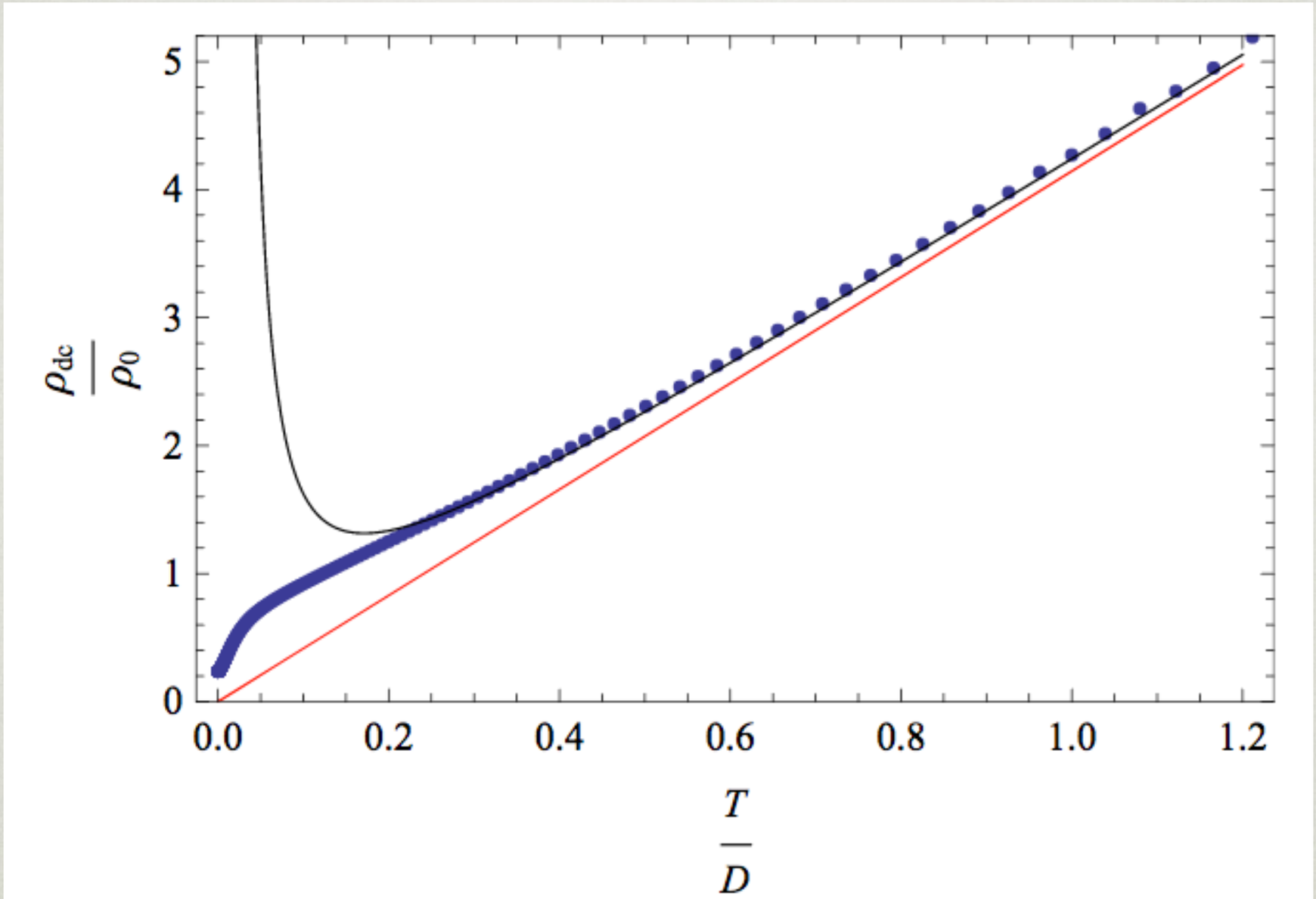
atomic-like?



very diffuse?

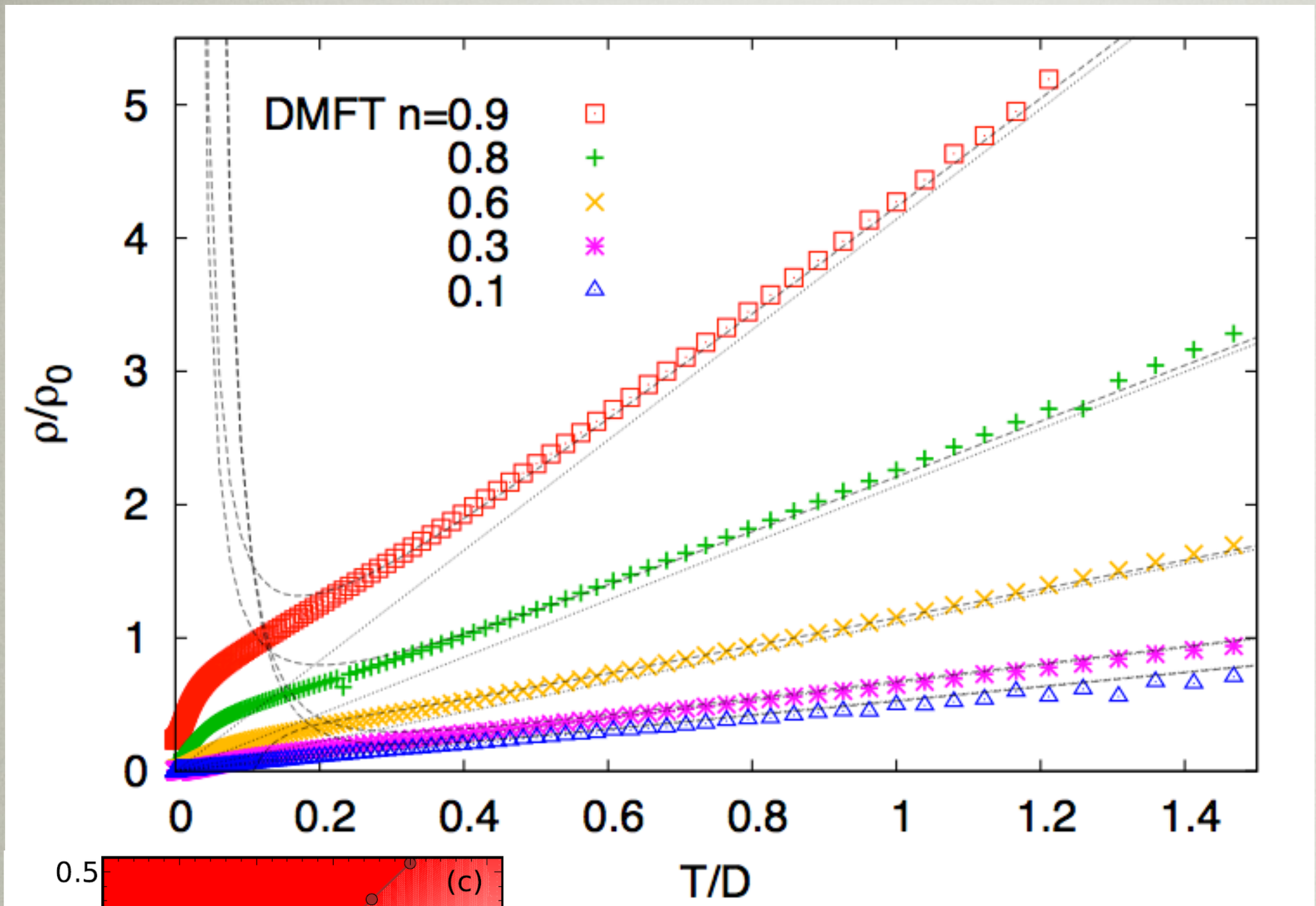
high-T asymptotics

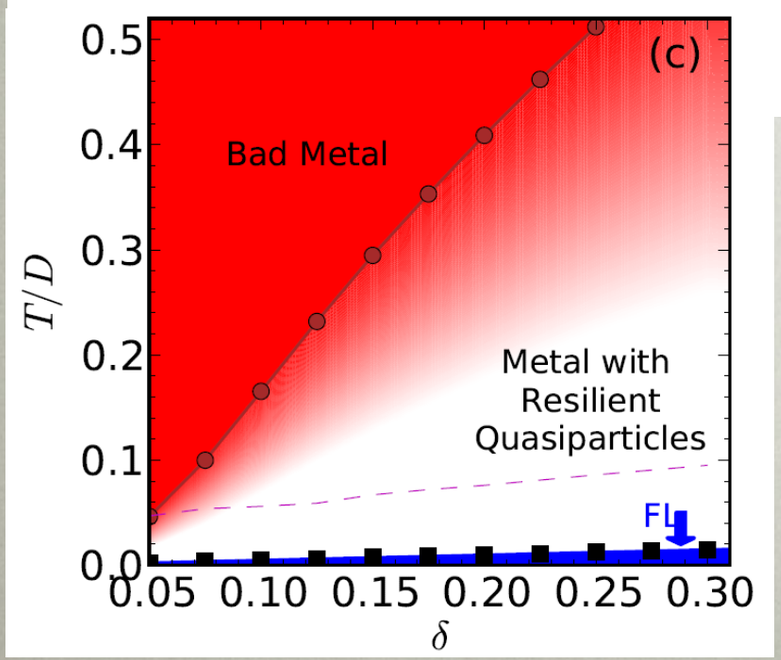




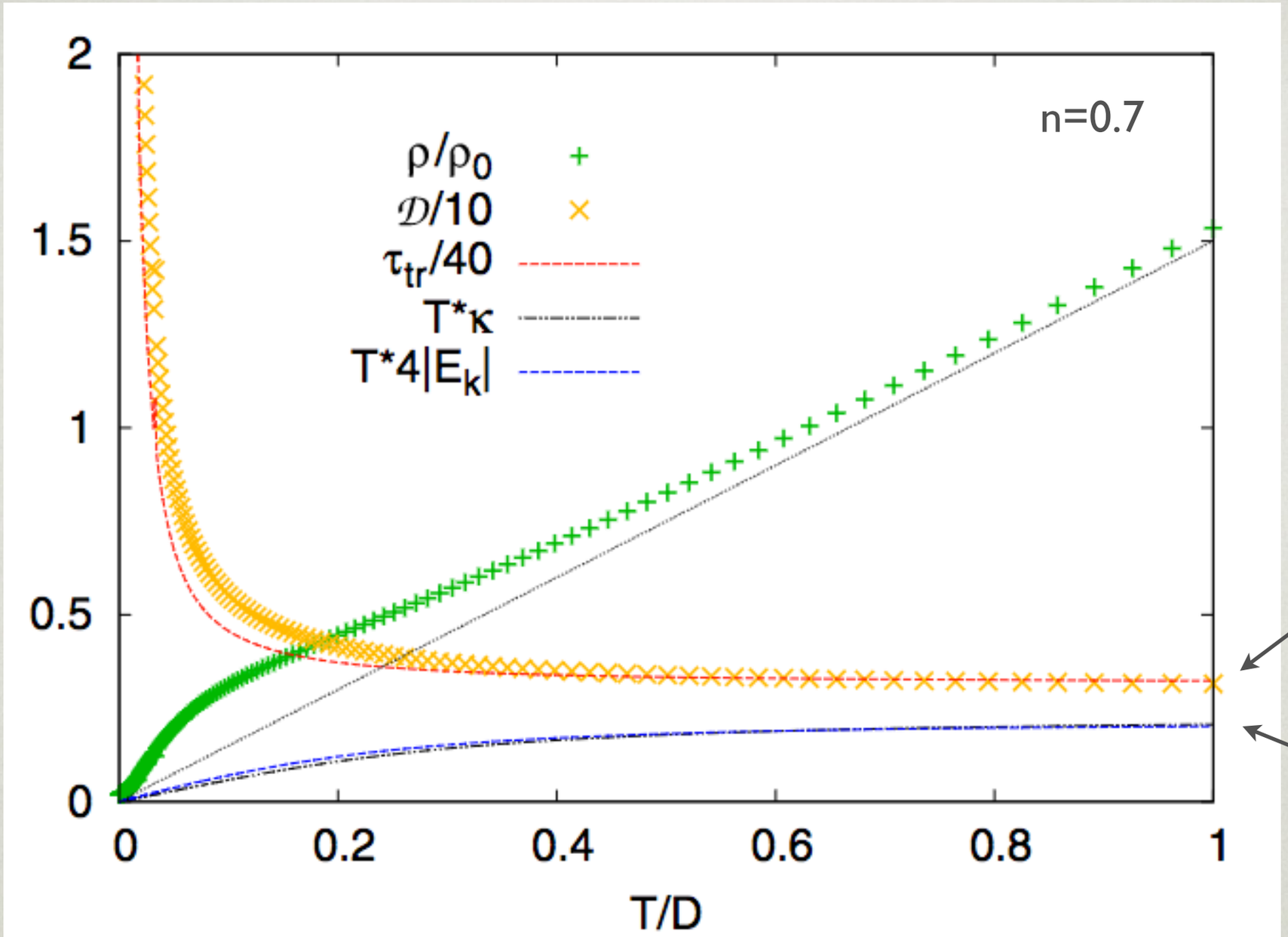
n=0.9

$$\rho = \frac{T}{1-n}\left[c_1 + \frac{1}{T^2}c_3(n)\right]$$





- dominant 1/T term agrees with DMFT at large T
- $1/T^3$ term describes corrections down to ρ_{MIR}



Einstein relation:

$$\sigma = e^2 \kappa \mathcal{D} \qquad \kappa \equiv \frac{\partial n}{\partial \mu}$$

Calandra, Gunnarsson, EPL 61 88 (2003)
Ohata, Kubo JPSJ 1970
J. Kokalj PRB 95 041110(R) (2017)

BIG PROBLEMS

- orbital degeneracy: big local Hilbert space, big Hilbert space at each shell of Wilson chains
- multiple quantum dots with multiple conduction leads
- lack of symmetry: diagonalization of big matrices scales as N^3

Parallelization

- Make use of multithreaded LAPACK routines, e.g. Intel MKL. Controlled by environment variables `MKL_NUMTHREADS`, `MKL_DYNAMIC`. Diagonalisation does not scale linearly, but the speed-up is substantial.
- Run diagonalisations in parallel using multithreading (OpenMP) on the same compute node, or using message-passing (MPI) across several compute nodes.

Note: nested OpenMP parallelism needs to be enabled using `OMP_NESTED=TRUE`. Often difficult to make it work (segmentation faults).

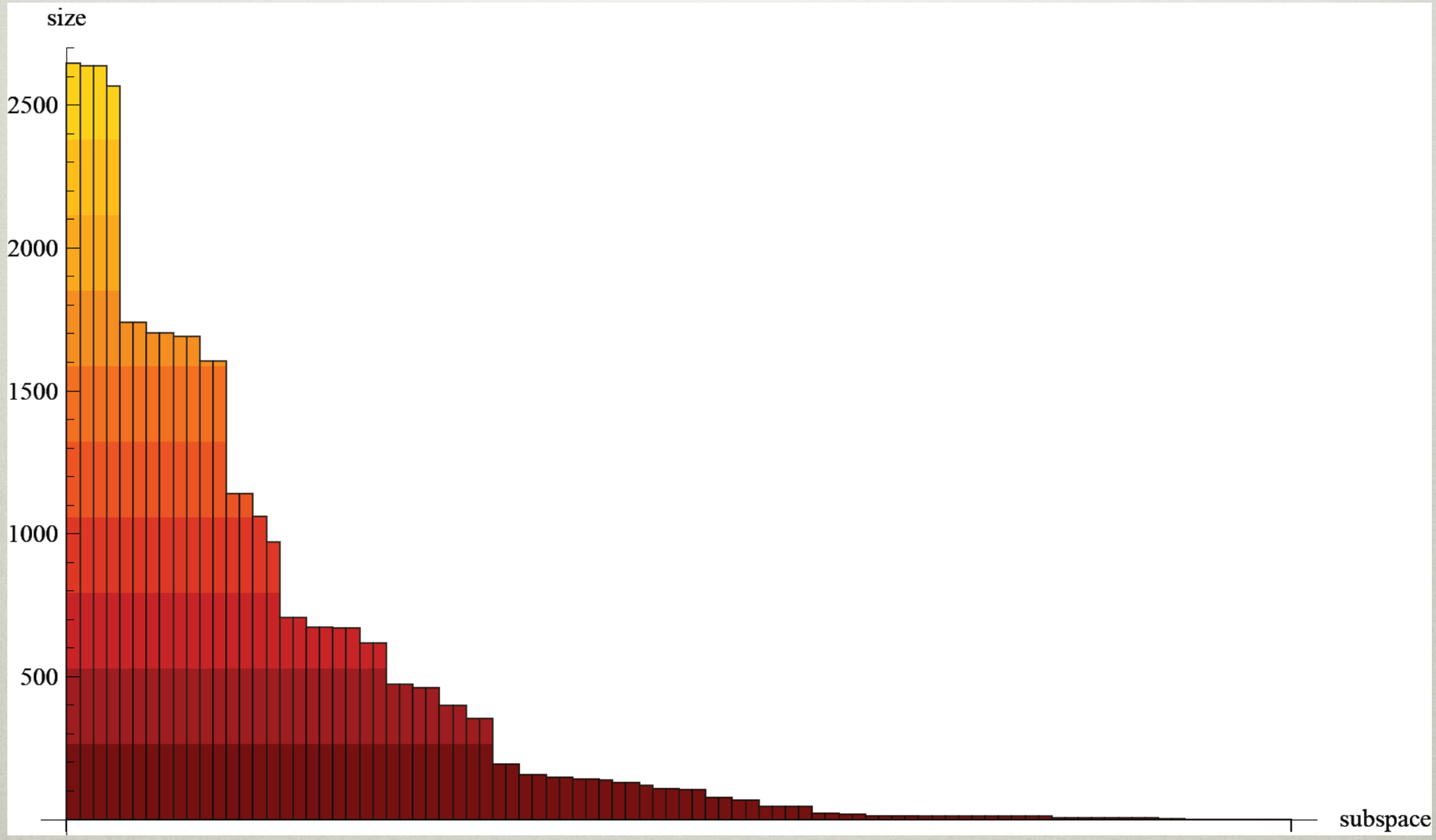
log

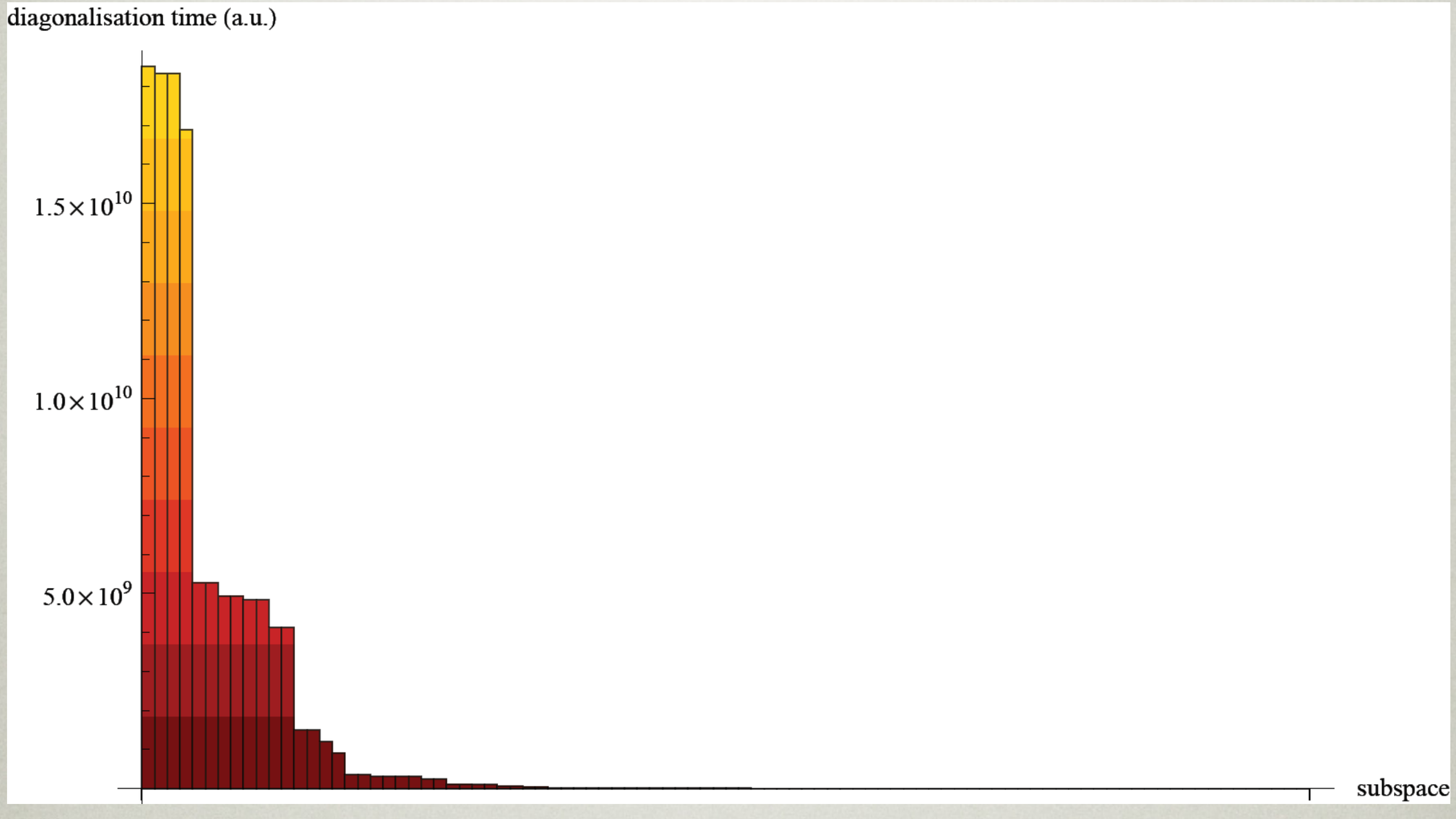
```
NRG Ljubljana 2.4.3.31 - (c) Rok Zitko <rok.zitko@ijs.si>
Timestamp: Mon Nov 13 12:55:52 2017
Compiled on Aug 14 2018 at 10:37:37
Compiled-in symmetry types: ANYJ DBLISOSZ DBLSU2 ISO ISO2 ISO2LR
ISOLR ISOSZ ISOSZLR NONE P PP QJ QS QSC3 QSLR QST QSTZ QSZ QSZLR
QSZTZ SL SL3 SPSU2 SPSU2C

No MPI: single node calculation.

[OMP] Max. number of threads: 1
[OMP] Number of processors: 32
[OMP] Dynamic thread adjustment: 0
[OMP] Nested parallelism: 0

Using Intel MKL library 11.3.2
Processor optimization: Intel(R) Advanced Vector Extensions 2
(Intel(R) AVX2) enabled processors
max_threads=8 blas_max_threads=8 dynamic=0
```

export MKL_NUM_THREADS=8

export MKL_DYNAMIC=FALSE

Matrix dimensions in different invariant subspaces.

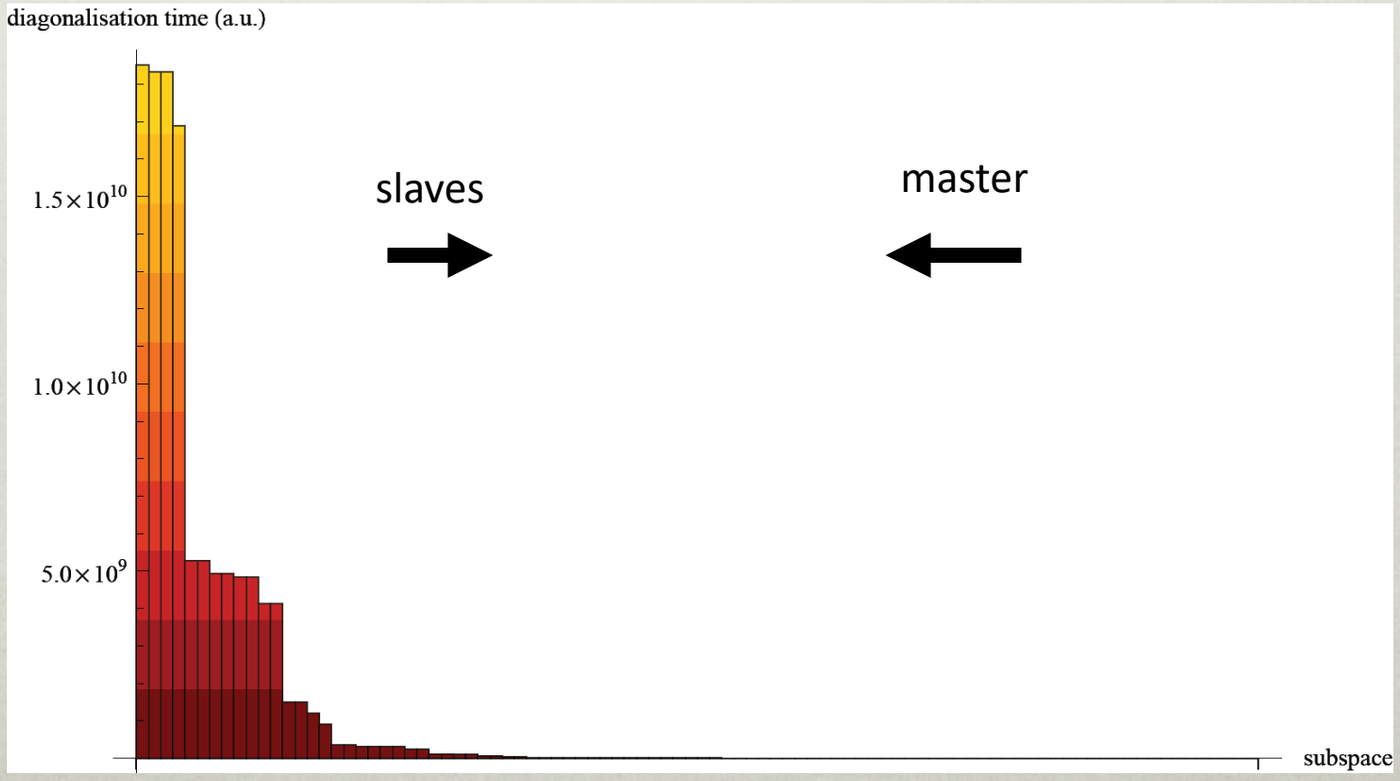




Conclusion: up to ~5-6 simultaneous diagonalisations.

Master-slave strategy

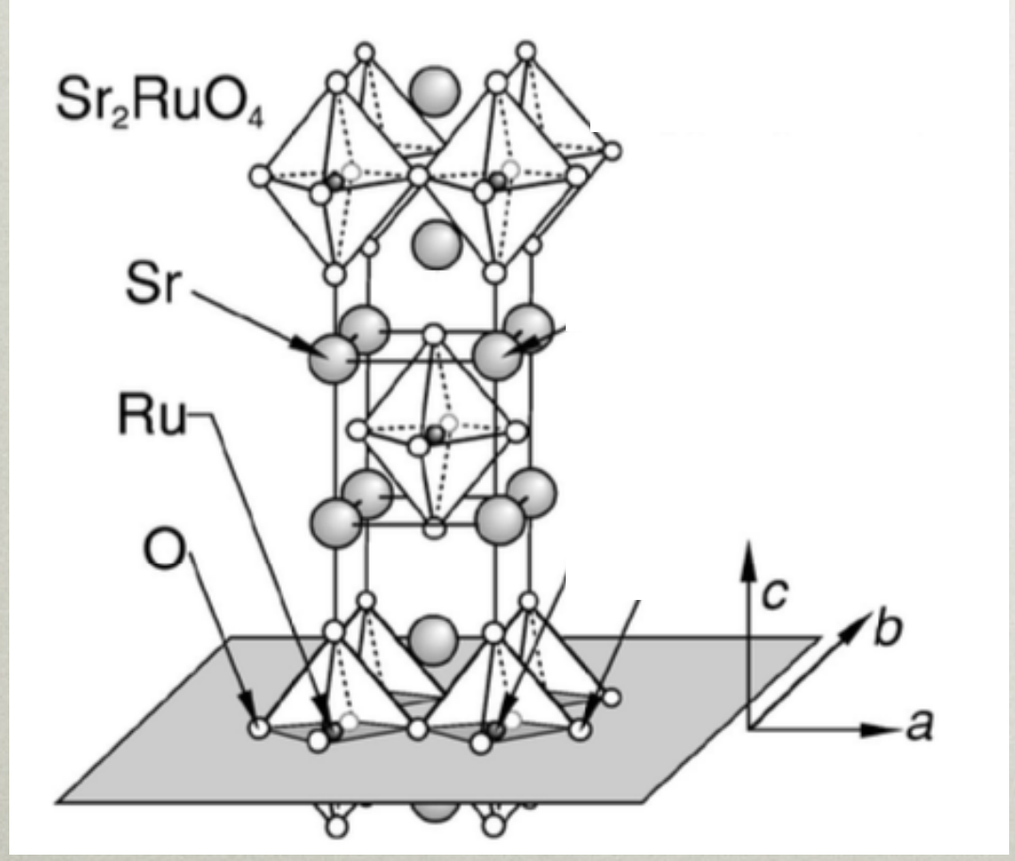
1. Master delegates diagonalisations of large matrices to slave nodes.
2. Master diagonalizes small matrices locally.

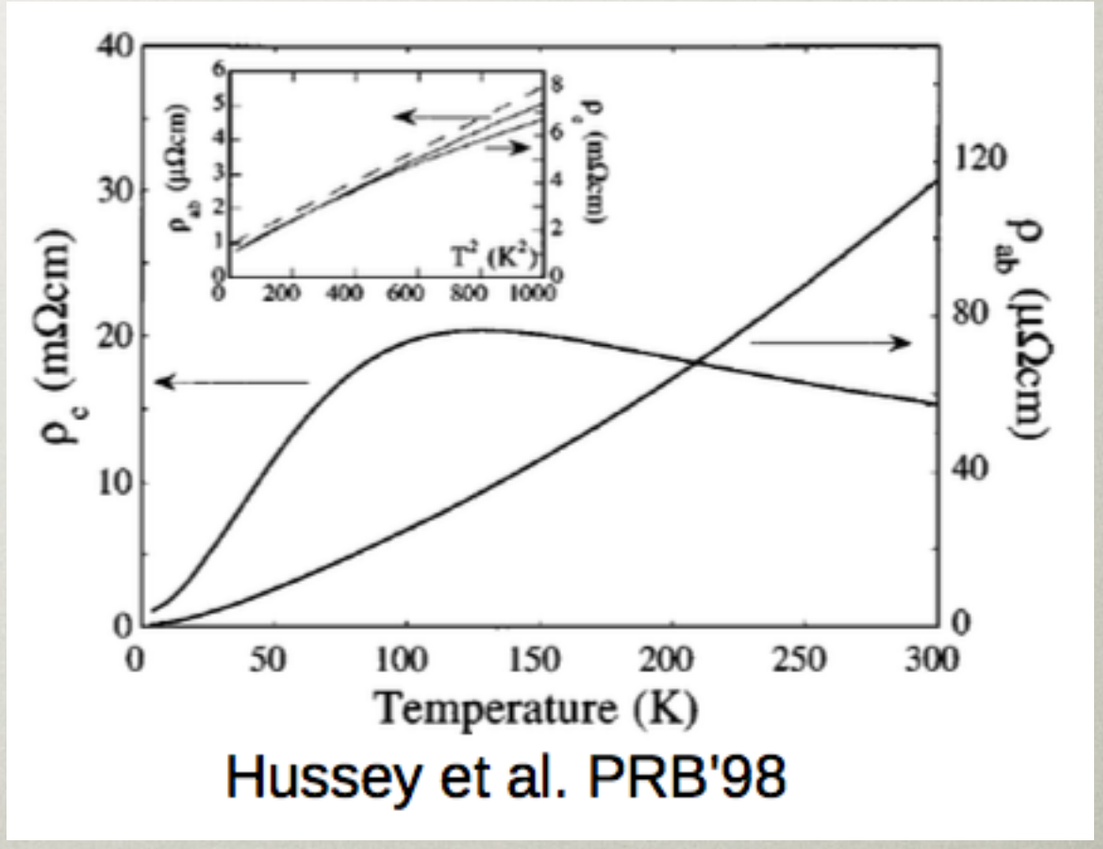


Hund's metal

Metal in which correlations are driven by Hund's coupling J.
Small coherence scale, even though U moderate.

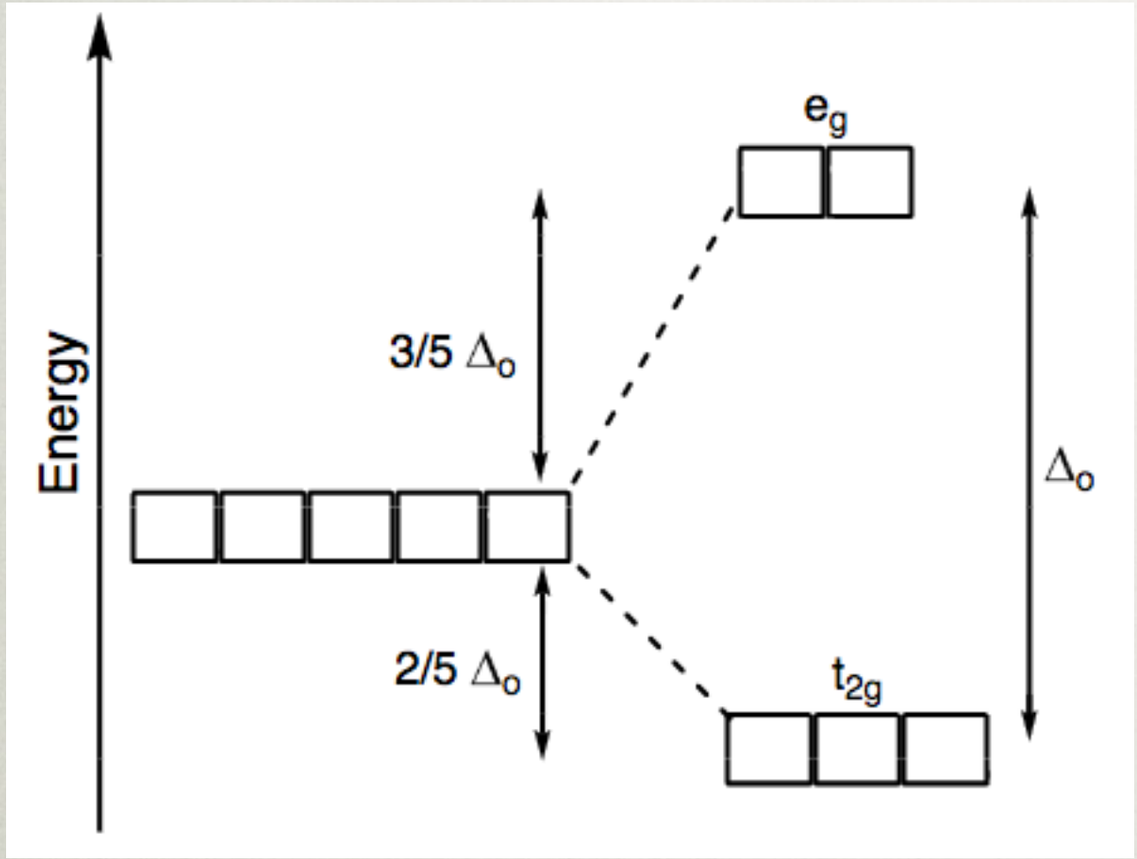
e.g. Sr_2RuO_4, $m^*/m \sim 4$, bad metal with $T_{coh} \sim 20K$ U~W



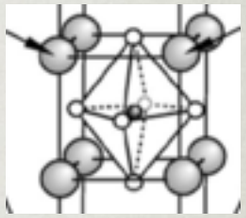


Haule, Kotliar, NJP'09; Werner, Gull, Troyer, Millis PRL'08;
de'Medici, Mravlje, Georges, PRL'11; Georges, de'Medici, Mravlje, Annu Rev CM'13

t_{2g} ORBITALS



crystal field splitting
in octahedral field



d_{xy}, d_{xz}, d_{yz}

Can be mapped to an effective orbital degree of freedom which transforms as the L=1 representation of SO(3).

Sr_2RuO_4 : 4 electrons in Ru t_{2g} orbitals

Interaction in three-orbital models

$$H = U \sum_m n_{m\uparrow} n_{m\downarrow}$$

intraorbital Coulomb

$$+U' \sum_{m<n,\sigma} n_{m\sigma} n_{n\bar{\sigma}}$$

interorbital Coulomb
opposite spin

$$+(U' - J) \sum_{m<n,\sigma} n_{m\sigma} n_{n\sigma}$$

interorbital Coulomb
parallel spin

$$-J \sum_{m<n,\sigma} c^\dagger_{m\sigma} c_{m\bar{\sigma}} c^\dagger_{n\bar{\sigma}} c_{n\sigma}$$

spin exchange

$$-J \sum_{m<n} [c^\dagger_{m\uparrow} c^\dagger_{m\downarrow} c_{n\uparrow} c_{n\downarrow} + \text{h.c.}]$$

pair hopping

"Rotationally invariant" for U'=U-2J

Interaction in three-orbital models

Kanamori interaction $\mathrm{U}(1) \times \mathrm{SU}(2) \times \mathrm{SO}(3)$

$$H_{\mathrm{imp}} = \frac{1}{2}(U - 3J)N_d(N_d - 1) - 2J\mathbf{S}^2 - \frac{J}{2}\mathbf{L}^2$$

1st Hund's rule

2nd Hund's rule

Dworin-Narath interaction $\mathrm{U}(1) \times \mathrm{SU}(2) \times \mathrm{SU}(3)$

$$H_{\mathrm{imp}} = \frac{1}{2}(U - 3J)N_d(N_d - 1) - 2J\mathbf{S}^2$$

Georges, de'Medici, Mravlje, Annu Rev CM'13

Nishikawa, Hewson, PRB'12: role of (non)conservation of orbital angular momentum

$$N_d = \sum_{m,\sigma} d^\dagger_{m\sigma} d_{m\sigma}$$

$$\mathbf{S} = \sum_{m} d^\dagger_{m\sigma} \left(\frac{1}{2}\boldsymbol{\sigma}_{\sigma\sigma'}\right) d_{m\sigma'}$$

$$\mathbf{L} = \sum_{\sigma} d^\dagger_{m\sigma} \mathcal{L}_{mm'} d_{m'\sigma}$$

- Dynamical symmetry enhancement: SO(3)→SU(3)
- Separate screening of L and S (non-Fermi-liquid physics?)
- Effects of spin-orbit coupling (3rd Hund's rule)

Multiplet structure (Kanamori interaction)

N	S	L	Degeneracy $= (2S+1)(2L+1)$	Energy
0,[6]	0	0	$\boxed{1}$	0
1,[5]	1/2	1	$\boxed{6}$	$-5J/2$,$[10\mathcal{U}-5J/2]$
2,[4]	1	1	$\boxed{9}$	$\mathcal{U}-5J$,$[6\mathcal{U}-5J]$
2,[4]	0	2	5	$\mathcal{U}-3J$,$[6\mathcal{U}-3J]$
2,[4]	0	0	1	$\mathcal{U}$,$[6\mathcal{U}]$
3	3/2	0	$\boxed{4}$	$3\mathcal{U}-15J/2$
3	1/2	2	10	$3\mathcal{U}-9J/2$
3	1/2	1	6	$3\mathcal{U}-5J/2$

Table 1: Eigenstates and eigenvalues of the t_{2g} Hamiltonian $\mathcal{U}\hat{N}(\hat{N}-1)/2 - 2J\vec{S}^2 - J\vec{L}^2/2$ in the atomic limit ($\mathcal{U} \equiv U - 3J$). The boxed numbers identifies the ground-state multiplet and its degeneracy, for $J > 0$.

Georges, de'Medici, Mravlje, Annu Rev CM'13

Effective Kondo model

$$H_{\mathrm{K}} = -P_n H_{\mathrm{hyb}} \left(\sum_a \frac{P^a_{n+1}}{\Delta E^a_{n+1}} + \sum_b \frac{P^b_{n-1}}{\Delta E^b_{n-1}} \right) H_{\mathrm{hyb}} P_n$$

N_d=2, S=1, L=1

$$H_K = J_p N_f + J_s \mathbf{S}\cdot\mathbf{s} + J_l \mathbf{L}\cdot\mathbf{l} + J_q \mathbf{Q}\cdot\mathbf{q} +$$
$$J_{ls}(\mathbf{L}\otimes\mathbf{S})\cdot(\mathbf{l}\otimes\mathbf{s}) + J_{qs}(\mathbf{Q}\otimes\mathbf{S})\cdot(\mathbf{q}\otimes\mathbf{s})$$

orbital quadrupole operators

$$Q^{bc}_{i,j} = \frac{1}{2}\left(L^b_{i,m}L^c_{m,j} + L^c_{i,m}L^b_{m,j}\right) - \frac{2}{3}\delta_{b,c}\delta_{i,j}$$

$$\mathrm{Tr}(Q^\alpha Q^\beta) = 2\delta_{\alpha,\beta}$$

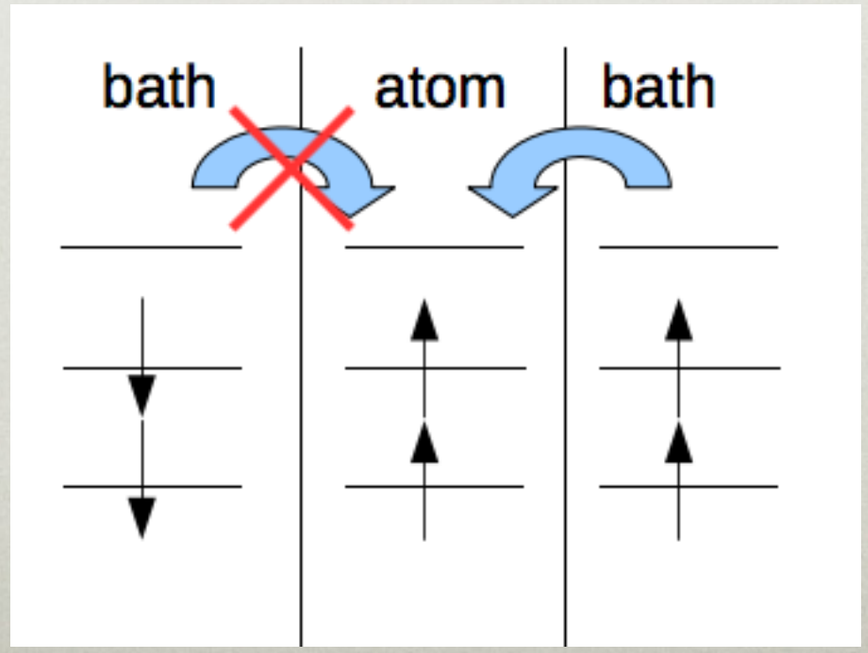
Horvat, Zitko, Mravlje PRB'16

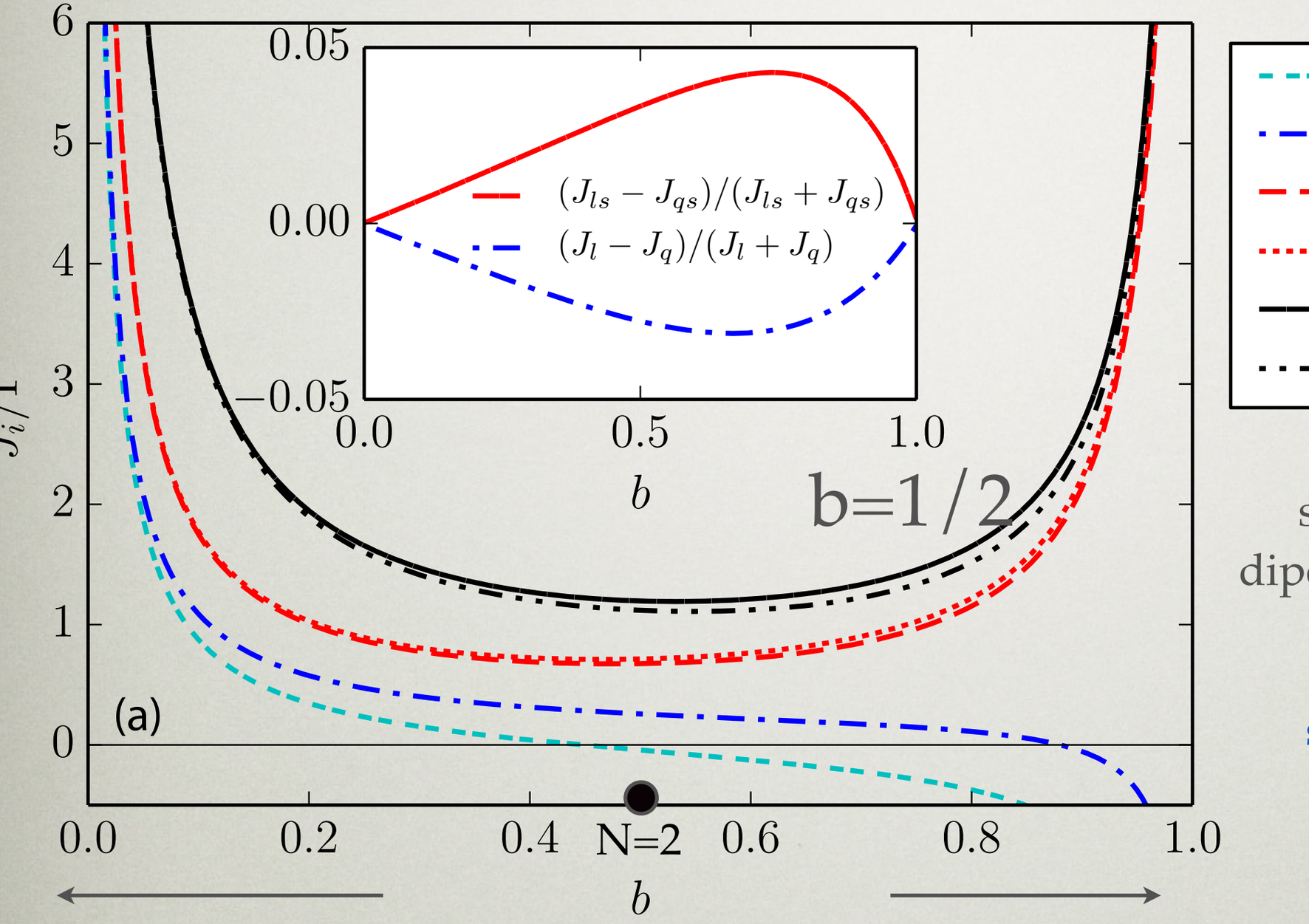
Yin, Haule, Kotliar PRB'12
Aron, Kotliar PRB'15
Stadler et al. PRL'15

Bare Kondo coupling constants

J_s is small or even ferromagnetic

Ferromagnetic alignment favored by fluctuation to N=3 (half-filled). This is in contrast to single-orbital problems.





spin

orbital

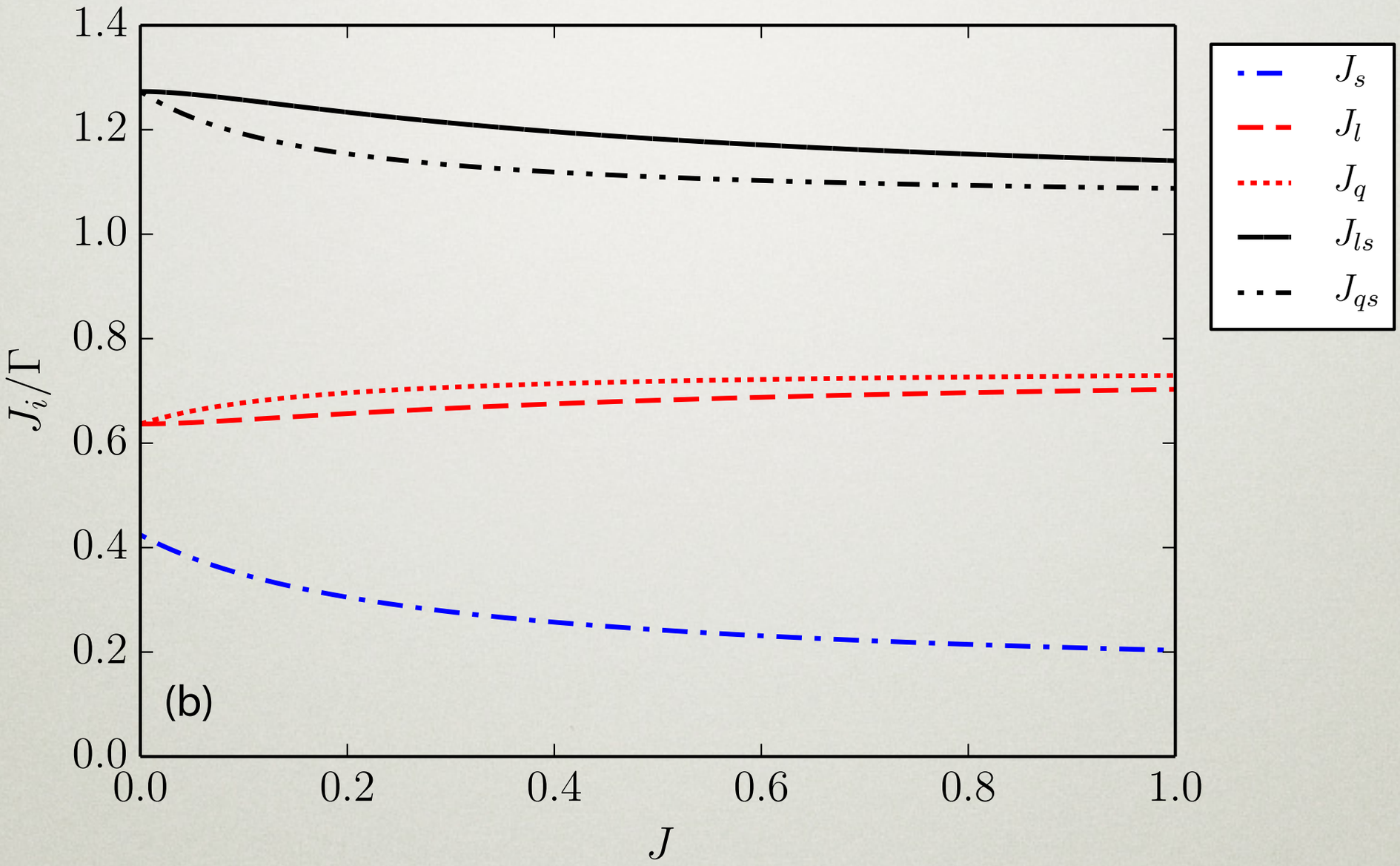
mixed

small splitting between dipole and quadrupole terms

small/ferromagnetic J_s

b = local potential

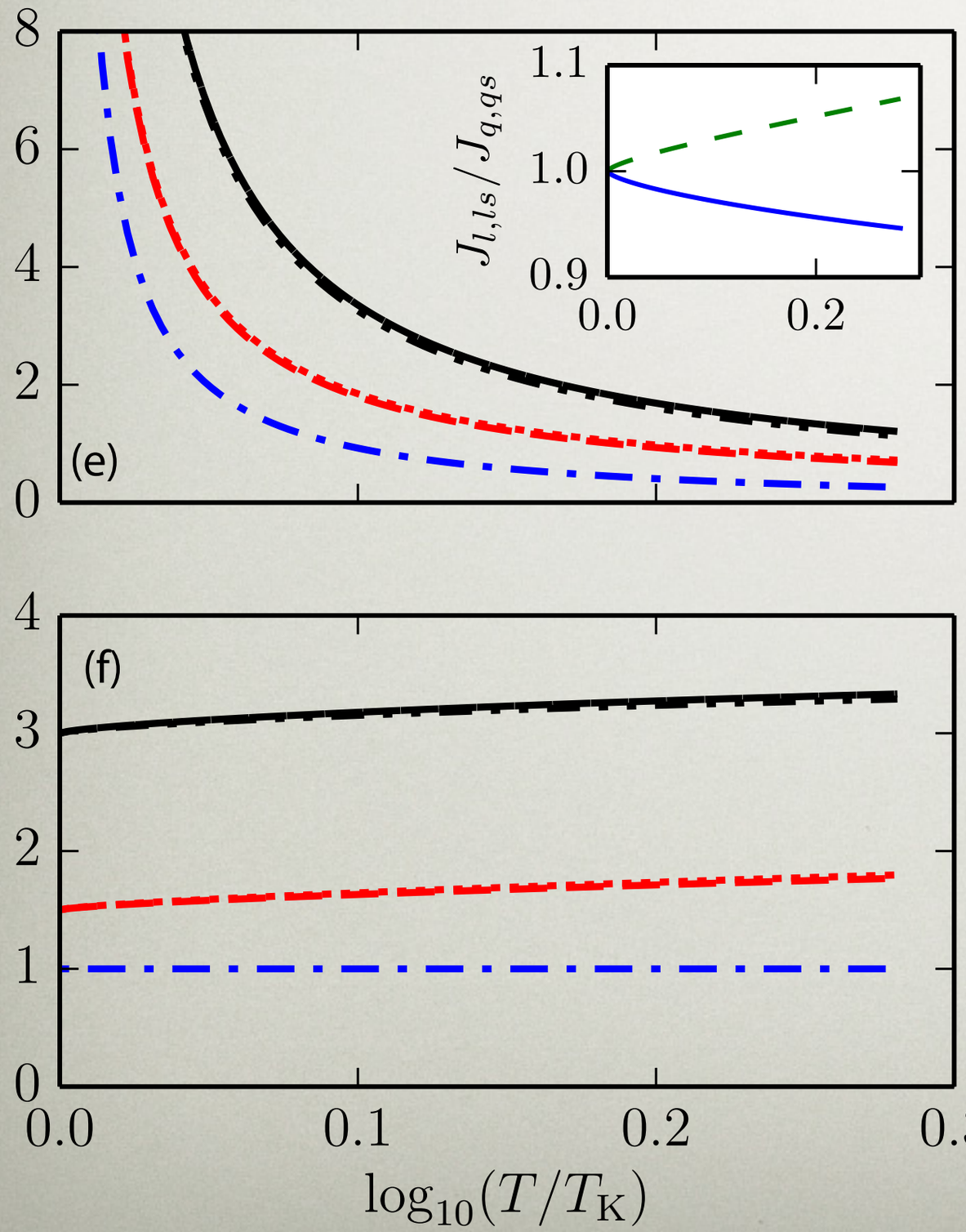
Splitting between dipolar and quadrupolar coupling



Driven by the orbital part of Hund's coupling term: $-\frac{J}{2}\mathbf{L}^2$

Dynamical symmetry enhancement

(within perturbative RG)



Splitting between the dipole and quadrupole orbital couplings goes to zero at low-T: SO(3) → SU(3) enhancement.

As if there were no $-(J/2)L^2$ term.

cf. also work by Kuzmenko, Kikoin, Kiselev, Avishai

3-orbital NRG with full symmetry

$$\underset{\text{charge}}{\mathrm{U}(1)} \times \underset{\text{spin}}{\mathrm{SU}(2)} \times \underset{\text{orbital}}{\mathrm{SO}(3)}$$ (Kanamori type)

Dramatic improvement!

Calculations with Λ=4 feasible... but still quite demanding (hybrid MPI+OpenMP parallelization on 4×4 cores, ~24h per run for 4000 multiplets ~ E_{cutoff}=8).

Real-frequency-axis spectra → transport calculations!

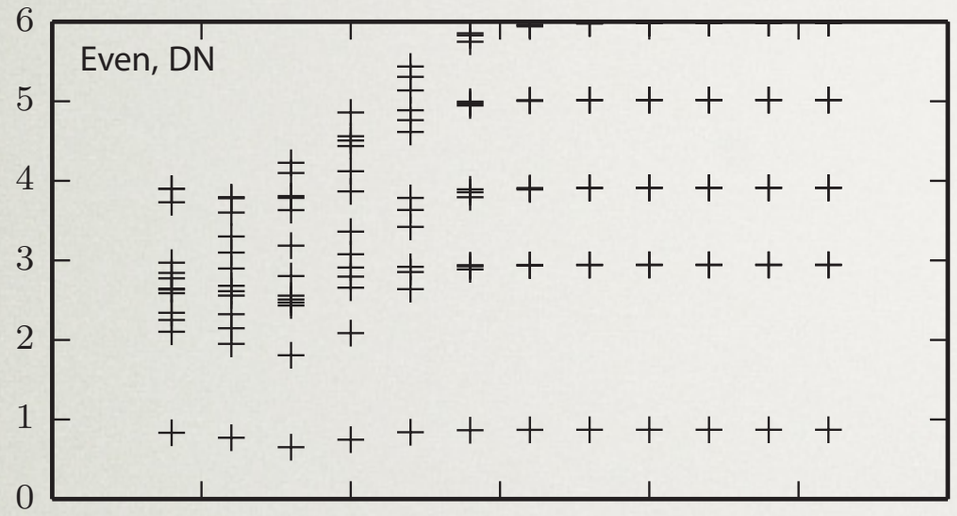
Weichselbaum et al. implement the larger SU(3) symmetry of the Dworin-Narath Hamiltonian without the L term (2nd Hund's rule).

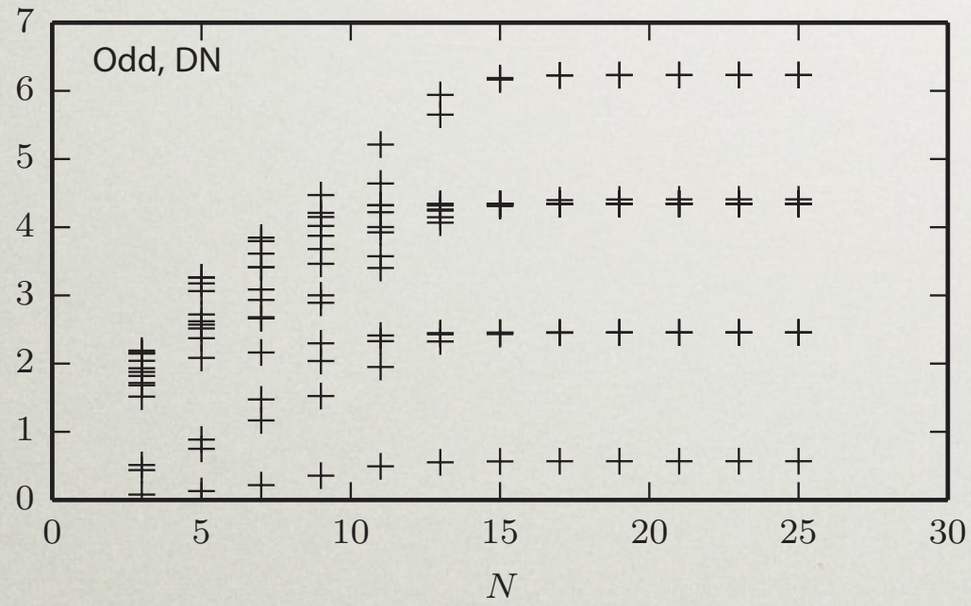
cf. Stadler et al. PRL'15, arxiv 2018

Horvat, Žitko, Mravlje PRB'16

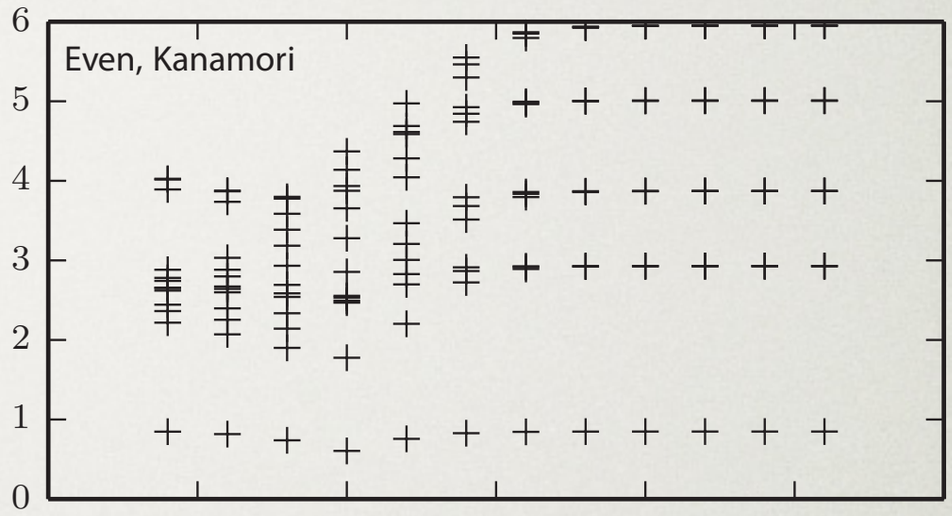
NRG flow diagrams

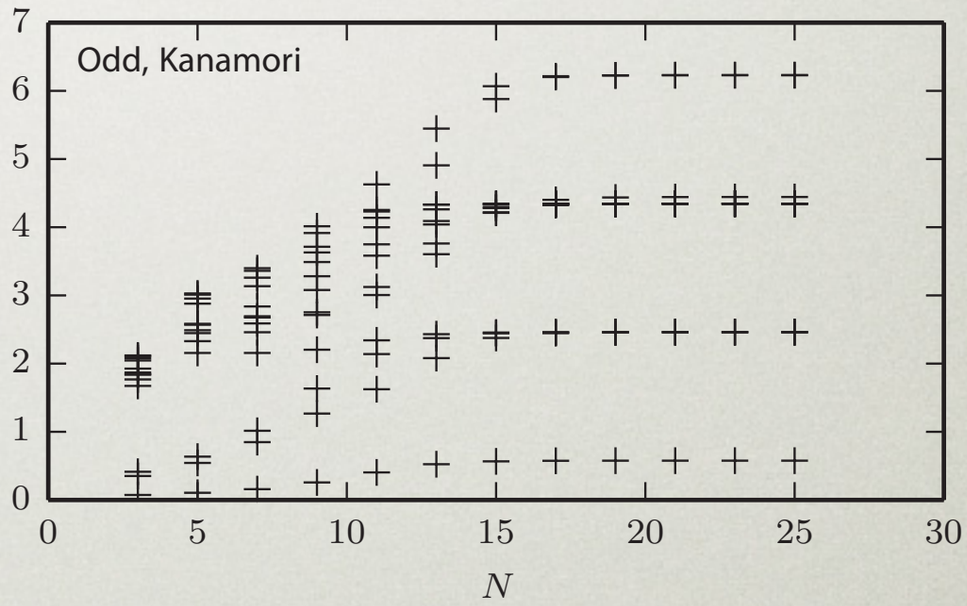
Dworin-Narath





Kanamori

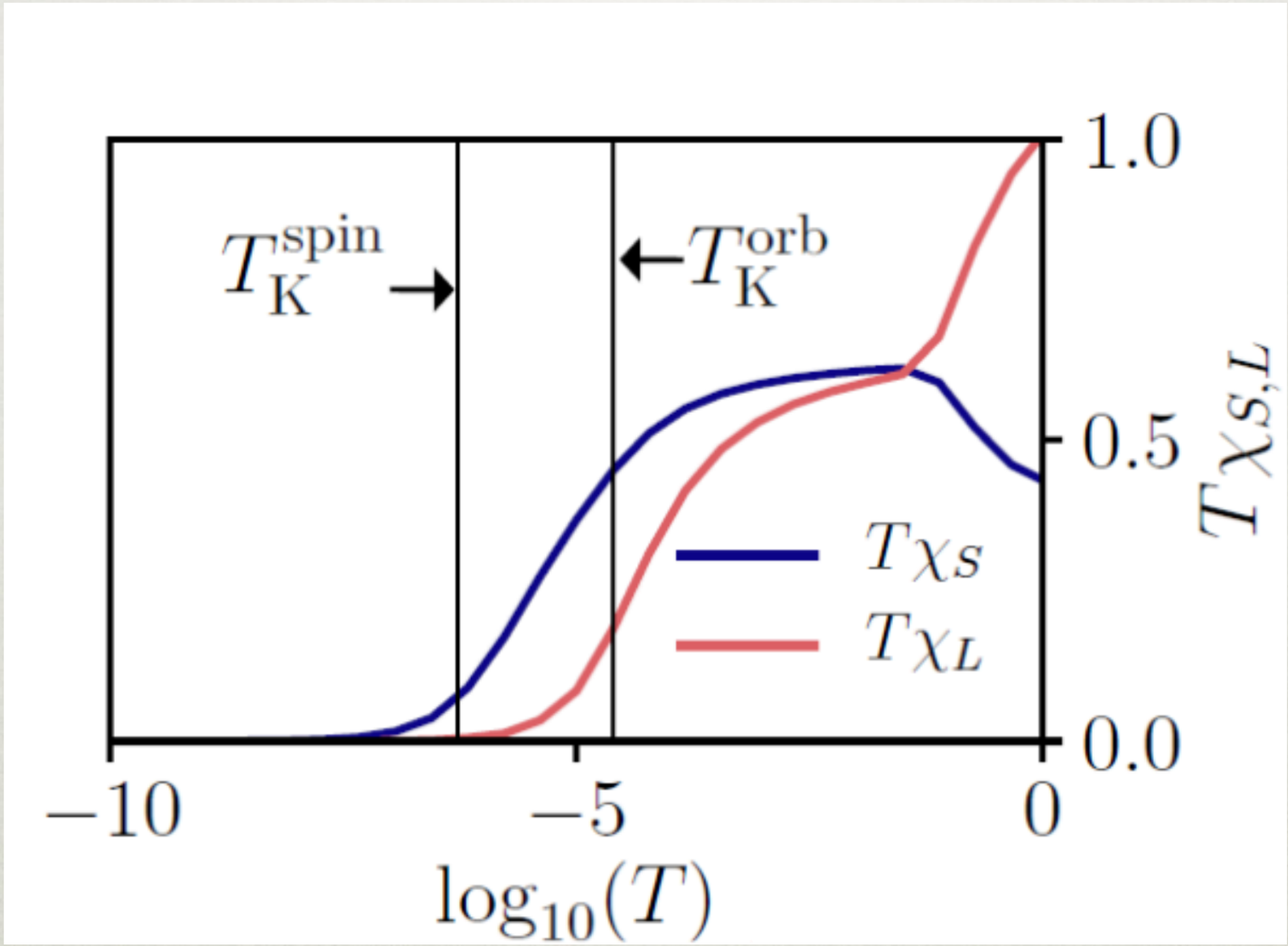




Same low-temperature strong-coupling fixed point!

Nishikawa, Hewson, PRB'12

Separation of orbital and spin Kondo temperatures



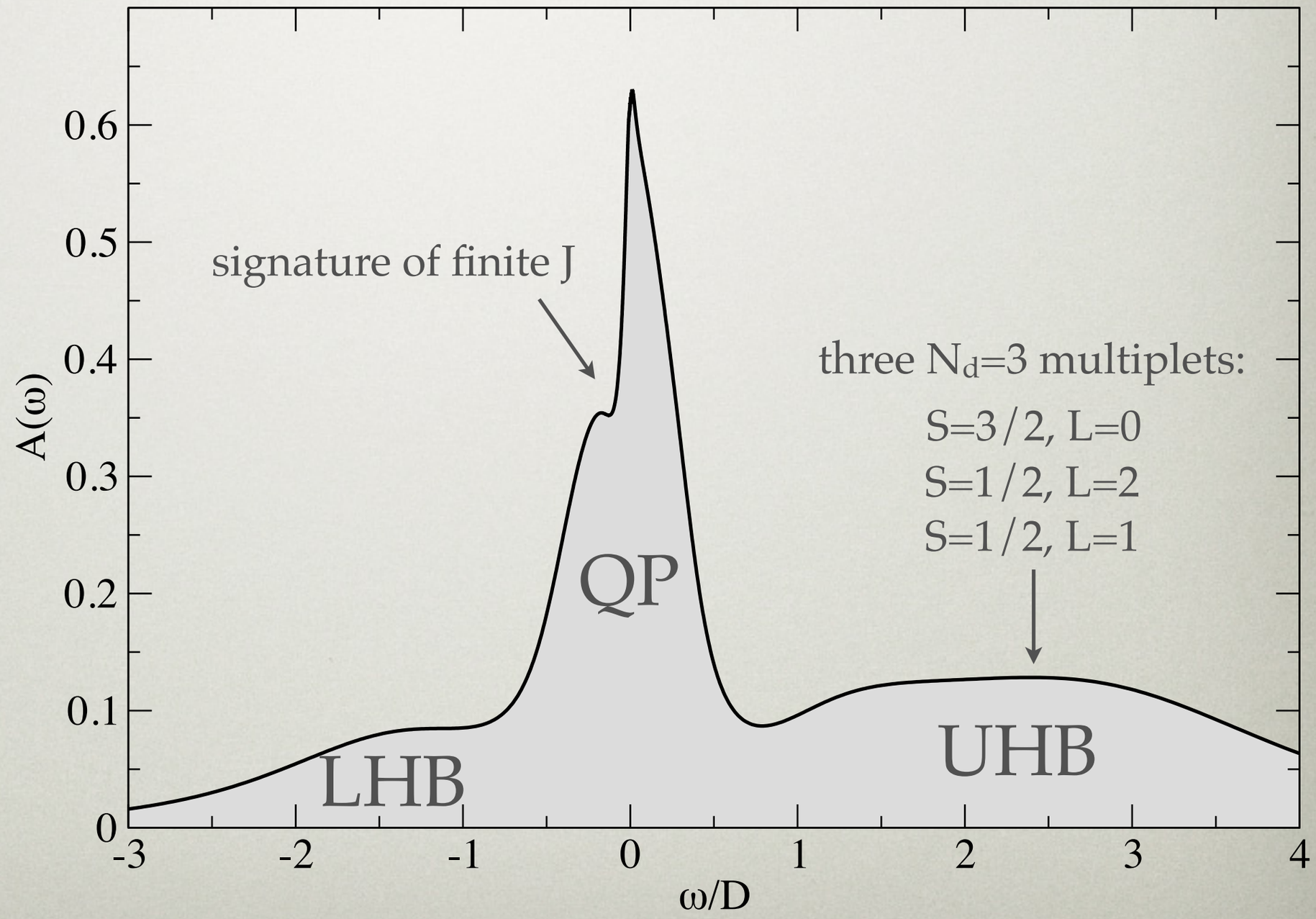
Generic: same behaviour found for Kanamori, Dworin-Narath, as well as their Schrieffer-Wolff-transformed variants.

Okada, Yosida, PTP'73
Yin, Haule, Kotliar PRB'12

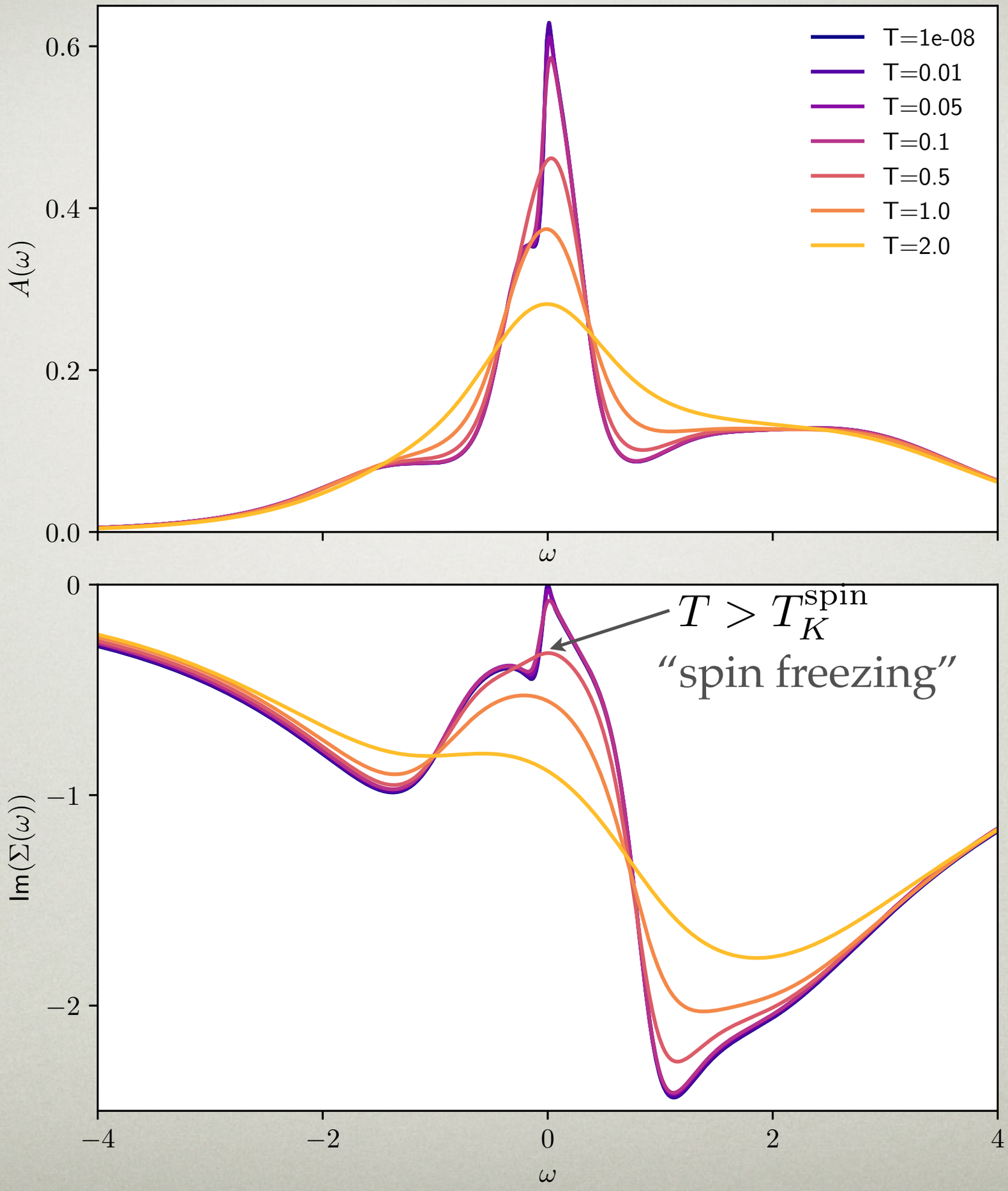
DMFT for Hubbard-Kanamori model

U/D=3.2
J/U=1/6
semi-circular DOS
no SOC

$\langle N_d \rangle = 2$
L=1, S=1 GS



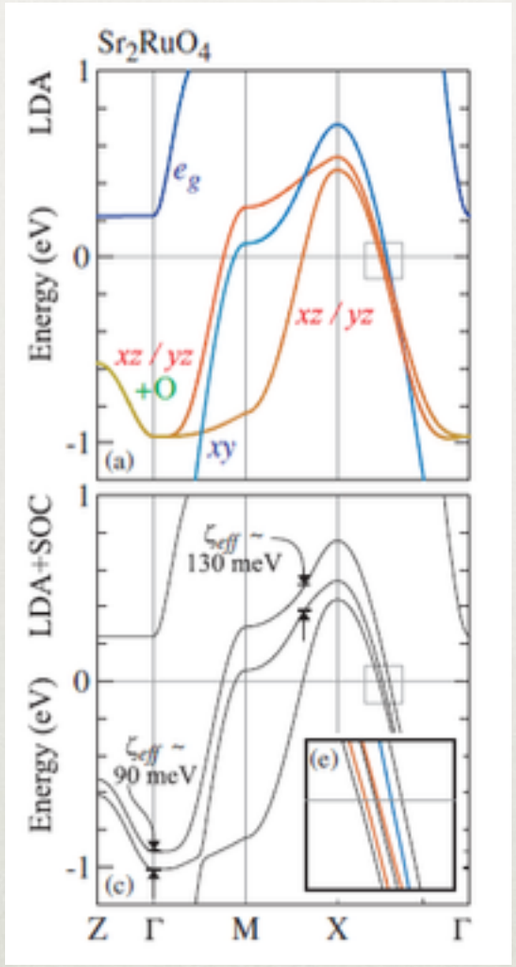
First seen in the minimal SU(3) model, Stadler et al. PRL'15


T=1e-08
T=0.01
T=0.05
T=0.1
T=0.5
T=1.0
T=2.0
$A(\omega)$
0.0
0.2
0.4
0.6
ω
$T > T_K^{\text{spin}}$
"spin freezing"
$\text{Im}(\Sigma(\omega))$
0
−1
−2
−4
−2
0
2
4
ω

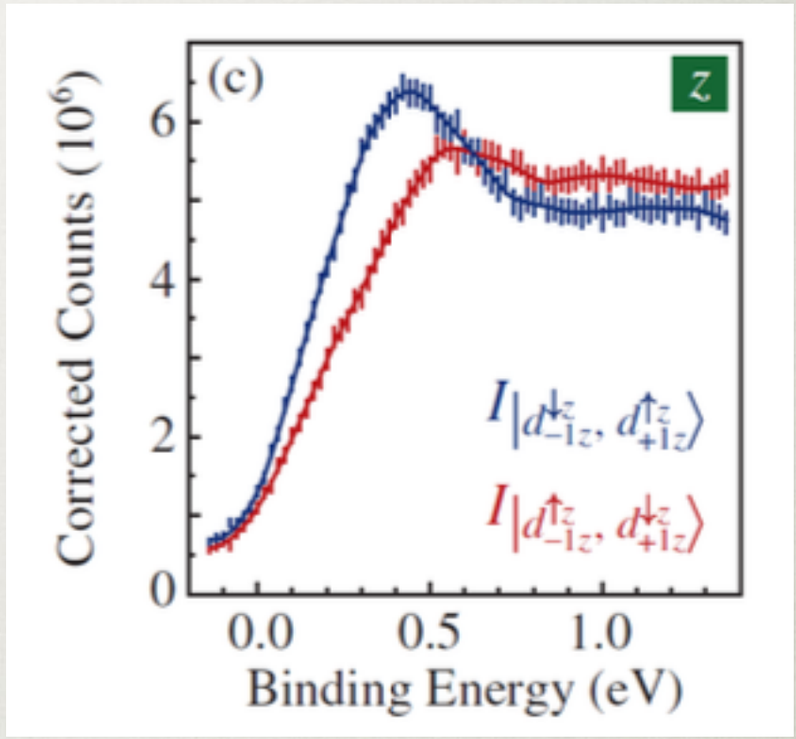
Spin-orbit coupling

SOC not small

$\lambda \sim 0.1\,\mathrm{meV} > T_{\mathrm{FL}}$



Haverkort et al. PRL'08



srARPES, splitting at Γ point

Veenstra et al. PRL'14

Important to account for the details in the band structure. Typically not included in LDA+DMFT calculations, but results still in good quantitative agreement with experiments. Why?

Schrieffer-Wolff transformation

$$\mathbf{J} = \mathbf{L} + \mathbf{S}$$

$$H_{LSJ} = \sum_{\Lambda\Sigma\Gamma} K_{\Lambda\Sigma\Gamma} \mathbf{T}^{\Lambda\Sigma\Gamma}(J) \cdot \mathbf{t}^{\Lambda\Sigma\Gamma}(J)$$

Kondo coupling

unit tensor operators
(impurity & band)

$$Q^{ij} = S(J_i, J_j)$$

$$R^{ijk} = S(J_i, J_j, J_k)$$

Can be expressed in terms of S,L,Q,LS,QS operators!

... but very lengthy expressions

3-orbital NRG with conserved J=L+S

$$\mathrm{U}(1) \times \mathrm{SU}(2)$$

charge total moment

Need to distinguish J=3/2 and J=1/2 species of fermions,
more book-keeping, but not too difficult to implement.

Dramatic improvement (compared to U(1) symmetry only)!

Calculations with Λ=6 feasible... but still quite demanding
(hybrid MPI+OpenMP parallelization on 4×4 cores,
~1-2 days per run for 6000 multiplets).

Horvat, Žitko, Mravlje PRB'17

$\lambda < 0$ $\lambda > 0$

$J = 2$ Hund Van Vleck J=0

$\log_{10}(T_K)$

0

−5

(a)

$\log_{10}(\chi_J)$

5

J^2

$\log_{10}(\chi_J(T=0))$

0

(b)

6

4

2

0

J^2

δ/π

1.0

0.5

0.0

j=1/2

j=3/2

(c)

−2 −4 −6 −4 −2

$\log_{10}(-\lambda)$ $\log_{10}(\lambda)$

$|\lambda| < T_K^{\mathrm{orb}}$

DMFT for Hubbard-Kanamori model with spin-orbit coupling

U/D=3.2

J/U=1/8

semi-circular DOS

λ<0 (J=2 metal regime)