Discretization, z-averaging, thermodynamics, flow diagrams

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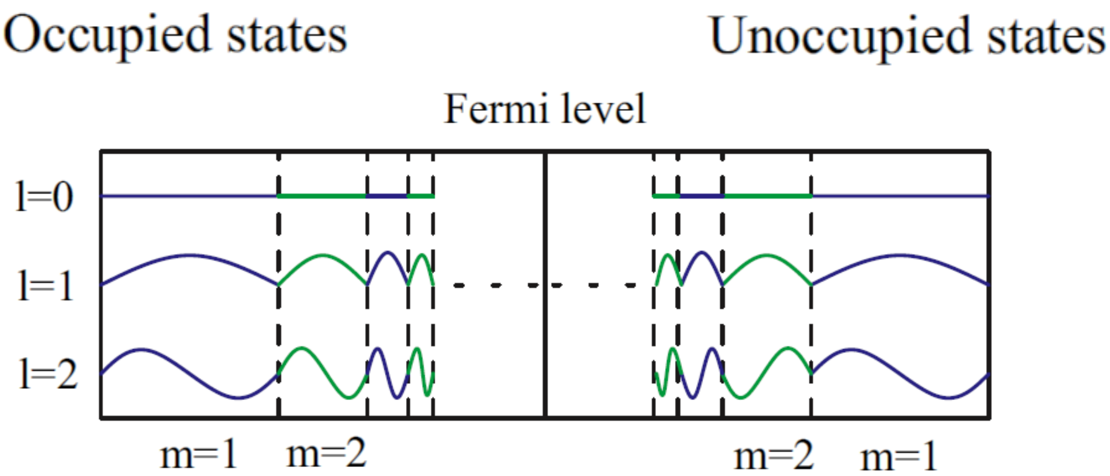
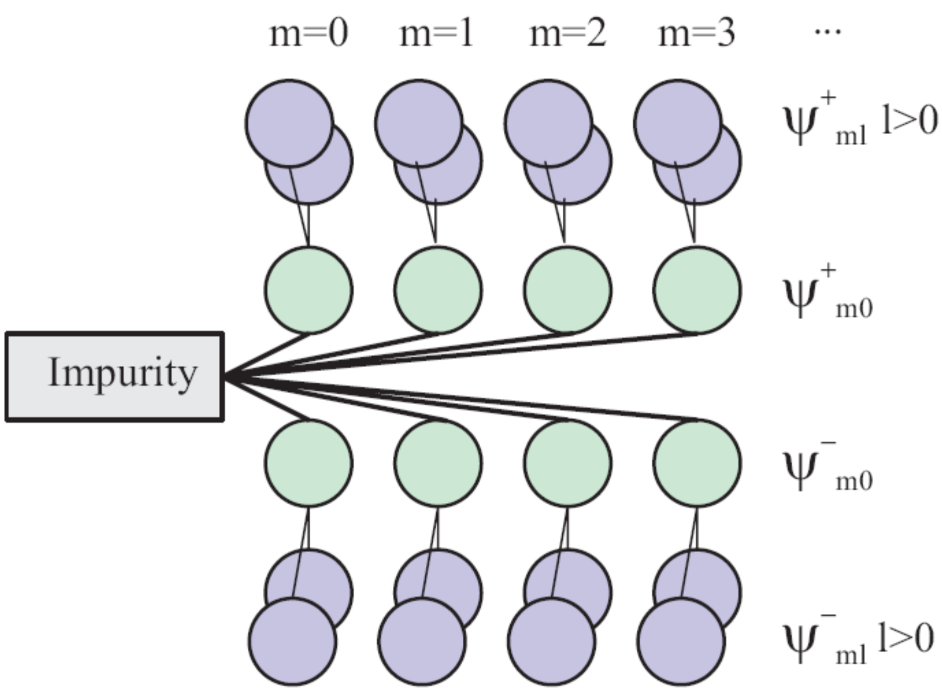
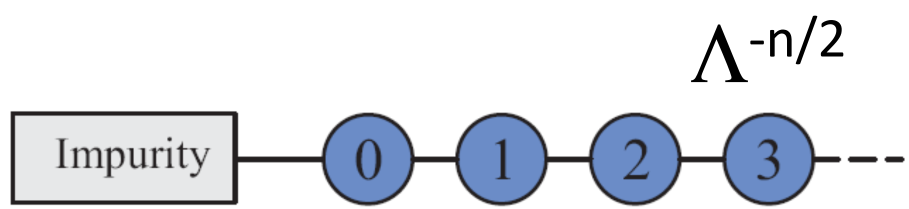
Numerical renormalization group (NRG)







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

f_0 – the 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 also the average state of all "representative states".

Gram-Schmidt orthogonalization

$$\mathrm{proj}_{\mathbf{u}}(\mathbf{v}) = \frac{\langle \mathbf{u}, \mathbf{v} \rangle}{\langle \mathbf{u}, \mathbf{u} \rangle} \mathbf{u}$$

$$\begin{aligned}
\mathbf{u}_1 &= \mathbf{v}_1, & \mathbf{e}_1 &= \frac{\mathbf{u}_1}{\|\mathbf{u}_1\|} \\
\mathbf{u}_2 &= \mathbf{v}_2 - \mathrm{proj}_{\mathbf{u}_1}(\mathbf{v}_2), & \mathbf{e}_2 &= \frac{\mathbf{u}_2}{\|\mathbf{u}_2\|} \\
\mathbf{u}_3 &= \mathbf{v}_3 - \mathrm{proj}_{\mathbf{u}_1}(\mathbf{v}_3) - \mathrm{proj}_{\mathbf{u}_2}(\mathbf{v}_3), & \mathbf{e}_3 &= \frac{\mathbf{u}_3}{\|\mathbf{u}_3\|} \\
\mathbf{u}_4 &= \mathbf{v}_4 - \mathrm{proj}_{\mathbf{u}_1}(\mathbf{v}_4) - \mathrm{proj}_{\mathbf{u}_2}(\mathbf{v}_4) - \mathrm{proj}_{\mathbf{u}_3}(\mathbf{v}_4), & \mathbf{e}_4 &= \frac{\mathbf{u}_4}{\|\mathbf{u}_4\|} \\
&\vdots & &\vdots \\
\mathbf{u}_k &= \mathbf{v}_k - \sum_{j=1}^{k-1} \mathrm{proj}_{\mathbf{u}_j}(\mathbf{v}_k), & \mathbf{e}_k &= \frac{\mathbf{u}_k}{\|\mathbf{u}_k\|}
\end{aligned}$$

http://en.wikipedia.org/wiki/Gram%E2%80%93Schmidt_process

Lanczos algorithm

H_{band} in truncated basis

We take f_0 instead of the random vector!

Algorithm Lanczos
  $v_1 \leftarrow$ random vector with norm 1.
  $v_0 \leftarrow 0$
  $\beta_1 \leftarrow 0$
  Iteration: for $j = 1, 2, \cdots, m$
    $w_j \leftarrow A v_j$
    $\alpha_j \leftarrow w_j \cdot v_j$
    $w_j \leftarrow w_j - \alpha_j v_j - \beta_j v_{j-1}$
    $\beta_{j+1} \leftarrow \|w_j\|$
    $v_{j+1} \leftarrow w_j / \beta_{j+1}$
  return

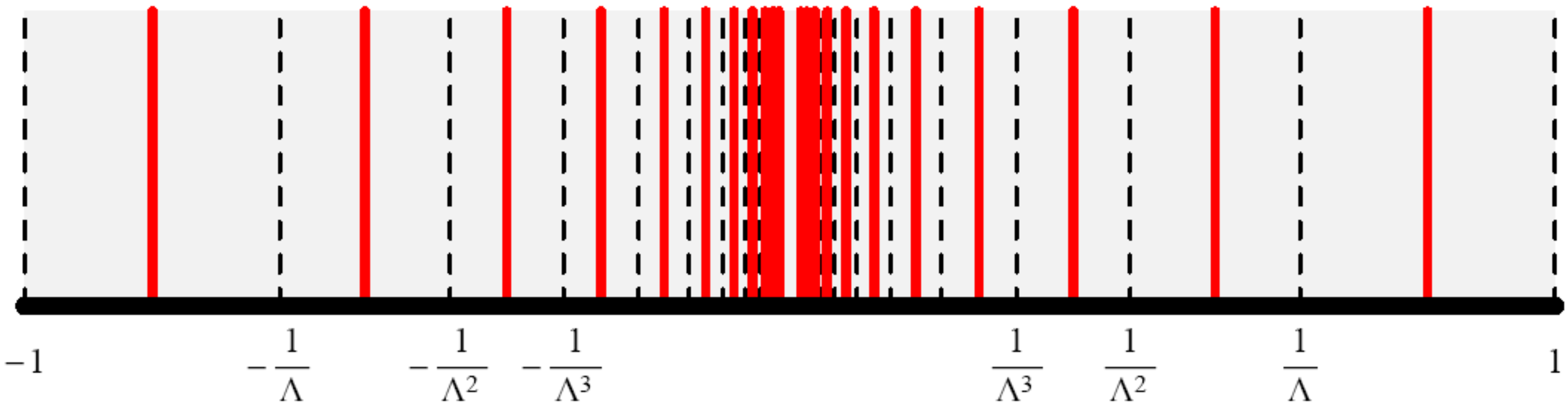
$$T_{mm} = \begin{pmatrix} \alpha_1 & \beta_2 & & & & 0 \\ \beta_2 & \alpha_2 & \beta_3 & & & \\ & \beta_3 & \alpha_3 & \ddots & & \\ & & \ddots & \ddots & \beta_{m-1} & \\ & & & \beta_{m-1} & \alpha_{m-1} & \beta_m \\ 0 & & & & \beta_m & \alpha_m \end{pmatrix}$$

- "←" is a shorthand for "changes to". For instance, "*largest* ← *item*" means that the value of *largest* changes to the value of *item*.
- "**return**" terminates the algorithm and outputs the value that follows.

The NRG Ljubljana contains a stand-alone tool `nrgchain` for tridiagonalization (in addition to the tridiagonalization code in initial.m and tridiag.h).

http://en.wikipedia.org/wiki/Lanczos_algorithm

Logarithmic discretization



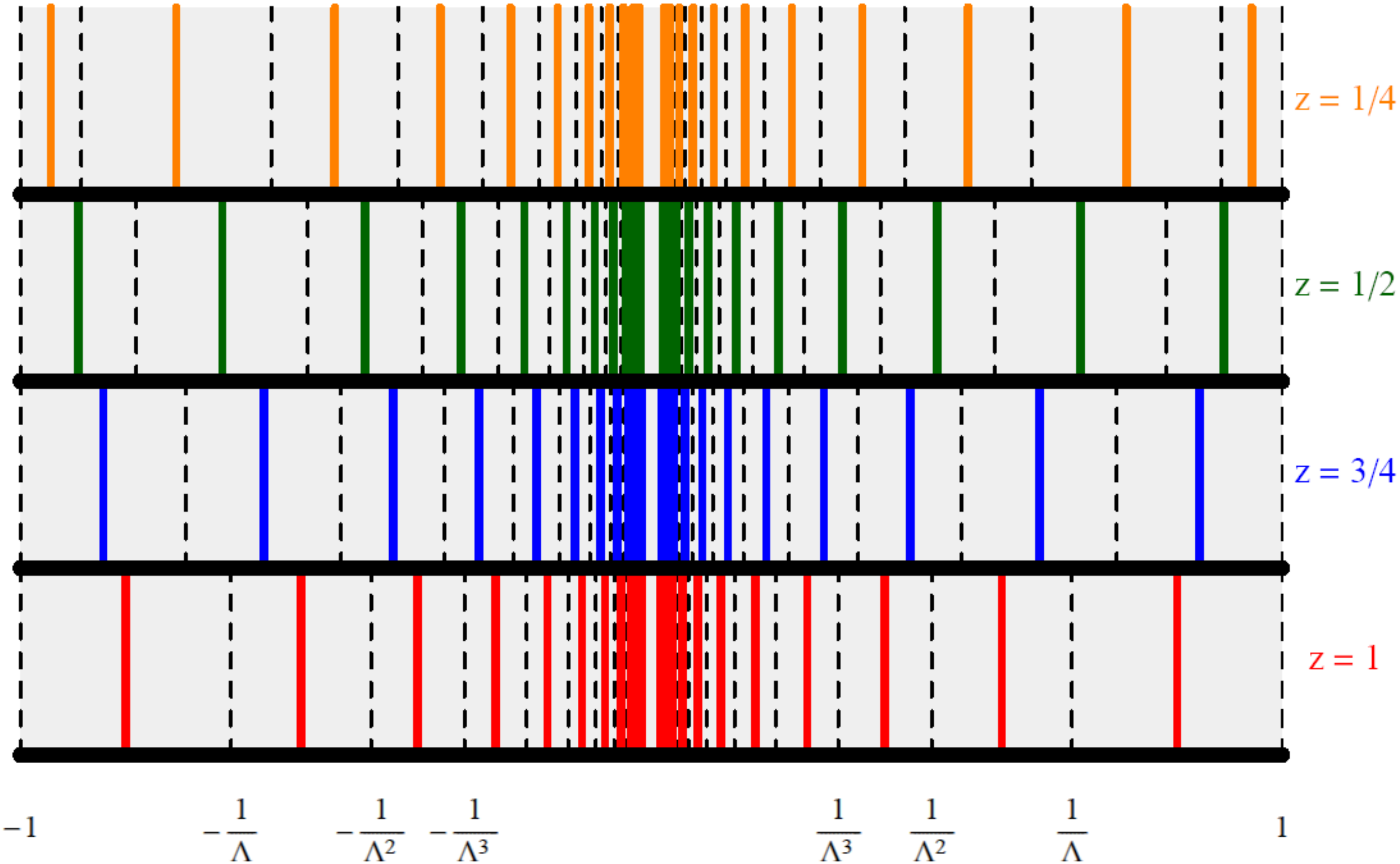
Good sampling of the states near the Fermi energy!

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

Correction:

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

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



$$\epsilon_1^z = D \qquad \epsilon_j^z = D\Lambda^{2-j-z} \quad (j = 2, 3, \ldots)$$

"*z*-averaging" or "interleaved method"

Frota, Oliveira, Phys. Rev. B **33**, 7871 (1986)
Oliveira, Oliveira: Phys. Rev. B **49**, 11986 (1994)

Discretization schemes

1) Conventional scheme

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

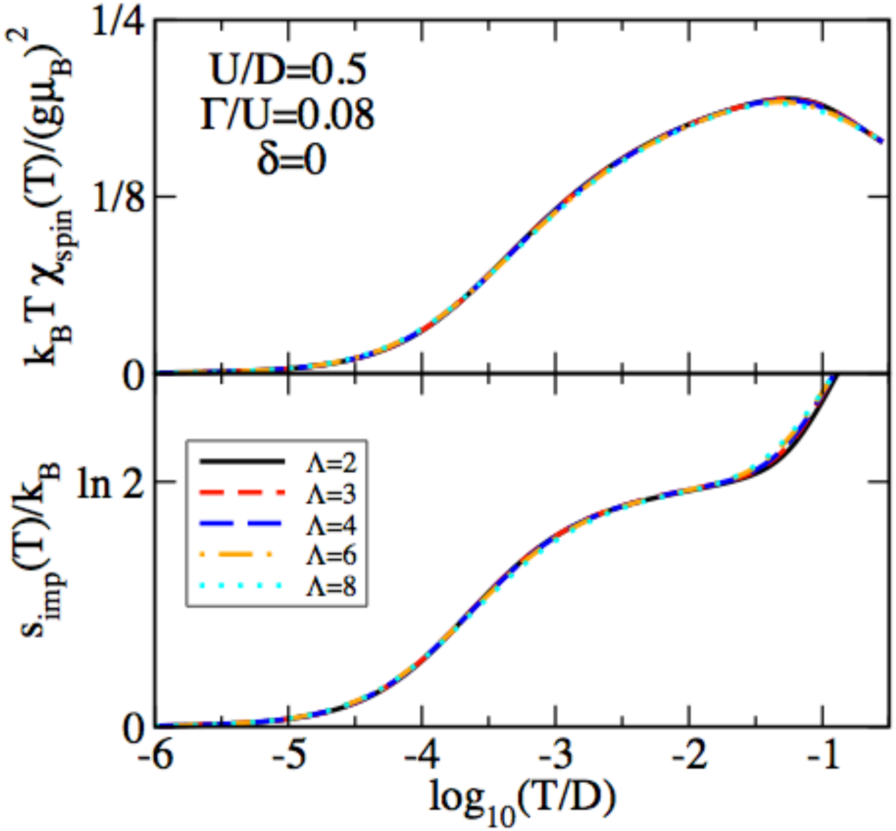
Chen, Jayaprakash, JPCM **7**, L491 (1995); Ingersent, PRB **54**, 11936 (1996); Bulla, Pruschke, Hewson, JPCM **9**, 10463 (1997).

2) Campo-Oliveira scheme

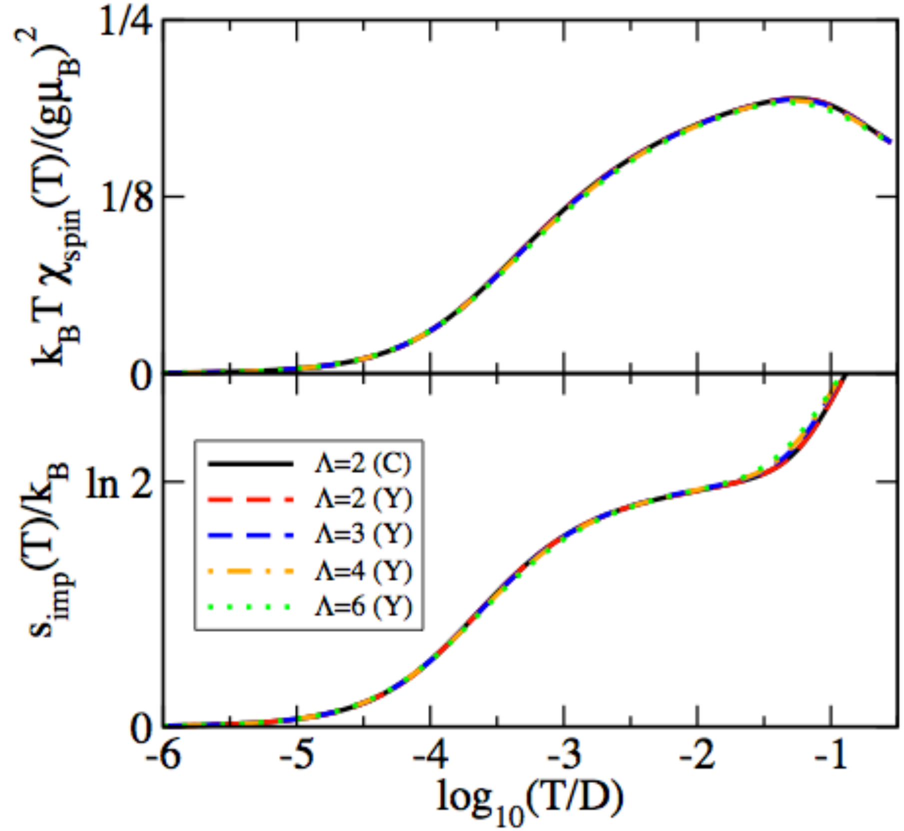
$$\mathcal{E}_j^z = \frac{\int_{I_j} \rho(\epsilon) d\epsilon}{\int_{I_j} \rho(\epsilon)/\epsilon \, d\epsilon}$$

Campo, Oliveira, PRB **72**, 104432 (2005).

$\rho(\varepsilon)$ = density of states in the band



(a) Campo's discretization, effect of increasing Λ



(b) Yoshida's discretization, effect of increasing Λ

With z-averaging it is possible to increase Λ quite significantly without introducing many artifacts in the results for thermodynamics (especially in the low-temperature limit).

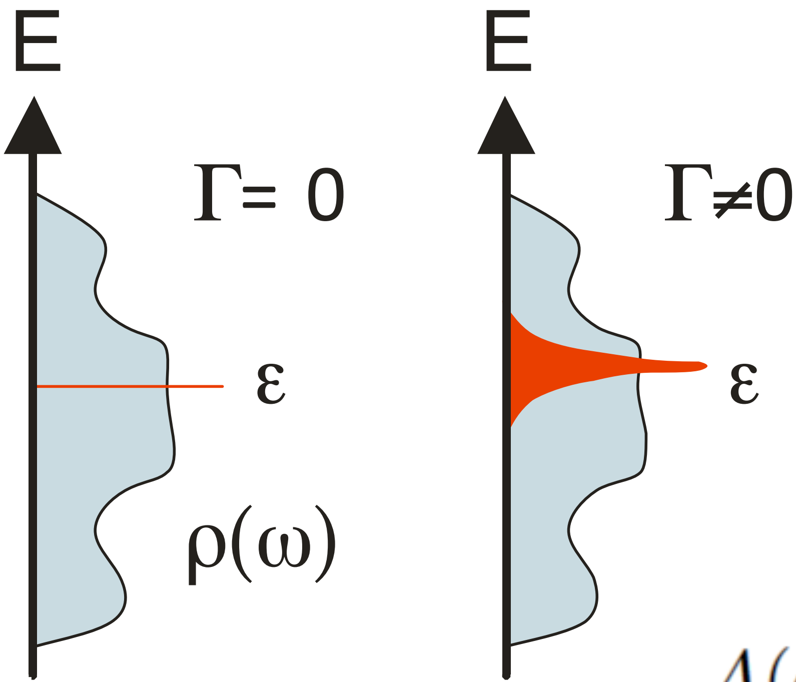
Can we obtain high-resolution spectral functions by using

1) many values of z

and

2) narrow Gaussian broadening?

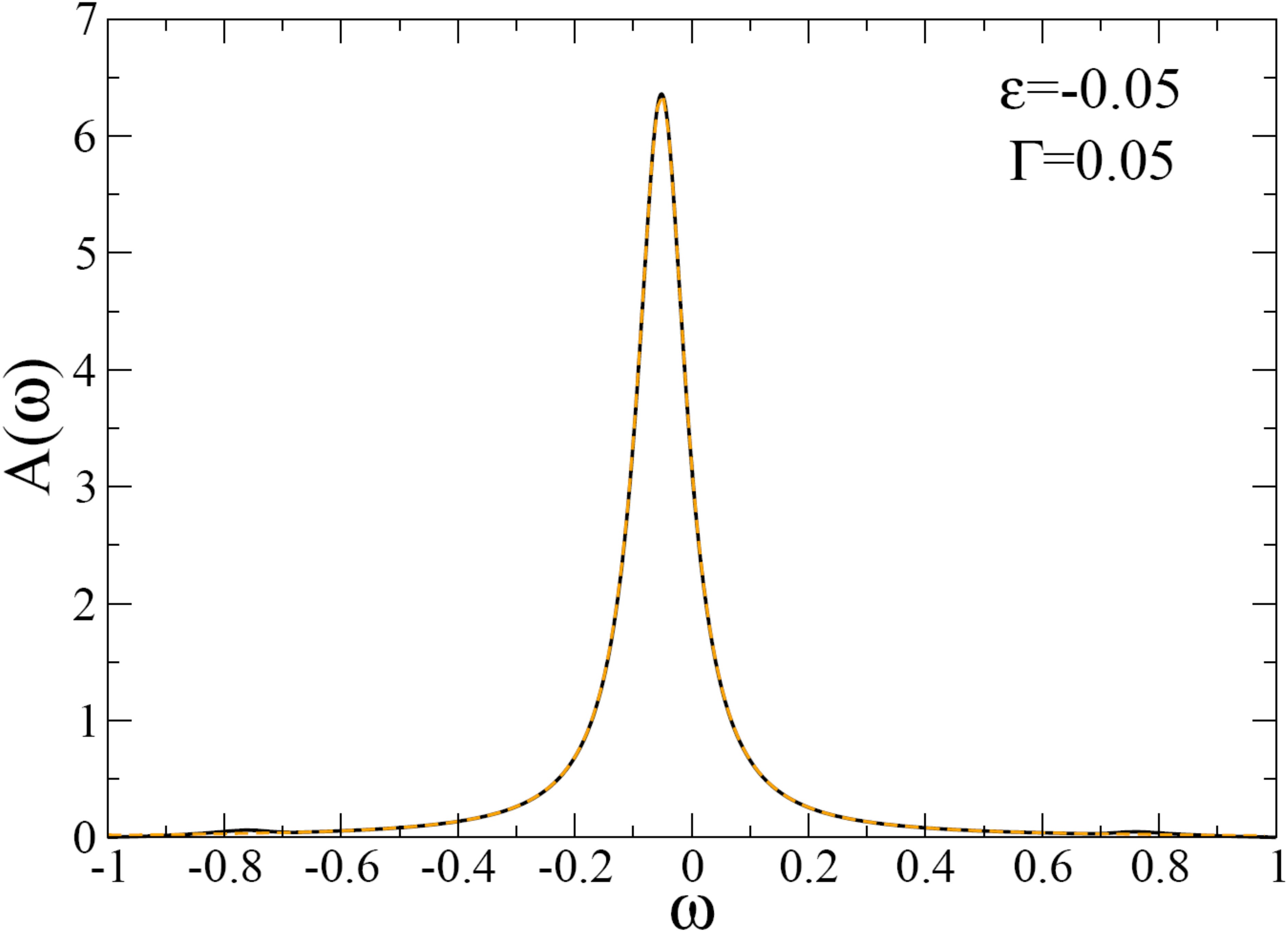
Test case: resonant-level model



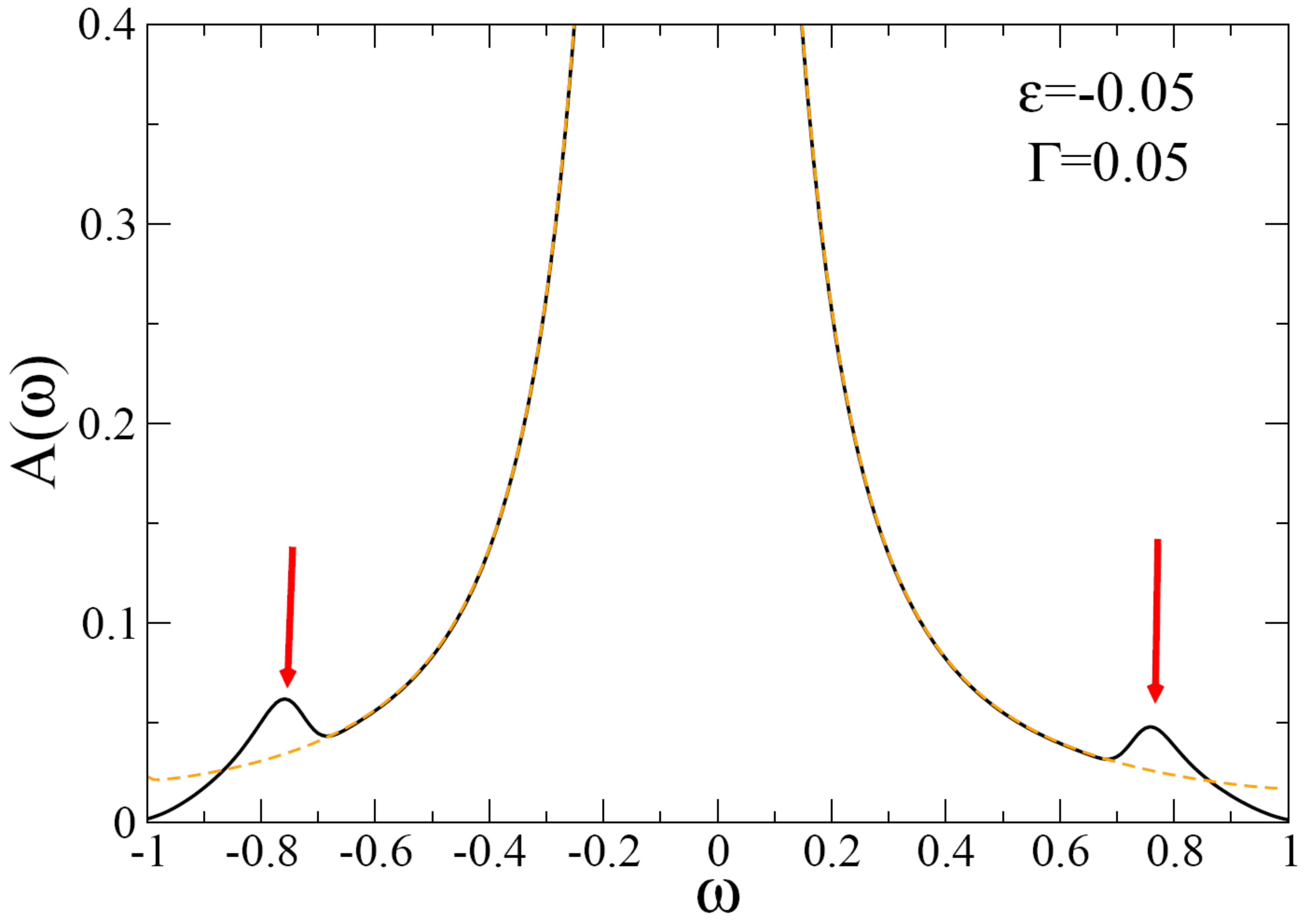
$$A(\omega) = -\frac{1}{\pi}\mathrm{Im}\left(\frac{1}{\omega - \epsilon + \Delta(\omega)}\right)$$

$$\Delta(\omega) = \Gamma\left[i + \frac{1}{\pi}\ln\left(\frac{1-\omega/D}{1+\omega/D}\right)\right]$$

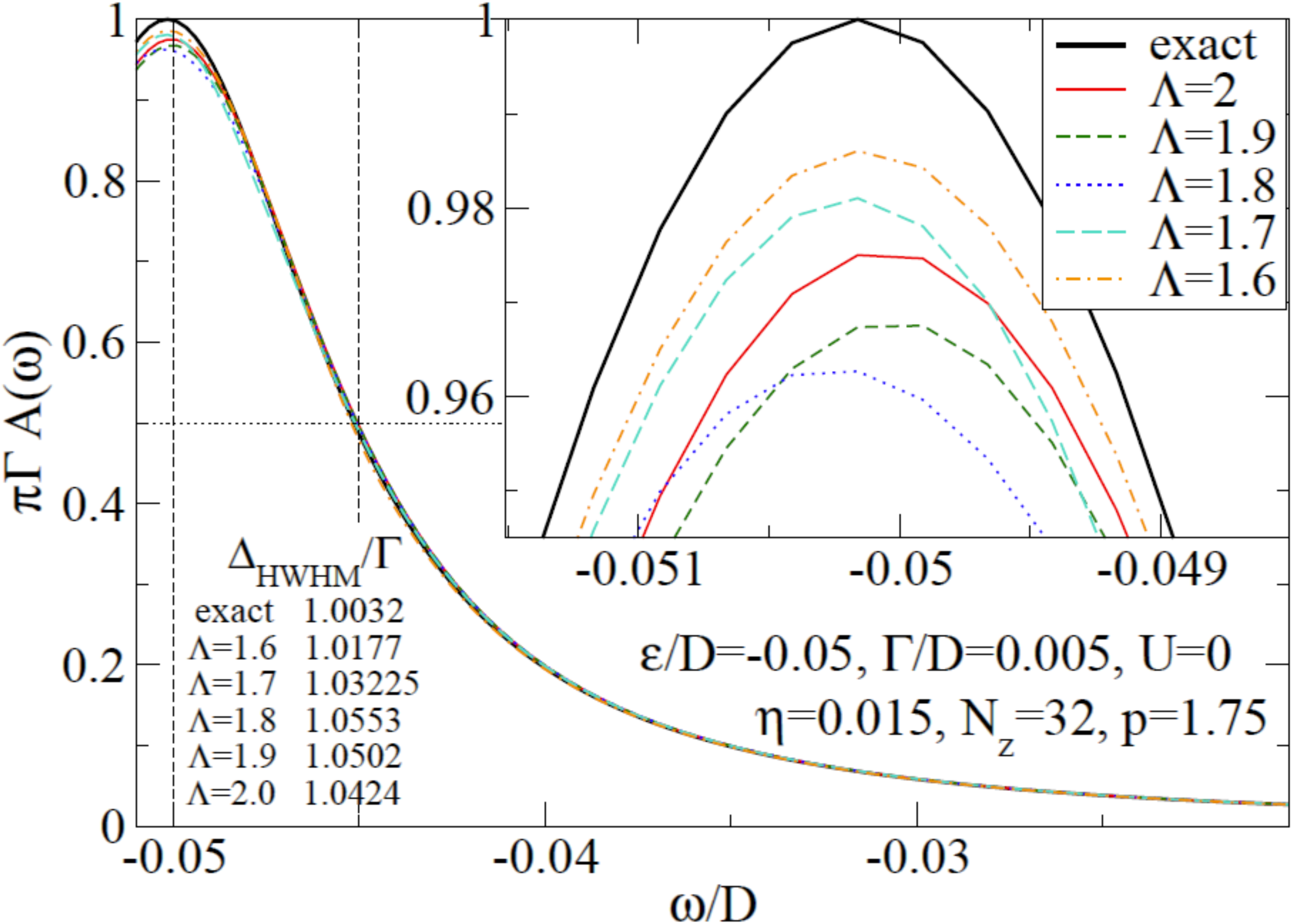
for a flat band, $\rho(\omega)$=const.



ε=-0.05
Γ=0.05
A(ω)
ω
0
1
2
3
4
5
6
7
-1
-0.8
-0.6
-0.4
-0.2
0
0.2
0.4
0.6
0.8
1



ε=-0.05
Γ=0.05
A(ω)
ω
0
0.1
0.2
0.3
0.4
-1
-0.8
-0.6
-0.4
-0.2
0
0.2
0.4
0.6
0.8
1



exact
Λ=2
Λ=1.9
Λ=1.8
Λ=1.7
Λ=1.6
Δ_HWHM/Γ
exact 1.0032
Λ=1.6 1.0177
Λ=1.7 1.03225
Λ=1.8 1.0553
Λ=1.9 1.0502
Λ=2.0 1.0424
ε/D=-0.05, Γ/D=0.005, U=0
η=0.015, N_z=32, p=1.75
πΓ A(ω)
ω/D

Higher-moment spectral sum rules

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

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

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

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

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

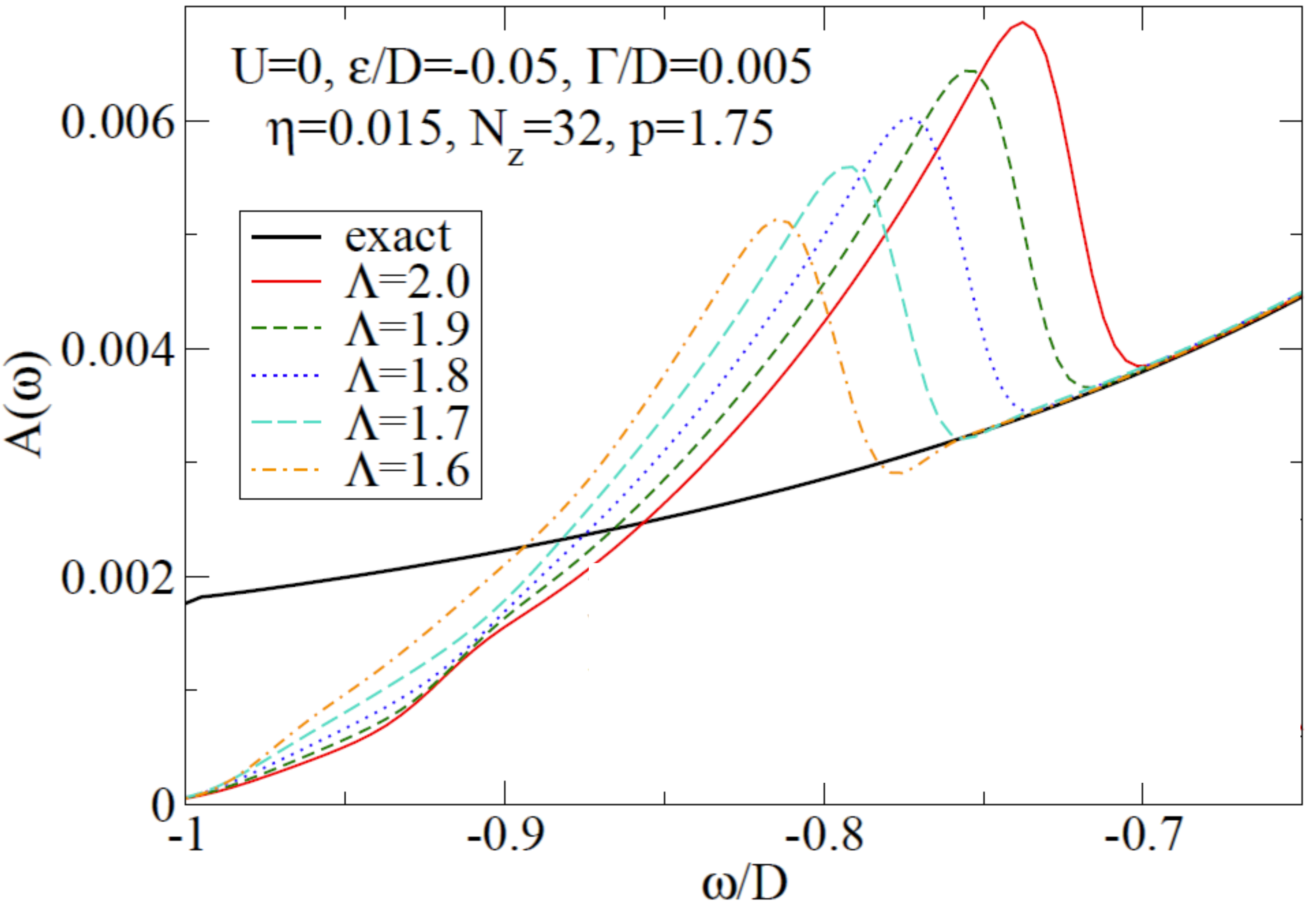
$$\begin{aligned}\mu_3 =& \epsilon^3 + 2\epsilon V^2 + U(3\epsilon^2 + 3\epsilon U + U^2 + 4V^2) \langle n_{-\sigma} \rangle \\ & - \frac{UV}{2} \left(4V \langle n_{f,-\sigma} \rangle + (U + 2\epsilon) \left\langle h^{(0)}_{-\sigma} \right\rangle \right) \\ & + t_0 UV \left\langle h^{(1)}_{-\sigma} \right\rangle\end{aligned}$$

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

Spectral moments for the resonant-level model

Moment	Exact, $\mu_i^{(e)}$	Static, $\mu_i^{(s)}$	Dynamic (delta peaks), $\mu_i^{(d)}$	Dynamic (broadened), $\mu_i^{(b)}$
μ_0	1		0.999442	0.999981
μ_1	-0.050000	-0.050000	-0.049983	-0.049999
μ_2	0.0056831	0.0056831	0.0056866	0.0056871
μ_3	-0.00044331	-0.00044331	-0.00044366	-0.00044389
μ_4	0.00110129	0.0010225	0.0010220	0.0010225

7 percent discrepancy!



U=0, ε/D=-0.05, Γ/D=0.005
η=0.015, N_z=32, p=1.75
exact
Λ=2.0
Λ=1.9
Λ=1.8
Λ=1.7
Λ=1.6
A(ω)
ω/D
0.006
0.004
0.002
0
-1
-0.9
-0.8
-0.7

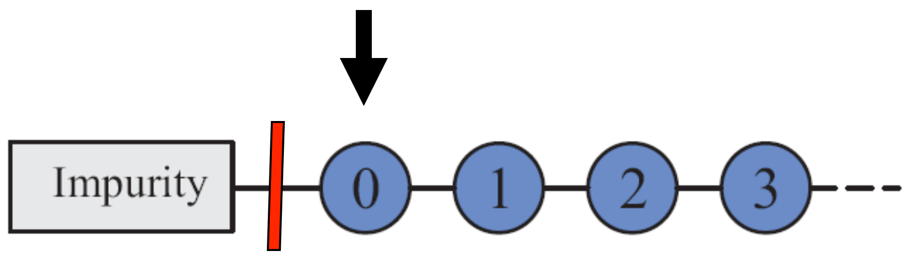
$$H = \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \epsilon\, n + U n_\uparrow n_\downarrow$$

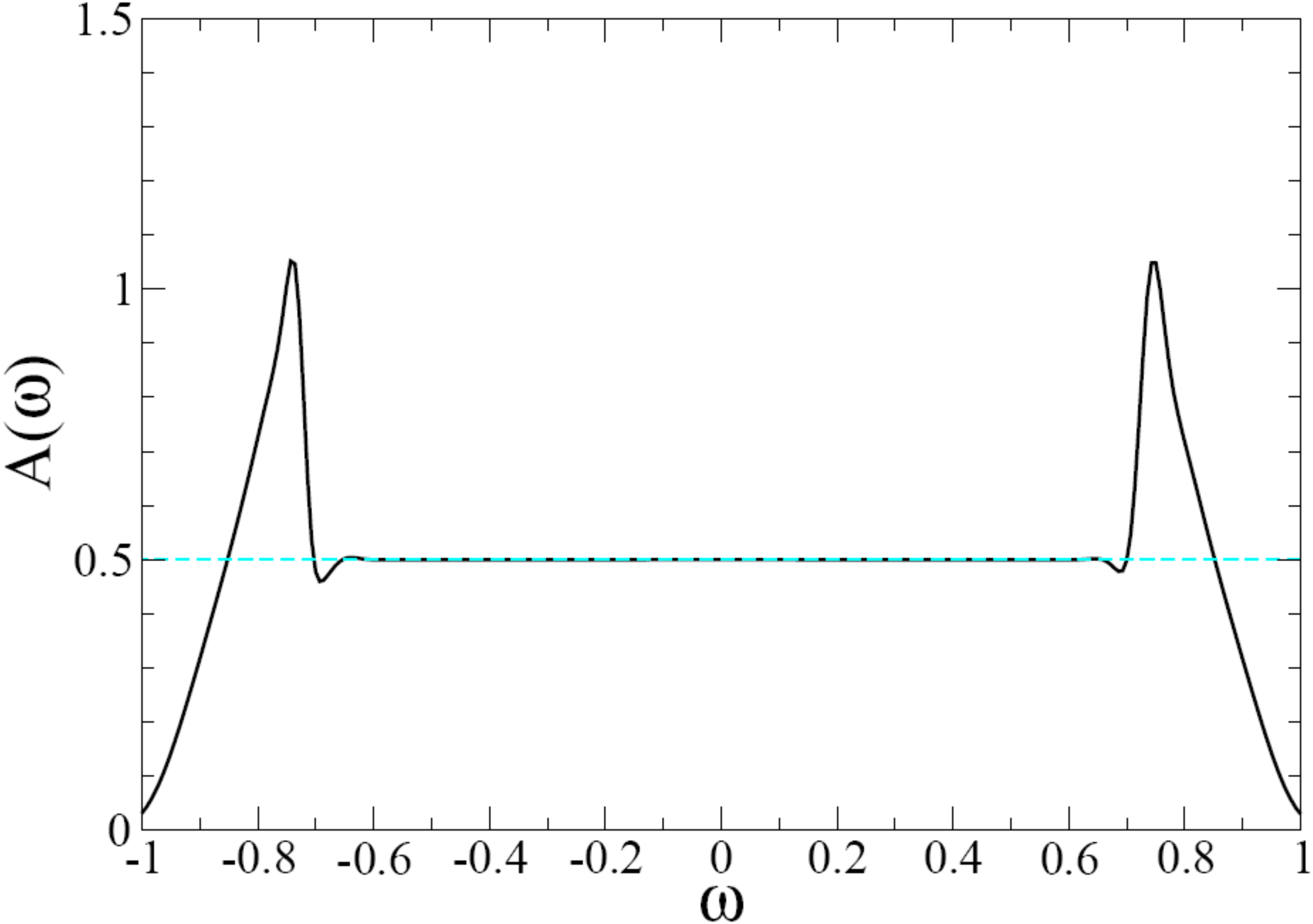
$$+ \frac{1}{\sqrt{N}} \sum_{k\sigma} V_k \left(c^\dagger_{k\sigma} d_\sigma + d^\dagger_\sigma c_{k\sigma} \right)$$

$$\downarrow$$

$$H_{\text{hyb}} = V \sum_\sigma \left(f^\dagger_{0\sigma} d_\sigma + d^\dagger_\sigma f_{0\sigma} \right)$$

$$V^2 = \frac{1}{N} \sum_k |V_k|^2 \qquad f_{0\sigma} = \frac{1}{\sqrt{N}} \sum_k \frac{V_k}{V} c_{k\sigma}$$

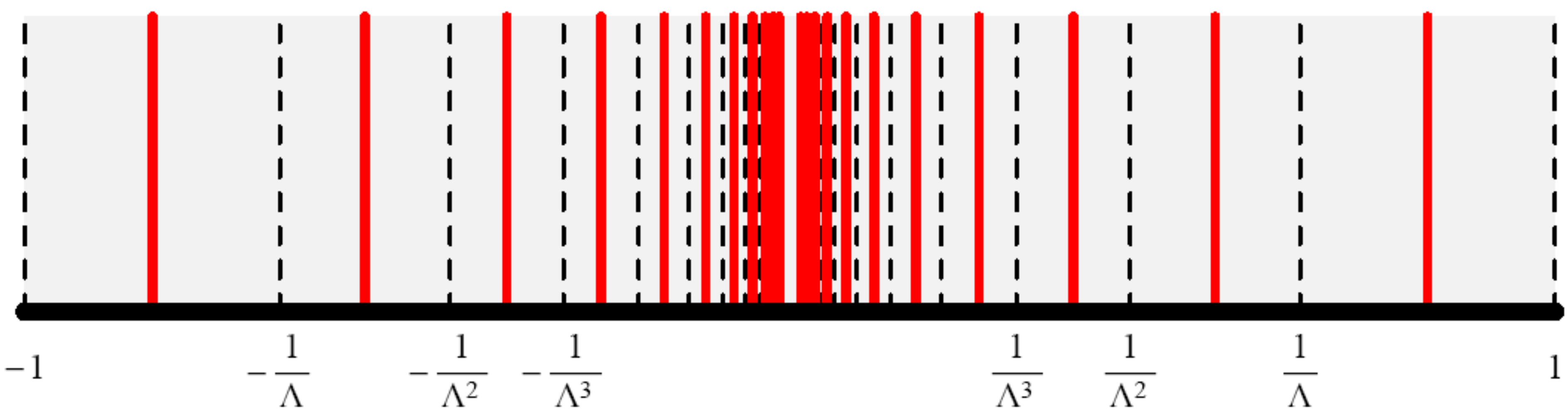




1.5
1
0.5
0
A(ω)
-1
-0.8
-0.6
-0.4
-0.2
0
0.2
0.4
0.6
0.8
1
ω

Origin of the band-edge artifacts

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



$$\mathcal{E}_1^z = D\frac{1-\Lambda^{-z}}{z\ln\Lambda} \qquad \mathcal{E}_j^z = D\frac{1-\Lambda^{-1}}{\ln\Lambda}\Lambda^{2-j-z}$$

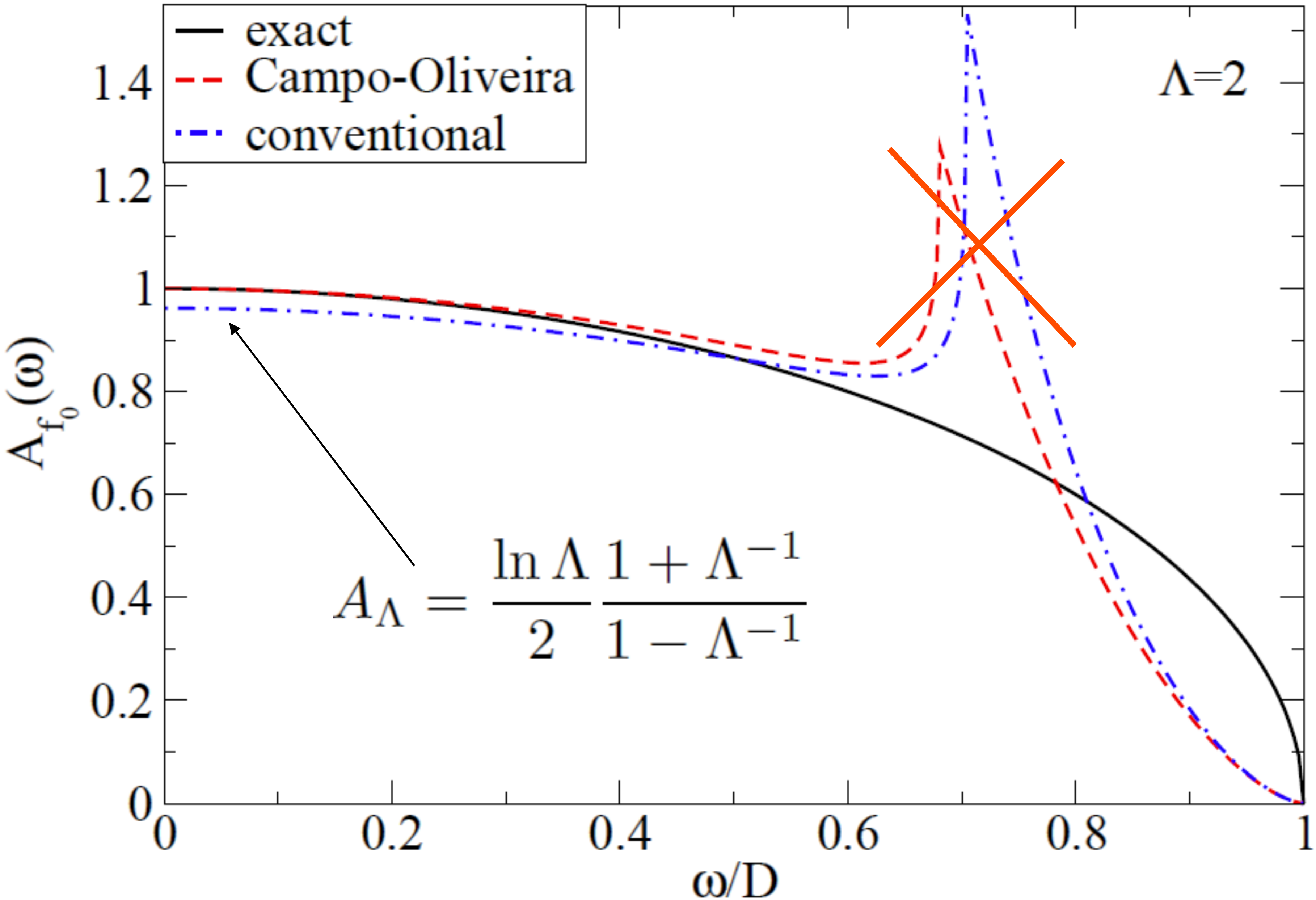
Campo, Oliveira, PRB **72**, 104432 (2005).

$$A_{f_0}(\omega) = 1/2D \qquad \omega \in \left[-\frac{1-\Lambda^{-1}}{\ln\Lambda}; +\frac{1-\Lambda^{-1}}{\ln\Lambda}\right]$$

$$A_{f_0}(\omega) = \frac{(1+\beta\omega)^2}{\omega\left(\omega+\frac{1+\beta\omega}{1-\omega^{\beta}+1/\omega}\right)\ln\Lambda}$$

for ω near band-edges

$$\beta = W\left[-e^{-1/\omega}/\omega\right]$$



NOTE: analytical results, not NRG.

Can we do better?

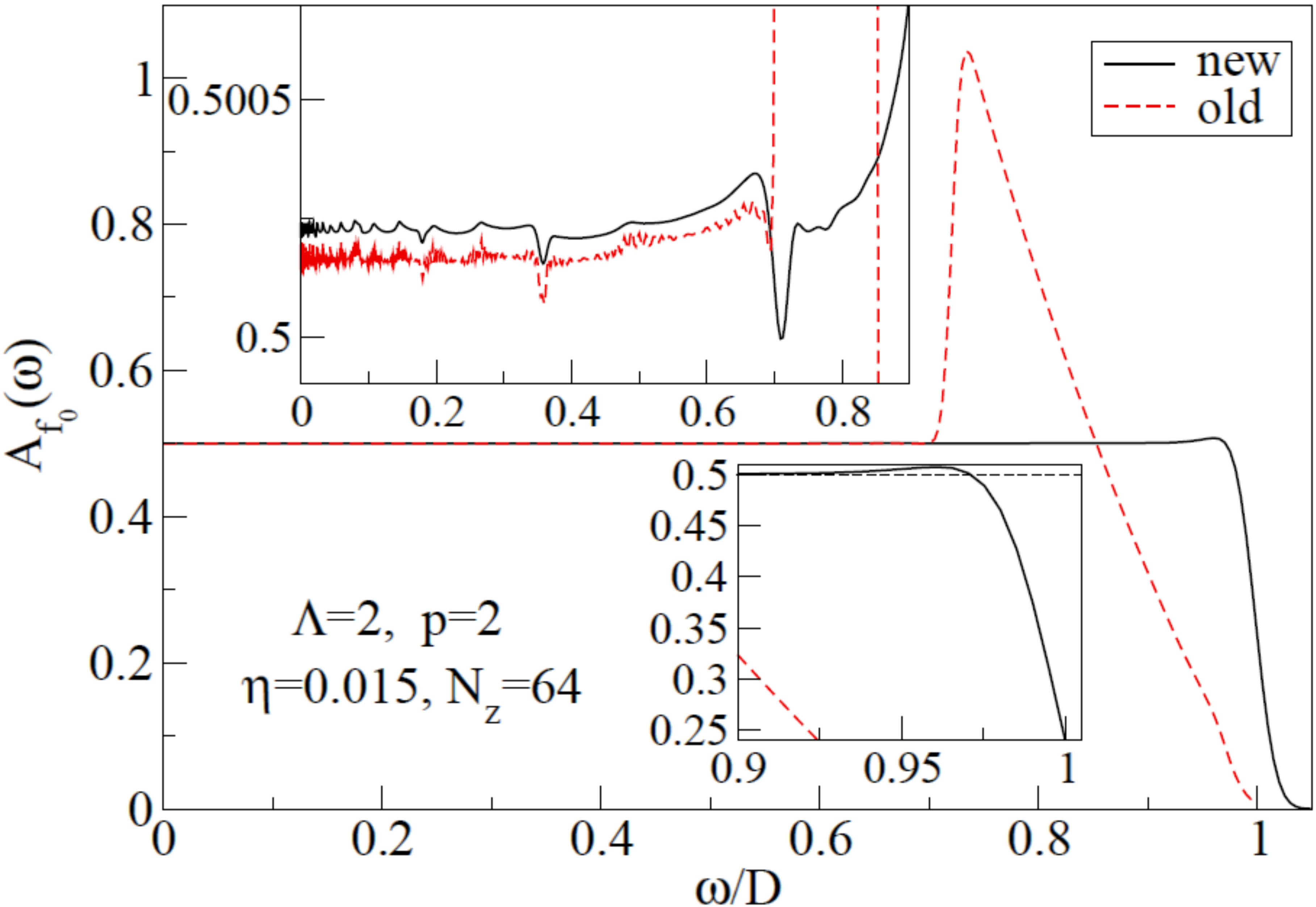
Yes! We **demand** $A_{f_0}(\omega) = \rho(\omega)$

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

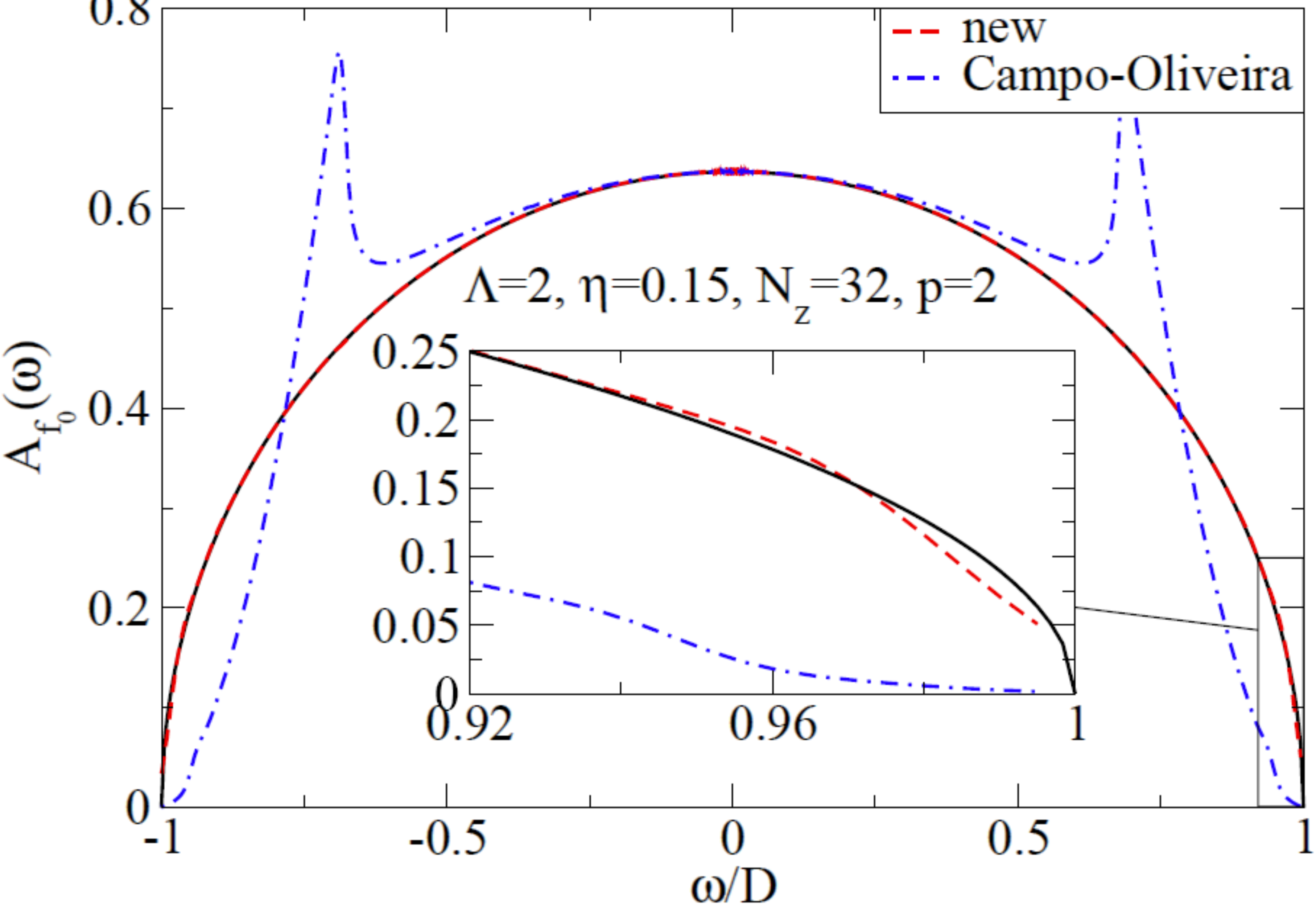
$$x = j + z \qquad \mathcal{E}(x) = D f(x) \Lambda^{2-x}$$

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

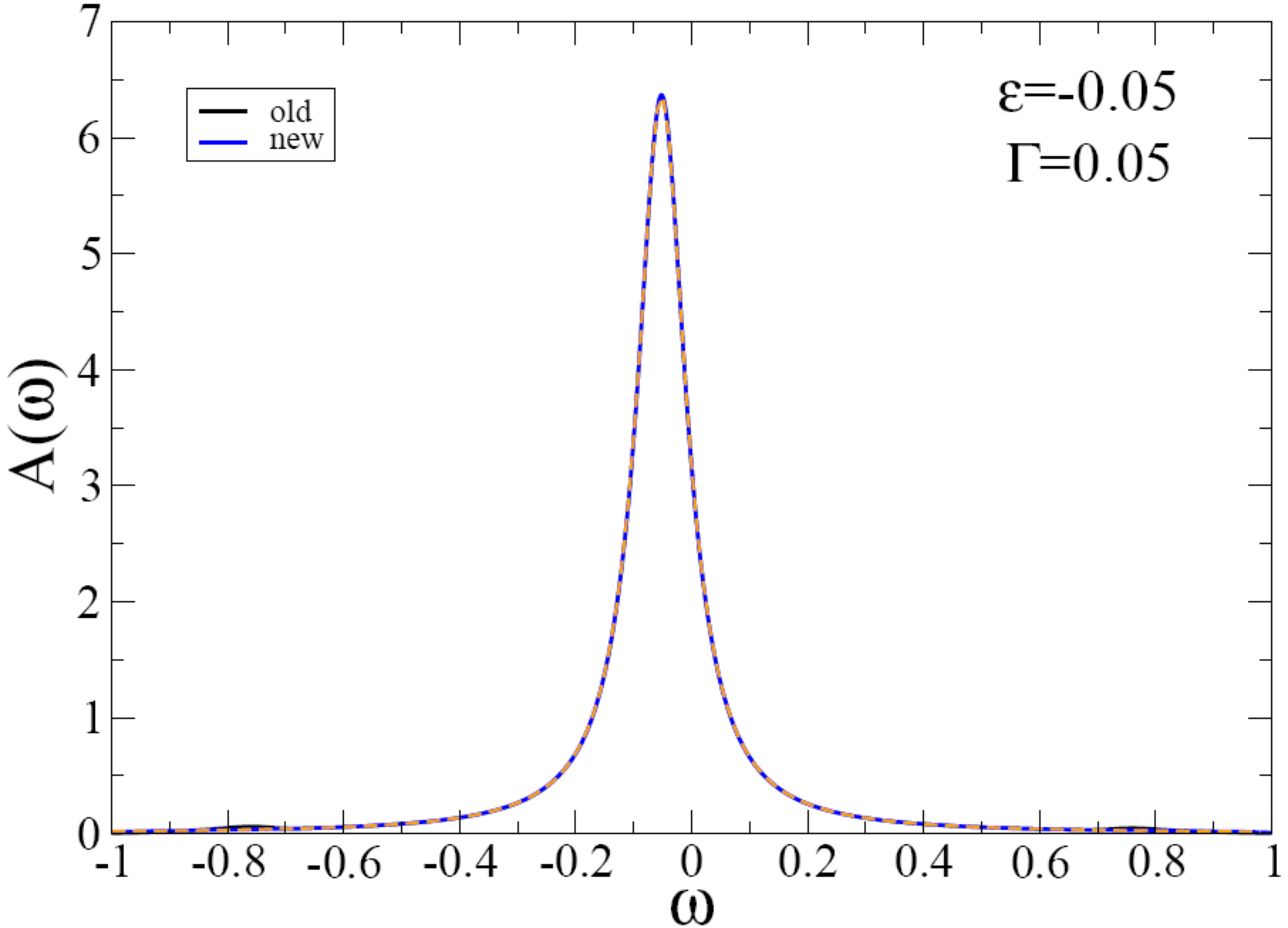
R. Žitko, Th. Pruschke, PRB **79**, 085106 (2009)
R. Žitko, Comput. Phys. Comm. **180**, 1271 (2009)

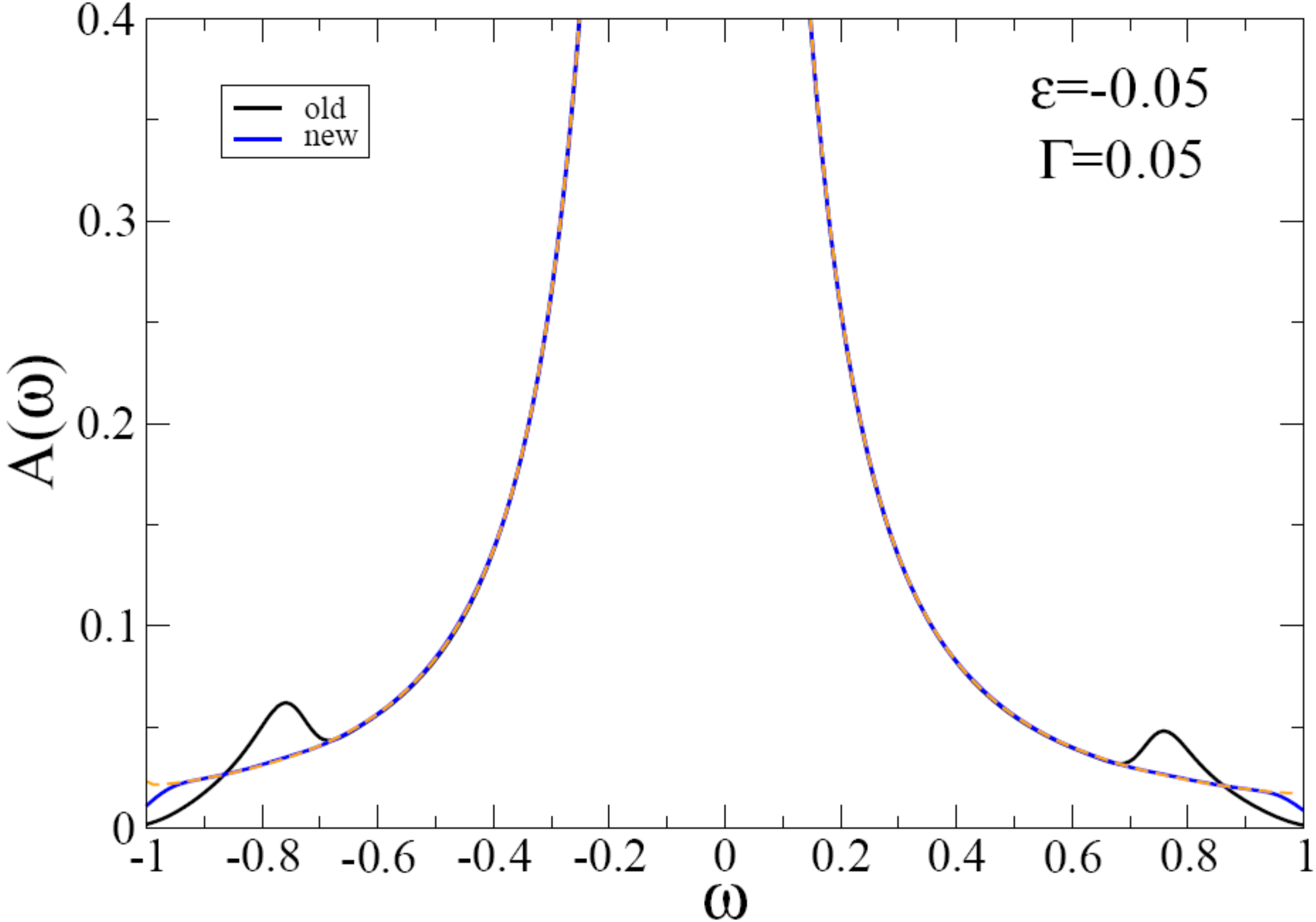


new
old
Λ=2, p=2
η=0.015, N_z=64
A_{f_0}(ω)
ω/D



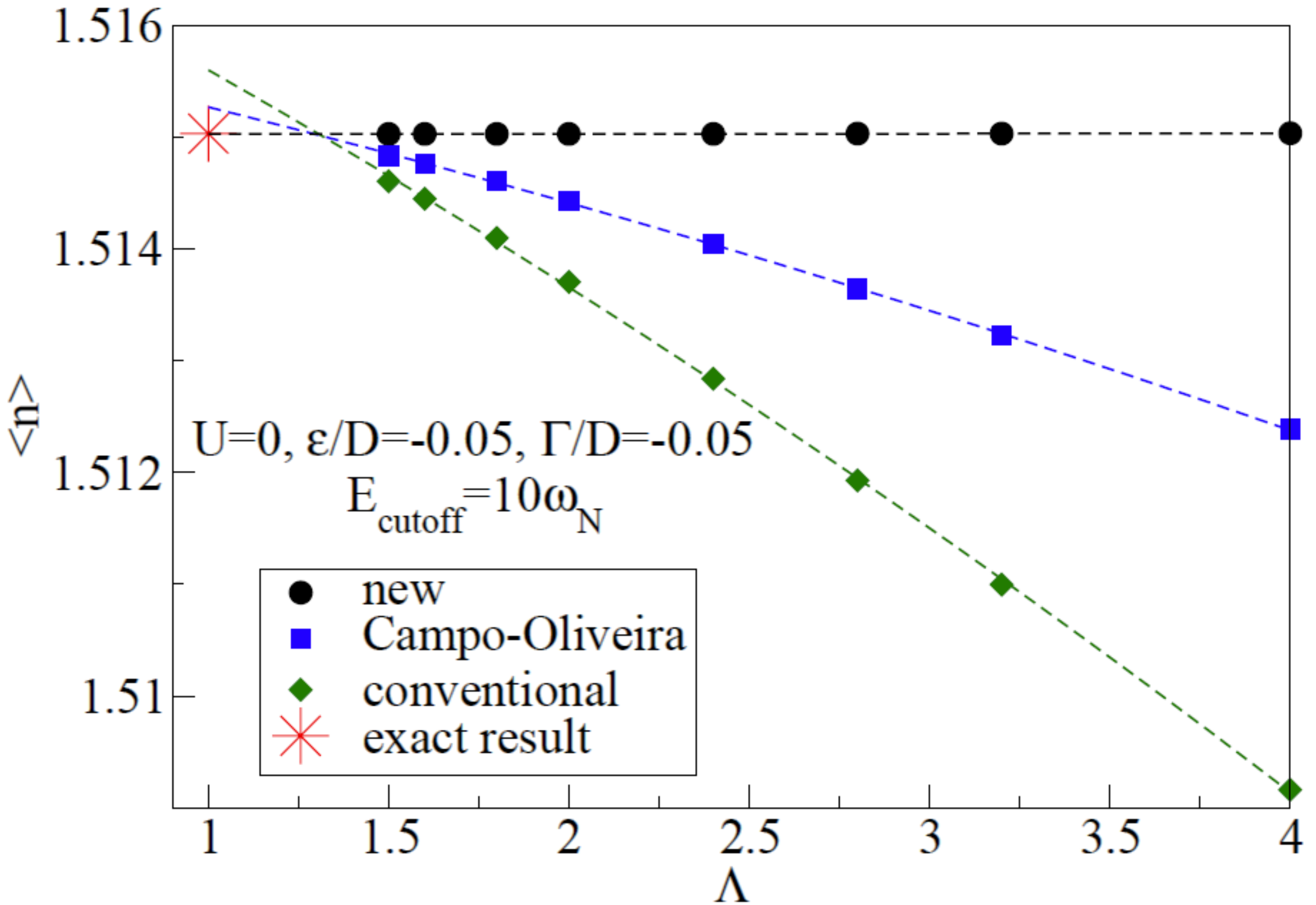
new
Campo-Oliveira
Λ=2, η=0.15, N_z=32, p=2
A_{f_0}(ω)
ω/D
0.8
0.6
0.4
0.2
0
-1
-0.5
0
0.5
1
0.25
0.2
0.15
0.1
0.05
0
0.92
0.96
1

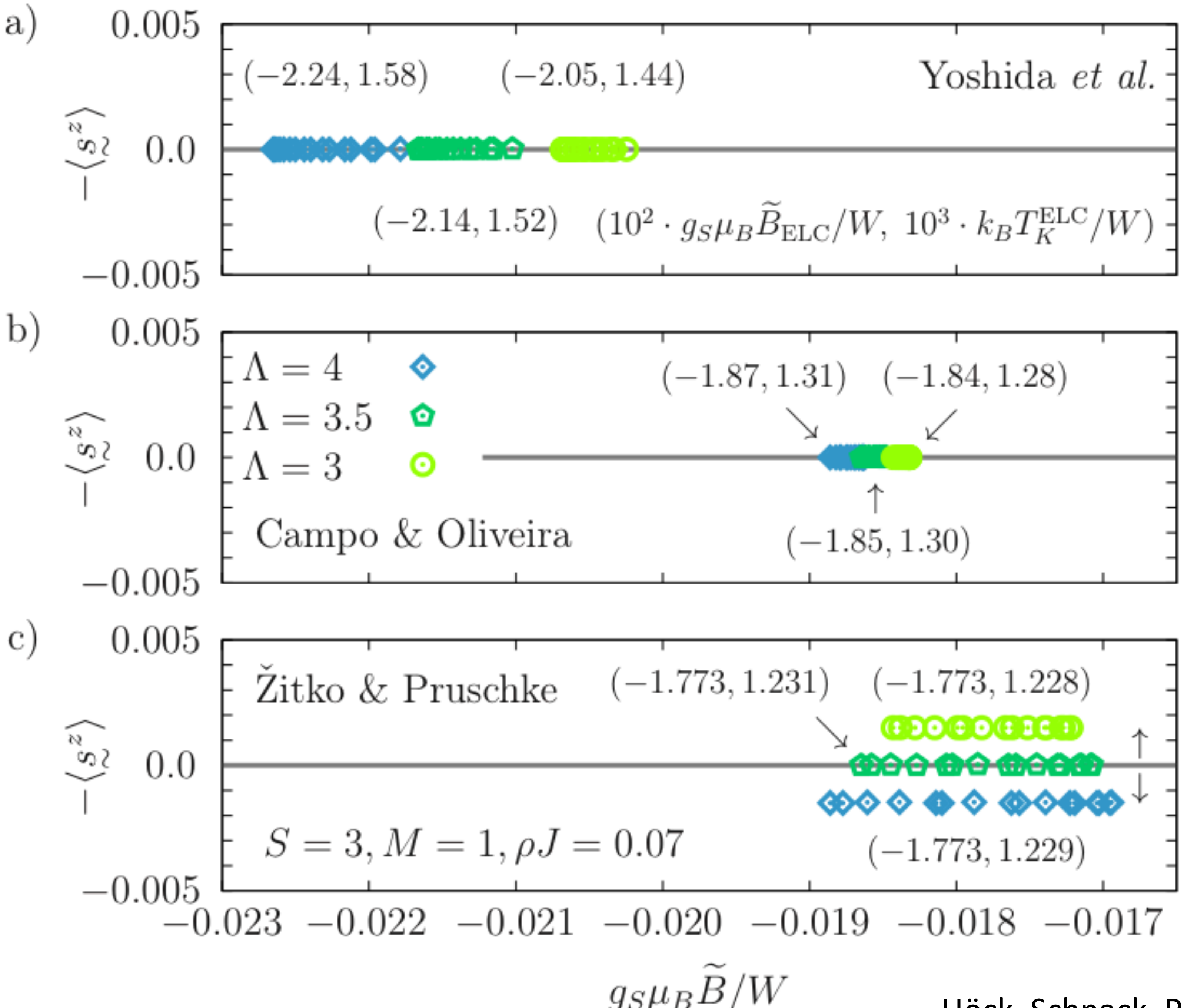

old
new
ε=-0.05
Γ=0.05
A(ω)
ω
7
6
5
4
3
2
1
0
-1
-0.8
-0.6
-0.4
-0.2
0
0.2
0.4
0.6
0.8
1



old
new
ε=-0.05
Γ=0.05
A(ω)
ω
0.4
0.3
0.2
0.1
0
-1
-0.8
-0.6
-0.4
-0.2
0
0.2
0.4
0.6
0.8
1

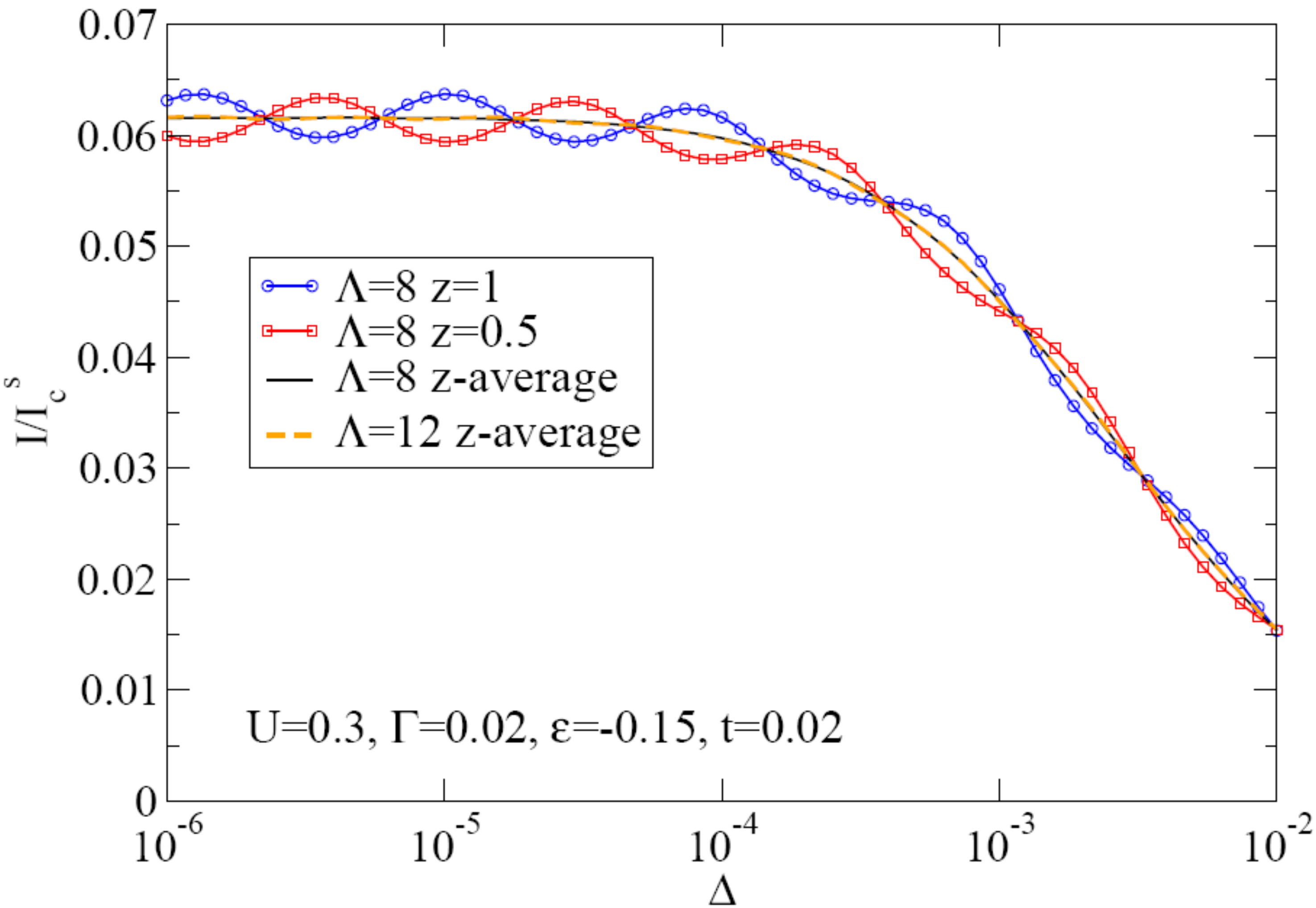
Main success: **excellent convergence** of various *expectation values*





Höck, Schnack, PRB 2013

Cancellation of Λ-periodic NRG discretization artifacts by the z-averaging



R. Žitko, M. Lee, R. Lopez, R. Aguado, M.-S. Choi, Phys. Rev. Lett. **105**, 116803 (2010)

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`.

Iterative diagonalization

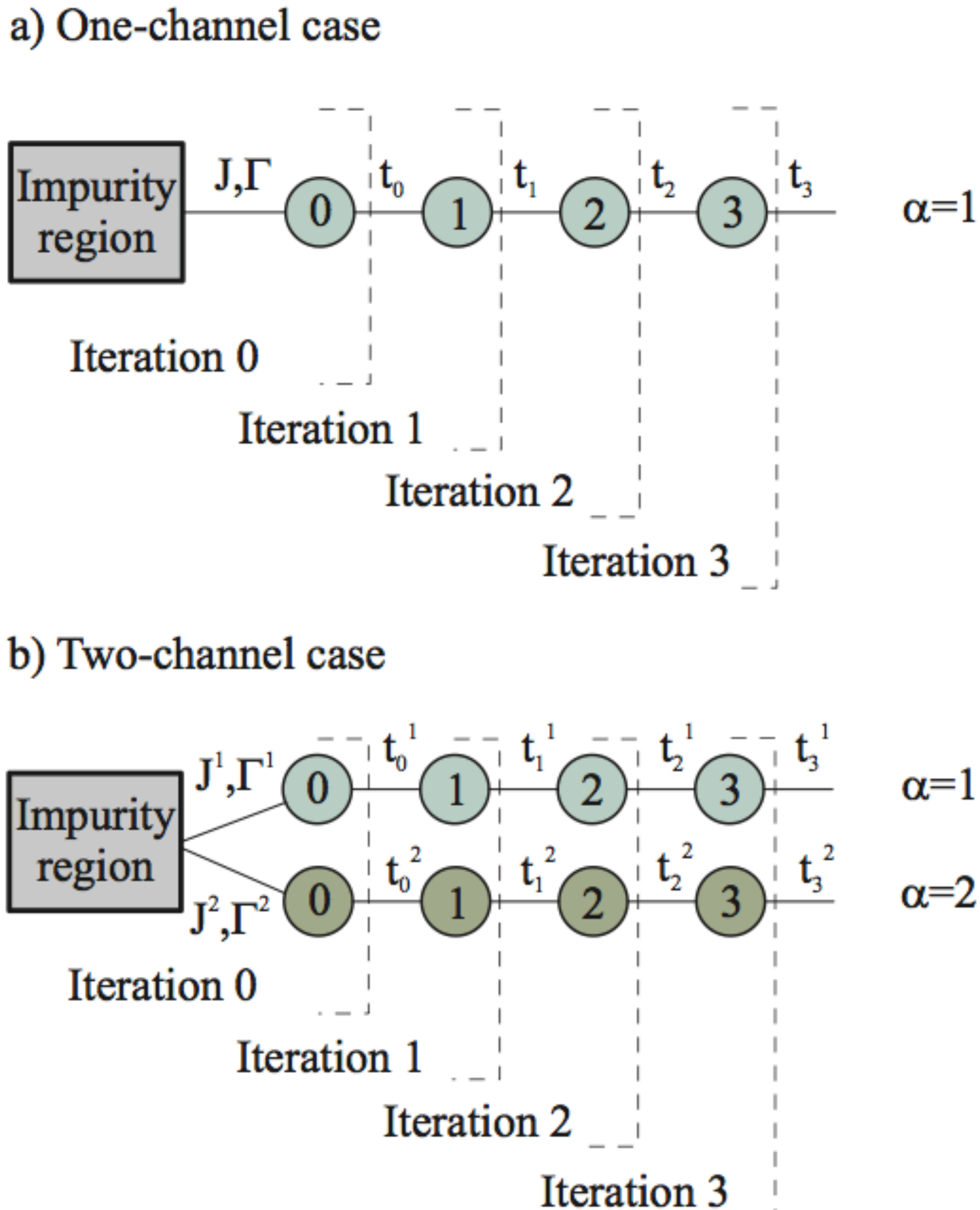
$$H = \lim_{N\to\infty} \left(\Lambda^{-N/2} H_N\right)$$

$$H_N = \Lambda^{N/2} \left[H_{\text{imp}} + H_{\text{C}} + \sum_{n=0}^{N} \sum_{\mu,\alpha} \Lambda^{-n/2} \xi_n \left(f^{\dagger}_{n,\mu,\alpha} f_{n+1,\mu,\alpha} + \text{H.c} \right) \right]$$

$$H_{N+1} = R\left\{H_N\right\} = \sqrt{\Lambda} H_N + \sum_{\mu,\alpha} \xi_N \left(f^{\dagger}_{n,\mu,\alpha} f_{n+1,\mu,\alpha} + \text{H.c} \right)$$

$$H_{N+2} = R^2 \left\{H_N\right\}$$

$$\ldots \to H_{N-2} \to H_N \to H_{N+2} \to \ldots$$


a) One-channel case
Impurity region
J,Γ
0
t0
1
t1
2
t2
3
t3
α=1
Iteration 0
Iteration 1
Iteration 2
Iteration 3
b) Two-channel case
Impurity region
J1,Γ1
J2,Γ2
0
t0 1
1
t1 1
2
t2 1
3
t3 1
α=1
0
t0 2
1
t1 2
2
t2 2
3
t3 2
α=2
Iteration 0
Iteration 1
Iteration 2
Iteration 3

$(\mathbf{q},\mathbf{s})$	States $(\mathbf{k})$
$(-1,0)$	1
$(0,\frac{1}{2})$	$a_\uparrow^\dagger$
$(1,0)$	$a_\downarrow^\dagger a_\uparrow^\dagger$

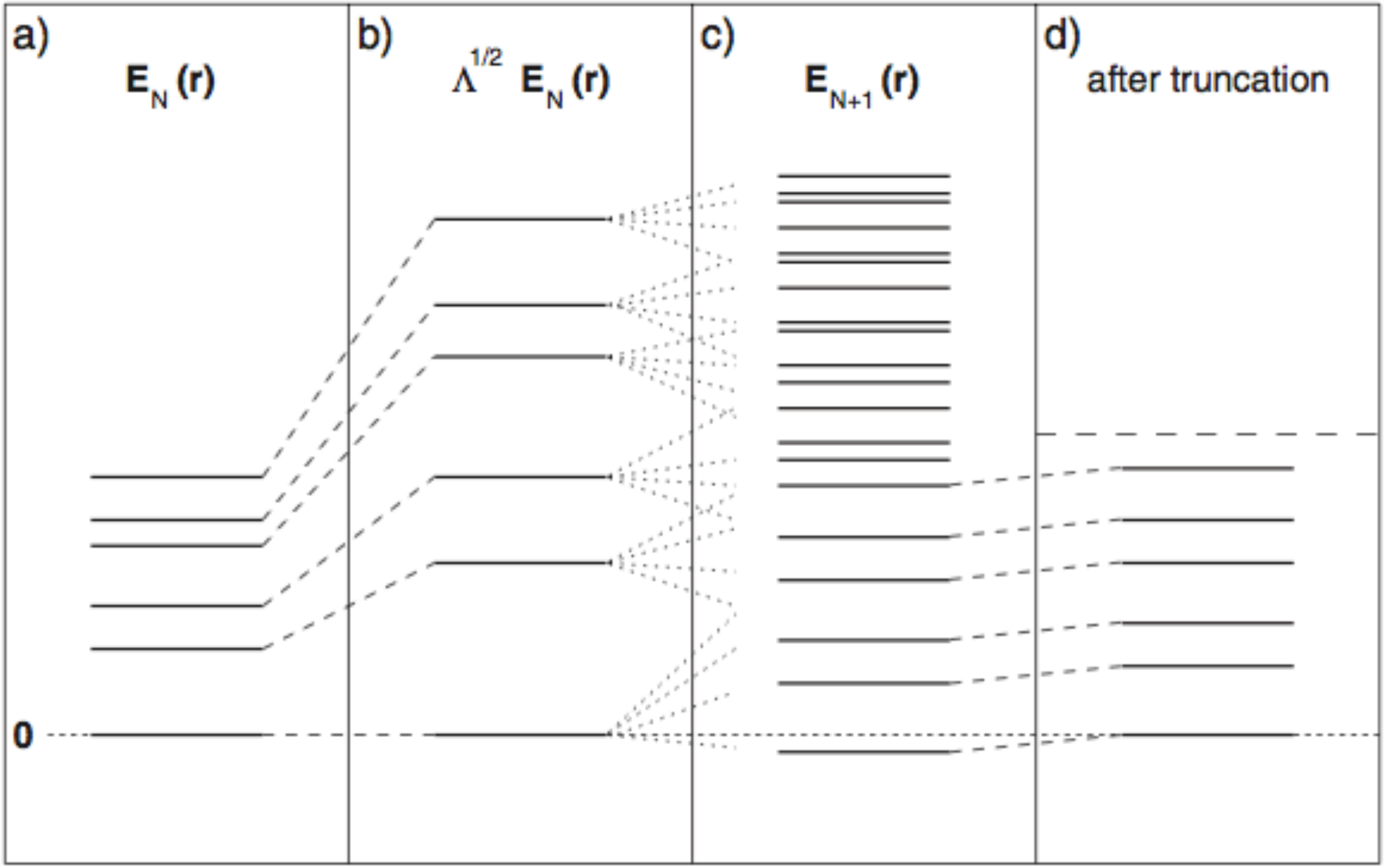
(a) One channel

$(\mathbf{q},\mathbf{s})$	States $(\mathbf{k})$
$(-2,0)$	1
$(-1,\frac{1}{2})$	$b_\uparrow^\dagger$, $a_\uparrow^\dagger$
$(0,0)$	$b_\downarrow^\dagger b_\uparrow^\dagger$, $\frac{1}{\sqrt{2}}\left(a_\downarrow^\dagger b_\uparrow^\dagger - a_\uparrow^\dagger b_\downarrow^\dagger\right)$, $a_\downarrow^\dagger a_\uparrow^\dagger$
$(0,1)$	$b_\uparrow^\dagger a_\uparrow^\dagger$
$(1,\frac{1}{2})$	$a_\uparrow^\dagger b_\downarrow^\dagger b_\uparrow^\dagger$, $b_\uparrow^\dagger a_\downarrow^\dagger a_\uparrow^\dagger$
$(2,0)$	$a_\uparrow^\dagger a_\downarrow^\dagger b_\uparrow^\dagger b_\downarrow^\dagger$

(b) Two channels

$$|QSS_z ri\rangle_{N+1} = \sum_{\mu=-S(i)}^{S(i)} \langle g_i^\mu(SS_z); S(i),\mu | SS_z\rangle \; |F_i(QS) f_i^\mu(S_z) r\rangle_N \otimes |i,\mu\rangle$$

$$|QS\omega\rangle = \sum_{ri} U_{QS}(\omega, ri) |QSri\rangle$$



Bulla, Costi, Pruschke, RMP 2008

$$T_N \propto \frac{D}{k_B} \Lambda^{-N/2} / \bar{\beta} \qquad \bar{\beta} \sim 1$$

Characteristic energy scale at the N-th step of the NRG iteration:

discretization=Y

$$\omega_N = \frac{1+\Lambda^{-1}}{2} \Lambda^{-(N-1)/2+1-z}$$

discretization=C or Z

$$\omega_N = \frac{1-\Lambda^{-1}}{\log \Lambda} \Lambda^{-(N-1)/2+1-z}$$

RG, fixed points, operators

$$H^* = R^2\{H^*\}$$

$$\delta H_{N+2} = R^2\{H^* + \delta H_N\} - H^* \approx \mathcal{L}^* \delta H_N$$

linear operator

$$\mathcal{L}^* O_l^* = \lambda_l^* O_l^*$$

$$\delta H_N = \sum_l C_l \lambda_l^{*N/2} O_l^*$$

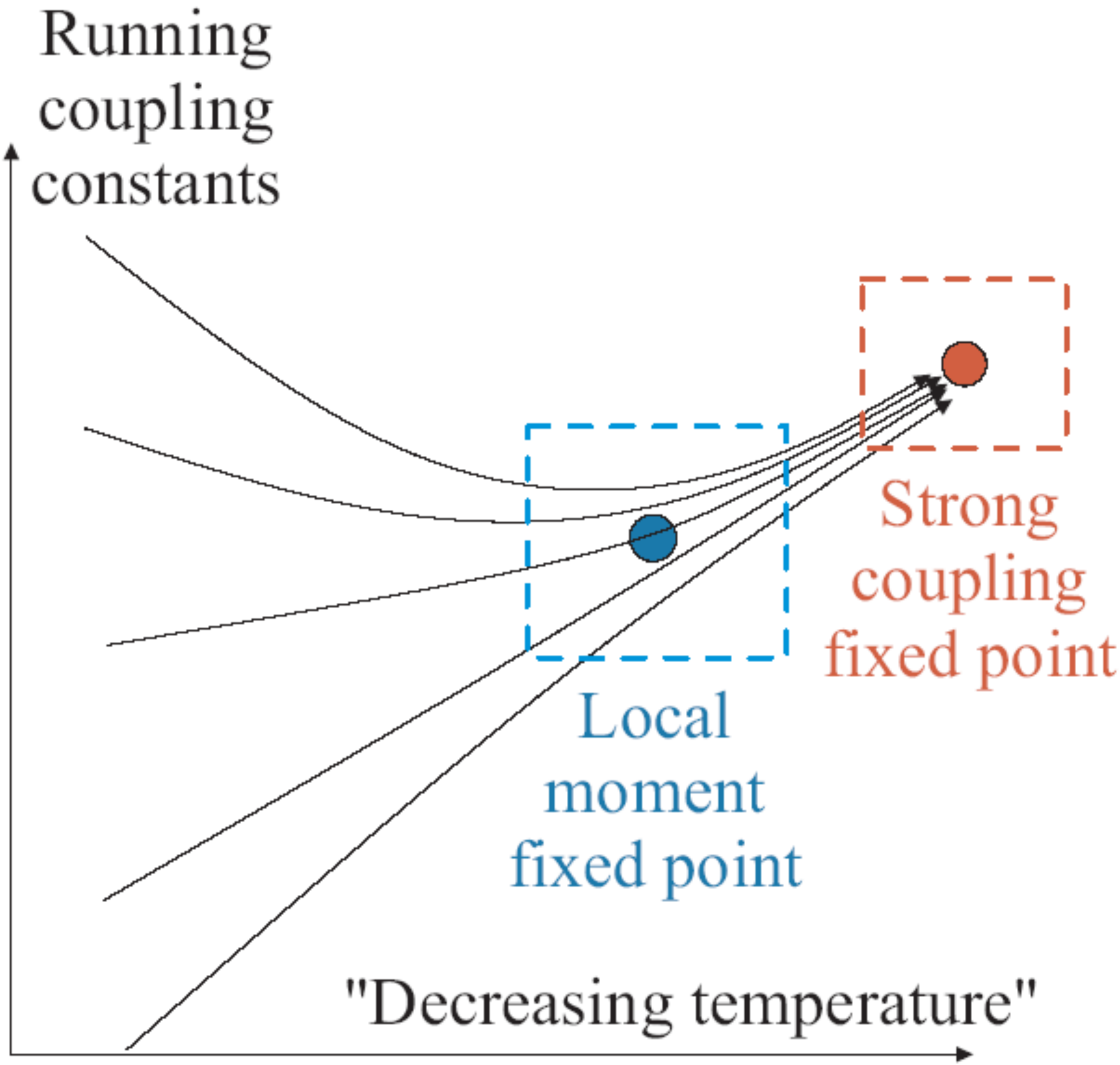
$\lambda_l^* > 1$ relevant operator

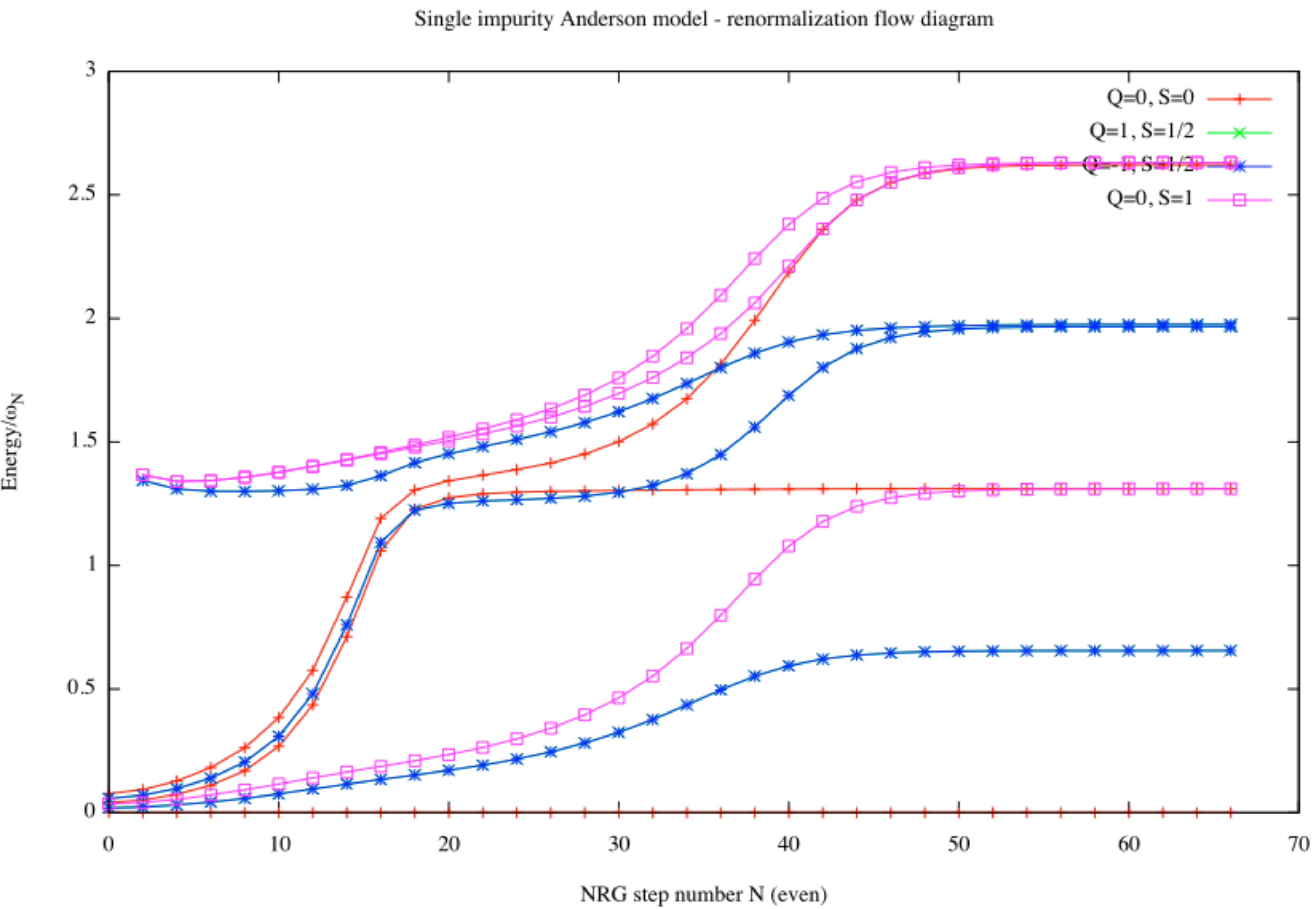
$\lambda_l^* < 1$ irrelevant operator

$\lambda_l^* = 1$ marginal operator

See Krishnamurthy, Wilkins, Wilson, PRB 1980 for a very detailed analysis of the fixed points in the SIAM.

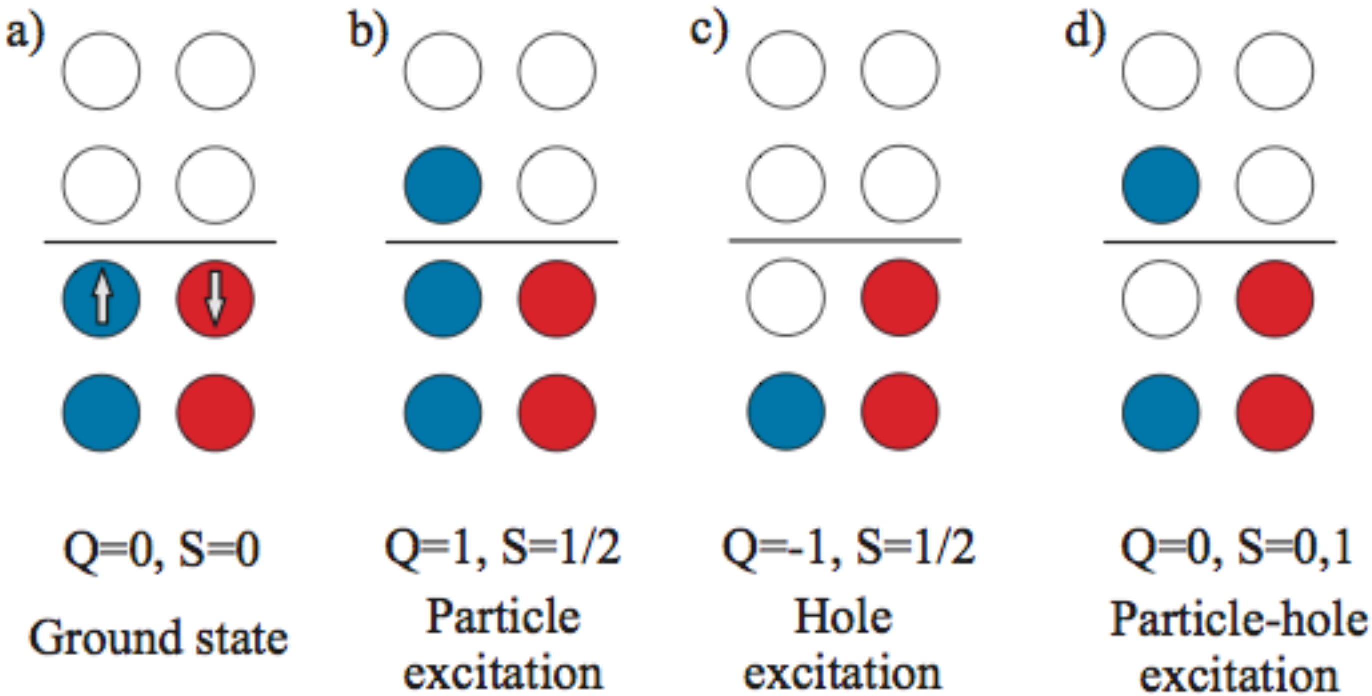
Universality

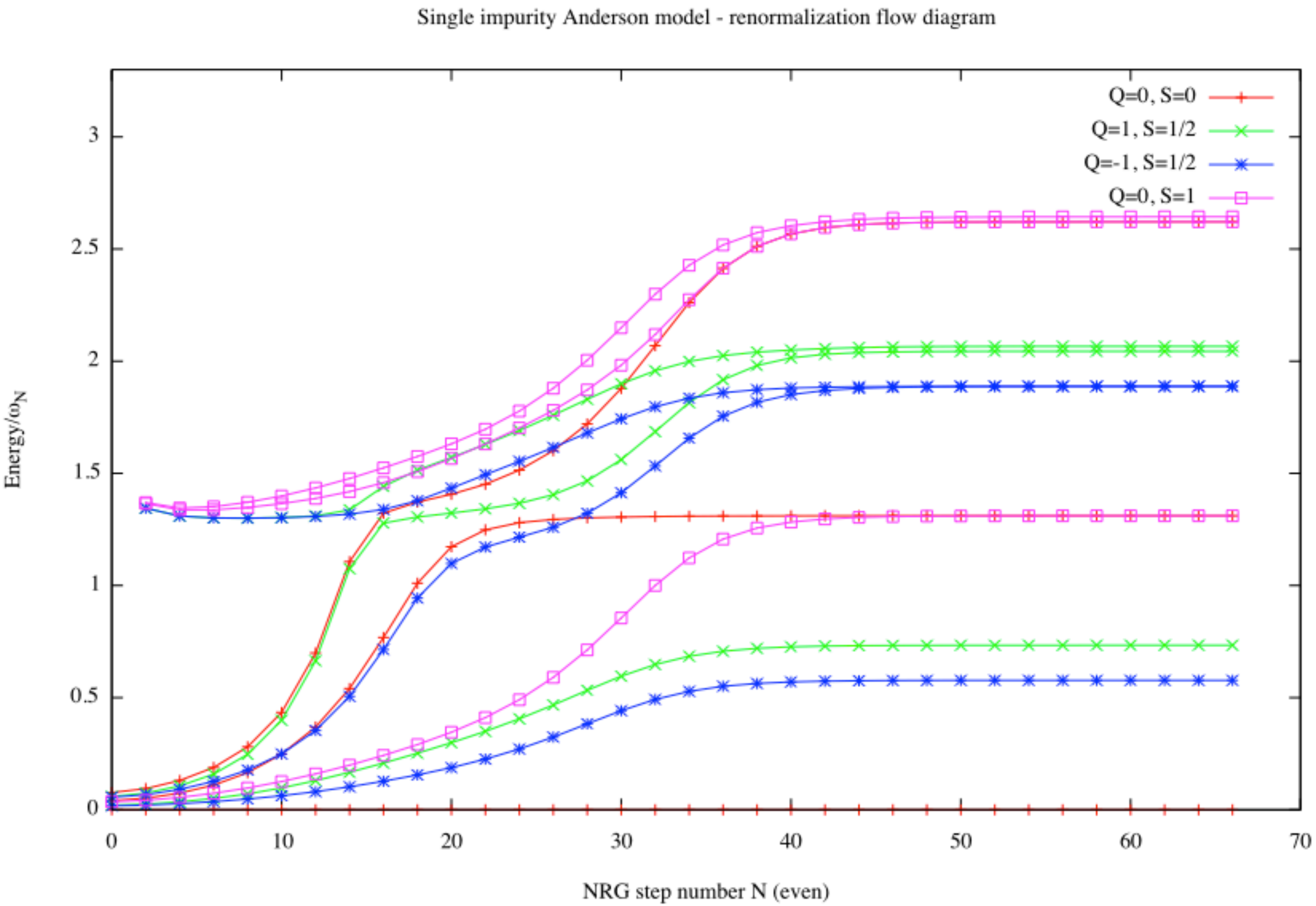




Single impurity Anderson model - renormalization flow diagram
Q=0, S=0
Q=1, S=1/2
Q=-1, S=1/2
Q=0, S=1
Energy/ω_N
NRG step number N (even)
0
0.5
1
1.5
2
2.5
3
0
10
20
30
40
50
60
70

Fermi-liquid fixed points





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70

Thermodynamic quantities

$$\chi_{\mathrm{imp}}(T) = \frac{(g\mu_B)^2}{k_B T}\Big(\langle S_z^2\rangle - \langle S_z^2\rangle_0\Big)$$

$$S_{\mathrm{imp}}(T) = \frac{(E-F)}{T} - \frac{(E-F)_0}{T}$$

$$E = \langle H\rangle = \mathrm{Tr}\left[He^{-H/k_B T}\right]$$

$$F = -k_B T \ln \mathrm{Tr}\left[e^{-H/k_B T}\right]$$

Computing the expectation values

$$\langle O \rangle = \mathrm{Tr}\left[O \exp(-\beta H)\right]/Z$$

$$Z = \mathrm{Tr}\left(e^{-\beta H}\right)$$

$$\beta = 1/k_B T$$

Conventional approach: use H_N as an approximation for full H at temperature scale T_N.

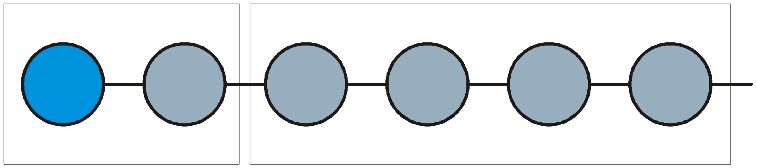
$$\beta H \approx \bar{\beta} H_N$$

Alternatively: use FDM for given T. Also works for thermodynamics: Merker, Weichselbaum, Costi, Phys. Rev. B 86, 075153 (2012)

Local vs. global operators

- Local operators: impurity charge, impurity spin, $d^{\dagger}_{\sigma}$. In general, any operator defined on the initial cluster.
- Global operators: total charge, total spin, etc. Example:

$$\hat{S}_z = \sum_{i=1}^{N} \hat{s}_z^i$$



(Magnetic) susceptibility

$$\chi_\alpha(T) = (g\mu_B)^2 \int_0^\beta d\tau \left(\langle S_\alpha(\tau) S_\alpha(0) \rangle - \langle S_\alpha \rangle^2 \right)$$

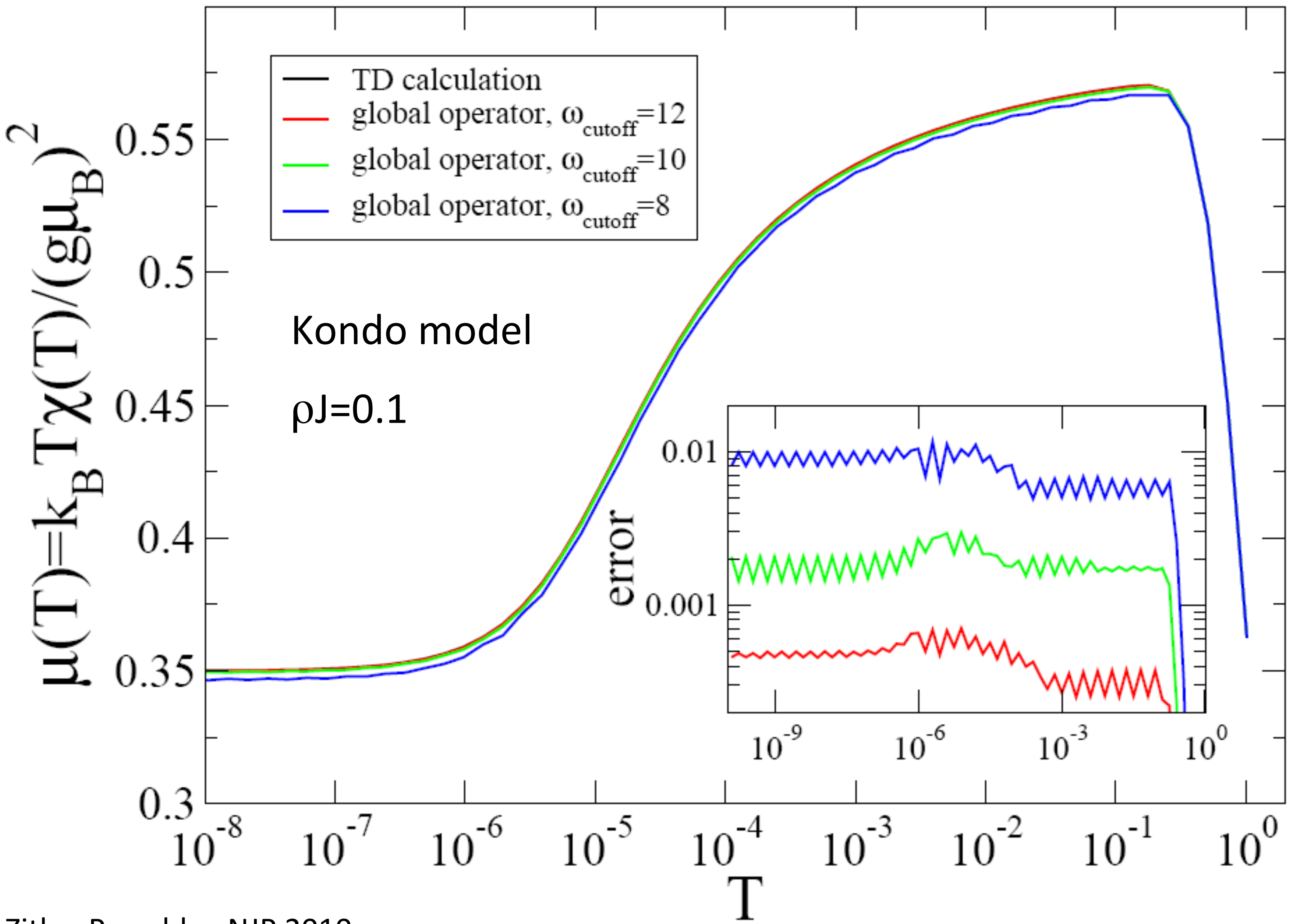
If $[H,S_z]=0$:

$$\chi_z(T) = (g\mu_B)^2 \beta \left(\langle S_z^2 \rangle (T) - [\langle S_z \rangle (T)]^2 \right)$$

General case:

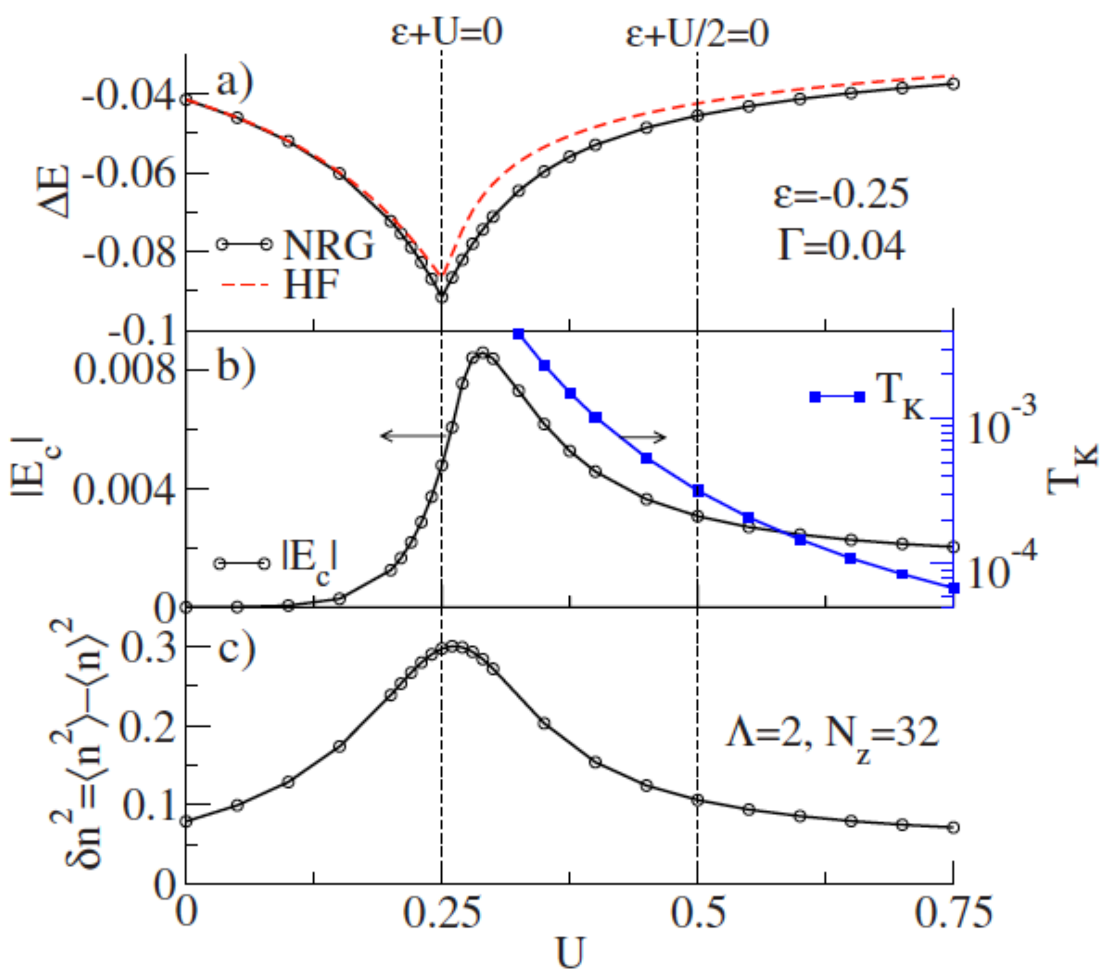
$$C(\tau) \;=\; \langle S_\alpha(\tau) S_\alpha(0) \rangle$$

$$\int_0^\beta C(\tau) \mathrm{d}\tau = \frac{1}{Z^{(N)}} \sum_{w,w'} \left(M^N_{ww'} \right)^* M^N_{w'w} \frac{e^{-\beta E_w} - e^{-\beta E_{w'}}}{\beta E_{w'} - \beta E_w}$$



Zitko, Pruschke, NJP 2010

Ground state energy (binding energy, correlation energy, Kondo singlet formation energy)



Zitko, PRB 2009