Spectral functions in NRG

Rok Žitko
Institute Jožef Stefan
Ljubljana, Slovenia

Green's functions - review

$$G_{AB}(t) = \langle\langle A; B \rangle\rangle_t := -i\theta(t)\langle [A(t), B(0)]_{\pm} \rangle$$

+ if A and B are fermionic operators
- if A and B are bosonic operators

$$A(t) = e^{iHt} A e^{-iHt}$$

$$\langle \hat{O} \rangle = \mathrm{Tr}\left[\rho \hat{O}\right] \qquad \rho = \frac{e^{-\beta H}}{Z}$$

NOTE: ħ=1

Also known as the **retarded** Green's function.

Following T. Pruschke: Vielteilchentheorie des Festkorpers

Laplace transformation:

$$G_{AB}(z) = \langle\langle A; B \rangle\rangle_z = \int_0^\infty \mathrm{d}t e^{izt} \langle\langle A; B \rangle\rangle_t, \quad \Im z > 0$$

Inverse Laplace transformation:

$$G_{AB}(t) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \mathrm{d}\omega e^{-i(\omega+i\delta)t} G_{AB}(\omega + i\delta)$$

Impurity Green's function (for SIAM):

$$G(z) = \langle\langle d; d^\dagger \rangle\rangle_z$$

Equation of motion

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\langle A;B\rangle\rangle_t = \langle\langle \dot{A};B\rangle\rangle_t - i\delta(t)\langle[A,B]_\pm\rangle$$

$$z\langle\langle A;B\rangle\rangle_z = \langle\langle [A,H];B\rangle\rangle_z + \langle[A,B]_\pm\rangle$$

Example 1: $$H = (\epsilon-\mu)d^\dagger d \qquad G(z) = \langle\langle d; d^\dagger\rangle\rangle_z$$

$$[d,H] = (\epsilon-\mu)[d,d^\dagger d] = (\epsilon-\mu)d$$

$$[d,d^\dagger]_+ = 1$$

$$zG(z) = (\epsilon-\mu)G(z) + 1$$

$$\boxed{G(z) = \frac{1}{z-(\epsilon-\mu)}}$$

Example 2: $$H = \sum_{k\sigma} (\epsilon_k - \mu) c^\dagger_{k\sigma} c_{k\sigma}$$

$$[c_{k\sigma}, H] = (\epsilon_{k\sigma} - \mu) c_{k\sigma}$$

$$[c_{k\sigma}, c^\dagger_{k'\sigma'}]_+ = \delta_{kk'}\delta_{\sigma\sigma'}$$

$$G_{k\sigma,k'\sigma'}(z) = \langle\langle c_{k\sigma}; c_{k'\sigma'} \rangle\rangle_z$$

$$\boxed{G_{k\sigma,k'\sigma'}(z) = \frac{\delta_{kk'}\delta_{\sigma\sigma'}}{z - (\epsilon_k - \mu)}}$$

Example 3: resonant-level model

$$H = \epsilon d^\dagger d + \sum_k \epsilon_k c_k^\dagger c_k + \sum_k V_k \left(d^\dagger c_k + c_k^\dagger d \right)$$

$$G_{dd} = \langle\langle d; d^\dagger \rangle\rangle \qquad G_{kk'} = \langle\langle c_k; c_{k'} \rangle\rangle$$

$$zG_{dd} = 1 + \langle\langle [d, H]; d^\dagger \rangle\rangle$$

$$[d, H] = \epsilon d + \sum_k V_k c_k$$

$$(z - \epsilon) G_{dd} = 1 + \sum_k V_k \underbrace{\langle\langle c_k; d^\dagger \rangle\rangle}_{G_{kd}}$$

$$zG_{kd} = \langle\langle [c_k, H]; d^\dagger \rangle\rangle$$

Here we have set **μ=0**. Actually, this convention is followed in the NRG, too.

$$[c_k, H] = \epsilon_k c_k + V_k d$$

$$(z - \epsilon_k) G_{kd} = V_k \langle\langle d; d^\dagger \rangle\rangle$$

$$G_{kd} = \frac{V_k}{z - \epsilon_k} G_{dd}$$

$$(z - \epsilon) G_{dd} = 1 + \sum_k V_k \frac{V_k}{z - \epsilon_k} G_{dd}$$

Hybridization function: **fully** describes the effect of the conduction band on the impurity

$$\Delta(z) = \sum_k \frac{V_k^2}{z - \epsilon_k}$$

$$\boxed{G_{dd}(z) = \frac{1}{z - \epsilon - \Delta(z)}}$$

Spectral decomposition

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

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

$$G_{AB}(t) = -i\theta(t)(C^{>}_{AB}(t) + \epsilon C^{<}_{AB}(t))$$

ε=+1 if A and B are fermionic, otherwise ε=-1.

$$G_{AB}(z) = \int_{-\infty}^{\infty} \mathrm{d}\omega \frac{\rho_{AB}(\omega)}{z - \omega}$$

spectral representation

$$\rho_{AB}(\omega) = \frac{1}{2\pi}\left(C^{>}_{AB}(\omega) + \varepsilon C^{<}_{AB}(\omega)\right)$$

spectral function

$$\rho_{AB}(\omega) = -\frac{1}{2\pi i}\left(G_{AB}(\omega + i\delta) - G_{AB}(\omega - i\delta)\right) = -\frac{1}{\pi} G''_{AB}(\omega)$$

$$\text{If } A = B^\dagger : G''_{AB}(\omega) = \mathrm{Im} G_{AB}(\omega + i\delta)$$

Relevant for $A = d, B = d^\dagger$

$$G(z) = -\frac{1}{\pi}\int_{-\infty}^{\infty} \frac{\mathrm{Im} G(\omega + i\delta)}{z - \omega}$$

$$p_n = e^{-\beta E_n}$$

$$C^{>}_{AB}(t) = \langle e^{iHt} A e^{-iHt} B \rangle = \sum_{nm} p_n A_{nm} B_{mn} e^{i(E_n - E_m)t}$$

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

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

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

Lehmann representation

Fluctuation-dissipation theorem

$$\langle AB \rangle = -\int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{\pi} \frac{G''_{AB}(\omega)}{1+\epsilon e^{-\beta\omega}}$$

Useful for testing the results of spectral-function calculations!

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

Dynamic quantities: Spectral density

Spectral density/function:

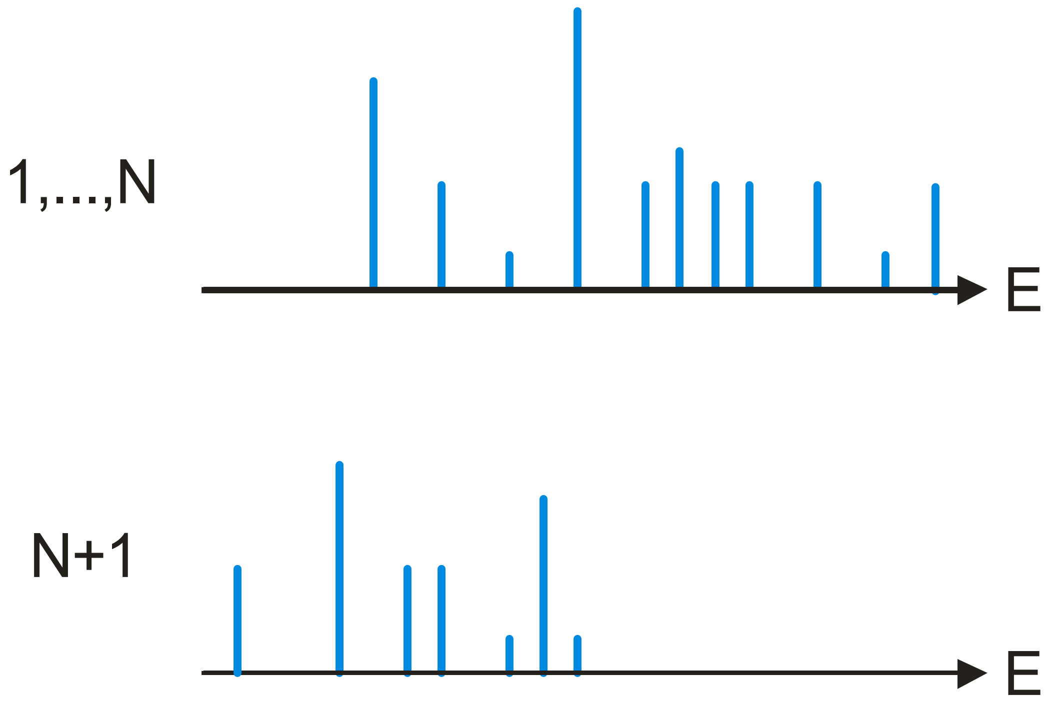
$$A(\omega) = -\frac{1}{\pi}\mathrm{Im}G(\omega + i\delta) = -\frac{1}{\pi}\mathrm{Im}G^R(\omega)$$

Describes single-particle excitations: at which energies it is possible to add an electron (ω>0) or a hole (ω<0).

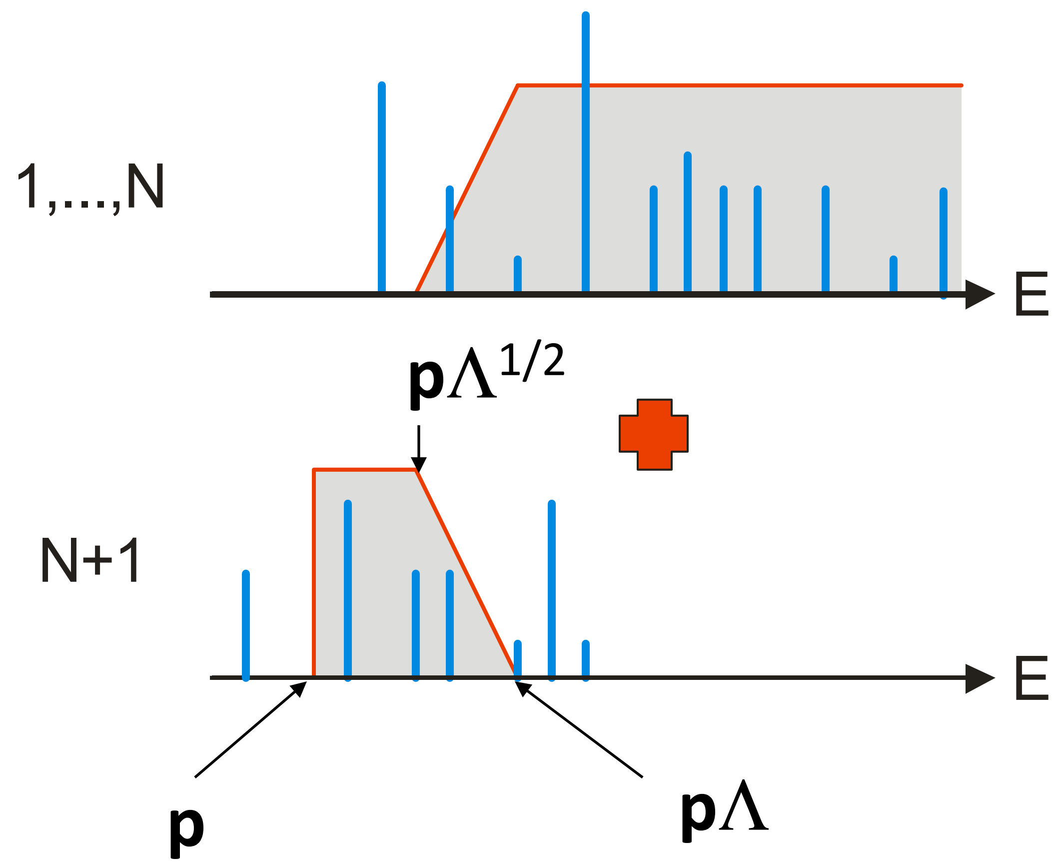
Traditional way: at NRG step N we take excitation energies in the interval [$a\,\omega_N$: $a\,\Lambda^{1/2}\,\omega_N$] or [$a\,\omega_N$: $a\,\Lambda\,\omega_N$], where a is a number of order 1. This defines the value of the spectral function in this same interval.

$$A(\omega) = \sum_{nm} \left| \langle m | d^\dagger | n \rangle \right|^2 \delta(\omega - E_m - E_n) \frac{e^{-\beta E_m} + e^{-\beta E_n}}{Z}$$

Patching



Patching



p: patching parameter (in units of energy scale at N+1-th iteration)

Broadening: traditional log-Gaussian

`smooth=old`

$$w(\omega, E) = lG(\omega, E)\theta(\omega E)\theta(|\omega| - \Omega) + G(\omega, E)\theta(\Omega - |\omega|)$$

$$lG(\omega, E) = \frac{e^{-b^2/4}}{bE\sqrt{\pi}} \exp\left[-\left(\frac{(\log\omega - \log E)}{b}\right)^2\right]$$

$$G(\omega, E) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{\omega - E}{\sigma}\right)^2\right]$$

Broadening: modified log-Gaussian

`smooth=wvd`

$$w(\omega, E) = mlG(\omega, E)h(|E|) + \tilde{G}(\omega, E)[1 - h(|E|)]$$

$$mLG(\omega, E) = \frac{\theta(\omega E)}{\alpha|\omega|\sqrt{\pi}} \exp\left[-\left(\frac{\log(\omega/E)}{\alpha} - \gamma\right)^2\right] \qquad \gamma = \alpha/4$$

$$\tilde{G}(\omega, E) = \frac{1}{\omega_0\sqrt{\pi}} \exp\left[-\left(\frac{\omega - E}{\omega_0}\right)^2\right]$$

$$h(x) = \exp\left[-\left(\frac{\ln(x/\omega_0)}{\alpha}\right)^2\right]$$ for x<ω0, 1 otherwise.

Broadening: modified log-Gaussian

`smooth=new`

$$w(\omega, E) = mlG(\omega, E)h(|\omega|) + \tilde{G}(\omega, E)[1 - h(|\omega|)]$$

Produces smoother spectral functions at finite temperatures (less artifacts at ω=T).

Other kernels

```
smooth=newsc
```

$$w(\omega,E)=mlG(\omega,E)\theta(|\omega|-\Omega)+\tilde{G}(\omega,E)\theta(\Omega-|\omega|)$$

For problems with a superconducting gap (below Ω).

```
smooth=lorentz
```

$$w(\omega,E)=L(\omega,E)$$

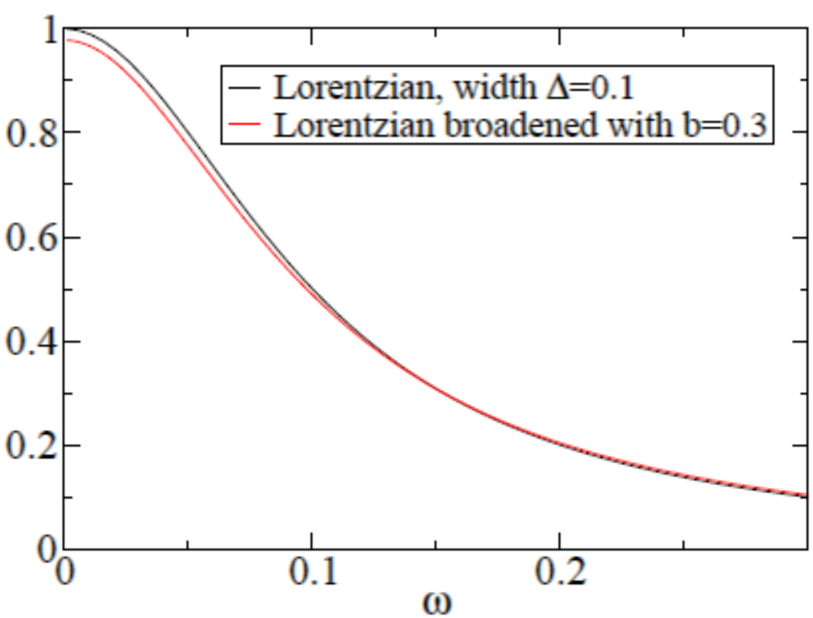
$$L(\omega,E)=\frac{\eta}{\pi}\frac{1}{(\omega-E)^2+\eta^2}$$

If a kernel with constant width is required (rarely!).

Log-Gaussian broadening

$$F_b(\omega, \omega_0) = \frac{e^{-b^2/4}}{b\sqrt{\pi}} \exp\left(-\frac{(\ln\omega - \ln\omega_0)^2}{b^2}\right)$$

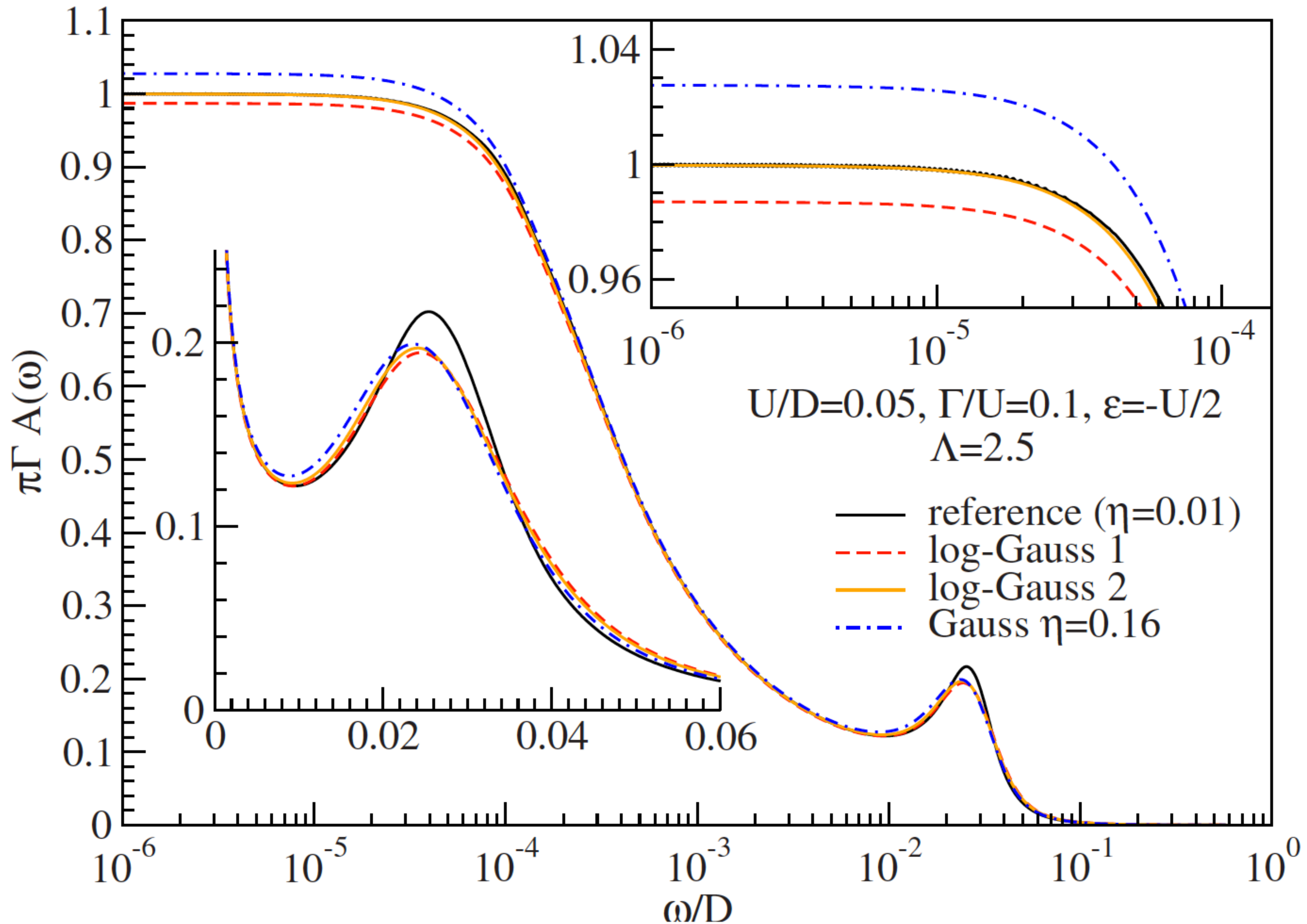
1) Features at ω=0



2) Features at ω≠0

$$\delta\omega_+ = \omega\left(e^{b\sqrt{\ln 2}} - 1\right)$$

$$\delta\omega_- = \omega\left(1 - e^{-b\sqrt{\ln 2}}\right)$$



πΓ A(ω)
ω/D
U/D=0.05, Γ/U=0.1, ε=-U/2
Λ=2.5
reference (η=0.01)
log-Gauss 1
log-Gauss 2
Gauss η=0.16

Equations of motion for SIAM:

$$H=\sum_{\sigma}\epsilon d_{\sigma}^{\dagger}d_{\sigma}+\sum_{k\sigma}\epsilon_k c_{k\sigma}^{\dagger}c_{k\sigma}+\sum_{k\sigma}V_k\left(d_{\sigma}^{\dagger}c_{k\sigma}+c_{k\sigma}^{\dagger}d_{\sigma}\right)+H_{\mathrm{int}}[d_{\sigma}^{\dagger},d_{\sigma}]$$

$$zG_{dd}=1+\langle\langle[d_{\sigma},H];d_{\sigma}^{\dagger}\rangle\rangle$$

$$[d_{\sigma},H]=\epsilon d_{\sigma}+\sum_{k}V_k c_{k\sigma}+[d_{\sigma},H_{\mathrm{int}}]$$

$$(z-\epsilon)G_{dd}=1+\sum_{k}V_k\langle\langle c_k;d^{\dagger}\rangle\rangle+\langle\langle[d_{\sigma},H_{\mathrm{int}}];d_{\sigma}^{\dagger}\rangle\rangle$$

$$(z-\epsilon)G_{dd}=1+\Delta(z)G_{dd}+\langle\langle[d_{\sigma},H_{\mathrm{int}}];d_{\sigma}^{\dagger}\rangle\rangle$$

$$G_{dd}(z)=\frac{1}{z-\epsilon-\boxed{\Sigma(z)}-\Delta(z)}$$

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

Self-energy trick

$$G_\sigma(\omega) = \langle\langle d_\sigma ; d_\sigma^\dagger \rangle\rangle_\omega$$

$$F_\sigma(\omega) = \langle\langle n_{-\sigma} d_\sigma ; d_\sigma^\dagger \rangle\rangle_\omega$$

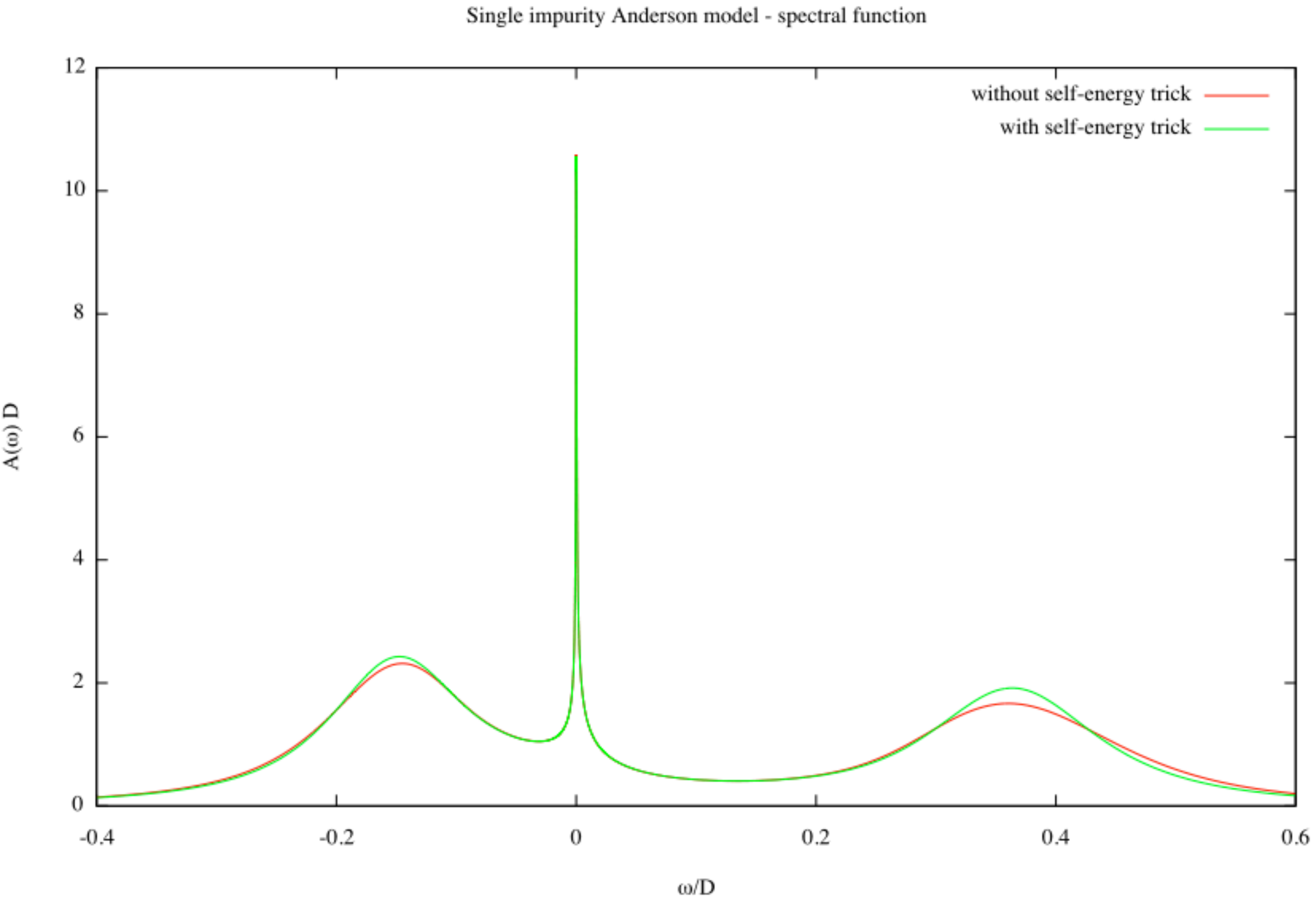
$$\Downarrow$$

$$\Sigma_\sigma(\omega) = U F_\sigma(\omega) / G_\sigma(\omega)$$

$$\Downarrow$$

$$G_\sigma^{\mathrm{improved}}(\omega) = \frac{1}{\omega - \epsilon - \Sigma(\omega) + \Delta(\omega)}$$

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


Single impurity Anderson model - spectral function
without self-energy trick
with self-energy trick
A(ω) D
ω/D
12
10
8
6
4
2
0
-0.4
-0.2
0
0.2
0.4
0.6

Non-orthodox approach: analytic continuation usng Padé approximants

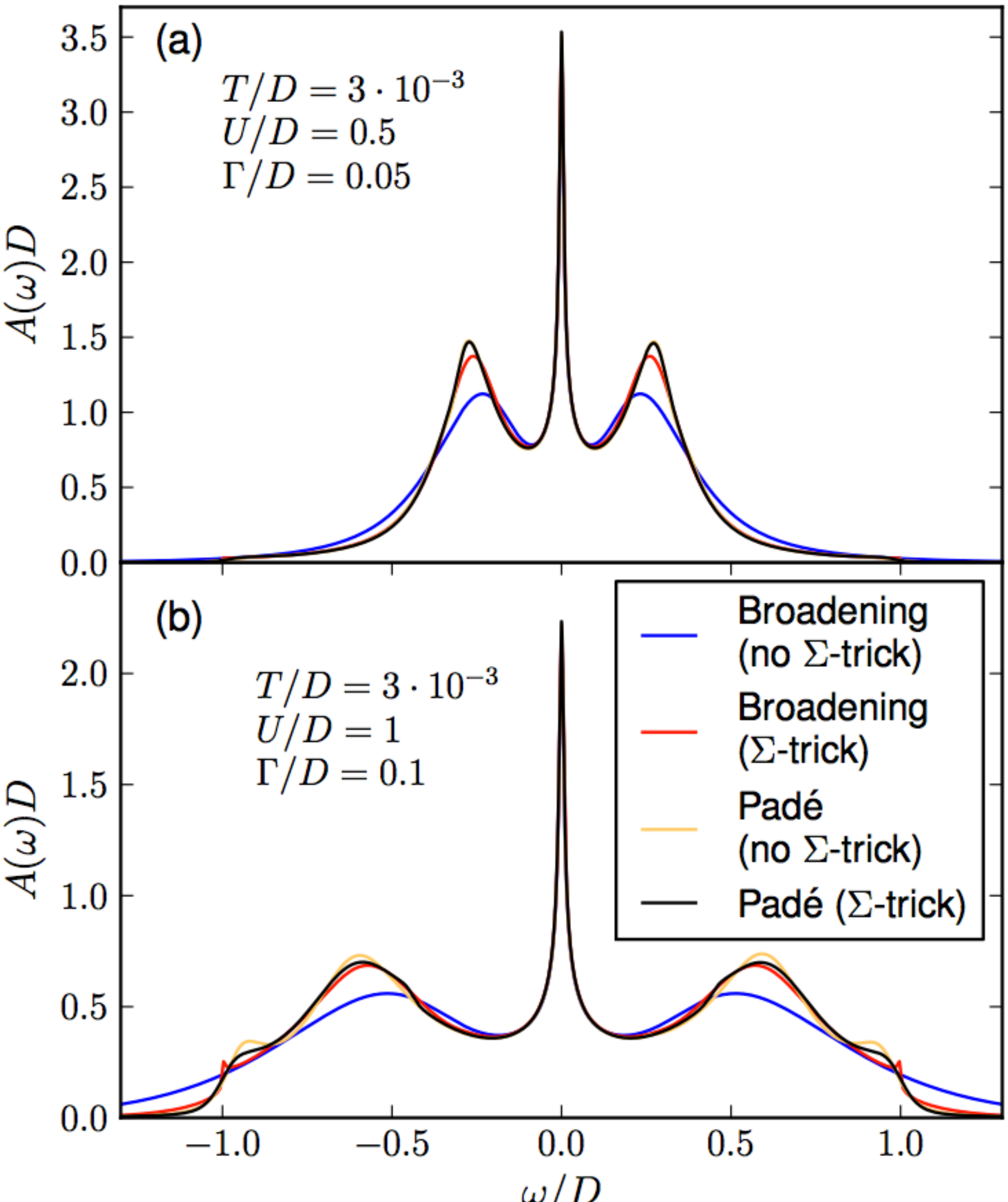
$$i\omega_n = i(2n+1)\pi T$$

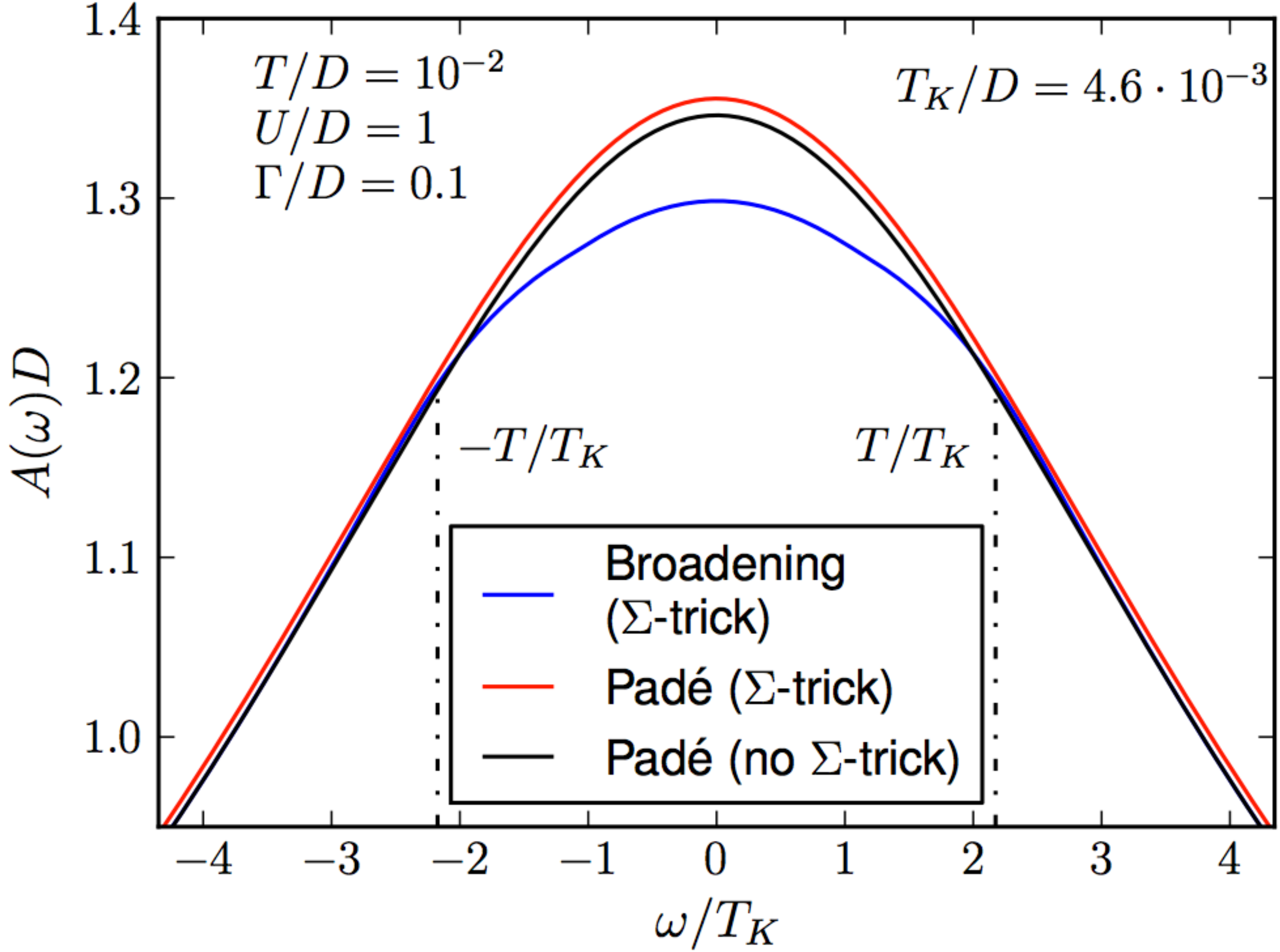
$$G(i\omega_n) = \int \frac{A_{NRG}(\omega)}{i\omega_n - \omega} \mathrm{d}\omega$$

$$G(i\omega_n) = \sum_j \frac{w_j}{i\omega_n - \omega_j}$$

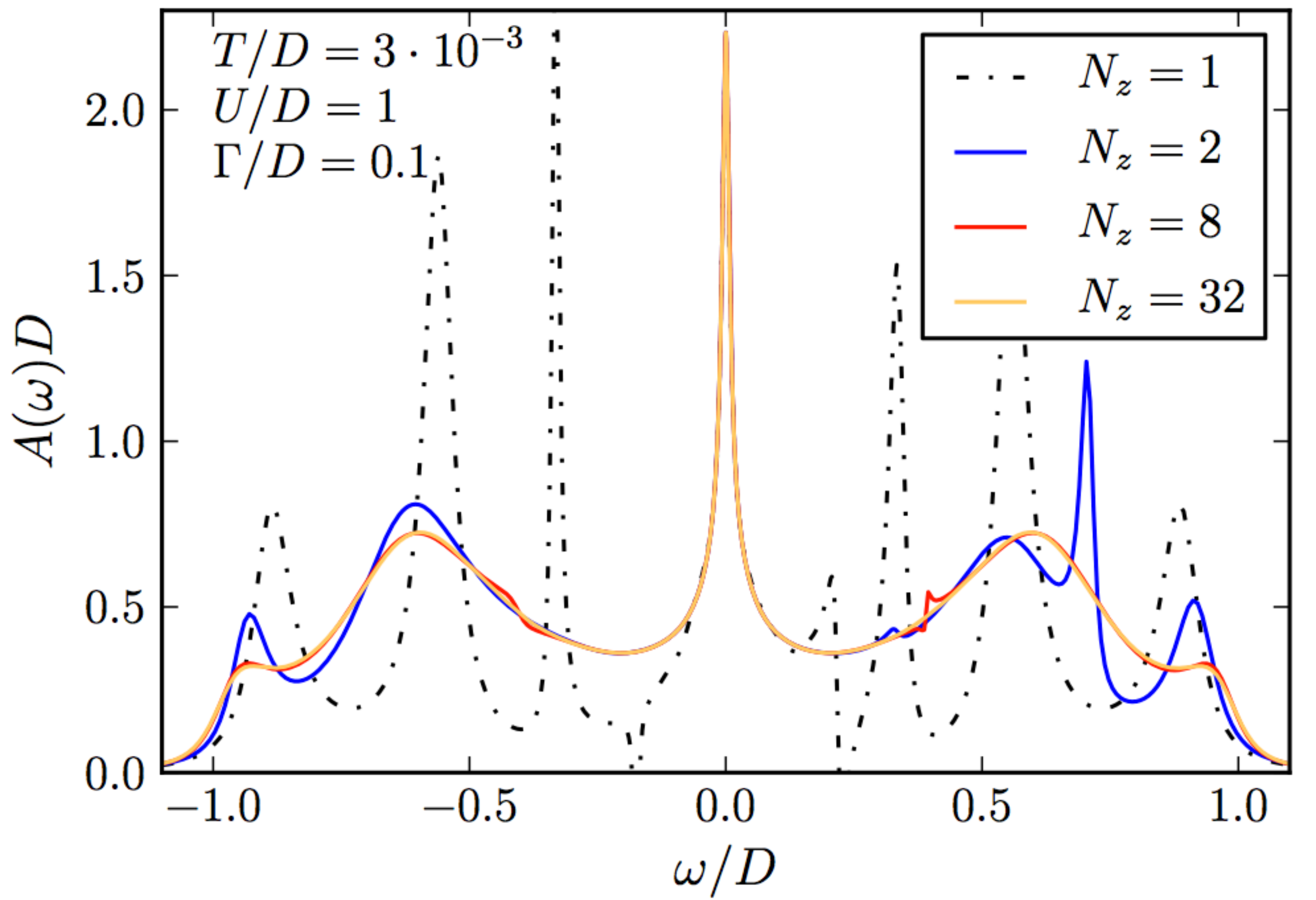
We want to reconstruct G(z) on the real axis. We do that by **fitting a rational function** to G(z) on the imaginary axis (the Matsubara points). This works better than expected. (This is an ill-posed numerical problem. Arbitrary-precision numerics is required.)

Ž. Osolin, R. Žitko, arXiv:1302.3334


(a)
$T/D = 3 \cdot 10^{-3}$
$U/D = 0.5$
$\Gamma/D = 0.05$
(b)
$T/D = 3 \cdot 10^{-3}$
$U/D = 1$
$\Gamma/D = 0.1$
Broadening (no Σ-trick)
Broadening (Σ-trick)
Padé (no Σ-trick)
Padé (Σ-trick)
$A(\omega)D$
ω/D



$T/D = 10^{-2}$
$U/D = 1$
$\Gamma/D = 0.1$
$T_K/D = 4.6 \cdot 10^{-3}$
$-T/T_K$
T/T_K
Broadening (Σ-trick)
Padé (Σ-trick)
Padé (no Σ-trick)
$A(\omega)D$
ω/T_K
1.4
1.3
1.2
1.1
1.0
−4
−3
−2
−1
0
1
2
3
4



$T/D = 3 \cdot 10^{-3}$
$U/D = 1$
$\Gamma/D = 0.1$
$N_z = 1$
$N_z = 2$
$N_z = 8$
$N_z = 32$
$A(\omega)D$
ω/D
0.0
0.5
1.0
1.5
2.0
−1.0
−0.5
0.0
0.5
1.0

Kramers-Kronig transformation

$$G'(\omega) = -\frac{1}{\pi} P \int_{-\infty}^{\infty} \mathrm{d}\omega' \frac{G''(\omega')}{\omega - \omega'}$$

$$G''(\omega) = \frac{1}{\pi} P \int_{-\infty}^{\infty} \mathrm{d}\omega' \frac{G'(\omega')}{\omega - \omega'}$$

Titchmarsh's theorem [edit]

A theorem due to Edward Charles Titchmarsh makes precise the relationship between the boundary values of holomorphic functions in the upper half-plane and the Hilbert transform (Titchmarsh 1948, Theorem 95). It gives necessary and sufficient conditions for a complex-valued square-integrable function $F(x)$ on the real line to be the boundary value of a function in the Hardy space $H^2(U)$ of holomorphic functions in the upper half-plane U.

The theorem states that the following conditions for a complex-valued square-integrable function $F : \mathbf{R} \to \mathbf{C}$ are equivalent:

- $F(x)$ is the limit as $z \to x$ of a holomorphic function $F(z)$ in the upper half-plane such that
$$\int_{-\infty}^{\infty} |F(x+iy)|^2 \, dx < K.$$
- $-\mathrm{Im}(F)$ is the Hilbert transform of $\mathrm{Re}(F)$, where $\mathrm{Re}(F)$ and $\mathrm{Im}(F)$ are real-valued functions with $F = \mathrm{Re}(F) + \mathrm{i}\,\mathrm{Im}(F)$.
- The Fourier transform $\mathcal{F}(F)(x)$ vanishes for $x < 0$.

PHYSICAL REVIEW B VOLUME 33, NUMBER 11 1 JUNE 1986

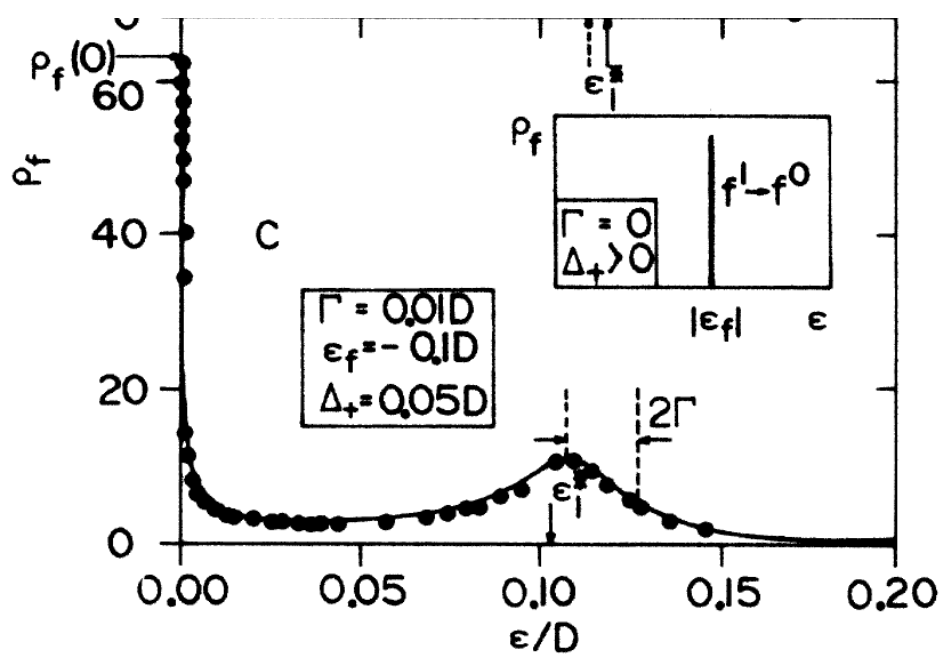
Photoemission spectroscopy for the spin-degenerate Anderson model

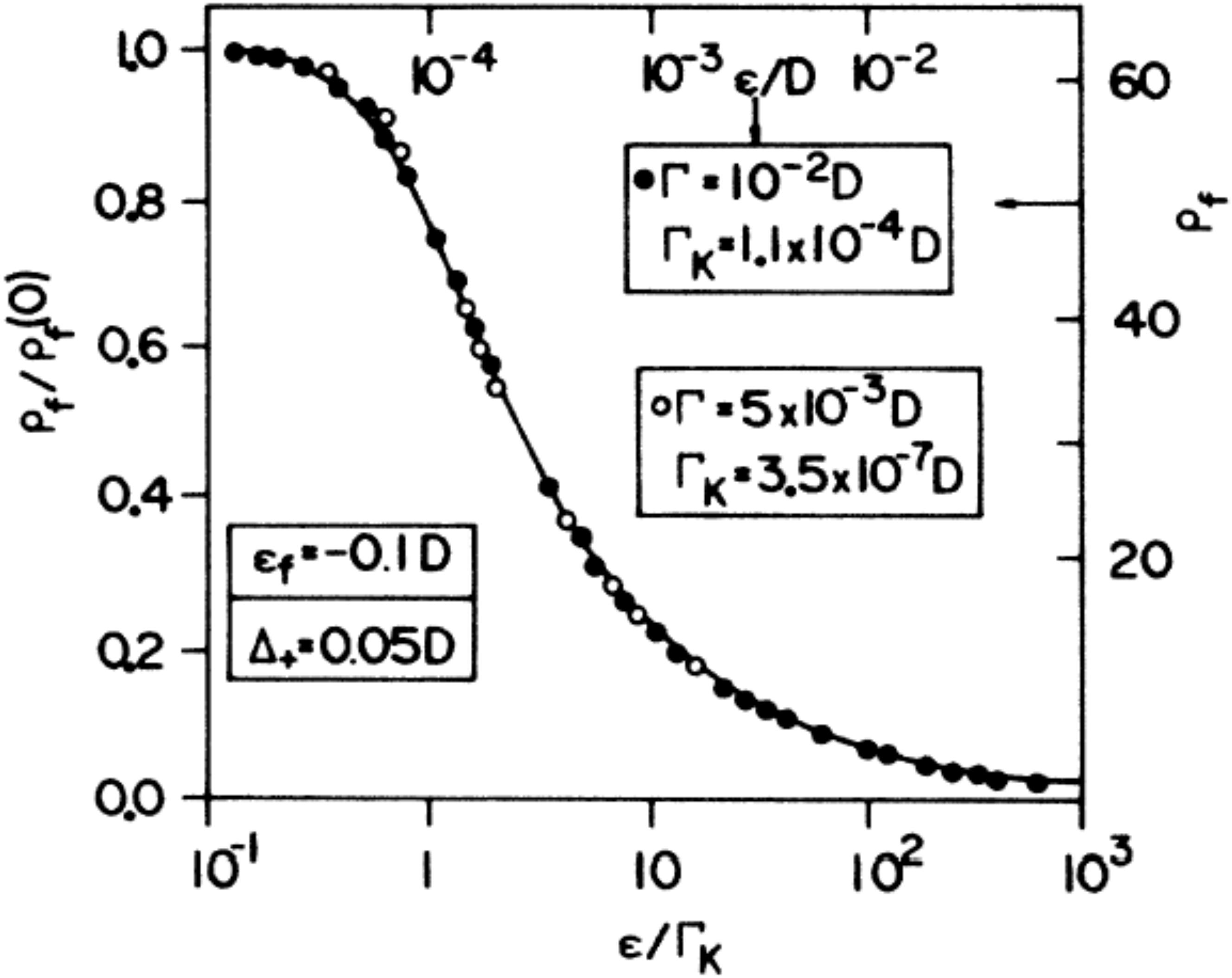
H. O. Frota* and L. N. Oliveira
Departamento de Física e Ciência dos Materiais, Instituto de Física e Química de São Carlos, Universidade de São Paulo, 13560 São Carlos, São Paulo, Brazil
(Received 17 March 1986)

PHYSICAL REVIEW B VOLUME 45, NUMBER 3 15 JANUARY 1992-I

Shape of the Kondo resonance

H. O. Frota*
Department of Physics and Astronomy, The University of Tennessee, Knoxville, Tennessee 37996-1200
(Received 6 August 1990; revised manuscript received 29 July 1991)





$$\rho_f(\epsilon) = \left(\tfrac{1}{2}\pi\Gamma\right) \mathrm{Re}\left[(\epsilon + i\Gamma_K)/i\Gamma_K\right]^{-1/2}$$

Inverse-square-root asymptotic behavior

Inverse square root behavior also found using the quantum Monte Carlo (QMC) approach:
Silver, Gubernatis, Sivia, Jarrell, Phys. Rev. Lett. **65** 496 (1990)

Anderson orthogonality catastrophe physics

Doniach, Šunjić 1970 *J. Phys. C: Solid State Phys.* **3** 285

Doniach-Šunjić: $\rho_f \sim E^{-\alpha}$, $\alpha = 1 - 2(\delta/\pi)^2$

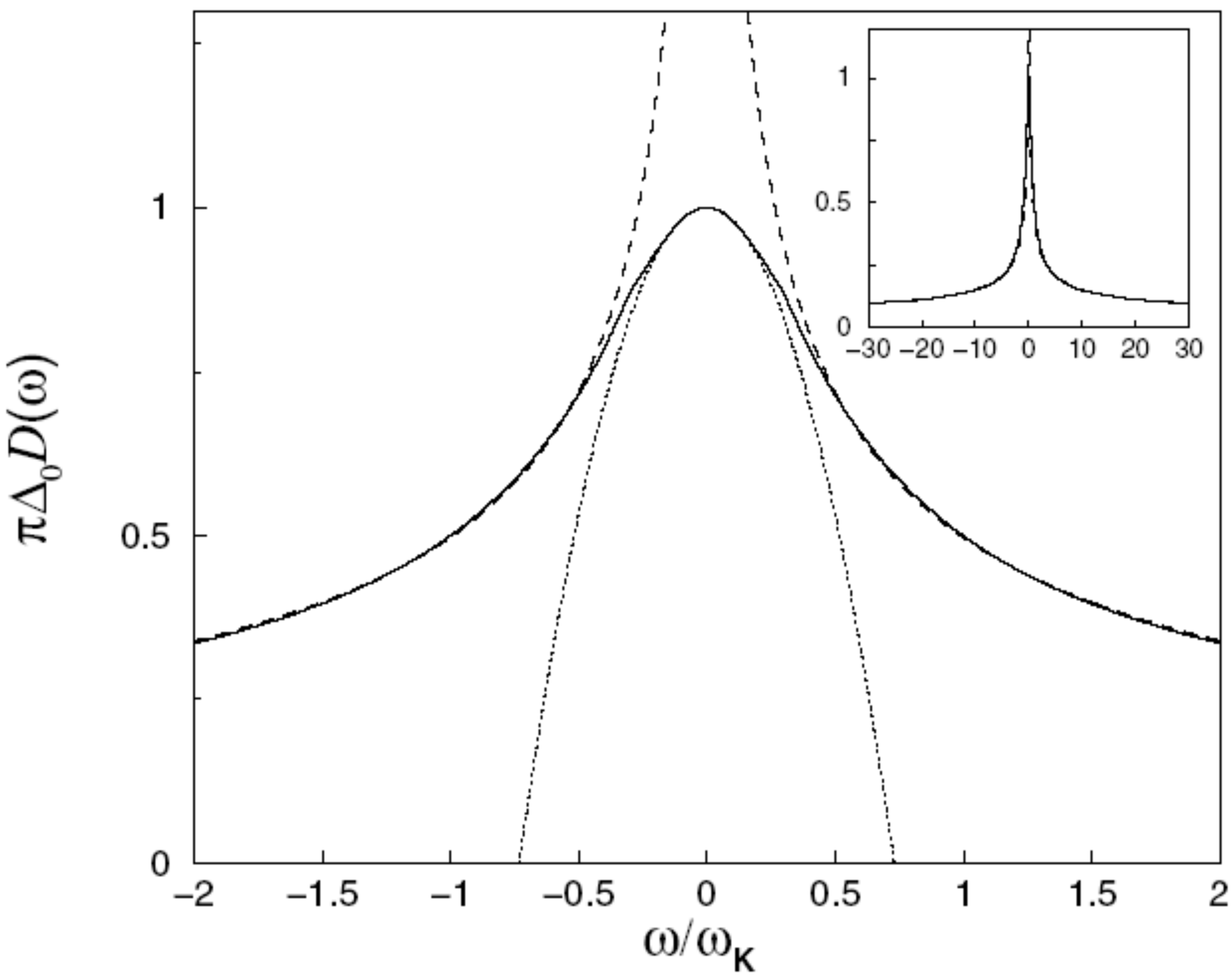
$\delta = \pi/2$ $E = \epsilon + i\Gamma_K$

$$\rho_f(\epsilon) = (\tfrac{1}{2}\pi\Gamma)\,\mathrm{Re}[(\epsilon + i\Gamma_K)/i\Gamma_K]^{-1/2}$$

J. Phys.: Condens. Matter **12** (2000) 4899–4921. Printed in the UK PII: S0953-8984(00)10831-8

The soft-gap Anderson model: comparison of renormalization group and local moment approaches

Ralf Bulla†, Matthew T Glossop‡, David E Logan‡ and Thomas Pruschke§



J. Phys.: Condens. Matter **13** (2001) 4505–4517 www.iop.org/Journals/cm PII: S0953-8984(01)23294-9

On the scaling spectrum of the Anderson impurity model

Nigel L Dickens and David E Logan

University of Oxford, Physical and Theoretical Chemistry Laboratory, South Parks Rd, Oxford OX1 3QZ, UK

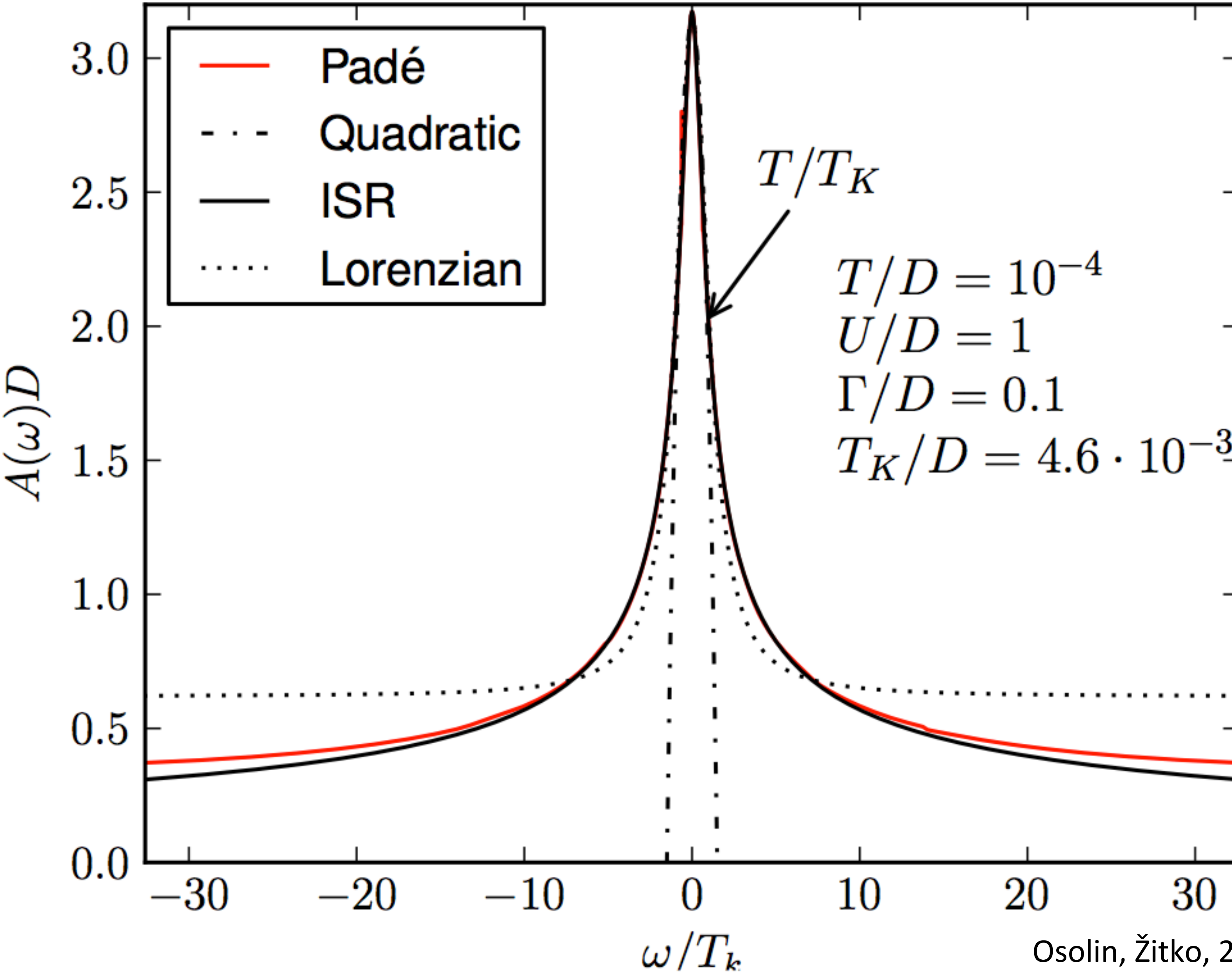
Received 23 March 2001

$$\pi \Delta_0 D(\omega) = \frac{1}{2}\left\{\frac{1}{[(4/\pi)\ln(|\omega'|)]^2+1} + \frac{5}{[(4/\pi)\ln(|\omega'|)]^2+25}\right\}$$

Arguments:

- Kondo model features characteristic logarithmic behavior, i.e., as a function of T, all quantities are of the form $[\ln(T/T_K)]^{-n}$.
- Better fit to the NRG data than the Doniach-Šunjić form.

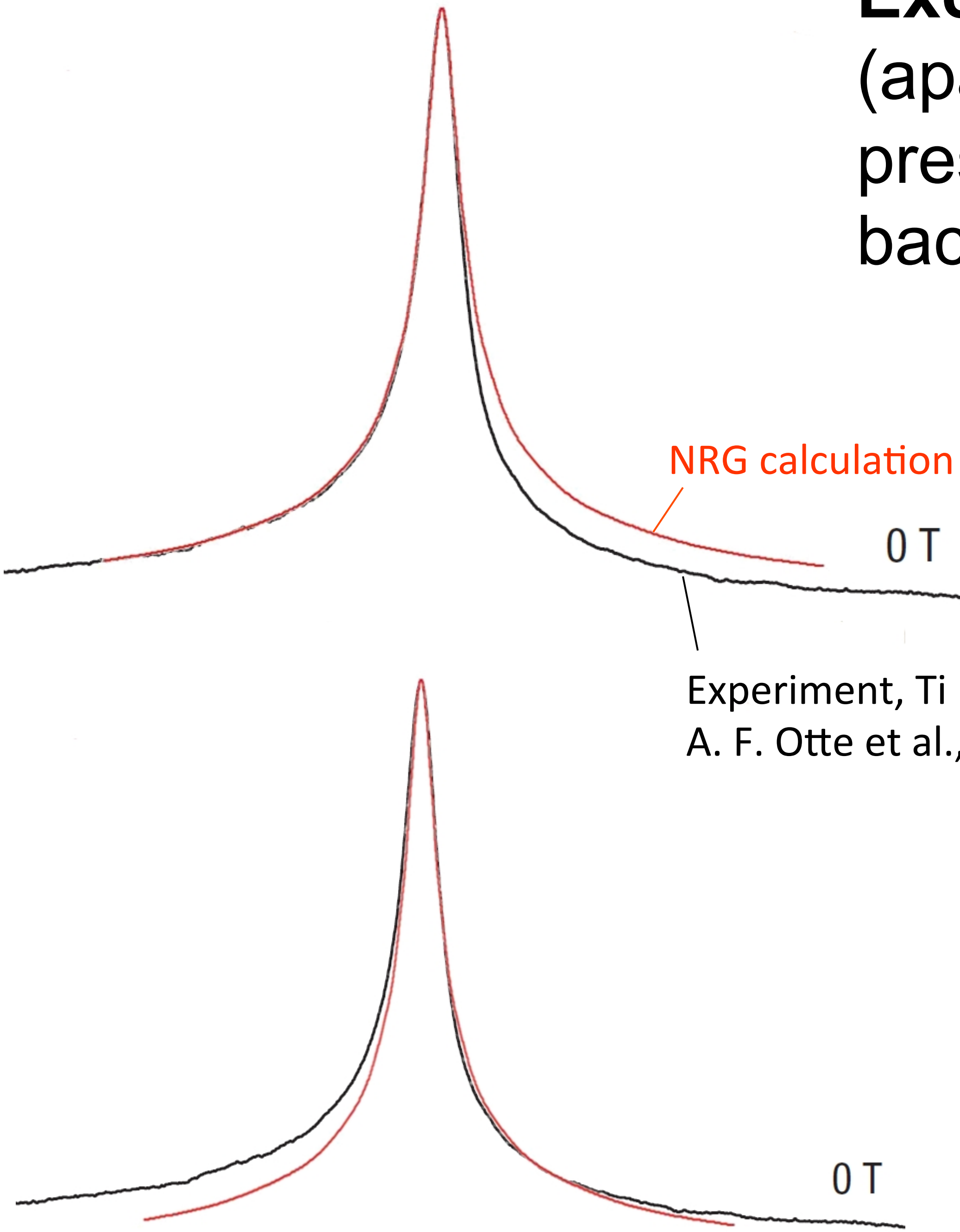
(No constant term has to be added, either.)



Osolin, Žitko, 2013

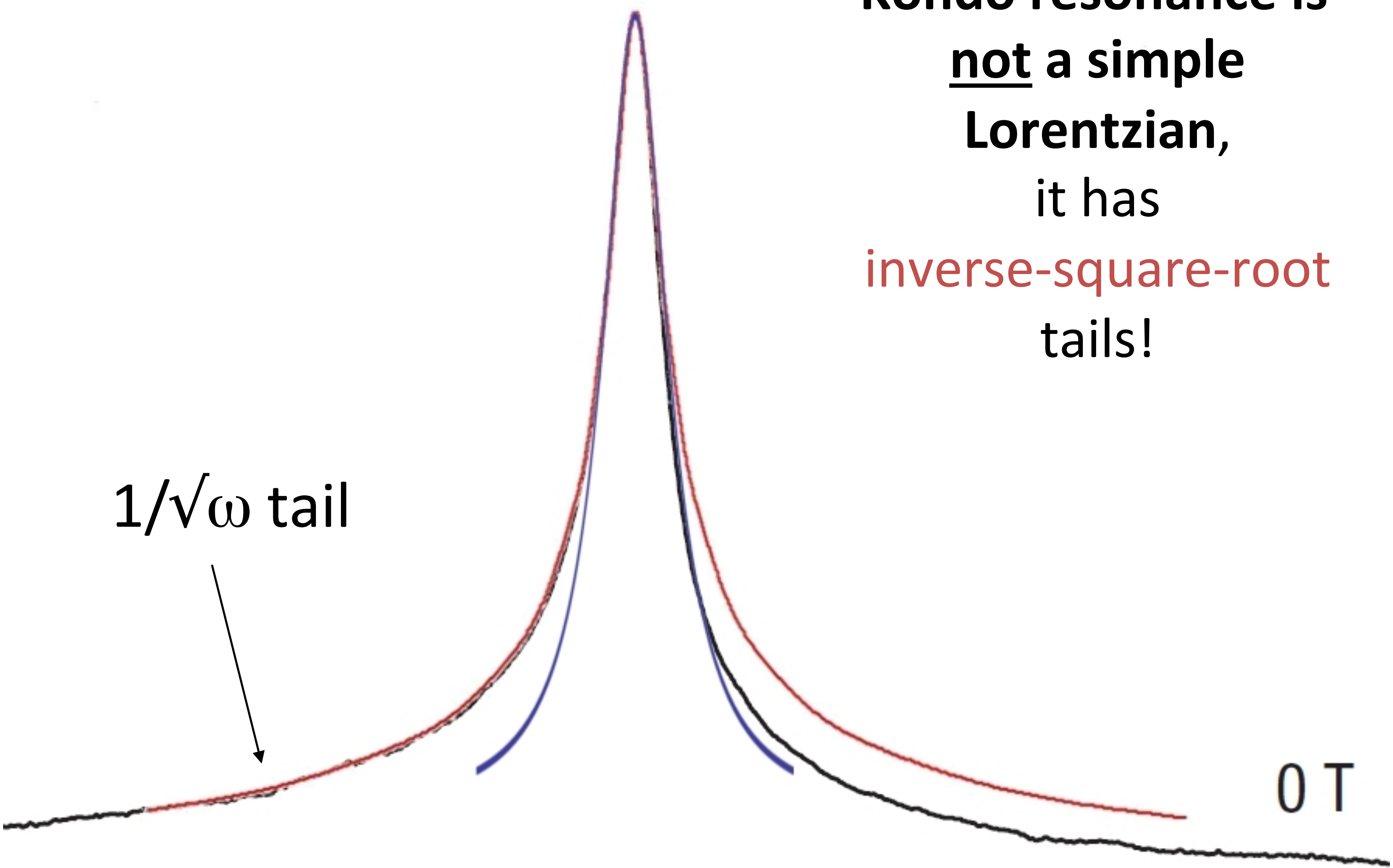
Comparison with experiment?

Excellent agreement
(apart from asymmetry, presumably due to some background processes)



Experiment, Ti (S=1/2) on CuN/Cu(100) surface
A. F. Otte et al., Nature Physics **4**, 847 (2008)

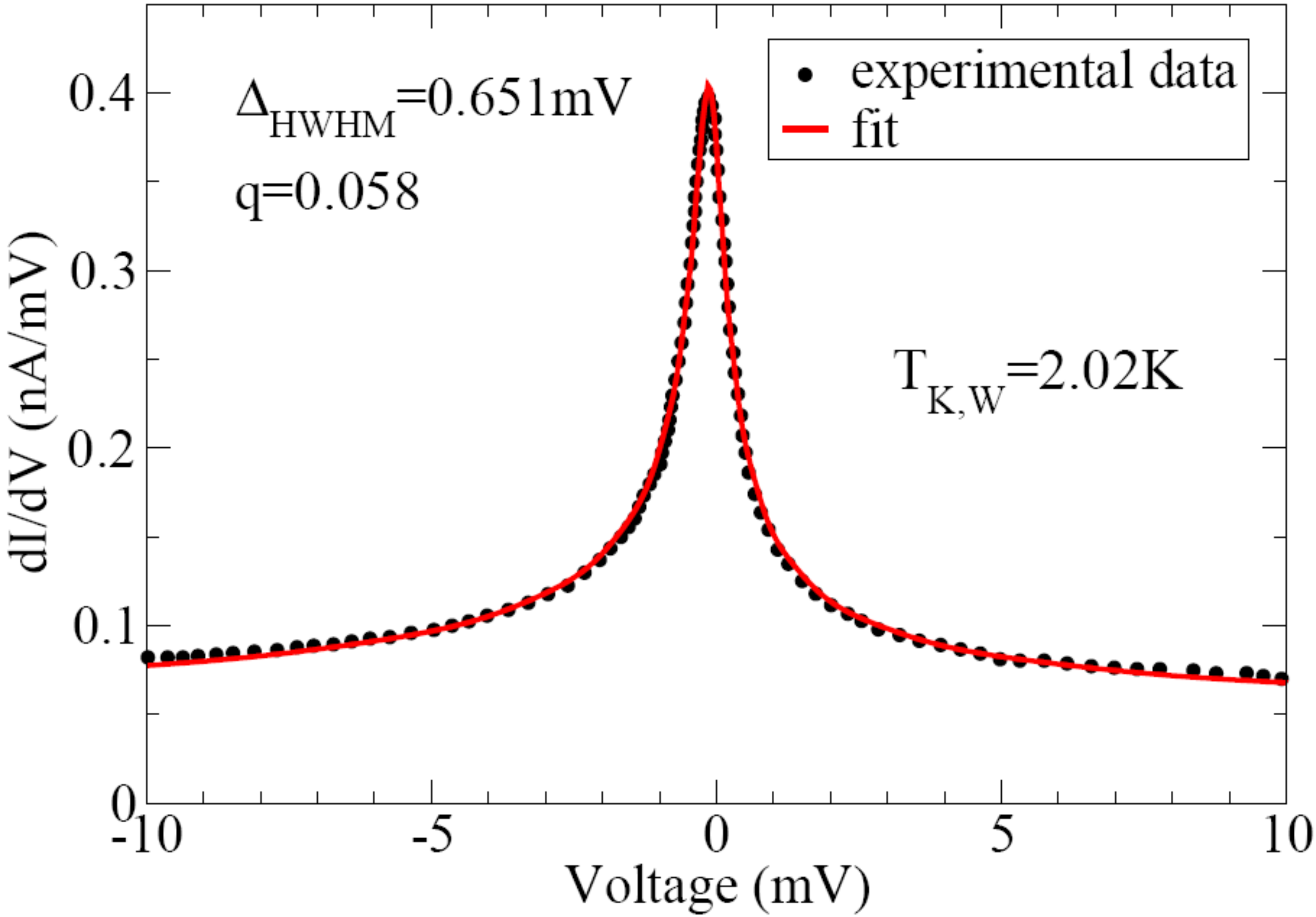
Kondo resonance is
<u>not</u> a simple
Lorentzian,
it has
inverse-square-root
tails!



Fano-like interference process between resonant and background scattering:

$$(\mathrm{d}I/\mathrm{d}V)(V) = a + b\left[(1-q^2)\mathrm{Im}\,G(eV) + 2q\mathrm{Re}\,G(eV)\right]$$

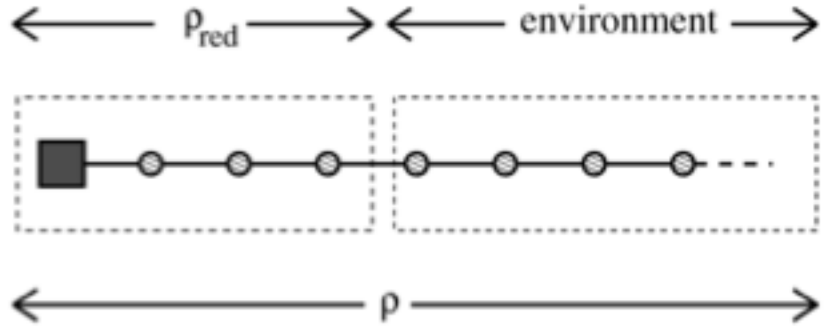
$$G(\omega) = G_{\mathrm{Kondo}}[(\omega - \omega_0)/\Delta_{\mathrm{HWHM}}]$$



RŽ, Phys. Rev. B 84, 195116 (2011)

Density-matrix NRG

- Problem: Higher-energy parts of the spectra calculated without knowing the true ground state of the system
- Solution: 1) Compute the density matrix at the temperature of interest. It contains full information about the ground state. 2) Evaluate the spectral function in an additional NRG run using the *reduced density matrix* instead of the simple Boltzmann weights.



$$\hat{\rho} = \sum_{m_1, m_2, n_1, n_2} \rho_{m_1 n_1 m_2 n_2} |m_1\rangle_{\mathrm{env}} |n_1\rangle_{\mathrm{sys}} \langle n_2|\langle m_2|$$

$$\hat{\rho}^{\mathrm{red}} = \sum_{n_1, n_2} \rho^{\mathrm{red}}_{n_1 n_2} |n_1\rangle_{\mathrm{sys}} \langle n_2|$$

$$\rho^{\mathrm{red}}_{n_1 n_2} = \sum_{m} \rho_{m n_1, m n_2}$$

W. Hofstetter, PRL 2000

$$\rho = \frac{1}{Z} \sum_{QSS_z\omega} \exp(-\beta E_{QS\omega}) |QSS_z\omega\rangle\langle QSS_z\omega|$$

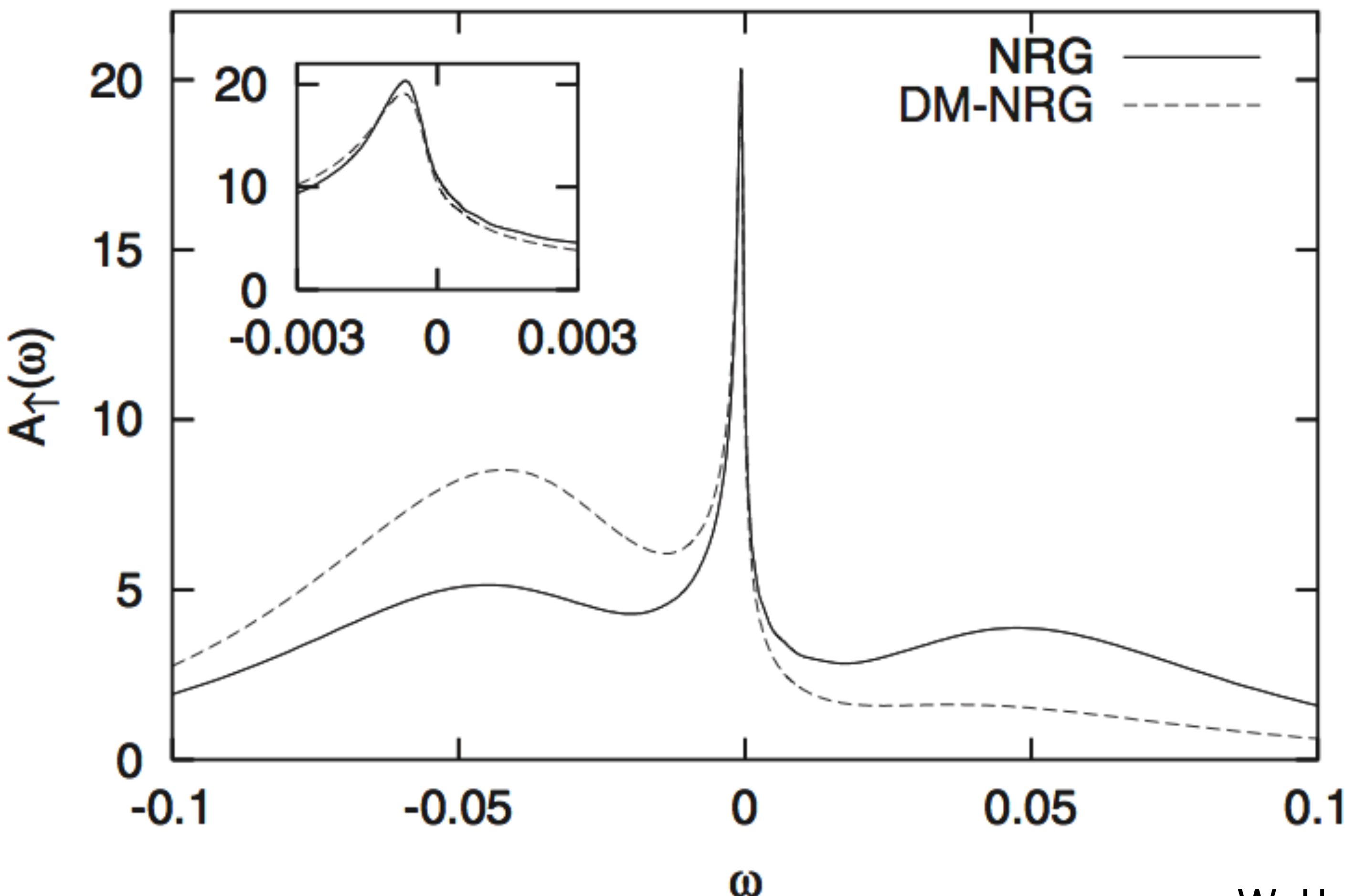
$$\rho^N_{\text{reduced}} = \sum_{QSS_z} \sum_{rr'} C^{QS,N}_{rr'} |QSS_z r\rangle_N \langle QSS_z r'|_N$$

$$\begin{aligned} C^{QS,N}_{rr'} = & \sum_{\omega\omega'} C^{Q-1,S,N+1}_{\omega\omega'} U_{Q-1,S}(\omega|r1) U_{Q-1,S}(\omega'|r'1) \\ & + \sum_{\omega\omega'} C^{Q+1,S,N+1}_{\omega\omega'} U_{Q+1,S}(\omega|r4) U_{Q+1,S}(\omega'|r'4) \\ & + \frac{2S+2}{2S+1} \sum_{\omega\omega'} C^{Q,S+\frac{1}{2},N+1}_{\omega\omega'} U_{Q,S+\frac{1}{2}}(\omega|r2) U_{Q,S+\frac{1}{2}}(\omega'|r'2) \\ & + \frac{2S}{2S+1} \sum_{\omega\omega'} C^{Q,S-\frac{1}{2},N+1}_{\omega\omega'} U_{Q,S-\frac{1}{2}}(\omega|r3) U_{Q,S-\frac{1}{2}}(\omega'|r'3) \end{aligned}$$

DMNRG for non-Abelian symmetries: Zitko, Bonca, PRB 2006

Spectral function computed as:

$$A_\mu^N(\omega) = \sum_{ijm} \left(\langle j|d_\mu^\dagger|m\rangle \langle j|d_\mu^\dagger|i\rangle \rho_{im}^{\mathrm{reduced}} + \langle j|d_\mu^\dagger|m\rangle \langle i|d_\mu^\dagger|m\rangle \rho_{ji}^{\mathrm{reduced}} \right) \delta(\omega - (E_j - E_m))$$



W. Hofstetter, PRL 2000

Construction of the complete basis set

$$|\alpha_{\mathrm{imp}}, \alpha_0, \ldots, \alpha_N\rangle$$

$$H_m|r\rangle = E_r|r\rangle$$

$$e = \{\alpha_{m+1}, \ldots, \alpha_N\}$$

$$\begin{tikzcd}
 & {|r, e; m\rangle} \arrow[dl] \arrow[d] \\
{|k, e; m\rangle_{\mathrm{kp}}} \arrow[d] & {|l, e; m\rangle_{\mathrm{dis}}} \\
{|k, \alpha_{m+1}, e'; m\rangle_{\mathrm{kp}}} &
\end{tikzcd}$$

$$\mathcal{F}_N = \mathrm{span}\{|l, e; m\rangle_{\mathrm{dis}}\}$$

Completeness relation:

$$\sum_{m}^{N} \sum_{l,e} |l,e;m\rangle_{\mathrm{dis}\ \mathrm{dis}}\langle l,e;m| = 1$$

Complete-Fock-space NRG:

$$\rho = \frac{1}{Z} e^{-\beta H} \approx \sum_{l} \rho_l |l;N\rangle\langle l;N|$$

$$\rho_l = \frac{e^{-\beta E_l^N}}{Z_N} \qquad Z_N = \sum_{l} e^{-\beta E_l^N}$$

Anders, Schiller, PRL 2005, PRB 2006

$$G^{i}_{A,B}(z) = \frac{1}{Z}\sum_{l,l'} \langle l;N|A|l';N\rangle\langle l';N|B|l;N\rangle \frac{e^{-\beta E^N_l} - s e^{-\beta E^N_{l'}}}{z + E^N_l - E^N_{l'}}$$

$$G^{ii}_{A,B}(z) = \sum_{m=m_{\min}}^{N-1} \sum_{l} \sum_{k,k'} A_{l,k'}(m)\rho^{\text{red}}_{k',k}(m) B_{k,l}(m) \frac{-s}{z + E_l - E_k}$$

$$G^{iii}_{A,B}(z) = \sum_{m=m_{\min}}^{N-1} \sum_{l} \sum_{k,k'} B_{l,k'}(m)\rho^{\text{red}}_{k',k}(m) A_{k,l}(m) \frac{1}{z + E_k - E_l}$$

$$\rho^{\text{red}}_{k,k'}(m) = \sum_{e} \langle k,e;m|\hat{\rho}|k',e;m\rangle$$

Peters, Pruschke, Anders, PRB 2006

Full-density-matrix NRG:

$$\rho = \sum_m \sum_{le} |le;m\rangle \frac{e^{-\beta E_l^m}}{Z} \langle le;m|$$

Weichselbam, von Dellt, PRL 2007

$$G(\omega) = \sum_{m'=m_0+1}^{N} \frac{w_{m'}}{Z_{m'}} \sum_{ll'} A_{ll'}^{m'} B_{l'l}^{m'} \frac{(e^{-\beta E_l^{m'}} + e^{-\beta E_{l'}^{m'}})}{\omega + E_l^{m'} - E_{l'}^{m'} + i\delta}$$

$$+ \sum_{m'=m_0+1}^{N-1} \frac{w_{m'}}{Z_{m'}} \sum_{lk} A_{lk}^{m'} B_{kl}^{m'} \frac{e^{-\beta E_l^{m'}}}{\omega + E_l^{m'} - E_k^{m'} + i\delta}$$

$$+ \sum_{m'=m_0+1}^{N-1} \frac{w_{m'}}{Z_{m'}} \sum_{kl} A_{kl}^{m'} B_{lk}^{m'} \frac{e^{-\beta E_l^{m'}}}{\omega + E_k^{m'} - E_l^{m'} + i\delta}$$

$$+ \sum_{m=m_0+1}^{N-1} \sum_{lkk'} A_{lk}^{m} \frac{\mathrm{R}_{\mathrm{red}}^{m}(k,k') B_{k'l}^{m}}{\omega + E_l^{m} - E_k^{m} + i\delta}$$

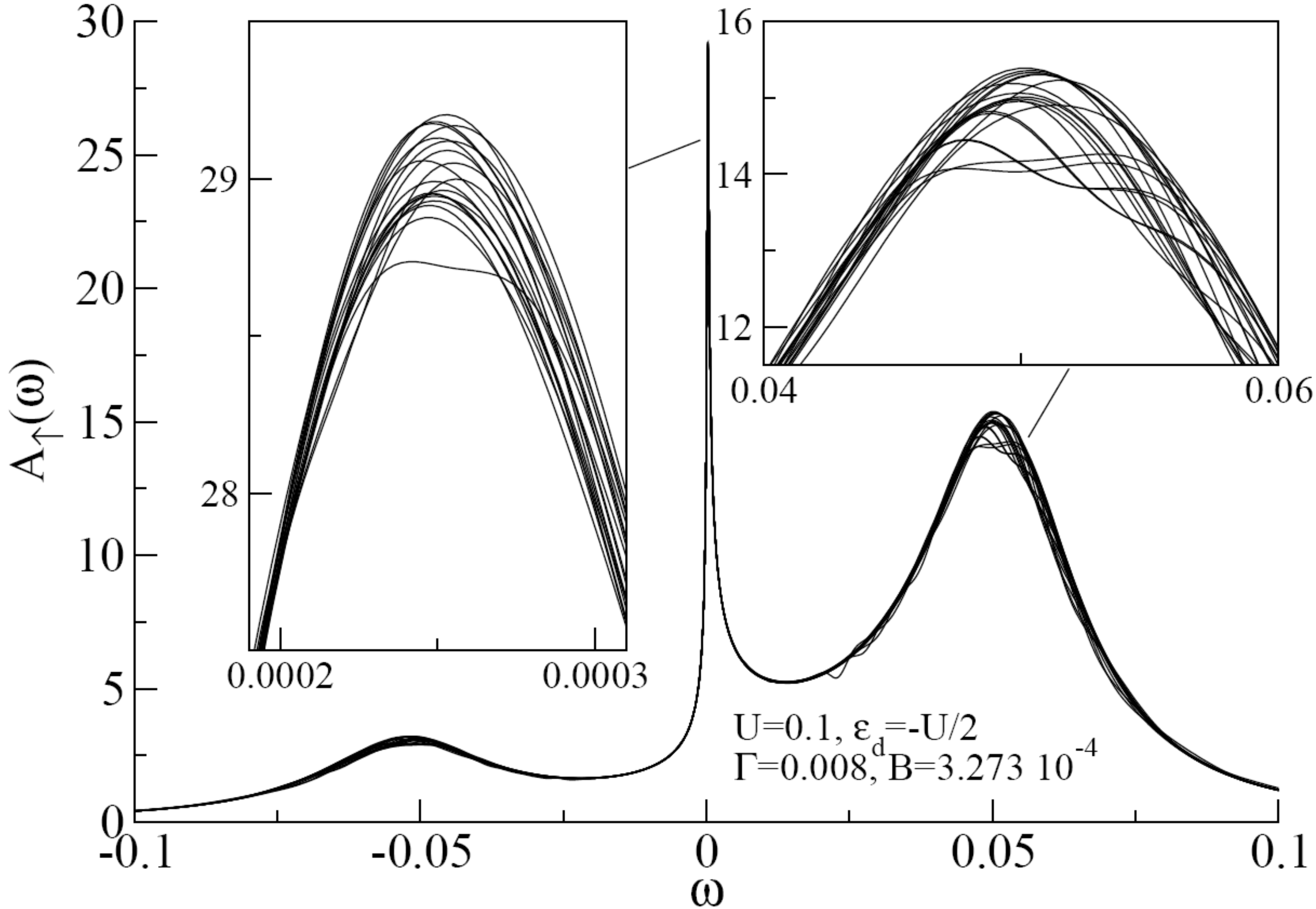
$$+ \sum_{m=m_0+1}^{N-1} \sum_{kk'l} A_{kl}^{m} \frac{\mathrm{R}_{\mathrm{red}}^{m}(k',k) B_{lk'}^{m}}{\omega + E_k^{m} - E_l^{m} + i\delta},$$

Costi, Zlatić, PRB 2010

CFS vs. FDM vs. DMNRG

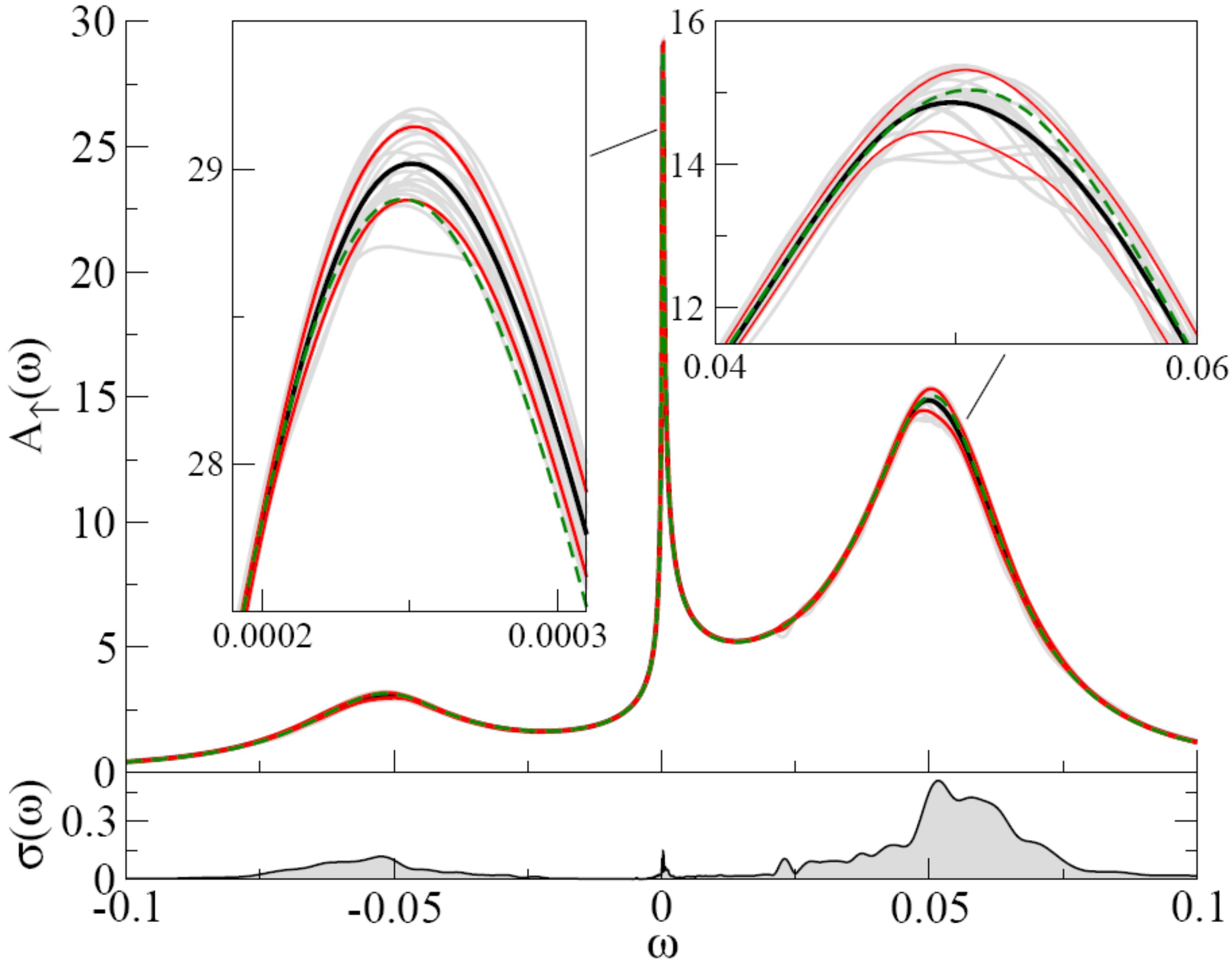
- CFS and FDM equivalent at T=0
- FDM recommended at T>0
- CFS and FDM are slower than DMNRG (all states need to be determined, more complex expressions for spectral functions)
- No patching, thus no arbitrary parameter as in DMNRG

Error bars in NRG?

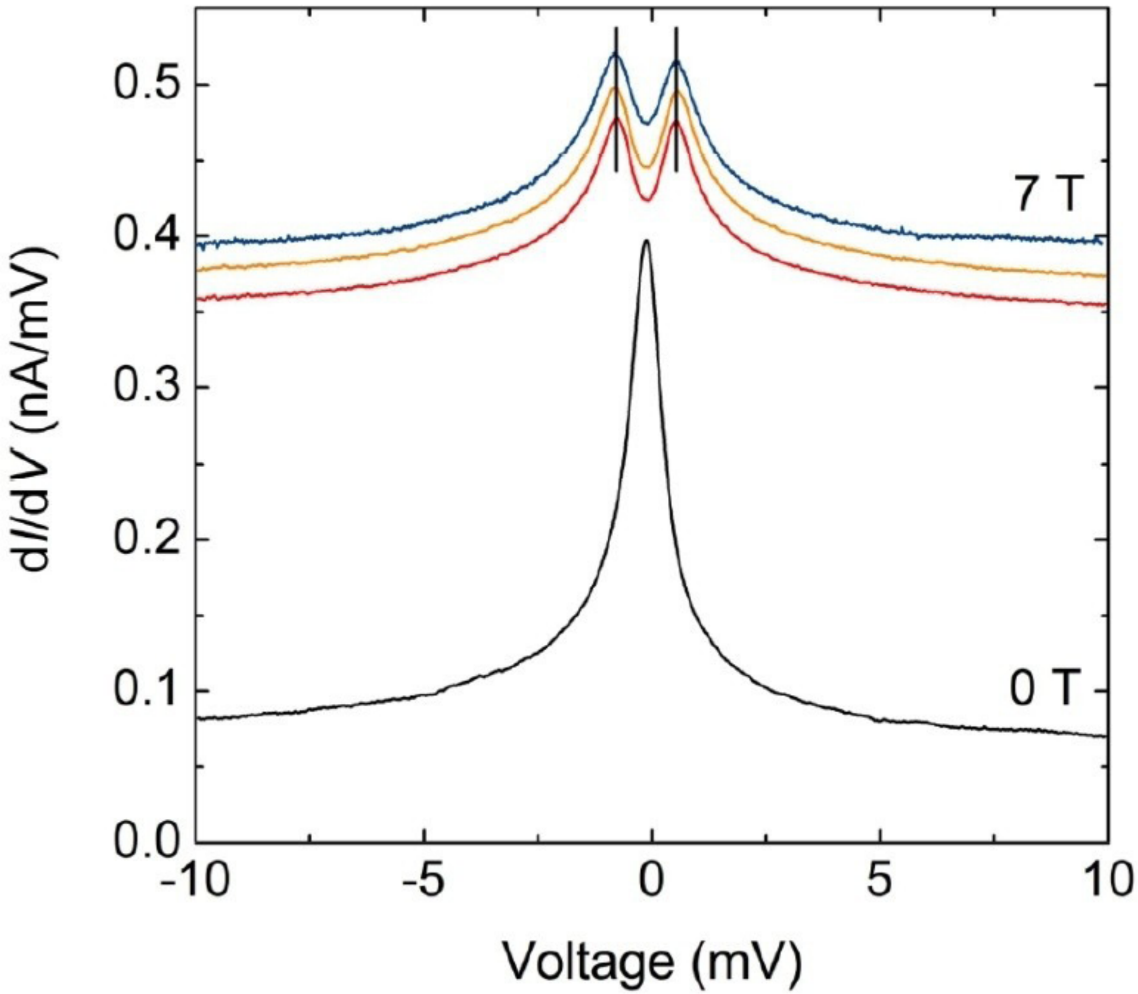


Rok Žitko, PRB **84**, 085142 (2011)

Average + confidence region!



Effect of the magnetic field: resonance splitting



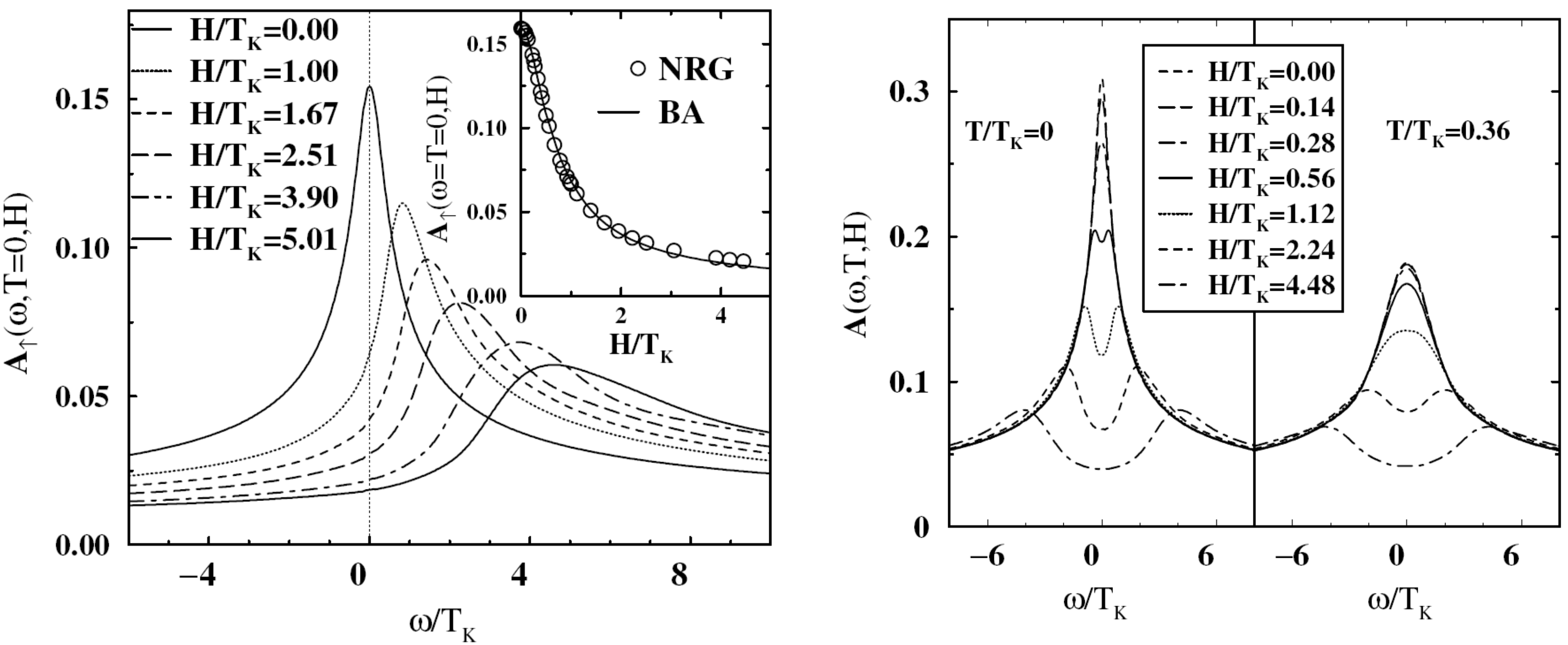
Ti atom

S=1/2

A. F. Otte et al., Nature Physics **4**, 847 (2008)

Kondo Effect in a Magnetic Field and the Magnetoresistivity of Kondo Alloys

T. A. Costi
Institut Laue-Langevin, 6 rue Jules Horowitz, B.P. 156, 38042 Grenoble Cedex 9, France
(Received 10 April 2000)

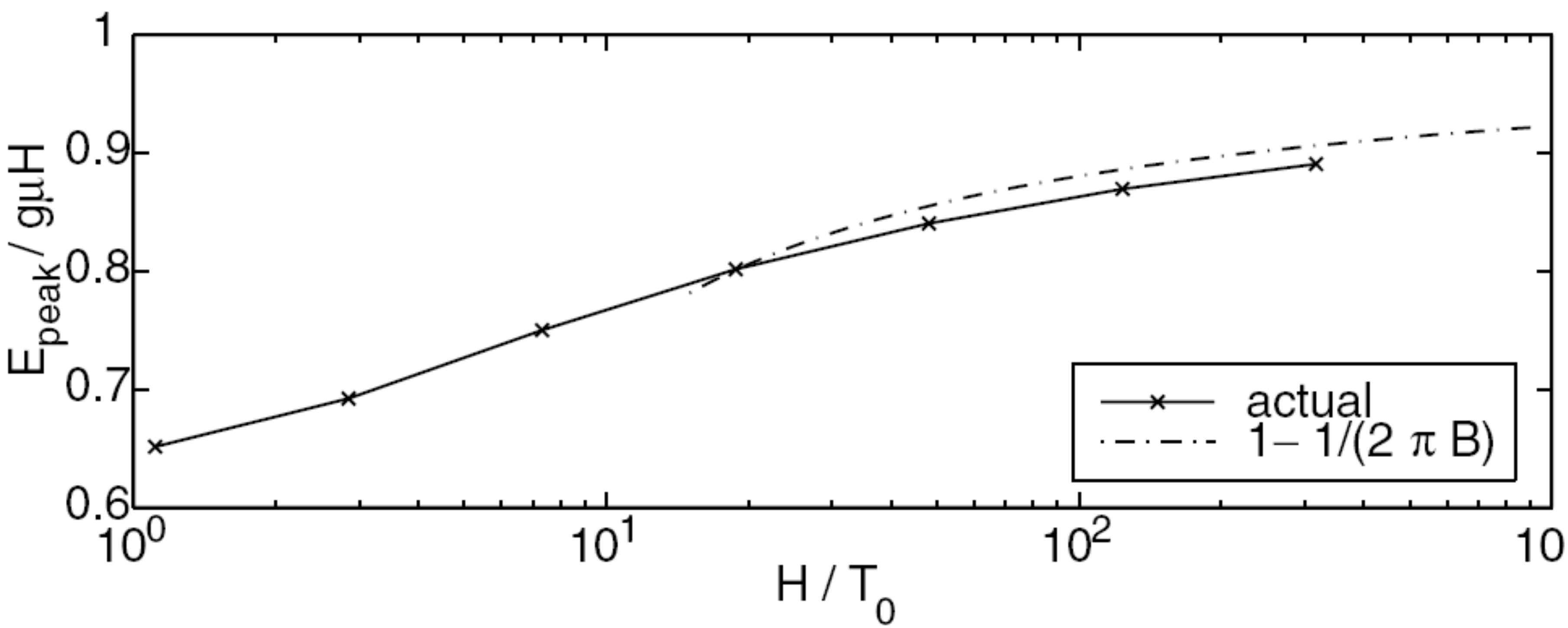


Numerical renormalization group (NRG) calculation

VOLUME 85, NUMBER 8 PHYSICAL REVIEW LETTERS 21 AUGUST 2000

Anomalous Magnetic Splitting of the Kondo Resonance

Joel E. Moore and Xiao-Gang Wen
Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139
(Received 4 November 1999)



Bethe Ansatz calculation using spinon density of states

J. Phys.: Condens. Matter **13** (2001) 9713–9738 PII: S0953-8984(01)26991-4

Field-dependent dynamics of the Anderson impurity model

David E Logan and Nigel L Dickens

Physical and Theoretical Chemistry Laboratory, University of Oxford, South Parks Road, Oxford OX1 3QZ, UK

Exact result for $B \to 0$: $\Delta = (\mathbf{2/3}) g\mu_B B$

Suggestion that for large B, Δ is larger than $g\mu_B B$.

PHYSICAL REVIEW B 73, 045117 (2006)

Field dependent quasiparticles in a strongly correlated local system

A. C. Hewson, J. Bauer, and W. Koller
Department of Mathematics, Imperial College, London SW7 2AZ, United Kingdom
(Received 26 August 2005; published 19 January 2006)

$$\lim_{h\to 0}\frac{\varepsilon_p(h)}{h} = \frac{R}{1+(R-1)^2/2}$$

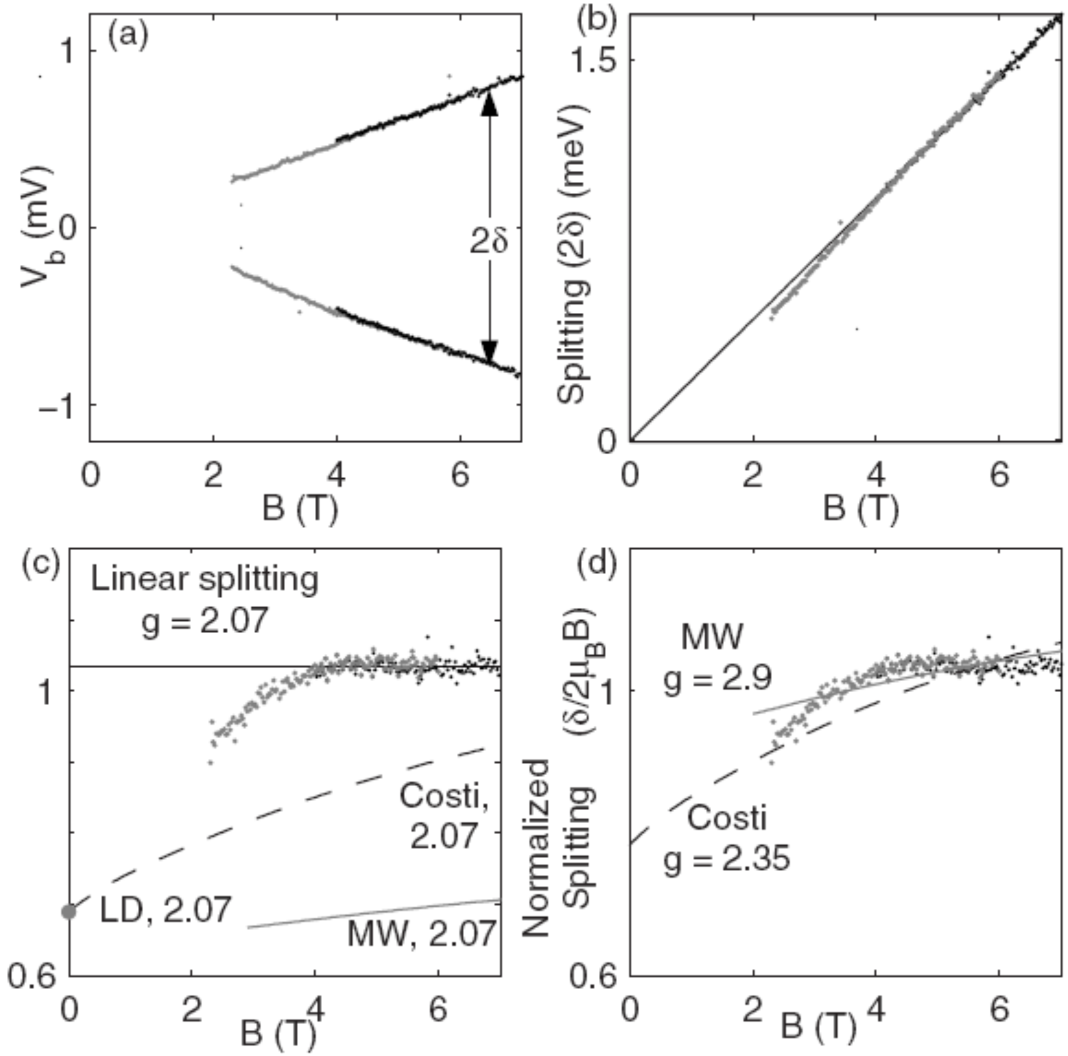
gives **2/3** for R=2, in agreement with Logan et al. (Factor 2 due to different convention.)

Also find that Δ > **1**$g\mu_B B$, but they note that this might be non-universal behavior due to charge fluctuations in the Anderson model (as opposed to the Kondo model).

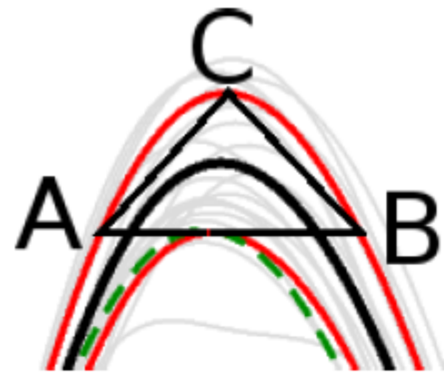
PHYSICAL REVIEW B **76**, 245311 (2007)

Magnetic field dependence of the spin-$\frac{1}{2}$ and spin-1 Kondo effects in a quantum dot

C. H. L. Quay,[1] John Cumings,[1,*] S. J. Gamble,[2] R. de Picciotto,[3] H. Kataura,[4] and D. Goldhaber-Gordon[1]

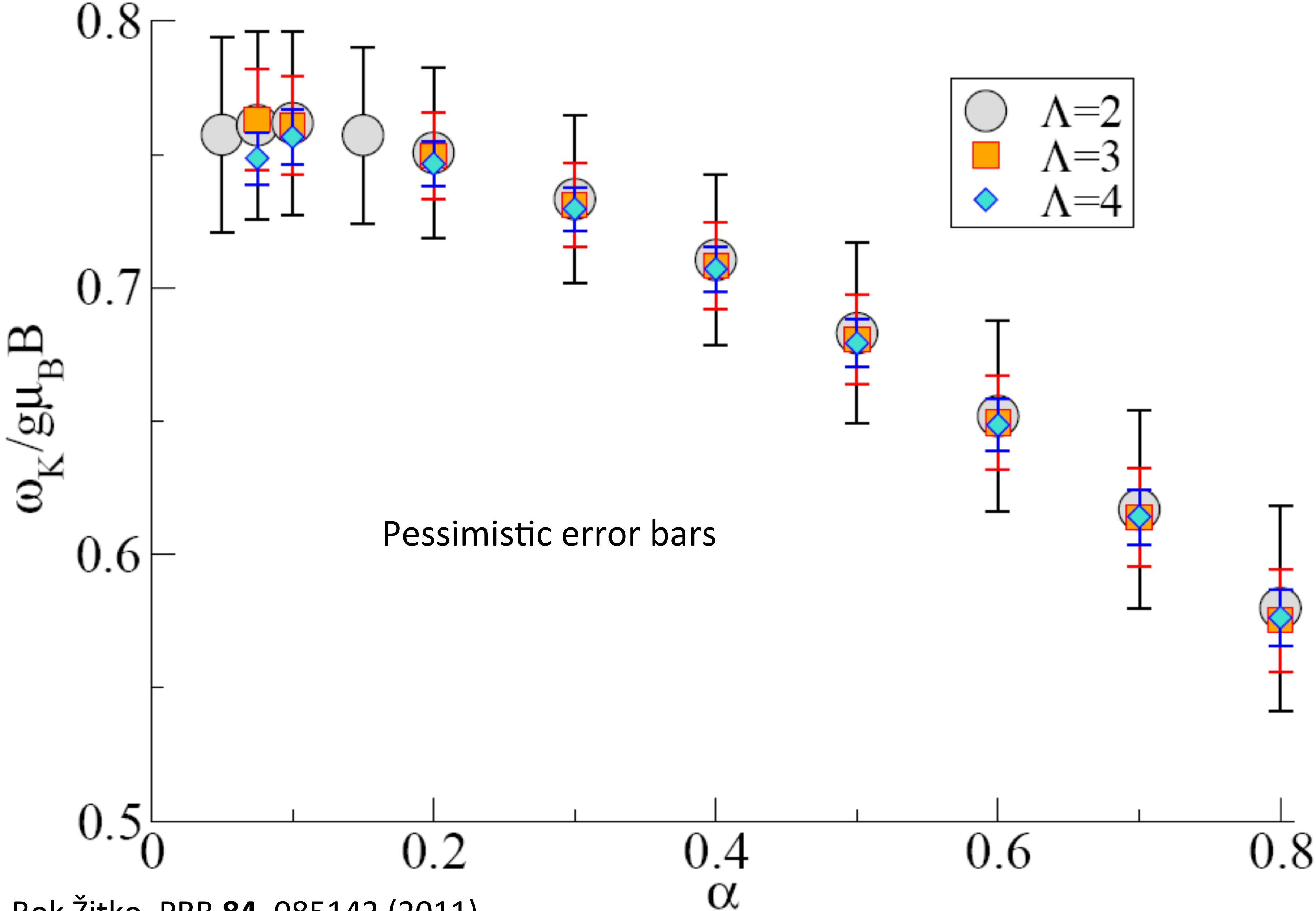


Interrelated problems: systematic discretization errors and spectral broadening



$$P(\omega,\omega') = \frac{\theta(\omega\omega')}{\sqrt{\pi}\alpha|\omega|}\exp\left[-\left(\frac{\log|\omega/\omega'|}{\alpha}-\frac{\alpha}{4}\right)^2\right]$$

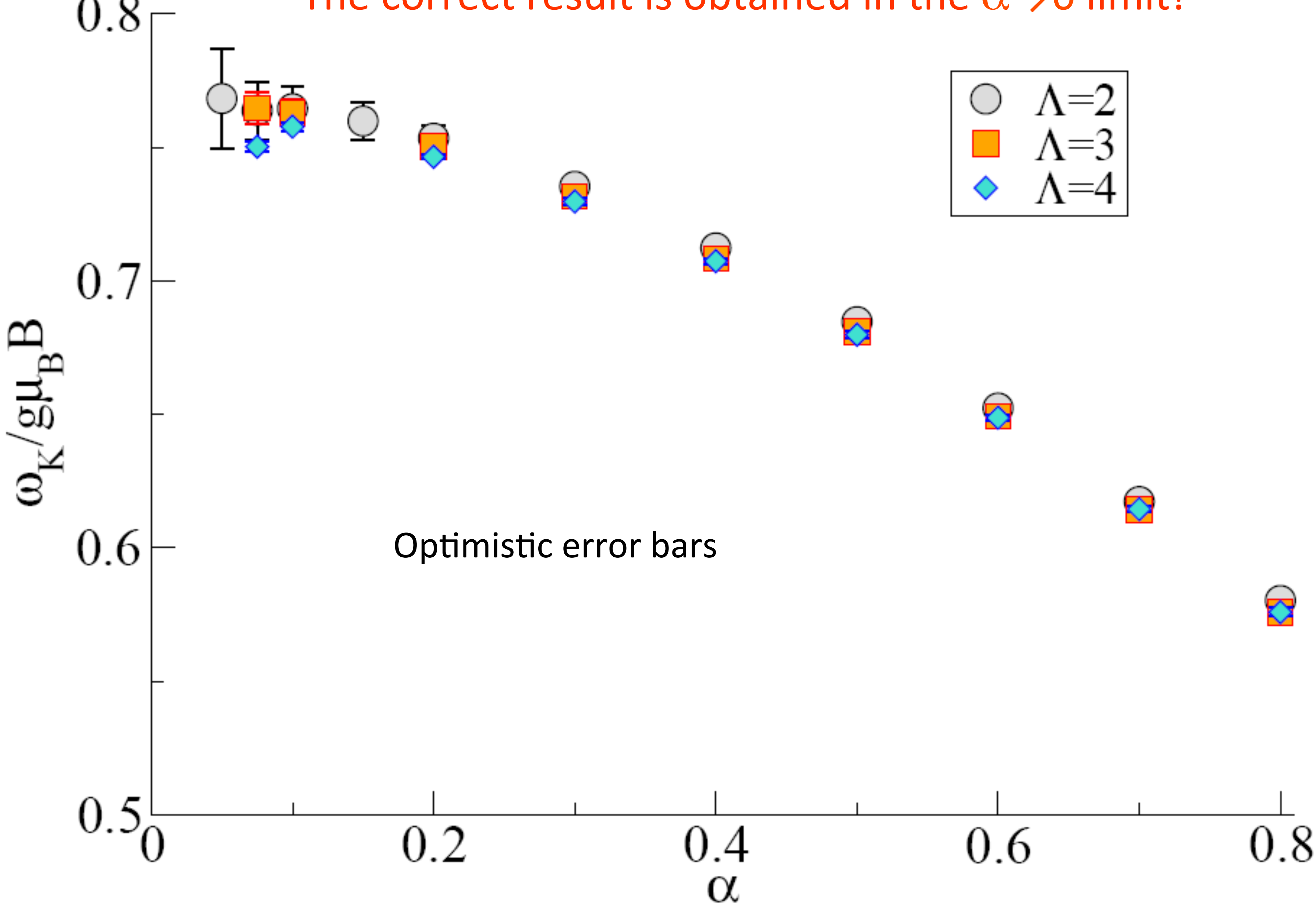
α determines how δ peaks are smoothed out!



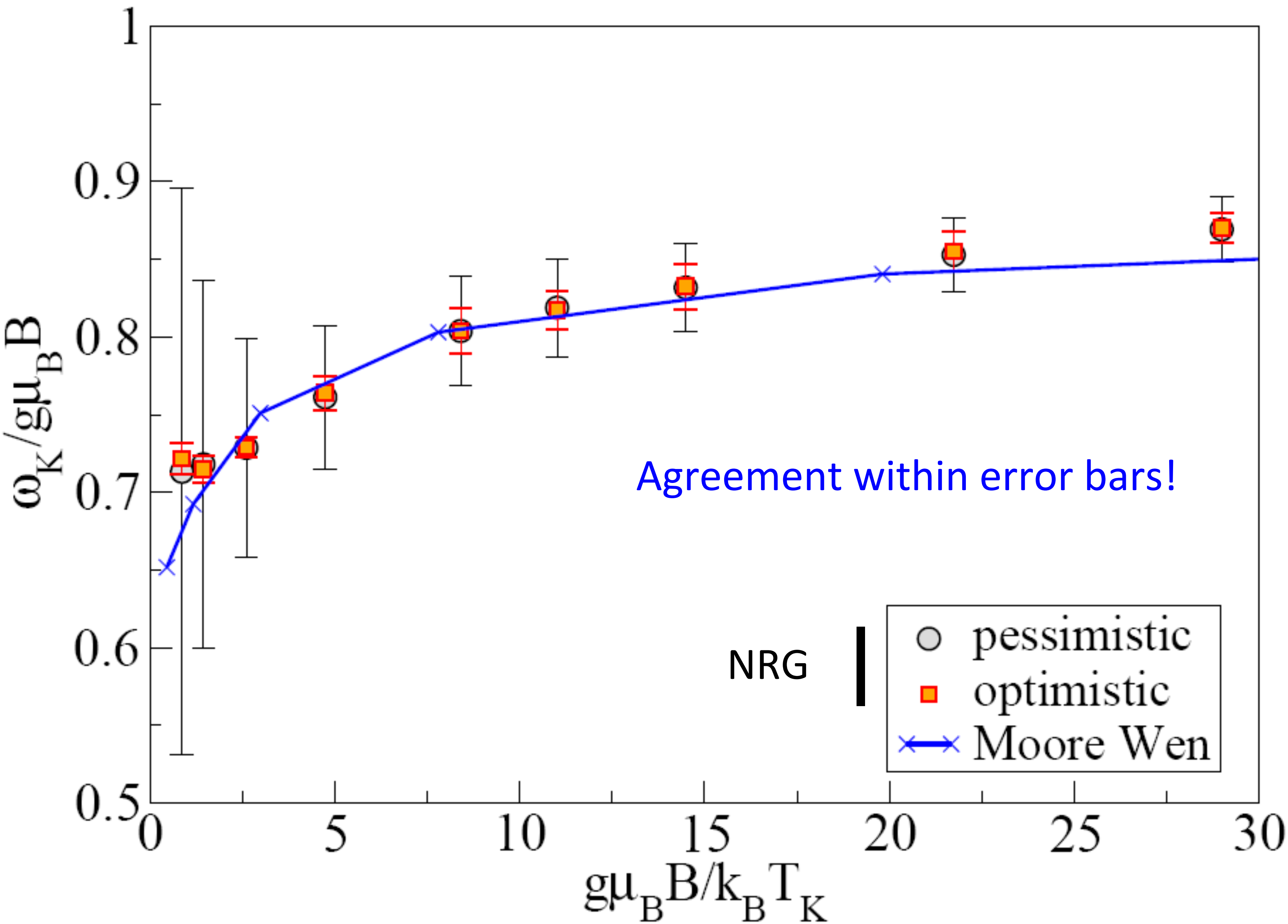
Pessimistic error bars

Rok Žitko, PRB **84**, 085142 (2011)

The correct result is obtained in the $\alpha \to 0$ limit!

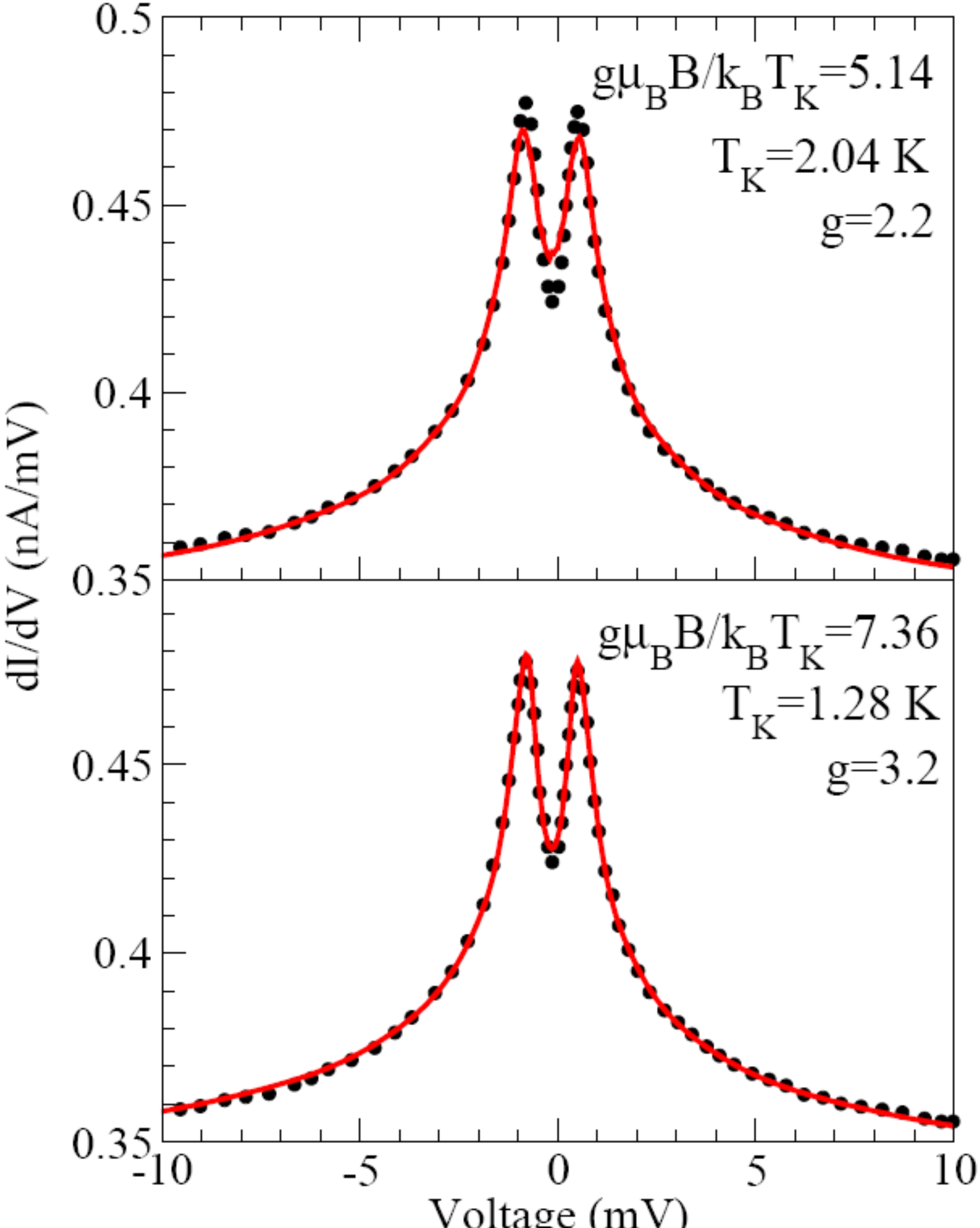


Optimistic error bars



$\omega_K/g\mu_B B$
$g\mu_B B/k_B T_K$
Agreement within error bars!
NRG
pessimistic
optimistic
Moore Wen

B=7 T



● Experimental results for Ti adatoms:

F. Otte et al., Nature Physics **4**, 847 (2008)

NRG calculation

R. Ž., submitted

Kondo model

$$G = G_0 + G_0 T G_0$$

$$T_\sigma = \langle\langle O_\sigma ; O_\sigma^\dagger \rangle\rangle$$

$$O_\sigma = [H_{\text{coupling}}, f_{0,\sigma}]$$

$$H_{\mathrm{K}} = \left(\frac{1}{2} f_{0,\alpha}^\dagger \boldsymbol{\sigma}_{\alpha\beta} f_{0,\beta} \right) \cdot \mathbf{S}$$

$$\boxed{O_\sigma = \left(\frac{1}{2} \boldsymbol{\sigma}_{\alpha\beta} f_{0,\beta} \right) \cdot \mathbf{S}}$$