The numerical renormalization group *as a DMFT impurity solver*

Fabian Kugler

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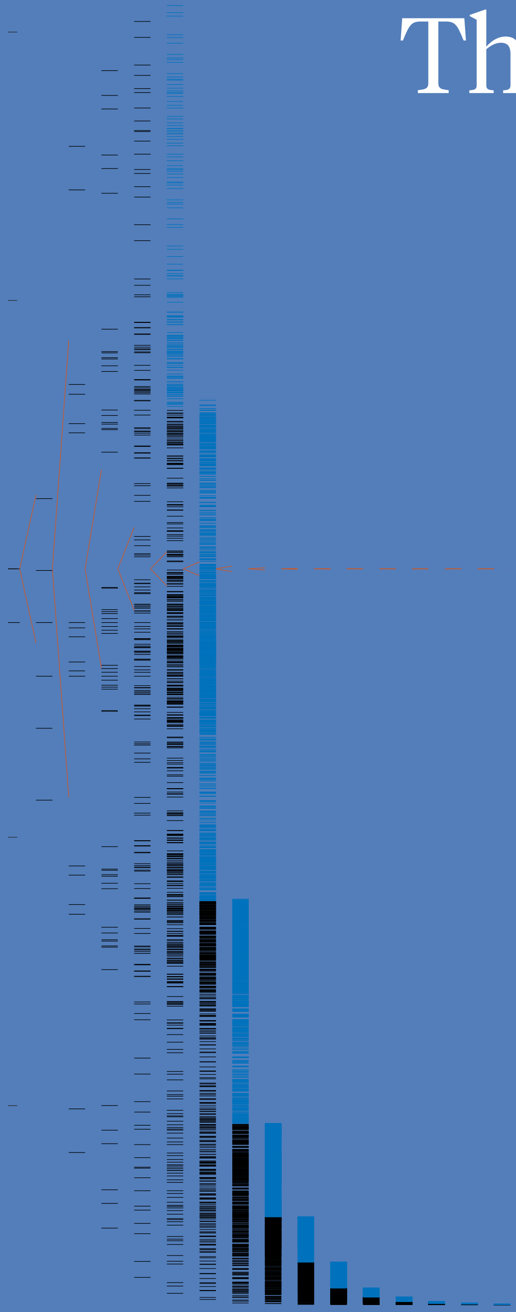
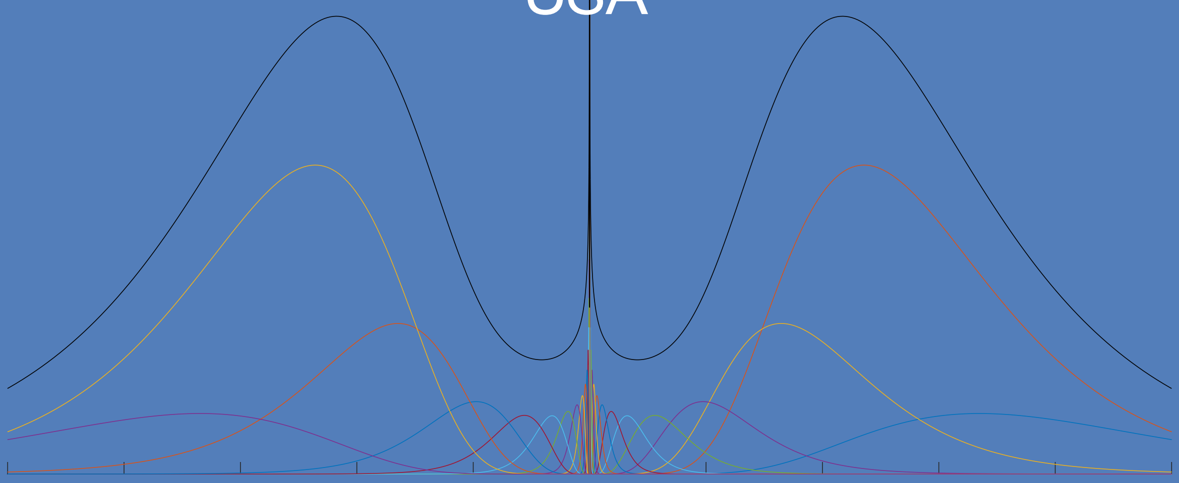
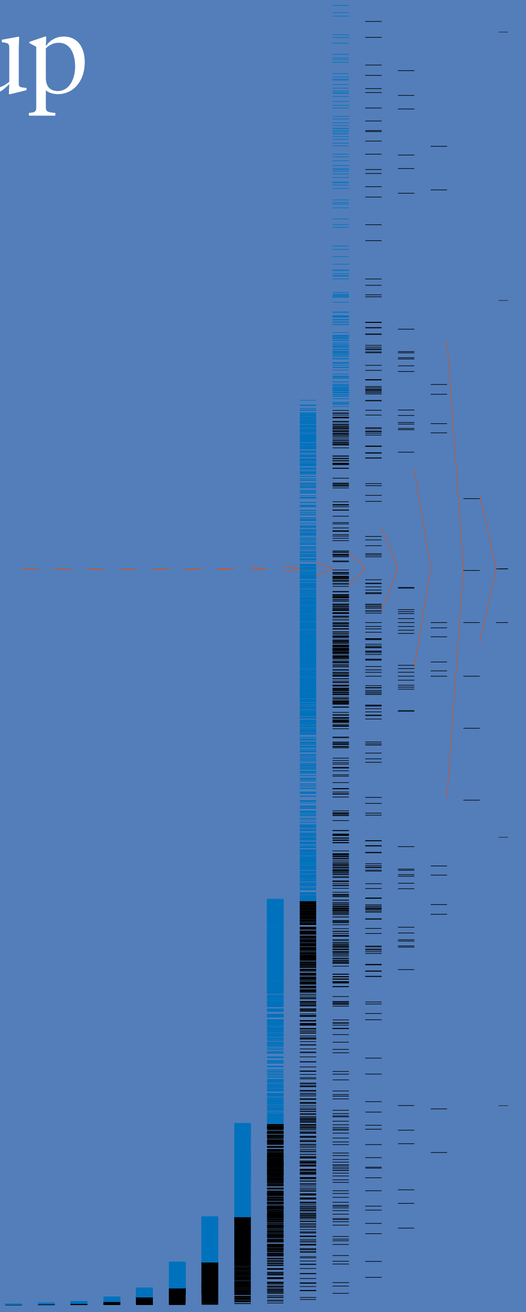
USA







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Formalism

Introduction

Logarithmic discretization

Mapping to Wilson chain

Iterative diagonalization

Complete basis

Log-Gaussian broadening

Self-energy estimators

Logarithmic discretization Mapping to Wilson chain Iterative diagonalization	Wilson, RMP 1975
Complete basis	Anders, Schiller, PRL 2005 Weichselbaum, von Delft, PRL 2008
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Applications

Orbital-selective Mott phase	Kugler et al., PRB 2019; Kugler, Kotliar, PRL 2022
DFT+DMFT+NRG for Sr$_2$RuO$_4$	Kugler et al., PRL 2020
Real-frequency two-particle vertex	Kugler, Lee, von Delft, PRX 2021; Lee, Kugler, von Delft, PRX 2021 Lihm, ..., Kugler, Lee, PRB 2024

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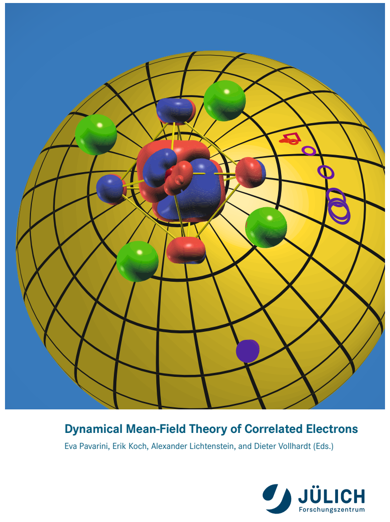
NRG reviews

Wilson, RMP 1975 (“a physics classic”)
http://dx.doi.org/10.1103/RevModPhys.47.773

Bulla, Costi, Pruschke, RMP 2008 (BCP08)
http://dx.doi.org/10.1103/RevModPhys.80.395

Von Delft, Lecture Notes 2022 (vD22)
https://www.cond-mat.de/events/correl22/manuscripts/vondelft.pdf



Dynamical Mean-Field Theory of Correlated Electrons

Eva Pavarini, Erik Koch, Alexander Lichtenstein, and Dieter Vollhardt (Eds.)

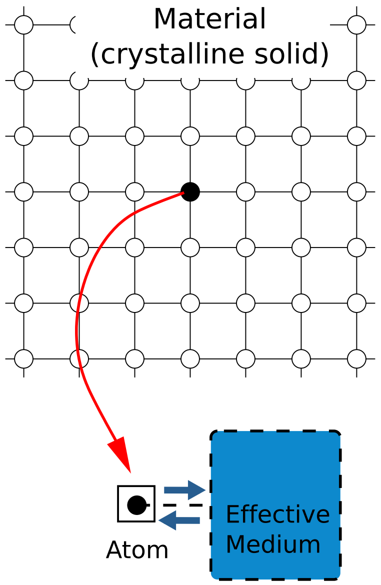
JÜLICH Forschungszentrum

Introduction

DMFT maps lattice model into impurity model:

Hubbard model (HM) $$H = \sum_i U n_{i\uparrow} n_{i\downarrow} + \sum_{\boldsymbol{k}} \xi_{\boldsymbol{k}} n_{\boldsymbol{k}} \qquad n_i = \sum_{\sigma=\uparrow,\downarrow} n_{i\sigma}, \quad n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$$

→ Anderson impurity model (AIM) $$H = \epsilon_d n_d + U n_{d\uparrow} n_{d\downarrow} + \sum_{\boldsymbol{k}\sigma} (V_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}\sigma} d_\sigma + \text{h.c.}) + \sum_{\boldsymbol{k}} \xi_{\boldsymbol{k}} n_{\boldsymbol{k}}$$



Georges, Comptes Rendus Physique 2016

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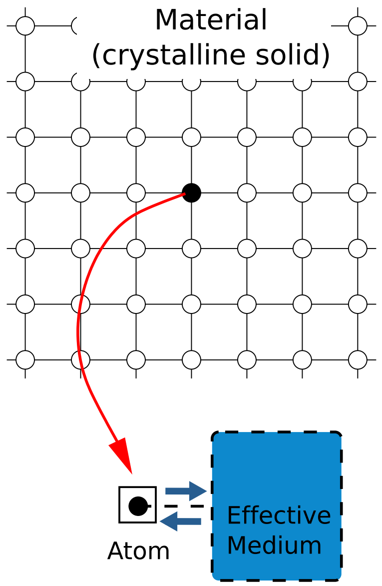
Why is AIM simpler than HM? Focusing on impurity correlation functions, the bath can be integrated out

$$S = -\sum_{\mathrm{i}\nu} \bar{d}_\sigma(\mathrm{i}\nu) \big[\mathrm{i}\nu - \epsilon_d - \Delta(\mathrm{i}\nu) \big] d_\sigma(\mathrm{i}\nu) + \int_0^\beta U n_{d\uparrow}(\tau) n_{d\downarrow}(\tau)$$



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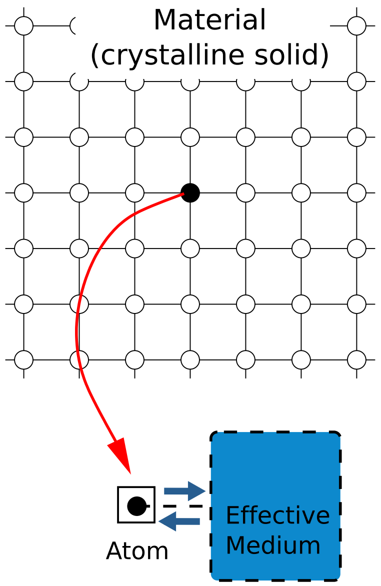

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Hybridization function $$\Delta(\mathrm{i}\nu) = \sum_{\boldsymbol{k}} \frac{|V_{\boldsymbol{k}}|^2}{\mathrm{i}\nu - \xi_{\boldsymbol{k}}}$$

with spectral representation $$\Delta(\mathrm{i}\nu) = \int \mathrm{d}\omega \frac{\Gamma(\omega)}{\mathrm{i}\nu - \omega}, \quad \Gamma(\omega) = \sum_{\boldsymbol{k}} |V_{\boldsymbol{k}}|^2 \delta(\omega - \xi_{\boldsymbol{k}}) \overset{\text{e.g.}}{=} \Gamma\Theta(D - |\omega|)$$

Why diagonalization?

Fully diagonalize Hamiltonian → expectation values and correlation functions (real or imaginary frequency) at any temperature in text-book fashion 🙂

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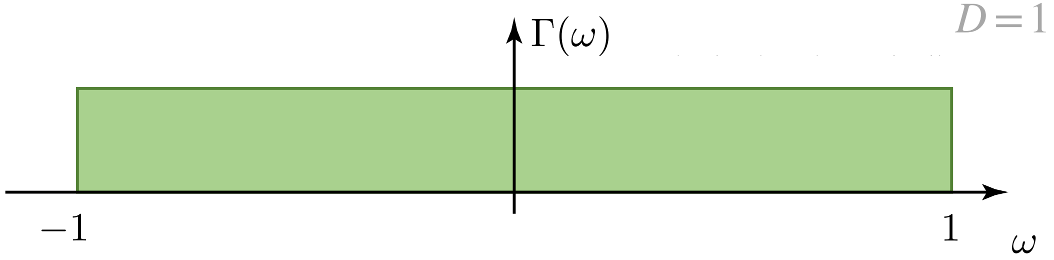

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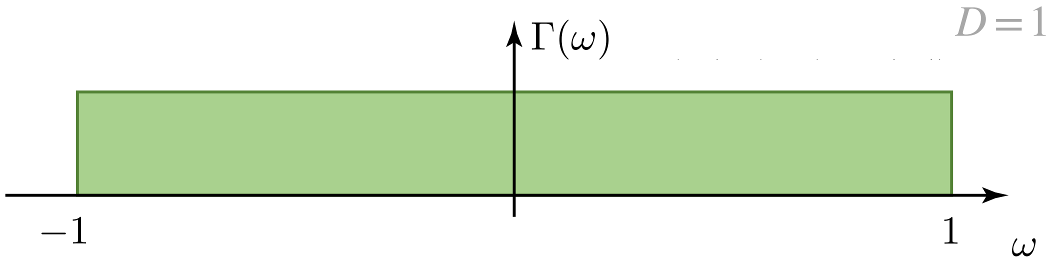

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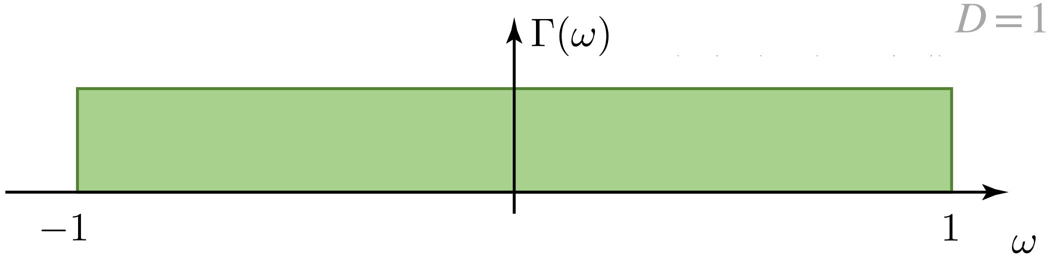
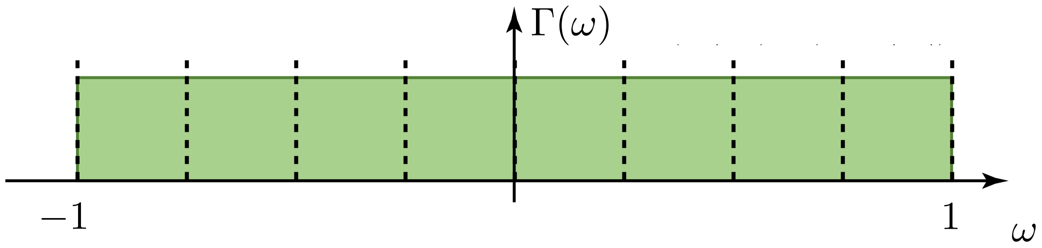


Discretization

Linear discretization: smallest energy scale $\sim \frac{D}{N}$

$D \sim \mathrm{eV}, T \sim \mathrm{K} \sim \mathrm{meV} \rightarrow N \sim 1000$ 🙁



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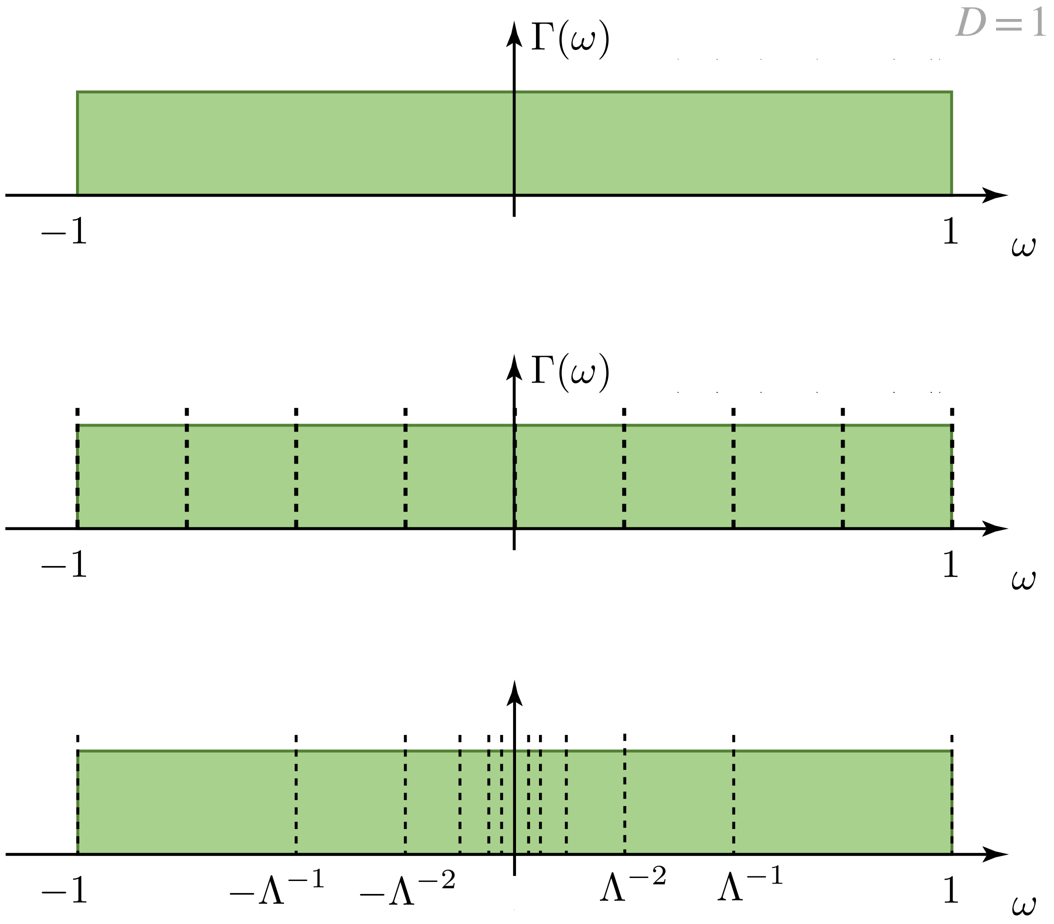
Logarithmic discretization ($\Lambda > 1$)

$D \sim \mathrm{eV}, T \sim \mathrm{K} \sim \mathrm{meV} \rightarrow N \sim \log_\Lambda 1000 \overset{\Lambda=2}{\sim} 10$ 🙂

“Be able to resolve small energies, accept coarse resolution at high energies”



Mapping to Wilson chain

$$\Gamma(\omega) \overset{\text{e.g.}}{=} \Gamma\Theta(D - |\omega|) = \sum_{\pm,n=1}^{N/2} V_{\pm n}^2 \delta(\omega - \xi_{\pm n})$$

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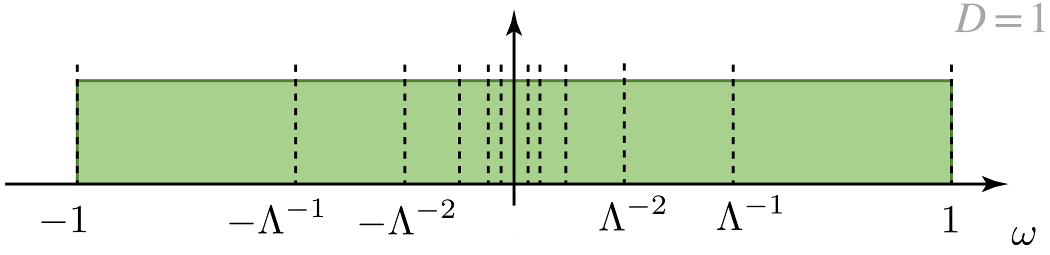
vD22

$D = 1$



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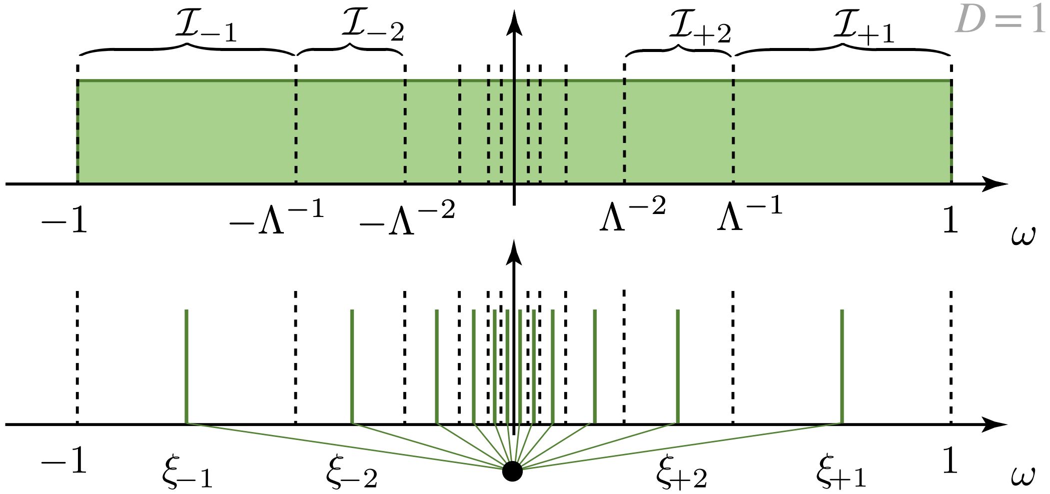

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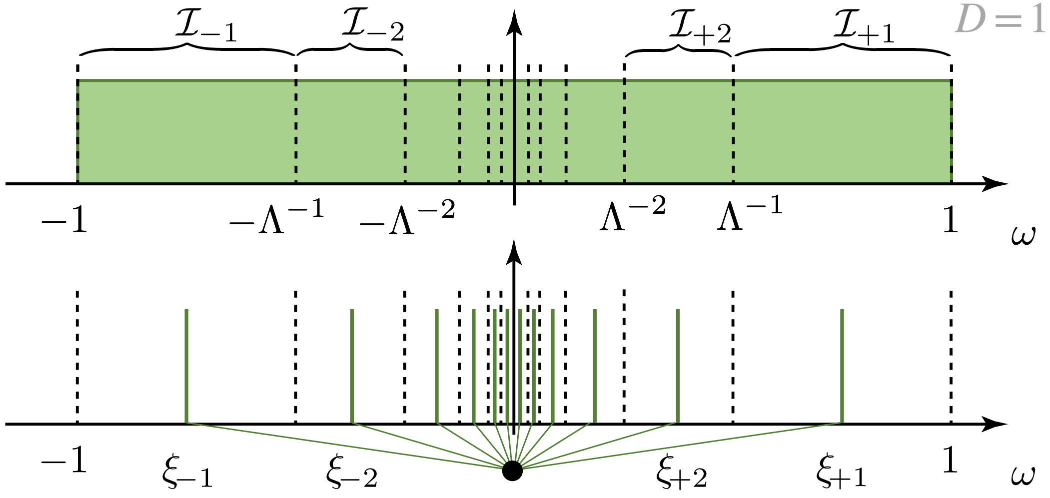

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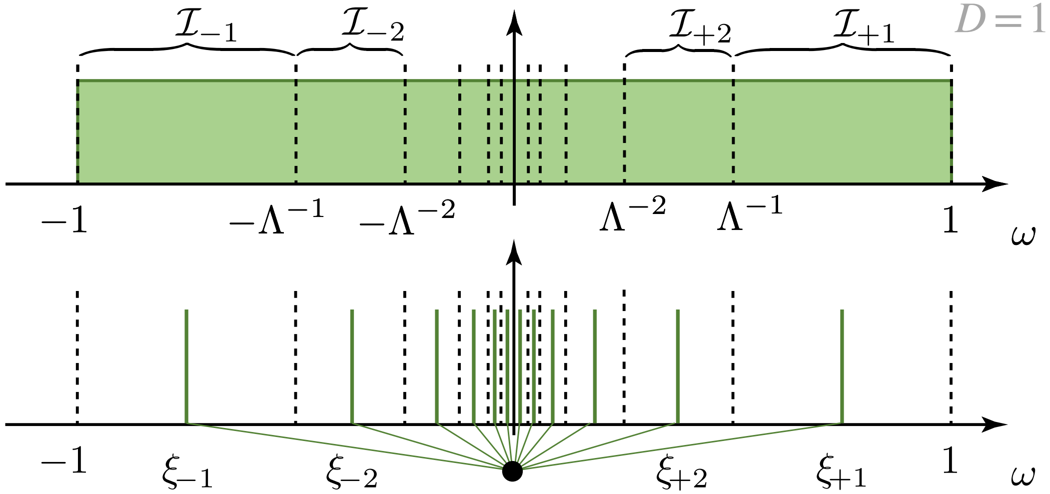

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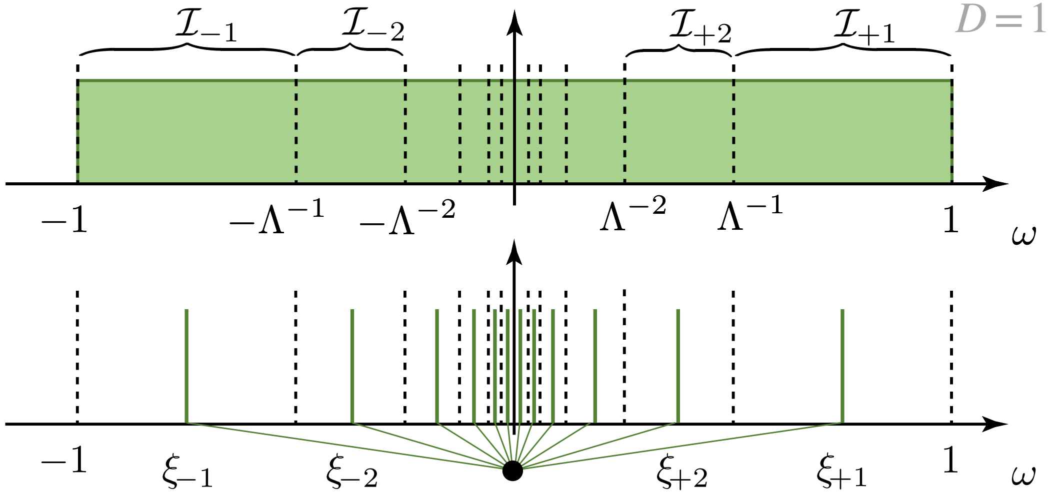

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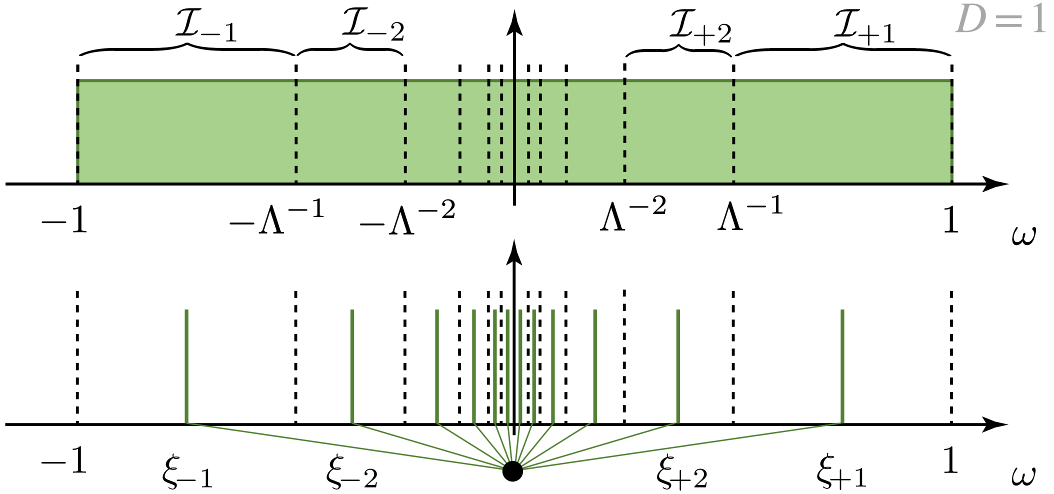

vD22
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Unitary traformation via tri-diagonalization (Lanczos)

$$\begin{array}{c|ccccc} & -2 & -1 & \text{imp} & 1 & 2 \\ \hline -2 & \xi_{-2} & 0 & V_{-2} & 0 & 0 \\ -1 & 0 & \xi_{-1} & V_{-1} & 0 & 0 \\ \text{imp} & V_{-2} & V_{-1} & 0 & V_1 & V_2 \\ 1 & 0 & 0 & V_1 & \xi_1 & 0 \\ 2 & 0 & 0 & V_2 & 0 & \xi_2 \end{array} \rightarrow \begin{array}{c|ccccc} & \text{imp} & 0 & 1 & 2 & 3 \\ \hline \text{imp} & 0 & t_d & 0 & 0 & 0 \\ 0 & t_d & \epsilon_0 & t_0 & 0 & 0 \\ 1 & 0 & t_0 & \epsilon_1 & t_1 & 0 \\ 2 & 0 & 0 & t_1 & \epsilon_2 & t_2 \\ 3 & 0 & 0 & 0 & t_2 & \epsilon_3 \end{array}$$

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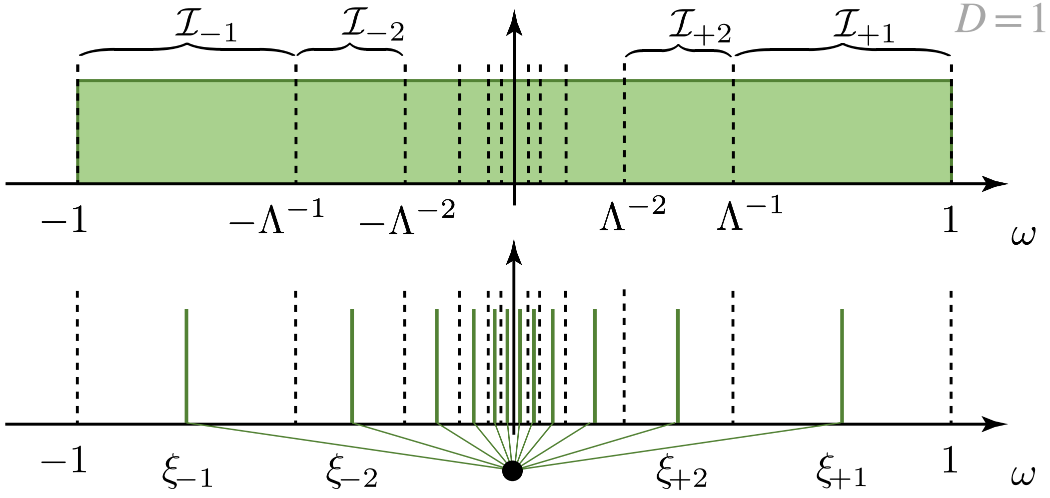

star geometry

Unitary traformation via tri-diagonalization (Lanczos)

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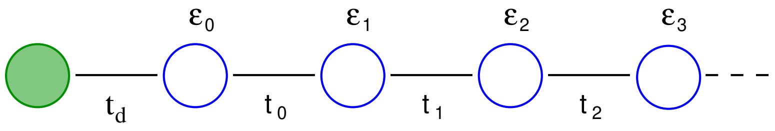

Wilson chain

BCP08

Mapping to Wilson chain

vD22
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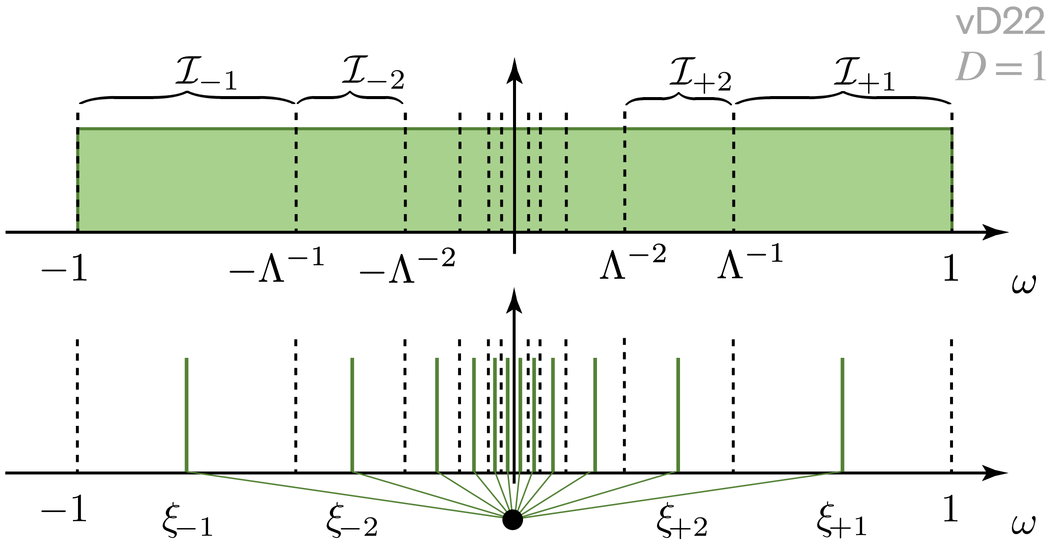


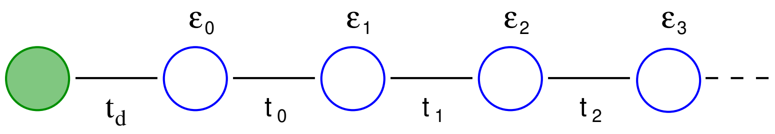
star geometry

$$t_n \overset{\text{e.g.}}{=} \frac{D(1+\Lambda^{-1})(1-\Lambda^{-n-1})}{2\sqrt{1-\Lambda^{-2n-1}}\sqrt{1-\Lambda^{-2n-3}}}\Lambda^{-n/2}, \qquad \epsilon_n \overset{\text{e.g.}}{=} 0$$

independent of $\int \Gamma(\omega)\mathrm{d}\omega$!

Unitary traformation via tri-diagonalization (Lanczos)

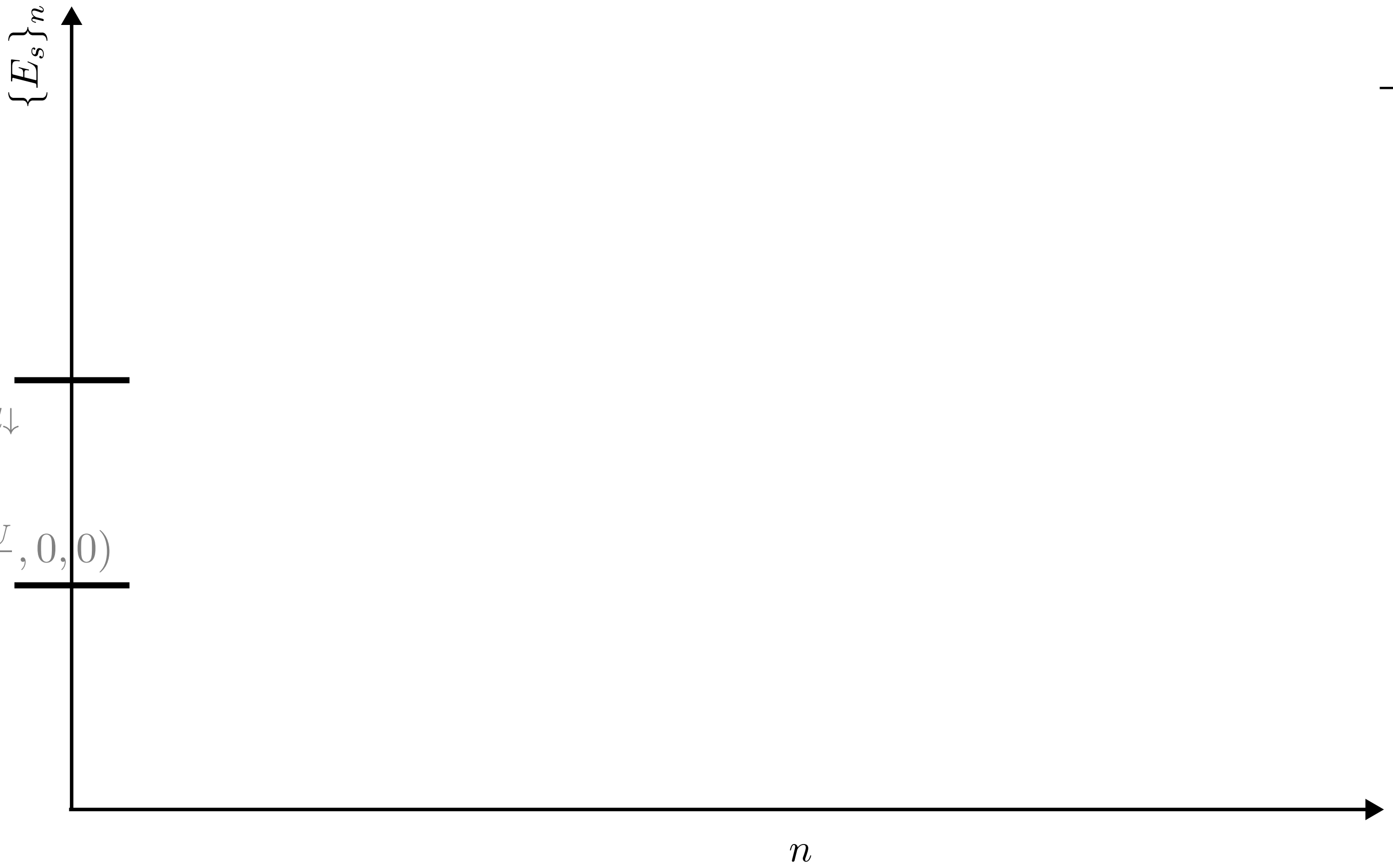
$$\begin{array}{c|ccccc} & -2 & -1 & \text{imp} & 1 & 2 \\ \hline -2 & \xi_{-2} & 0 & V_{-2} & 0 & 0 \\ -1 & 0 & \xi_{-1} & V_{-1} & 0 & 0 \\ \text{imp} & V_{-2} & V_{-1} & 0 & V_1 & V_2 \\ 1 & 0 & 0 & V_1 & \xi_1 & 0 \\ 2 & 0 & 0 & V_2 & 0 & \xi_2 \end{array} \rightarrow \begin{array}{c|ccccc} & \text{imp} & 0 & 1 & 2 & 3 \\ \hline \text{imp} & 0 & t_d & 0 & 0 & 0 \\ 0 & t_d & \epsilon_0 & t_0 & 0 & 0 \\ 1 & 0 & t_0 & \epsilon_1 & t_1 & 0 \\ 2 & 0 & 0 & t_1 & \epsilon_2 & t_2 \\ 3 & 0 & 0 & 0 & t_2 & \epsilon_3 \end{array}$$



Wilson chain

BCP08

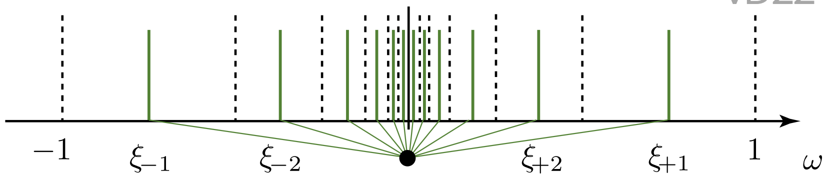
Iterative diagonalization



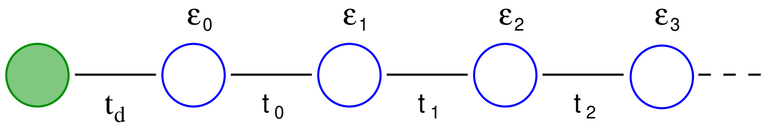
$-\frac{U}{2}n_d + U n_{d\uparrow} n_{d\downarrow}$
$= (U^\dagger D U)_{\mathrm{imp}},$
$D = \mathrm{diag}(\frac{-U}{2}, \frac{-U}{2}, 0, 0)$

$\dim\mathcal{H}:$ d

vD22

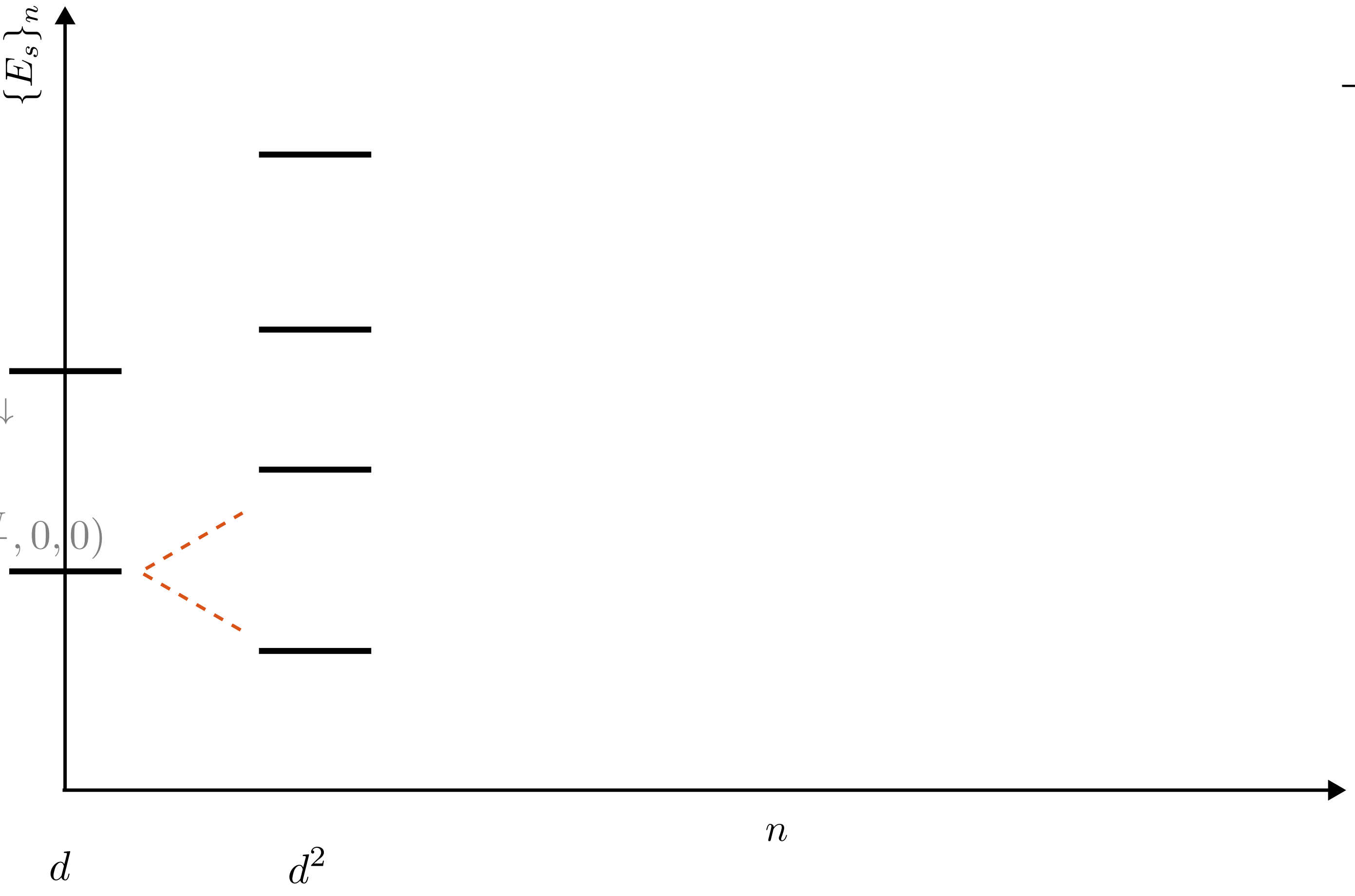


BCP08



“Be able to resolve small energies, accept coarse resolution at high energies”

Iterative diagonalization



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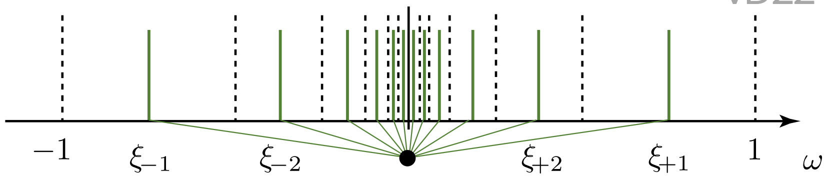
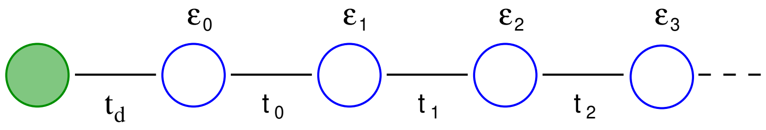
$D = \mathrm{diag}(\frac{-U}{2}, \frac{-U}{2}, 0, 0)$

$\dim\mathcal{H}:$ d d^2

vD22



BCP08



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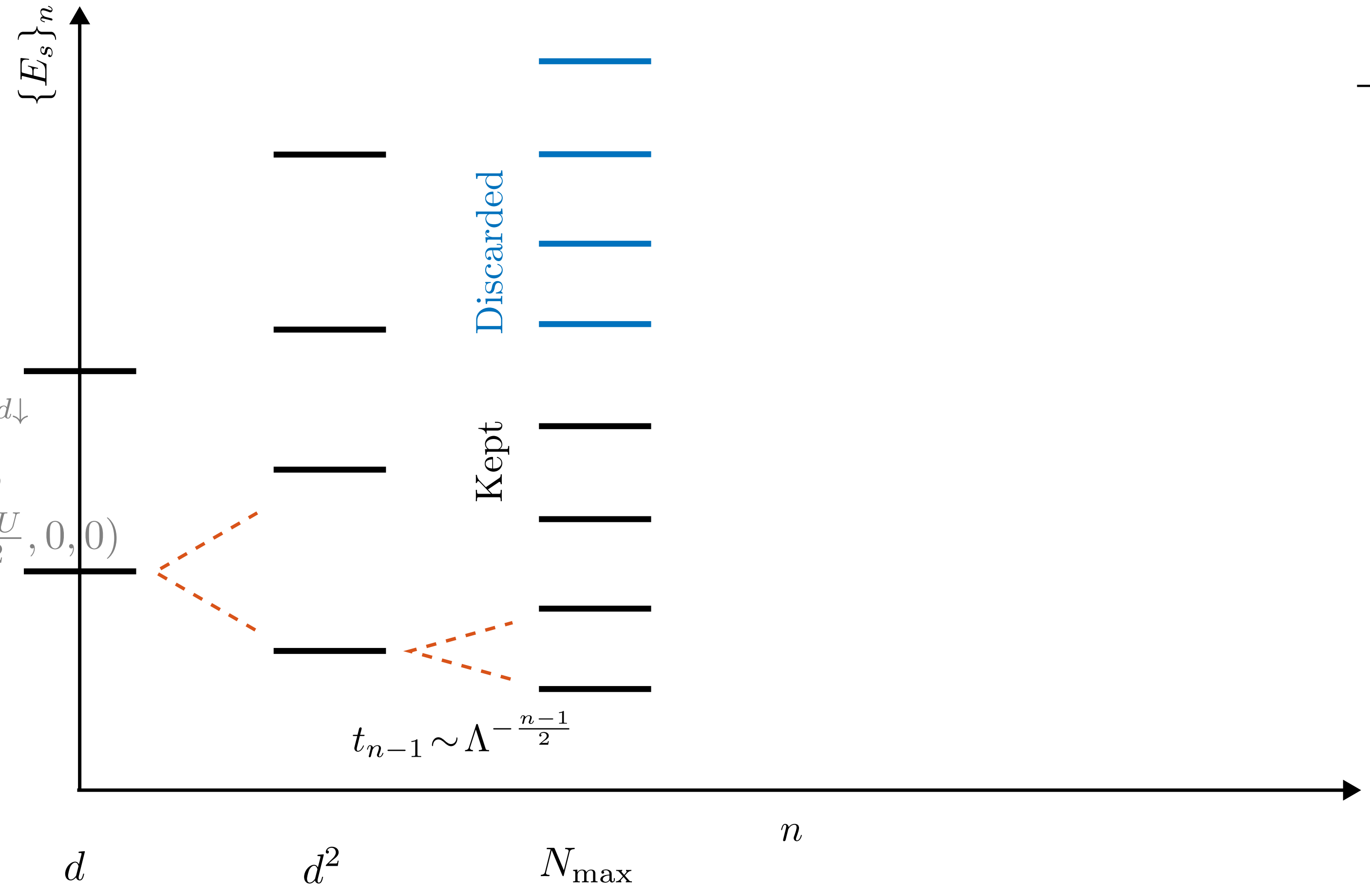
Iterative diagonalization



$-\frac{U}{2}n_d + U n_{d\uparrow} n_{d\downarrow}$
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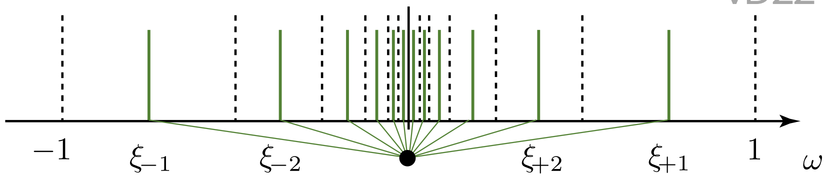
$D = \mathrm{diag}(\frac{-U}{2}, \frac{-U}{2}, 0, 0)$

vD22



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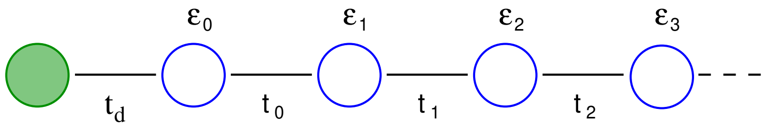
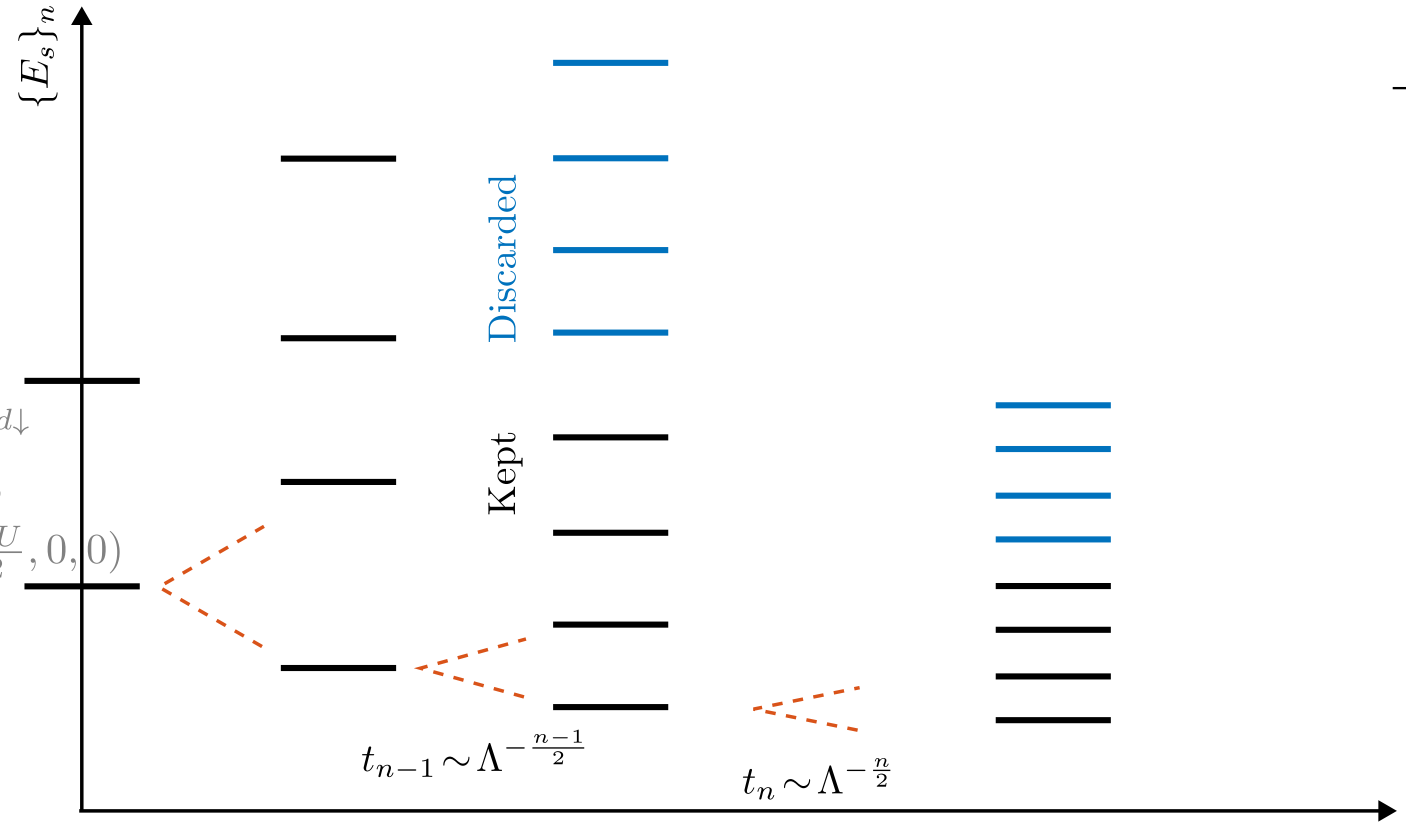


> *“Be able to resolve small energies,*
> *accept coarse resolution at high energies”*

Iterative diagonalization

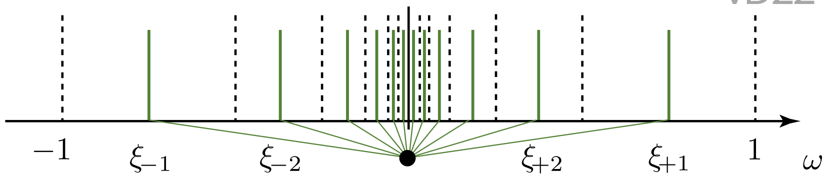


$-\frac{U}{2}n_d+Un_{d\uparrow}n_{d\downarrow}$
$=(U^\dagger DU)_{\text{imp}},$
$D=\text{diag}(\frac{-U}{2},\frac{-U}{2},0,0)$

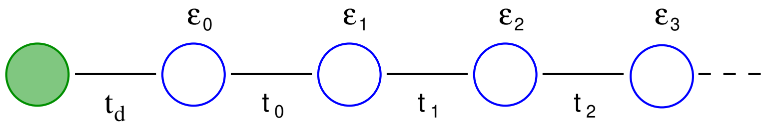
$\dim\mathcal{H}$: d d^2 N_{max} N_{max}

$$(U^\dagger DU)^{\text{K}}_{n-1}+\epsilon_n n_n$$
$$+(t_n c_n^\dagger c_{n-1}+\text{h.c.})$$

vD22



BCP08



“Be able to resolve small energies,
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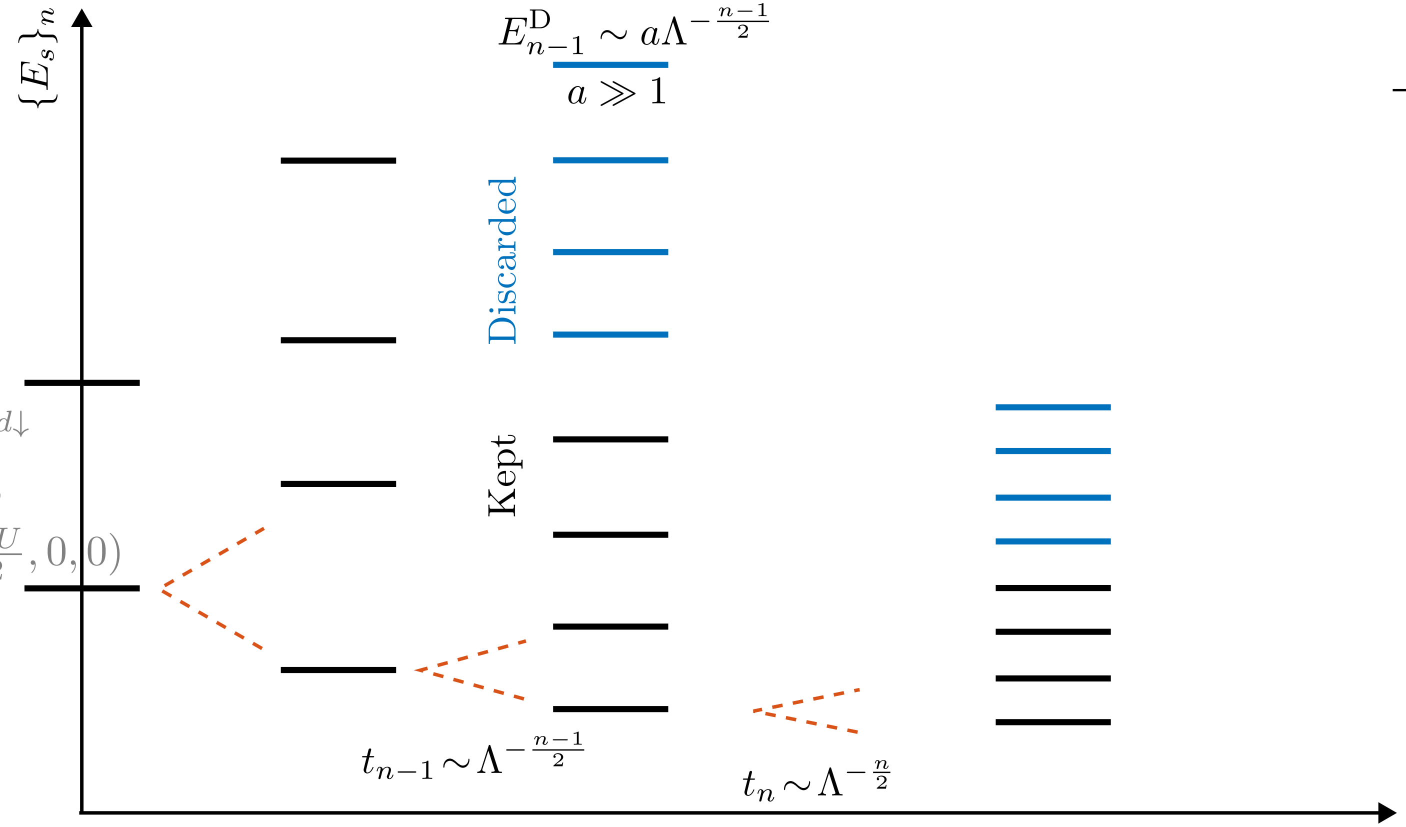
Iterative diagonalization



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$\dim\mathcal{H}$: d d^2 $N_{\max}$ $N_{\max}$

$$(U^\dagger D U)^{\mathrm{K}}_{n-1} + \epsilon_n n_n$$
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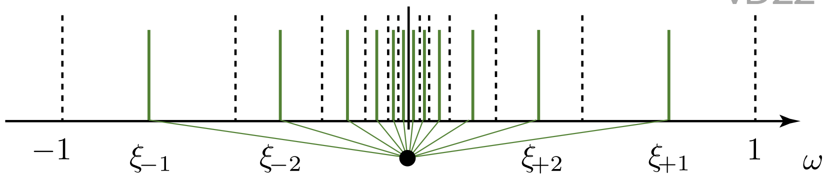
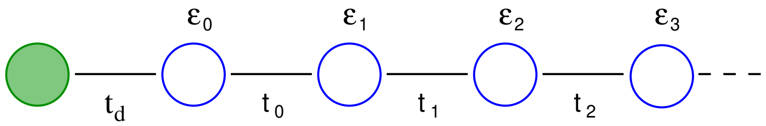
vD22



BCP08



“Be able to resolve small energies,
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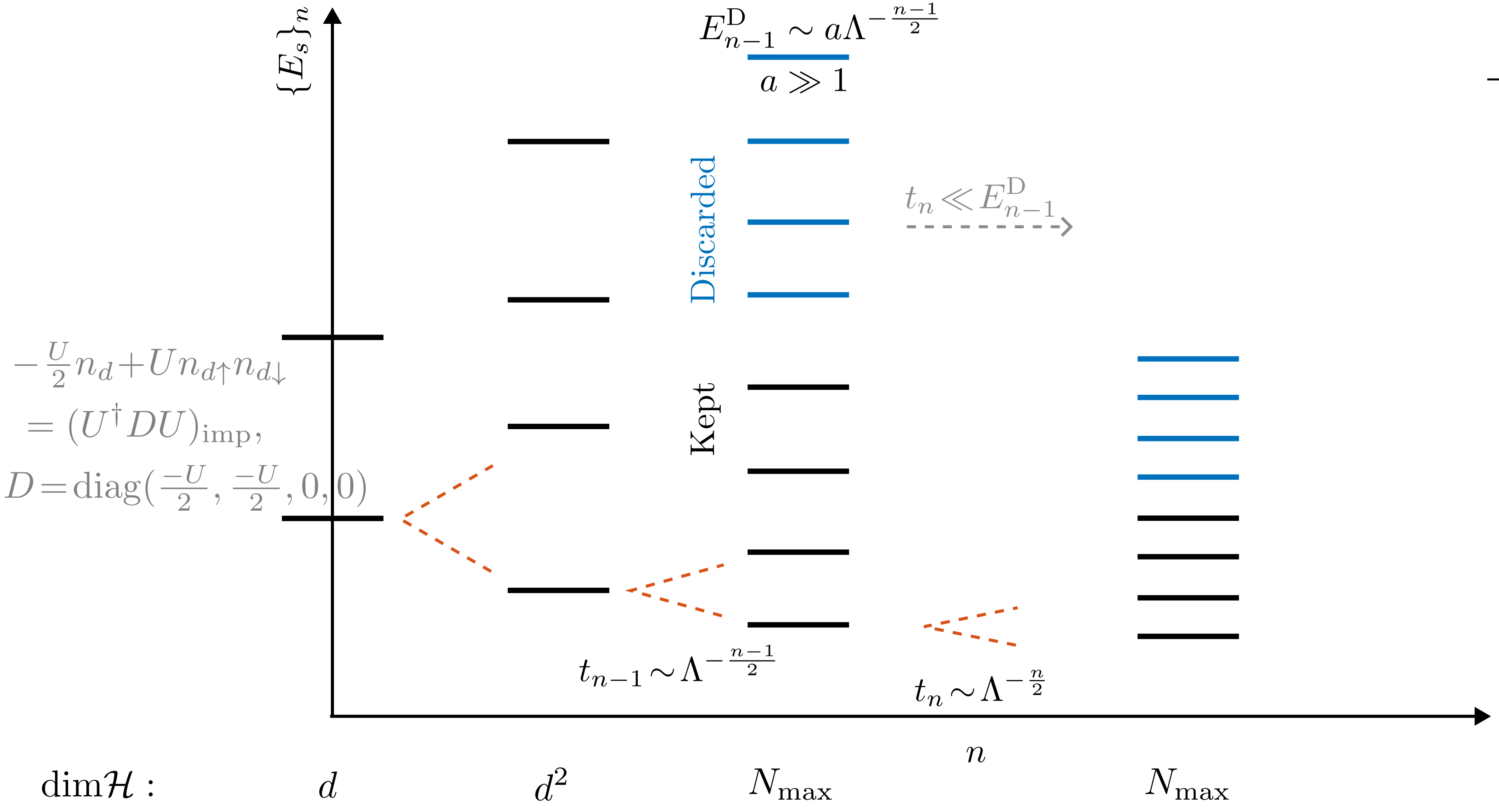
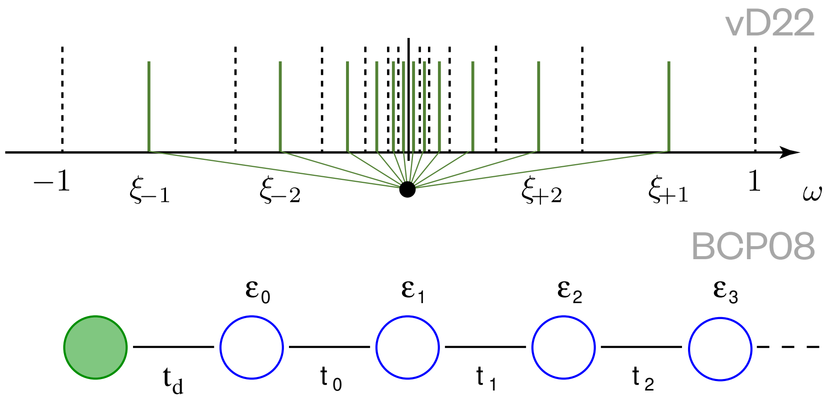
Iterative diagonalization



$$-\tfrac{U}{2}n_d + U n_{d\uparrow}n_{d\downarrow} = (U^\dagger D U)_{\mathrm{imp}},$$

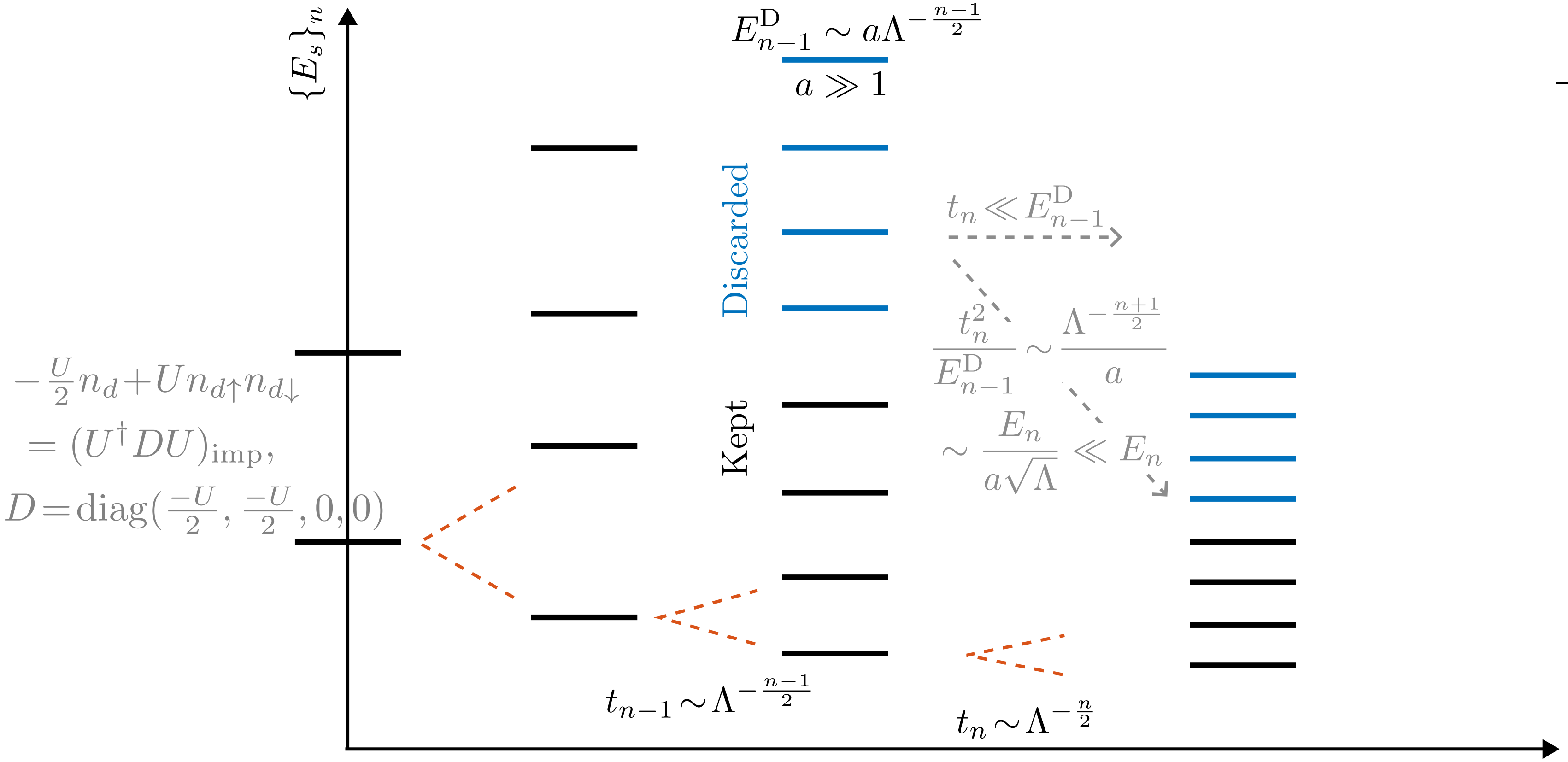
$$D = \mathrm{diag}(\tfrac{-U}{2}, \tfrac{-U}{2}, 0, 0)$$

$$(U^\dagger D U)^{\mathrm{K}}_{n-1} + \epsilon_n n_n$$
$$+ (t_n c^\dagger_n c_{n-1} + \mathrm{h.c.})$$



"Be able to resolve small energies, accept coarse resolution at high energies"

Iterative diagonalization



$E^{\mathrm{D}}_{n-1} \sim a\Lambda^{-\frac{n-1}{2}}$

$a \gg 1$

$t_n \ll E^{\mathrm{D}}_{n-1}$

$\frac{t_n^2}{E^{\mathrm{D}}_{n-1}} \sim \frac{\Lambda^{-\frac{n+1}{2}}}{a} \sim \frac{E_n}{a\sqrt{\Lambda}} \ll E_n$

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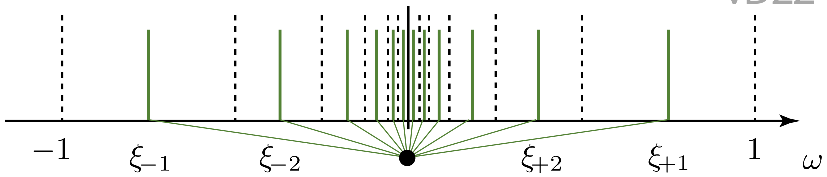
$t_{n-1} \sim \Lambda^{-\frac{n-1}{2}}$

$t_n \sim \Lambda^{-\frac{n}{2}}$

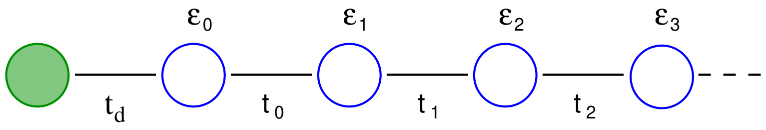
$\dim\mathcal{H}$: d d^2 $N_{\max}$ $N_{\max}$

$$(U^\dagger D U)^{\mathrm{K}}_{n-1} + \epsilon_n n_n + (t_n c_n^\dagger c_{n-1} + \mathrm{h.c.})$$

vD22



BCP08



“Be able to resolve small energies,
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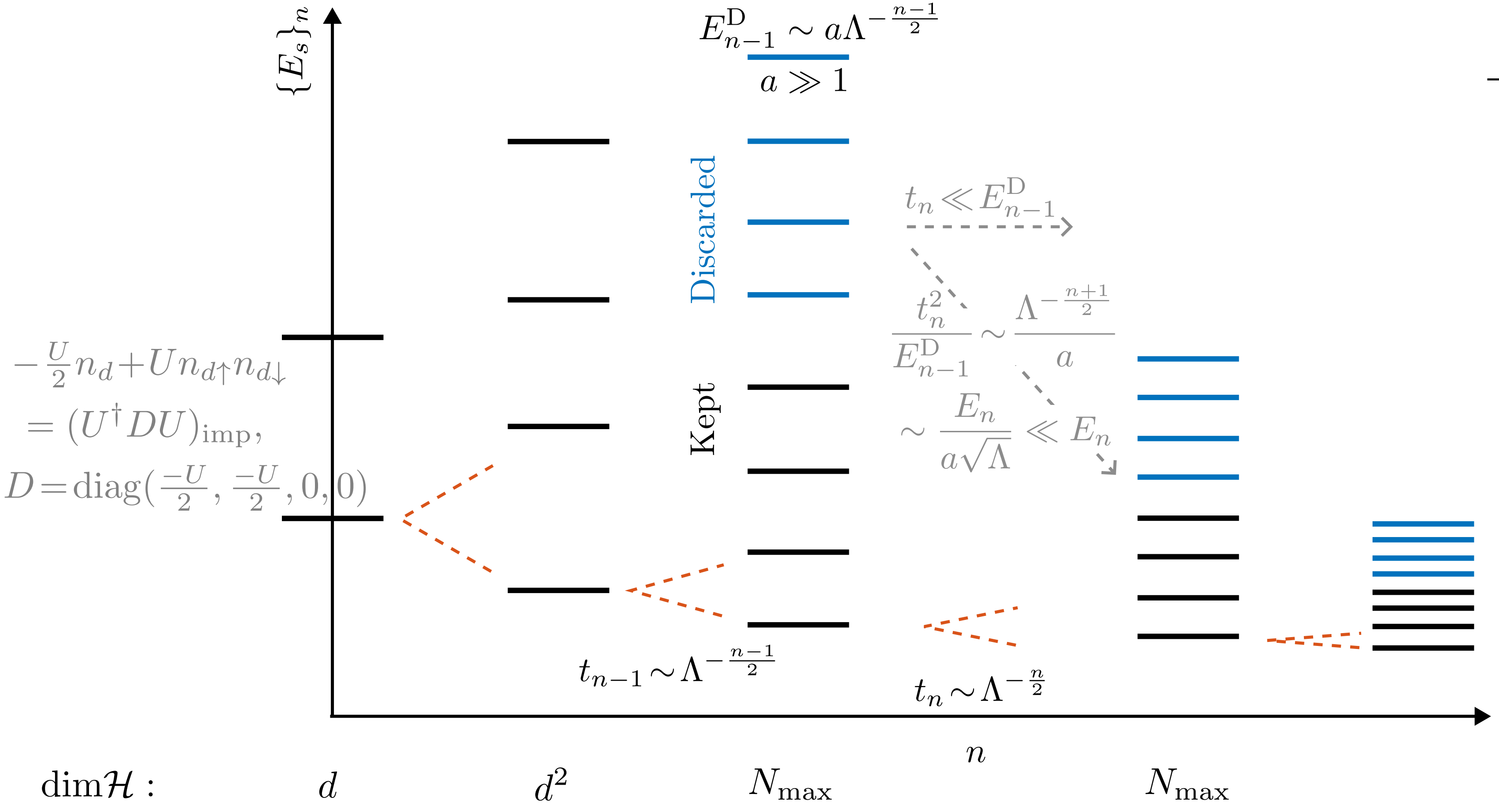
Iterative diagonalization



$\{E_s\}_n$

$E^{\mathrm{D}}_{n-1} \sim a\Lambda^{-\frac{n-1}{2}}$

$a \gg 1$

Discarded

Kept

$t_n \ll E^{\mathrm{D}}_{n-1}$

$\frac{t_n^2}{E^{\mathrm{D}}_{n-1}} \sim \frac{\Lambda^{-\frac{n+1}{2}}}{a} \sim \frac{E_n}{a\sqrt{\Lambda}} \ll E_n$

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$t_{n-1} \sim \Lambda^{-\frac{n-1}{2}}$

$t_n \sim \Lambda^{-\frac{n}{2}}$

n

$\dim\mathcal{H}:$ d d^2 $N_{\max}$ $N_{\max}$

$$(U^\dagger D U)^{\mathrm{K}}_{n-1} + \epsilon_n n_n$$
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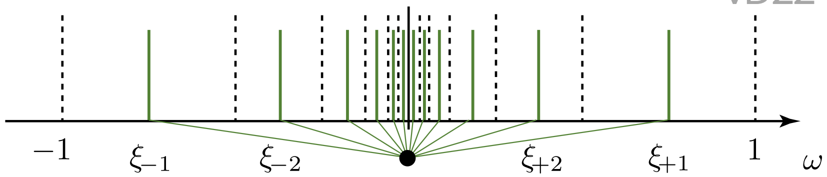
vD22



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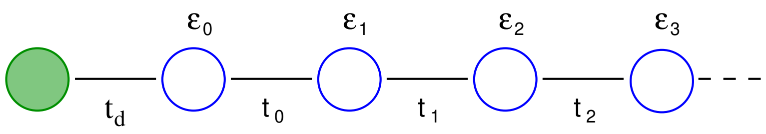

"Be able to resolve small energies,
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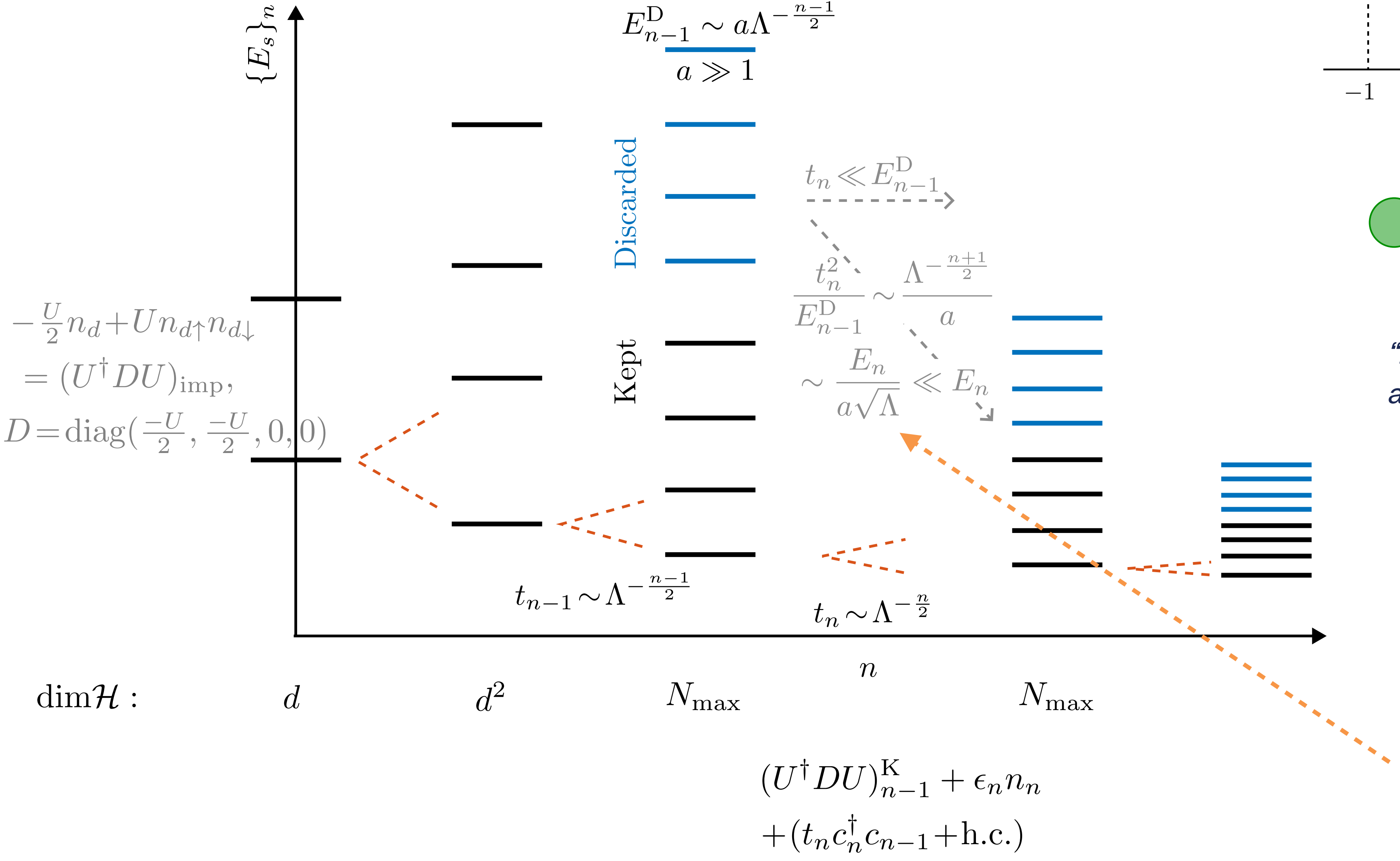
Iterative diagonalization



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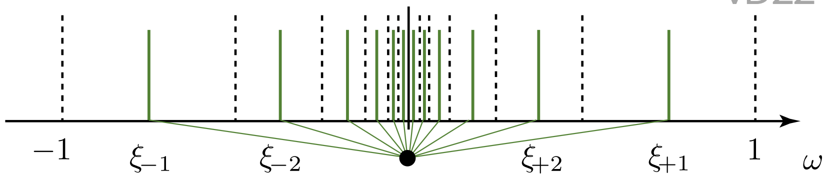
vD22



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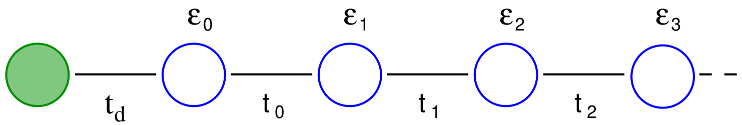

"Be able to resolve small energies,
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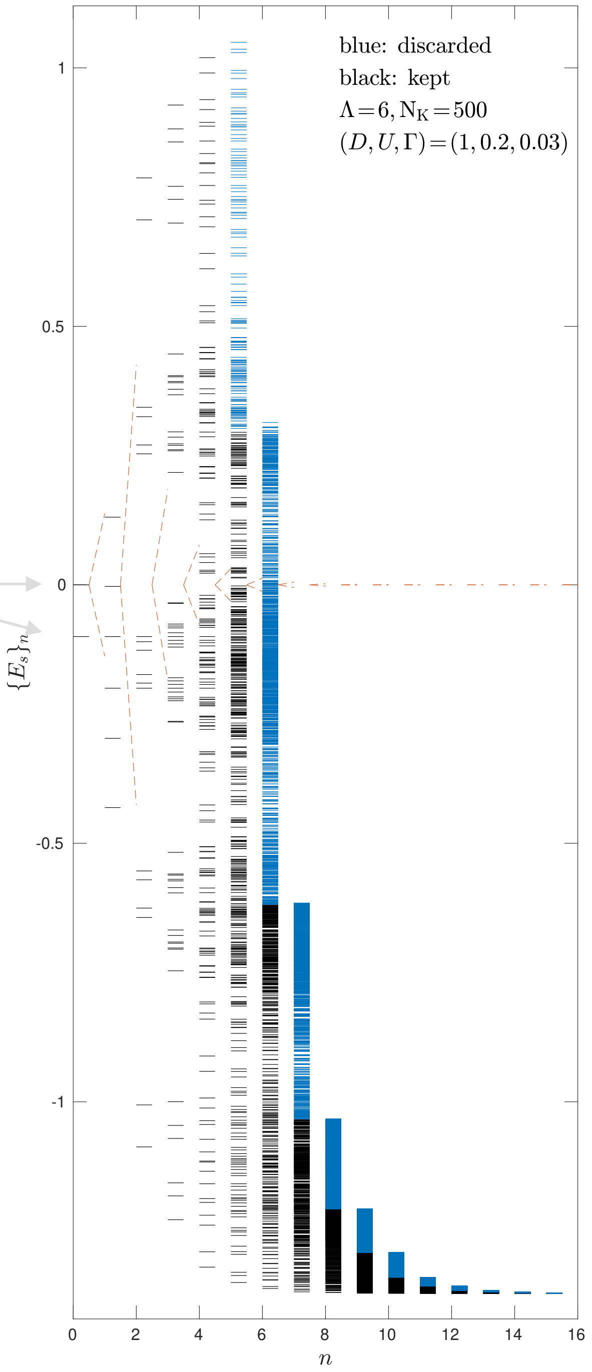
Interplay of control parameters
Λ, N_{K} $(a \sim N_{\mathrm{K}})$

... in practice

$$-\frac{U}{2}n_d+Un_{d\uparrow}n_{d\downarrow}$$
$$=(U^\dagger DU)_{\mathrm{imp}},$$
$$D=\mathrm{diag}(\frac{-U}{2},\frac{-U}{2},0,0)$$



... in practice

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$$=(U^{\dagger}DU)_{\text{imp}},$$
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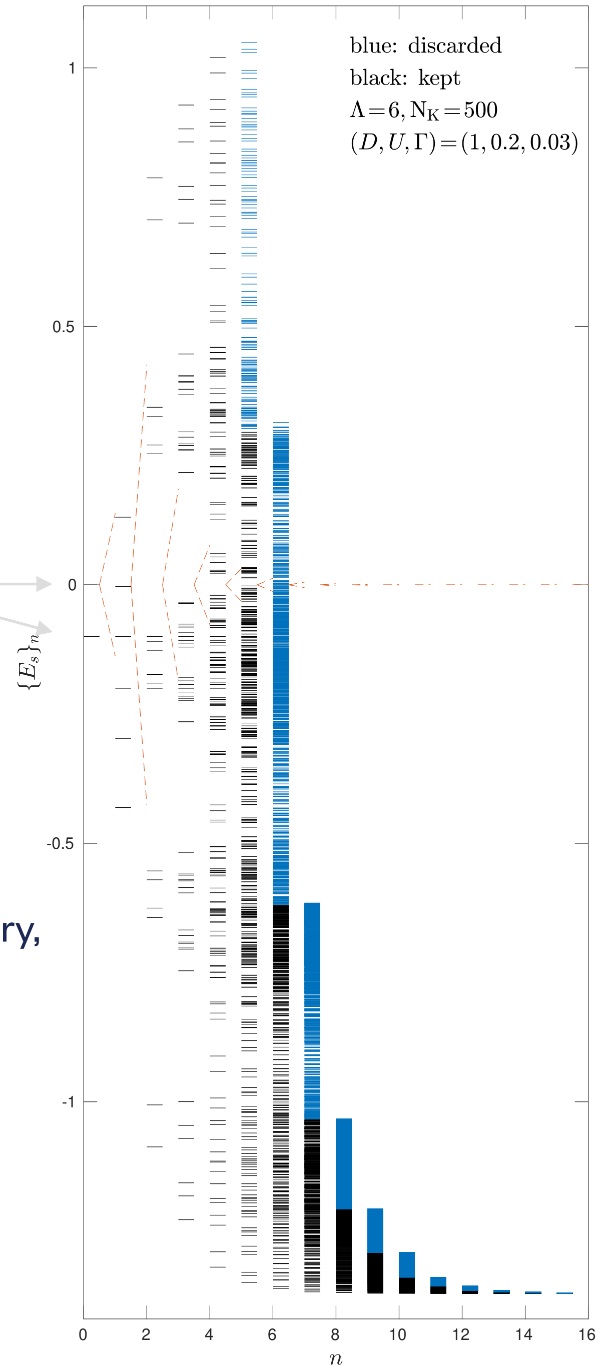

Exploit $\mathrm{SU(2)_{charge}\times SU(2)_{spin}}$ symmetry, (could fully diagonalize 9 sites, corresponding to $>2\times10^6$ states)

Using QSpace tensor library by Andreas Weichselbaum (BNL) for Abelian + non-Abelian symmetries

… in practice

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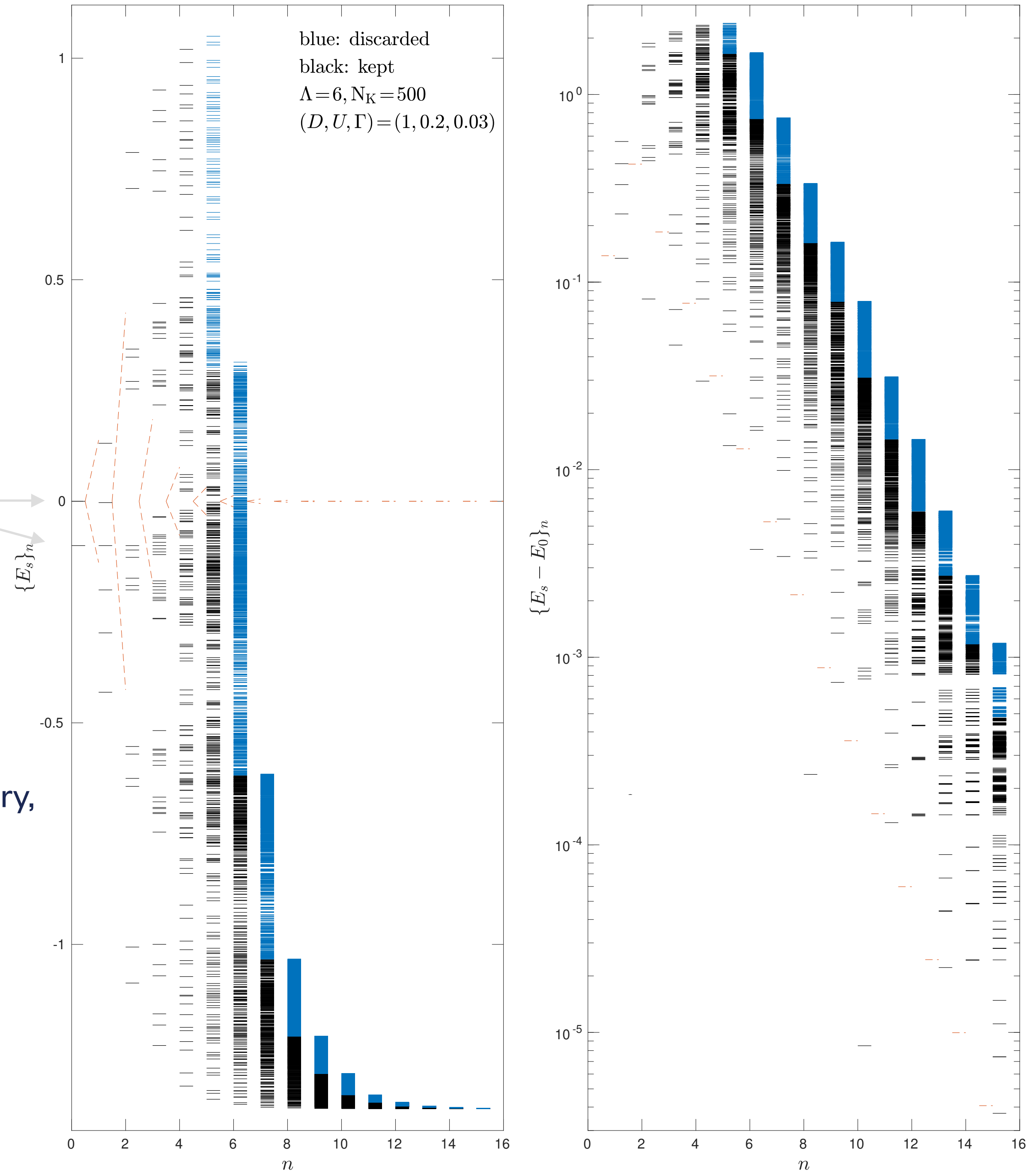

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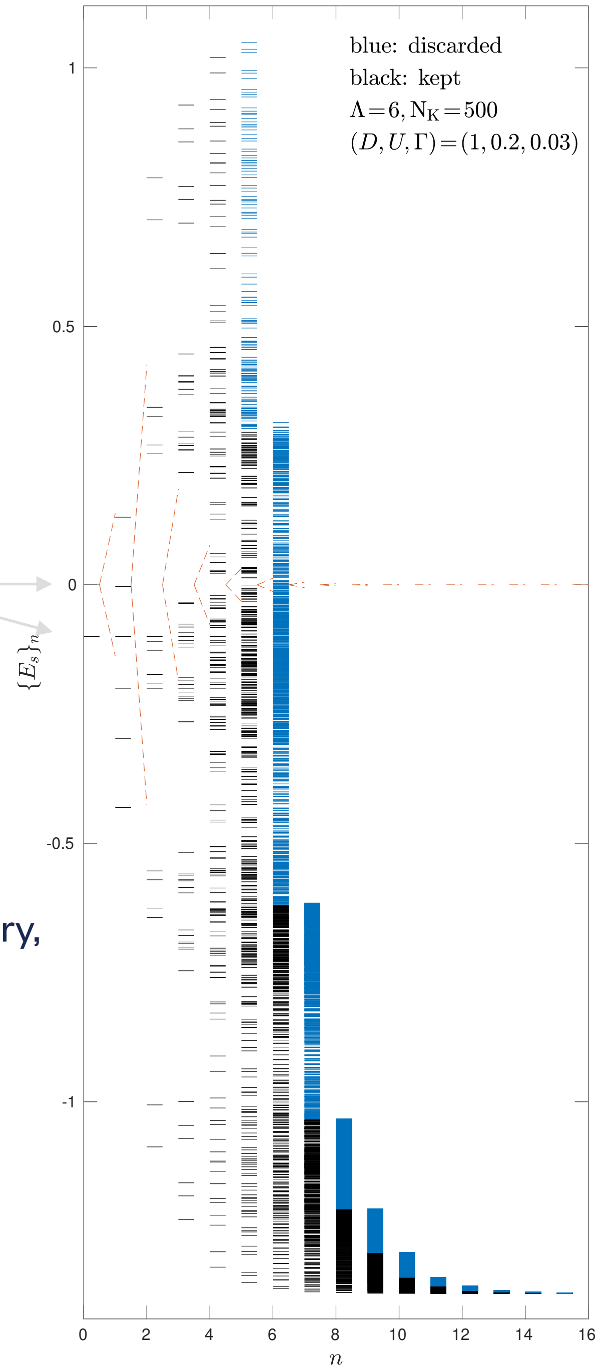

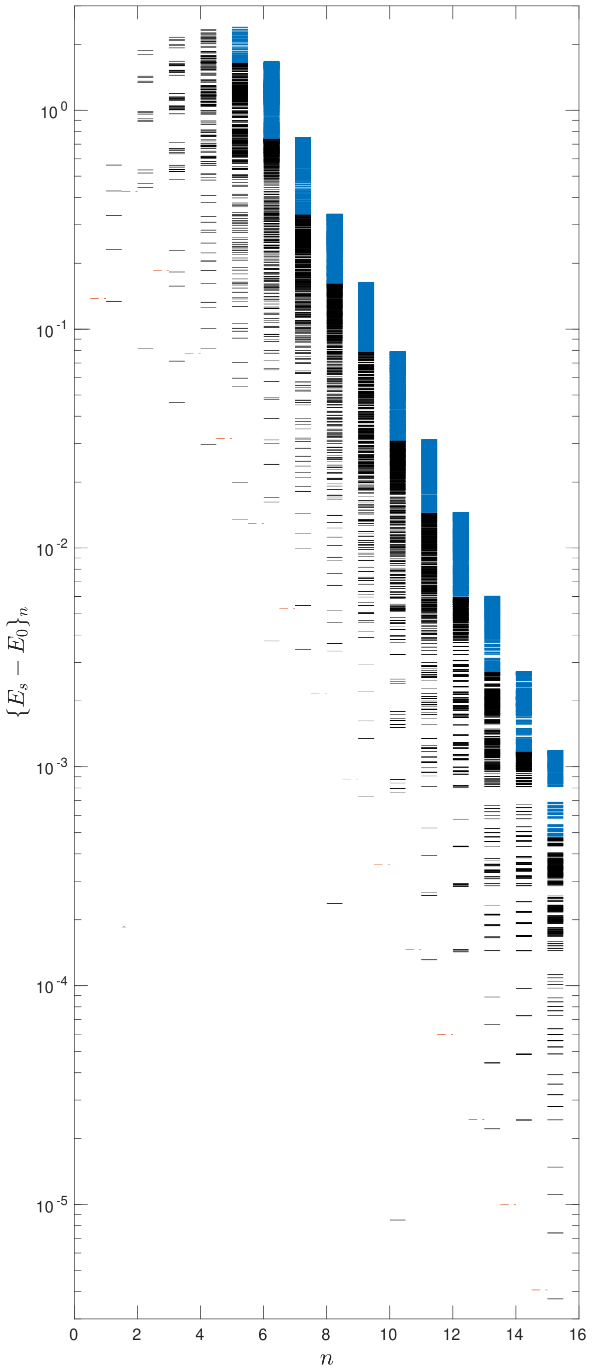

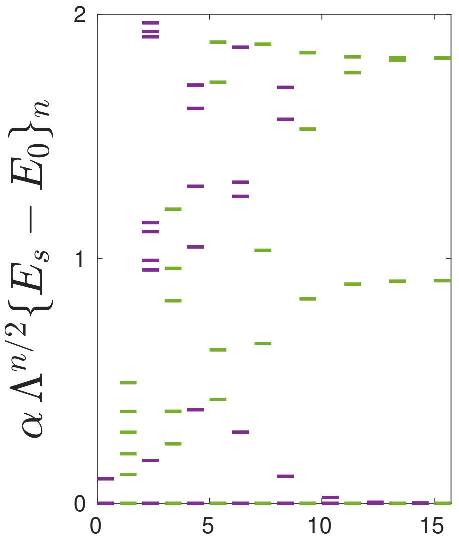

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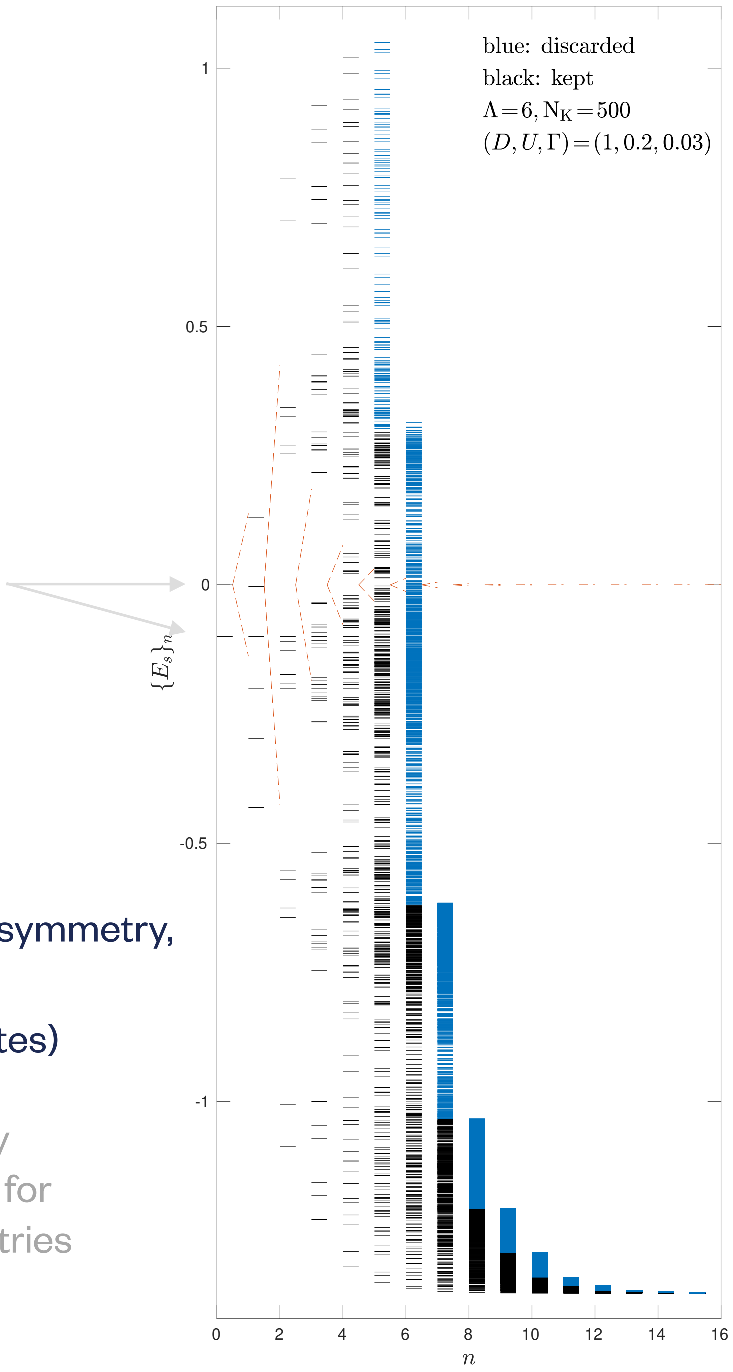
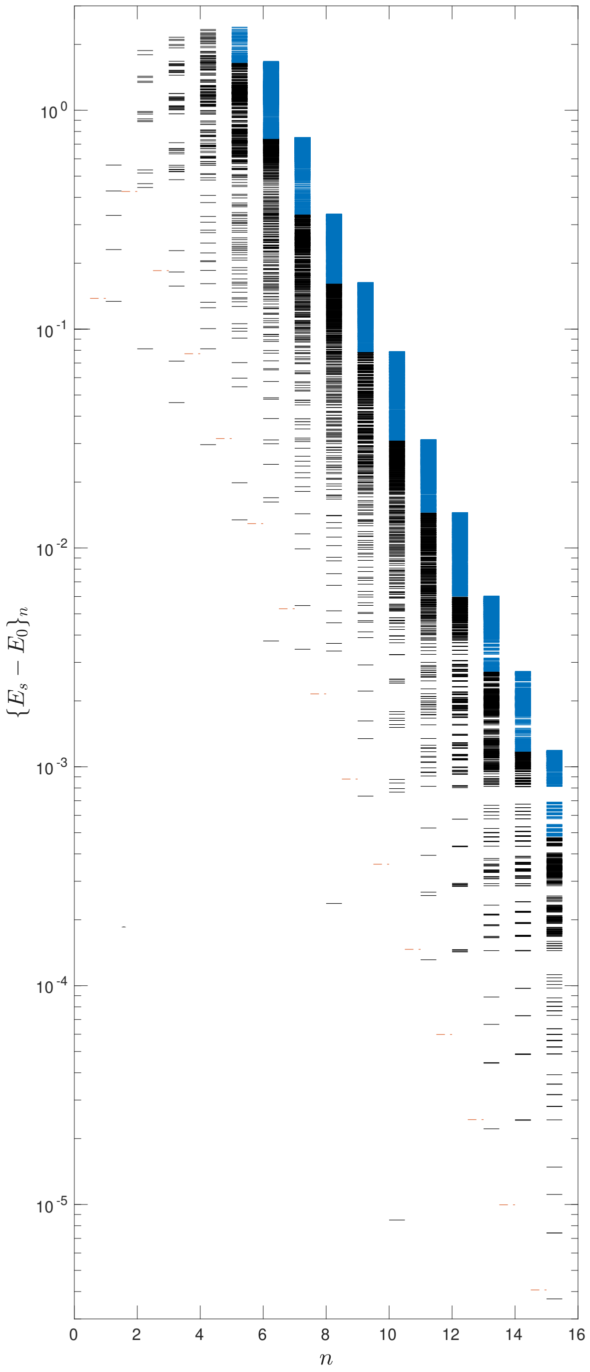
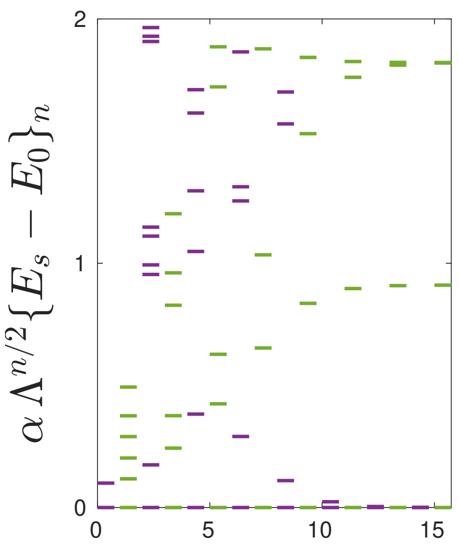
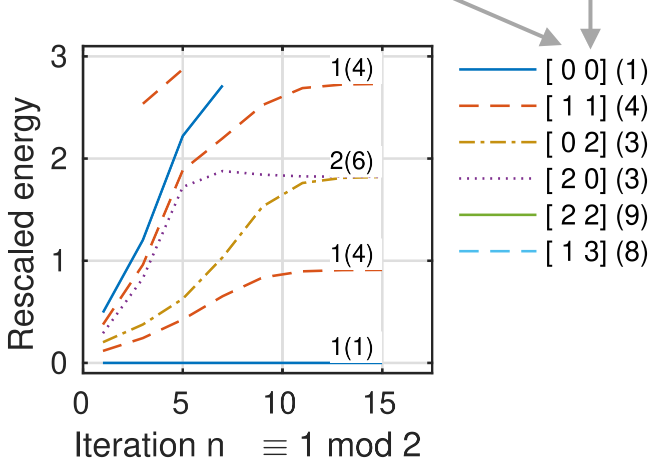






Charge: absolute deviation from half filling

Spin $2\,|S^z|$



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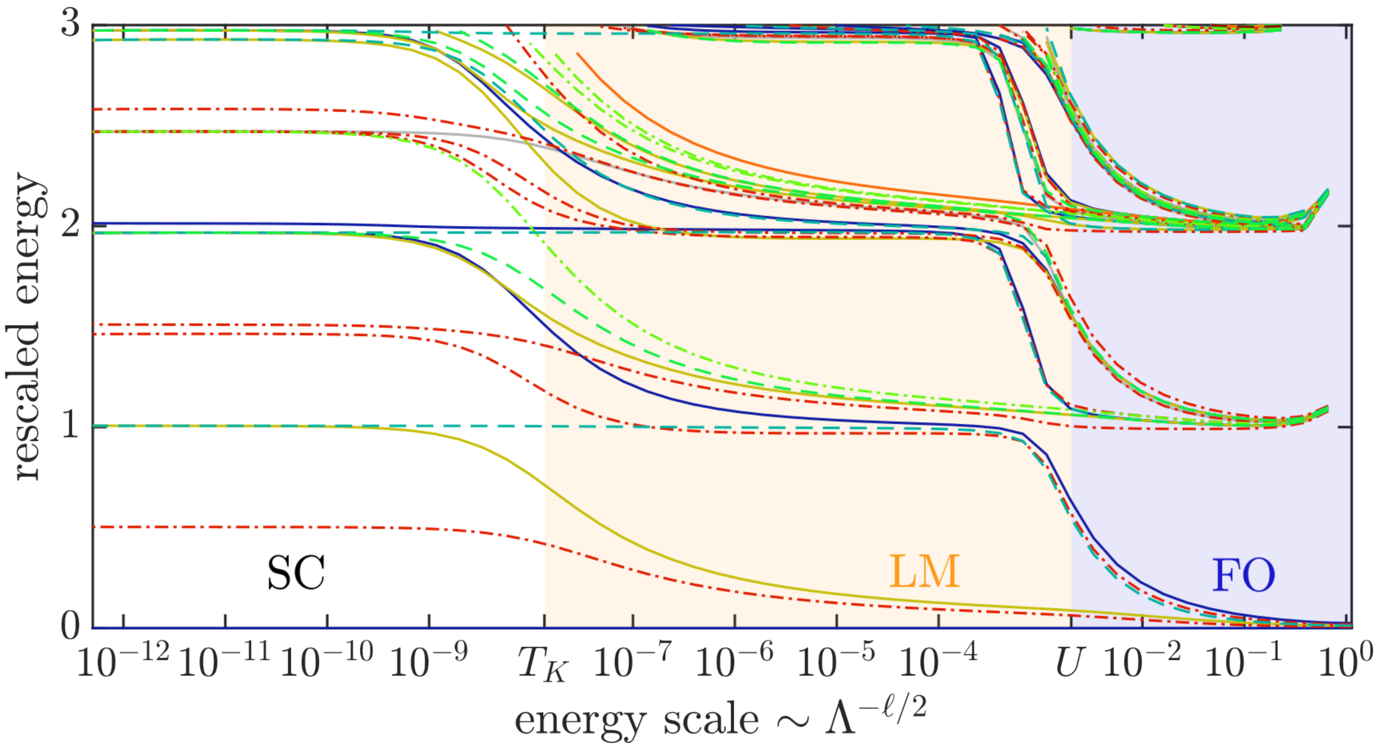
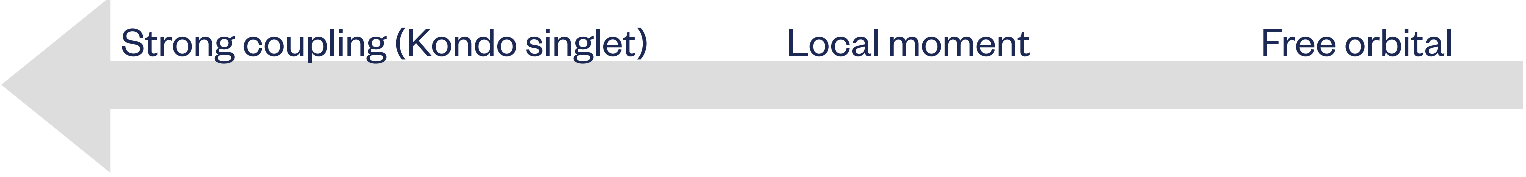
NRG flow diagram



Kondo model $J_K \vec{S} \cdot \vec{s}_{\text{bath}}$



Strong coupling (Kondo singlet)

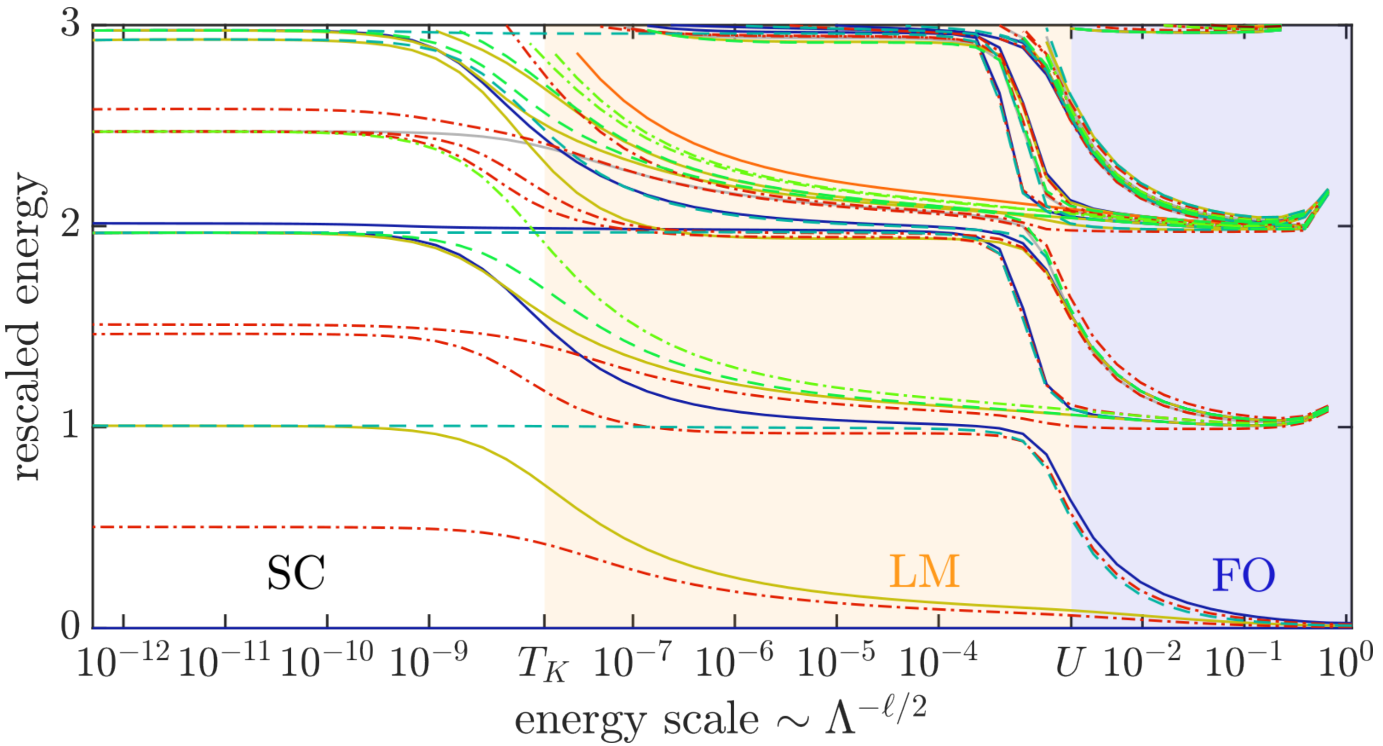
Local moment

Free orbital

RG flow

vD22

NRG flow diagram



$\frac{|\uparrow\rangle|\downarrow\rangle_{\text{bath}} - |\downarrow\rangle|\uparrow\rangle_{\text{bath}}}{\sqrt{2}} \otimes |N-1\rangle_{\text{bath}}$

$(|\uparrow\rangle, |\downarrow\rangle) \otimes |N\rangle_{\text{bath}}$

$(|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle) \otimes |N\rangle_{\text{bath}}$

Kondo model $J_K \vec{S} \cdot \vec{s}_{\text{bath}}$

Strong coupling (Kondo singlet) Local moment Free orbital

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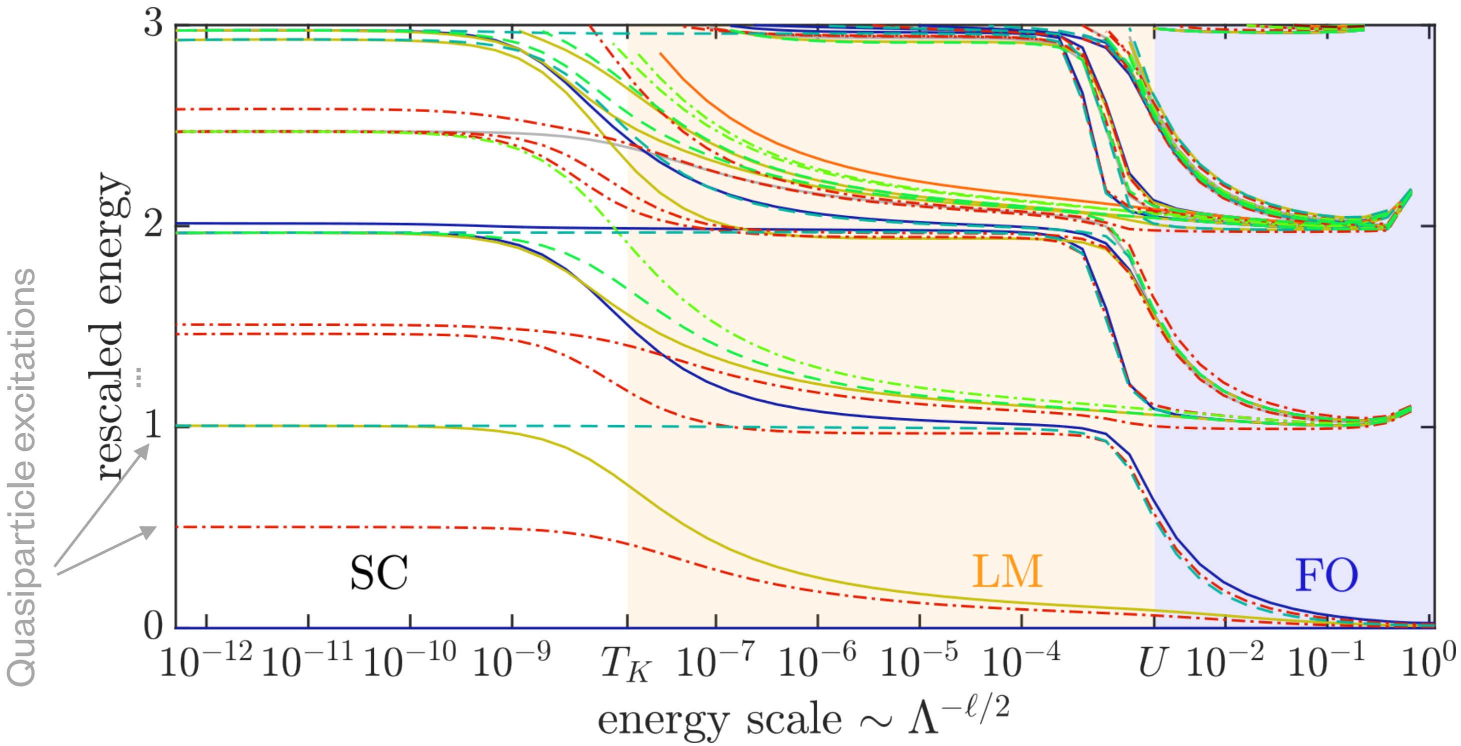

$$\frac{|\uparrow\rangle|\downarrow\rangle_{\text{bath}} - |\downarrow\rangle|\uparrow\rangle_{\text{bath}}}{\sqrt{2}} \otimes |N-1\rangle_{\text{bath}}$$

$$(|\uparrow\rangle, |\downarrow\rangle) \otimes |N\rangle_{\text{bath}}$$

$$(|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle) \otimes |N\rangle_{\text{bath}}$$

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Strong coupling (Kondo singlet) Local moment Free orbital

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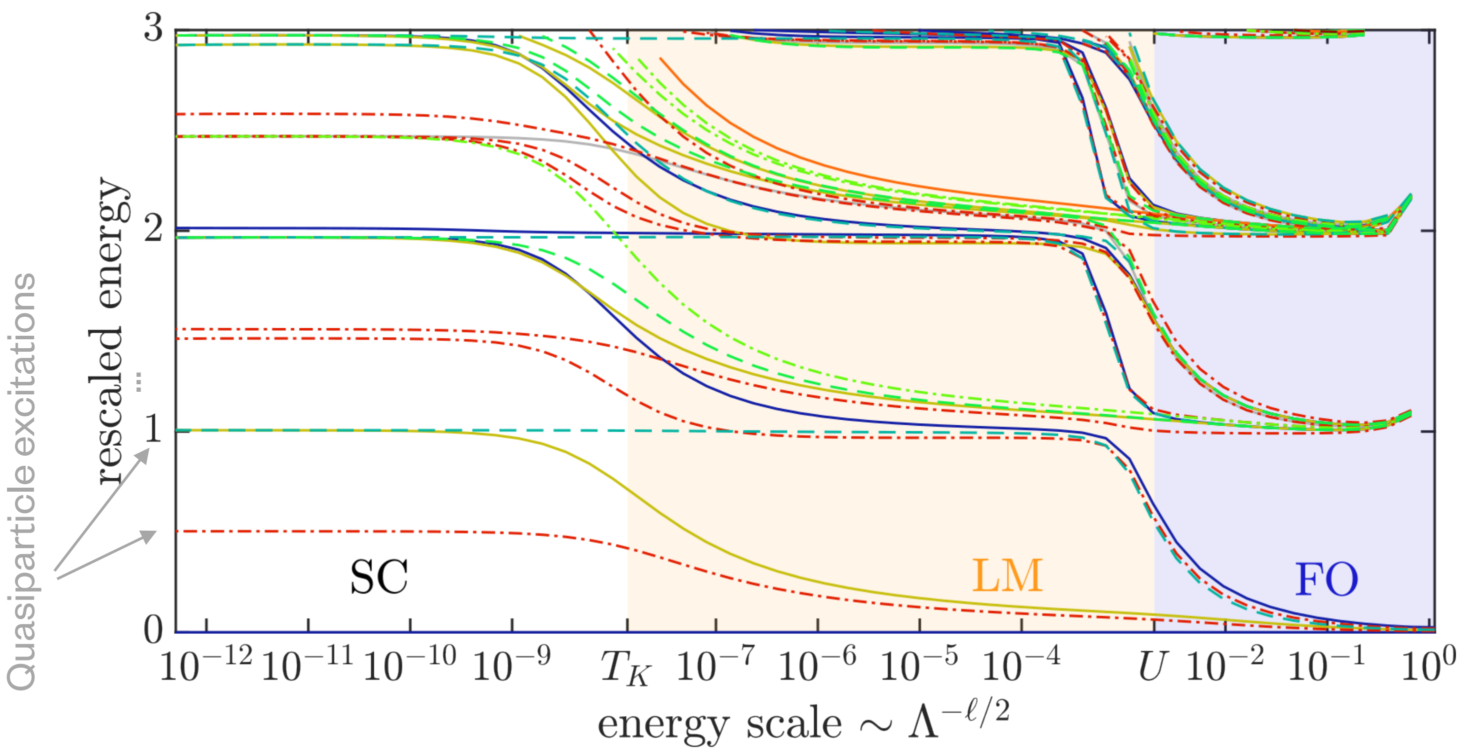

$$\frac{|\uparrow\rangle|\downarrow\rangle_{\text{bath}}-|\downarrow\rangle|\uparrow\rangle_{\text{bath}}}{\sqrt{2}}\otimes|N-1\rangle_{\text{bath}}$$

$$(|\uparrow\rangle,|\downarrow\rangle)\otimes|N\rangle_{\text{bath}}$$

$$(|0\rangle,|\uparrow\rangle,|\downarrow\rangle,|\uparrow\downarrow\rangle)\otimes|N\rangle_{\text{bath}}$$

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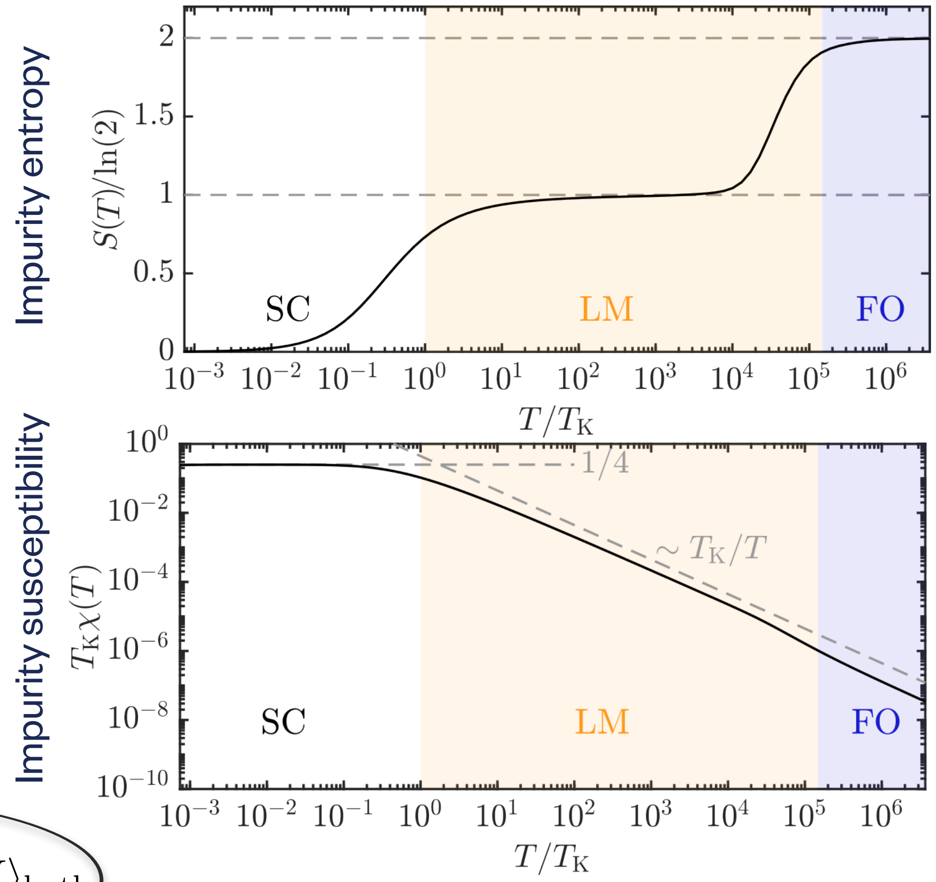
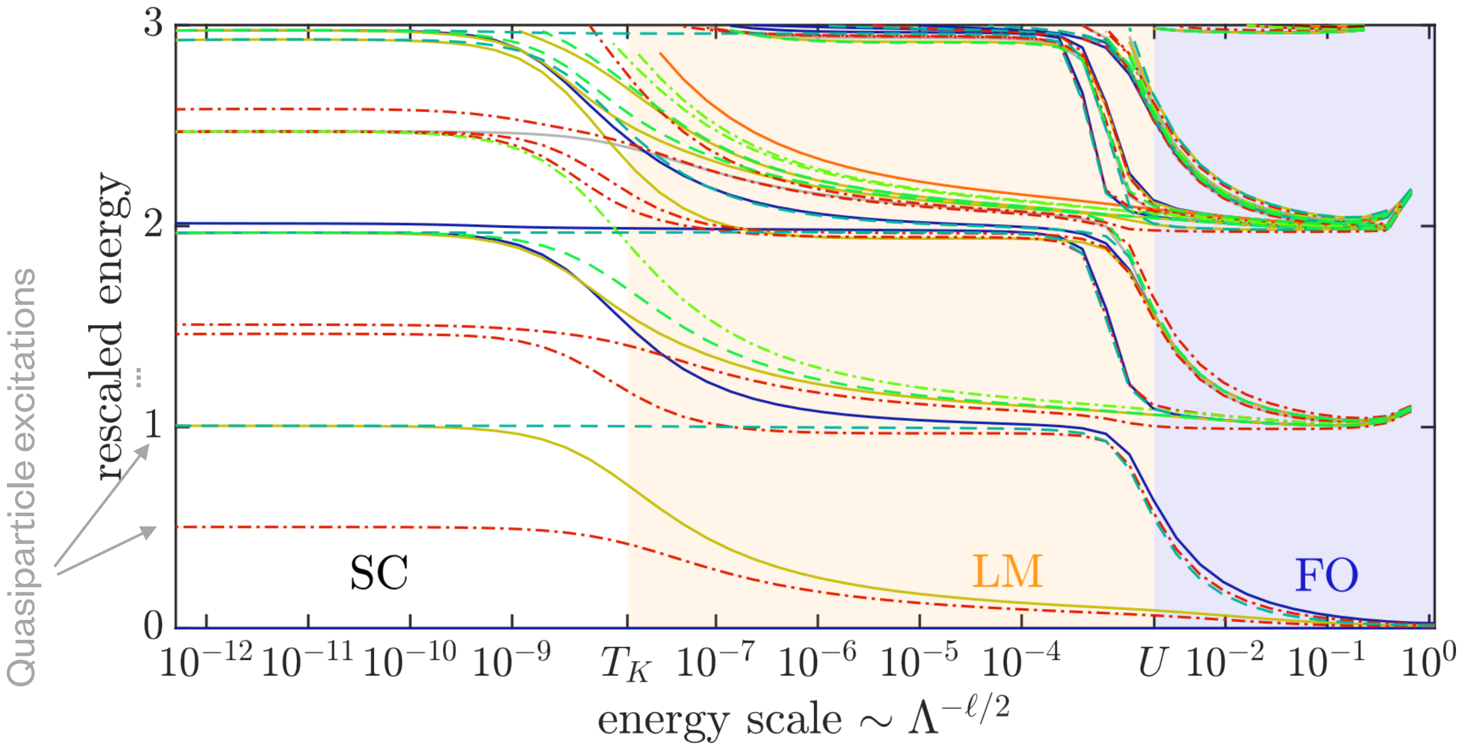
RG flow



RG flow reflected in other quantities
(here: thermodynamic/static properties)

vD22

NRG flow diagram



$\frac{|\uparrow\rangle|\downarrow\rangle_{\text{bath}} - |\downarrow\rangle|\uparrow\rangle_{\text{bath}}}{\sqrt{2}} \otimes |N-1\rangle_{\text{bath}}$

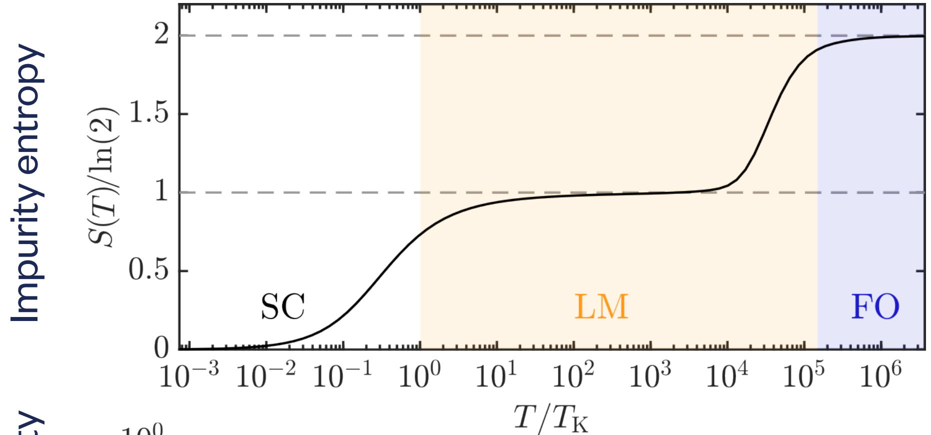
$(|\uparrow\rangle, |\downarrow\rangle) \otimes |N\rangle_{\text{bath}}$

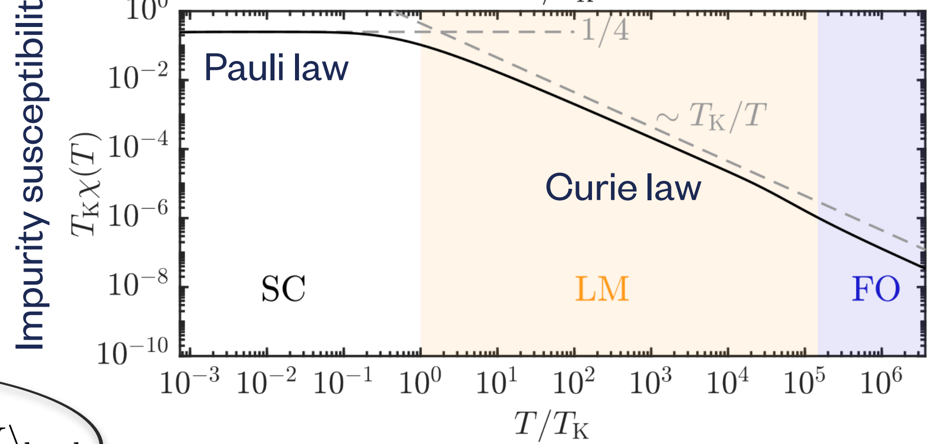
$(|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle) \otimes |N\rangle_{\text{bath}}$

Kondo model $J_K \vec{S} \cdot \vec{s}_{\text{bath}}$

Strong coupling (Kondo singlet) Local moment Free orbital

RG flow



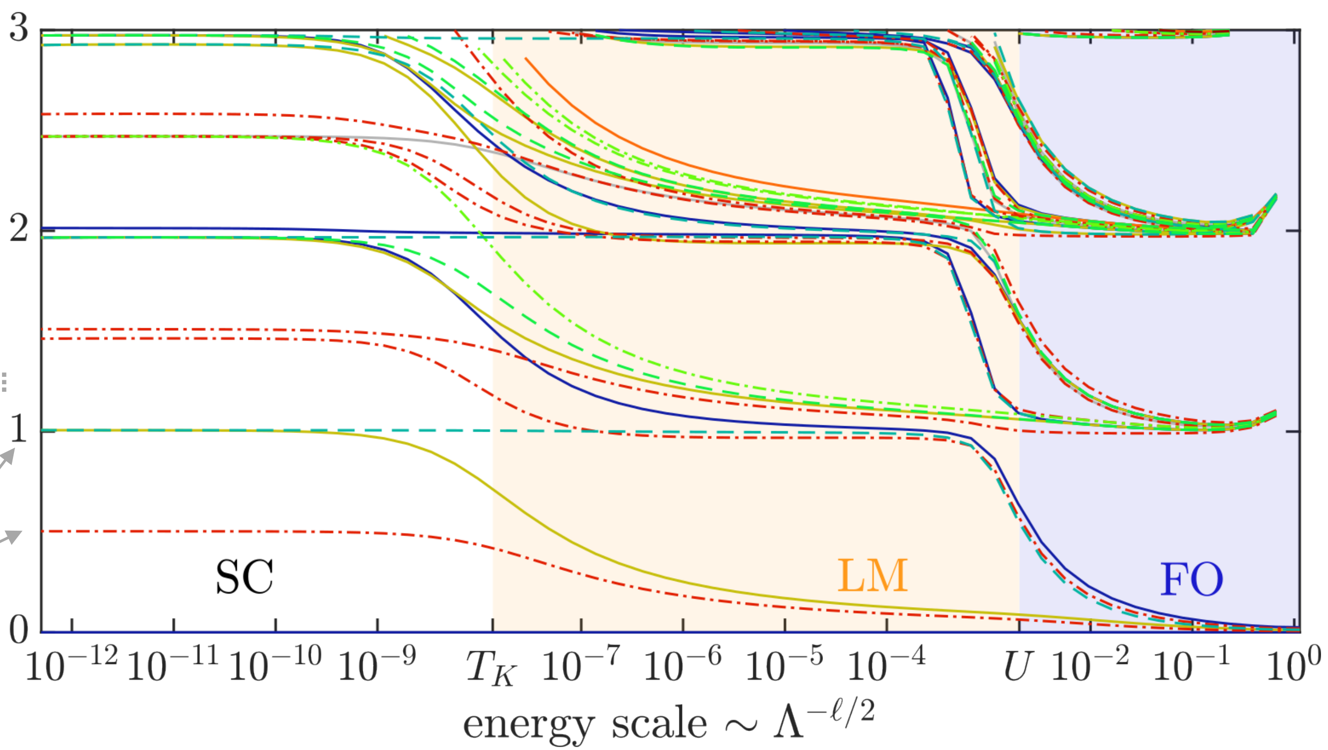


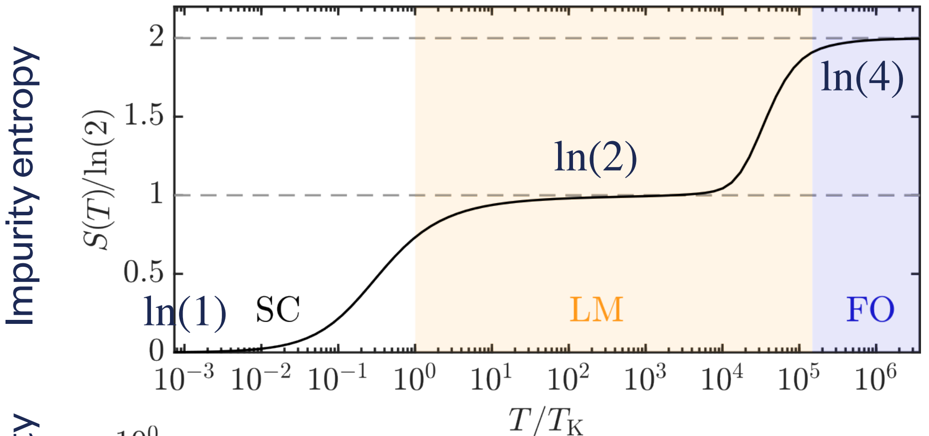
RG flow reflected in other quantities
(here: thermodynamic/static properties)

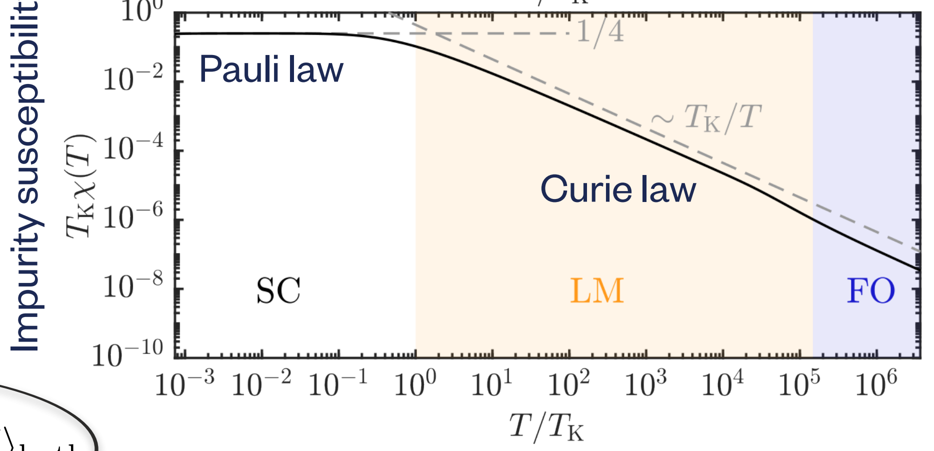
vD22

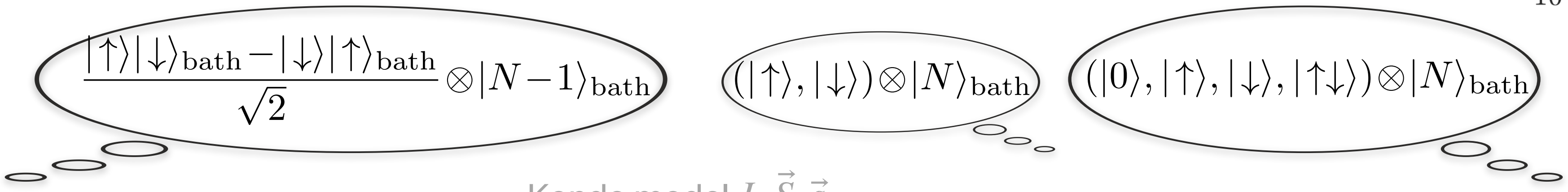
NRG flow diagram

Quasiparticle excitations









$$\frac{|\uparrow\rangle|\downarrow\rangle_{\text{bath}} - |\downarrow\rangle|\uparrow\rangle_{\text{bath}}}{\sqrt{2}} \otimes |N-1\rangle_{\text{bath}}$$

$$(|\uparrow\rangle, |\downarrow\rangle) \otimes |N\rangle_{\text{bath}}$$

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RG flow reflected in other quantities (here: thermodynamic/static properties)

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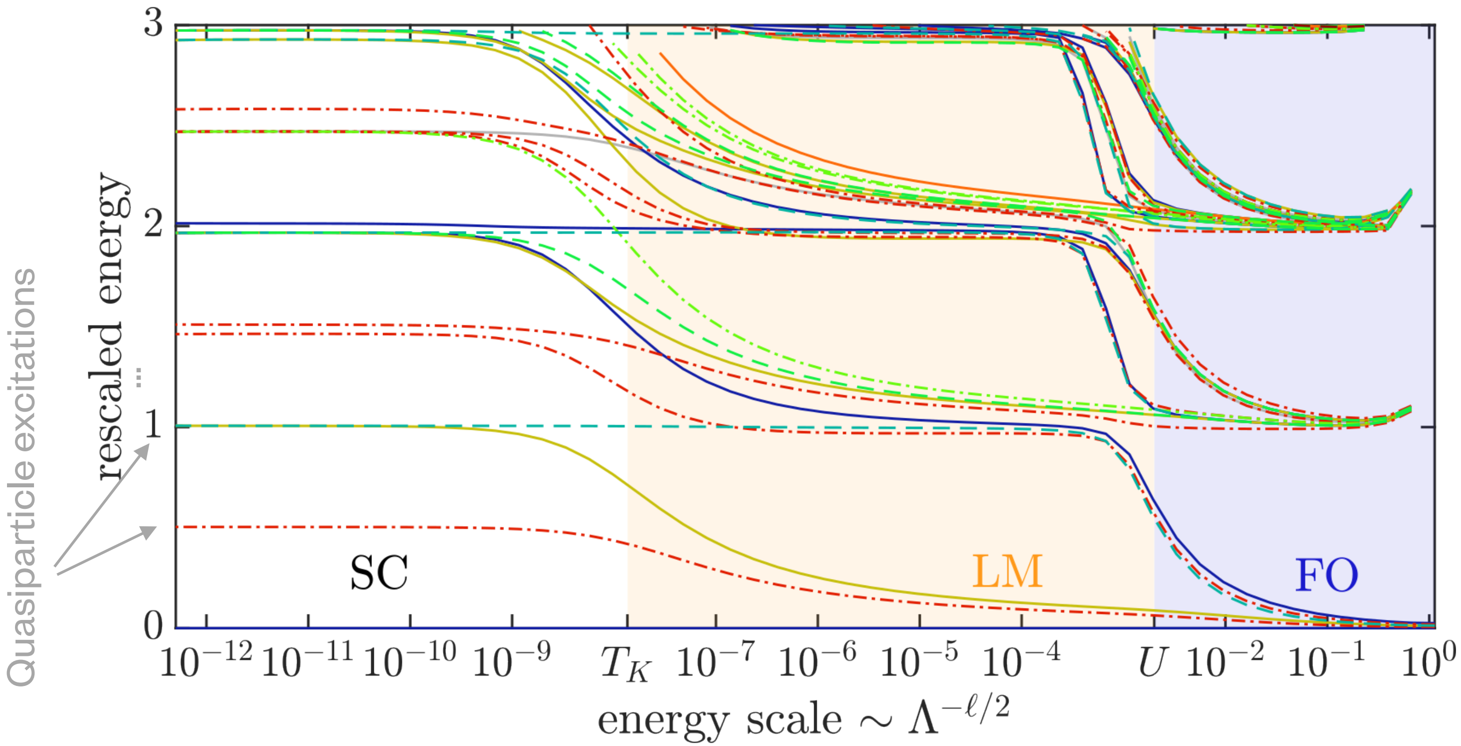
Strong coupling (Kondo singlet)

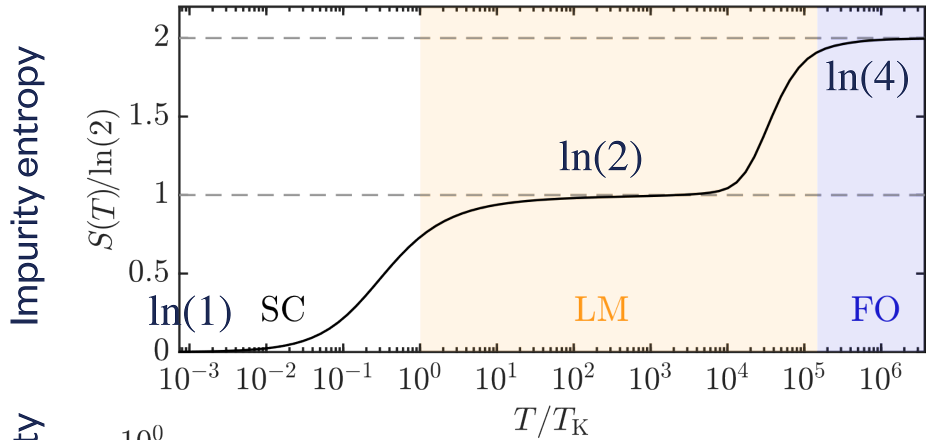
Local moment

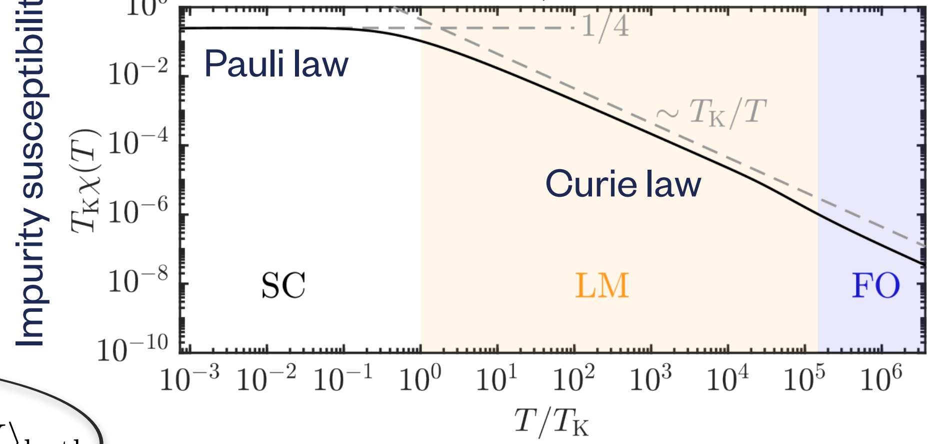
Free orbital

RG flow

NRG flow diagram







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RG flow

DMFT: Fermi-liquid (spin zero) metal independent atoms

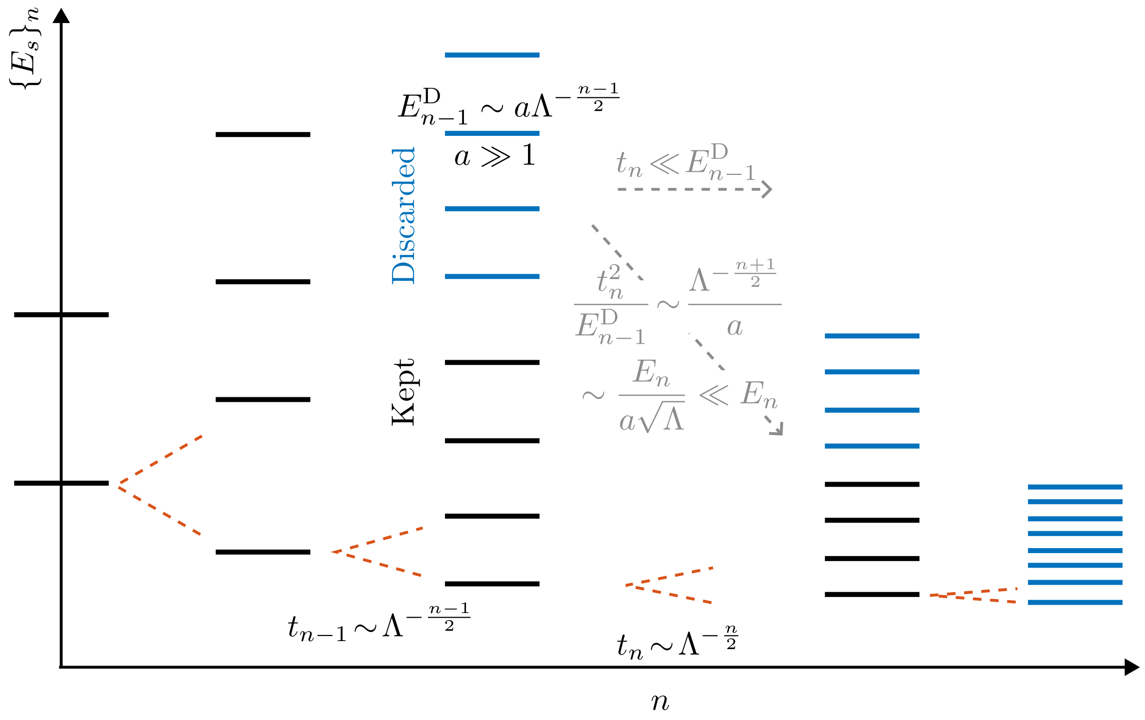
RG flow reflected in other quantities
(here: thermodynamic/static properties)

vD22

Anders-Schiller basis

Anders, Schiller, PRL 2005, PRB 2006

Change of perspective:
Complete basis of entire chain, iteratively refined for low-energy resolution!



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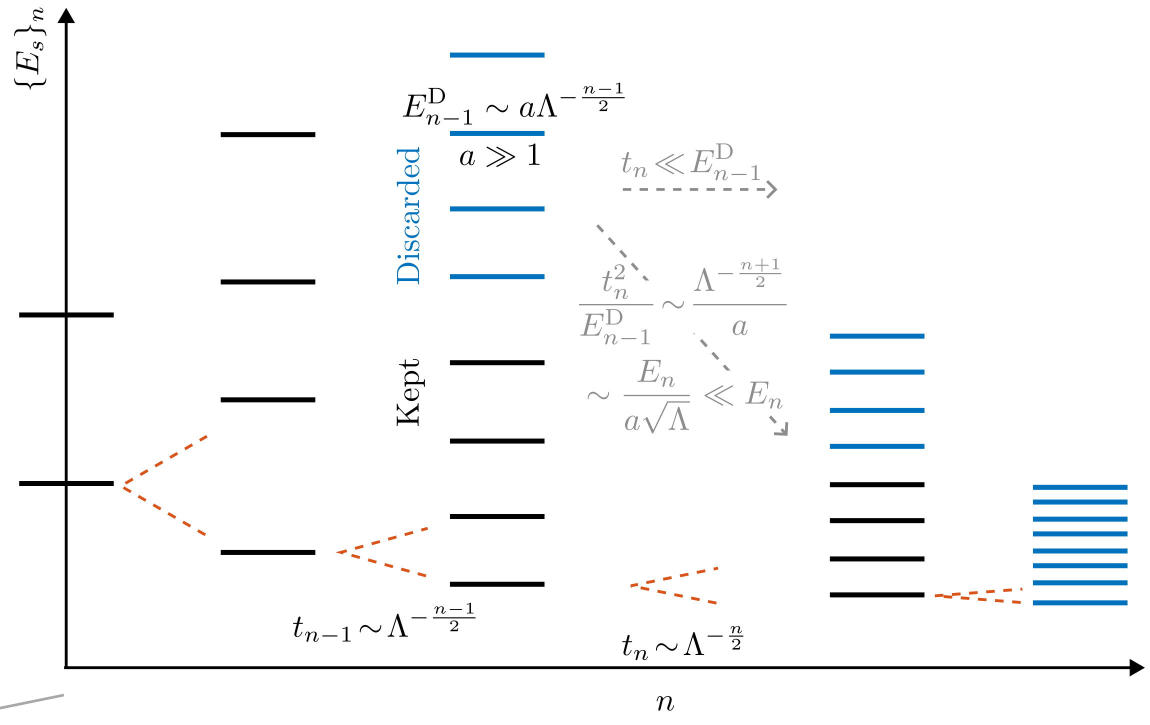

Eigenstates after diagonalization

Trivial product states of environment

$$\{|s\rangle_{\mathrm{imp}} \otimes |e\rangle_{0123}\}$$

$$= \{|se\rangle_{\mathrm{imp}}\}$$

$$d \times d^4$$

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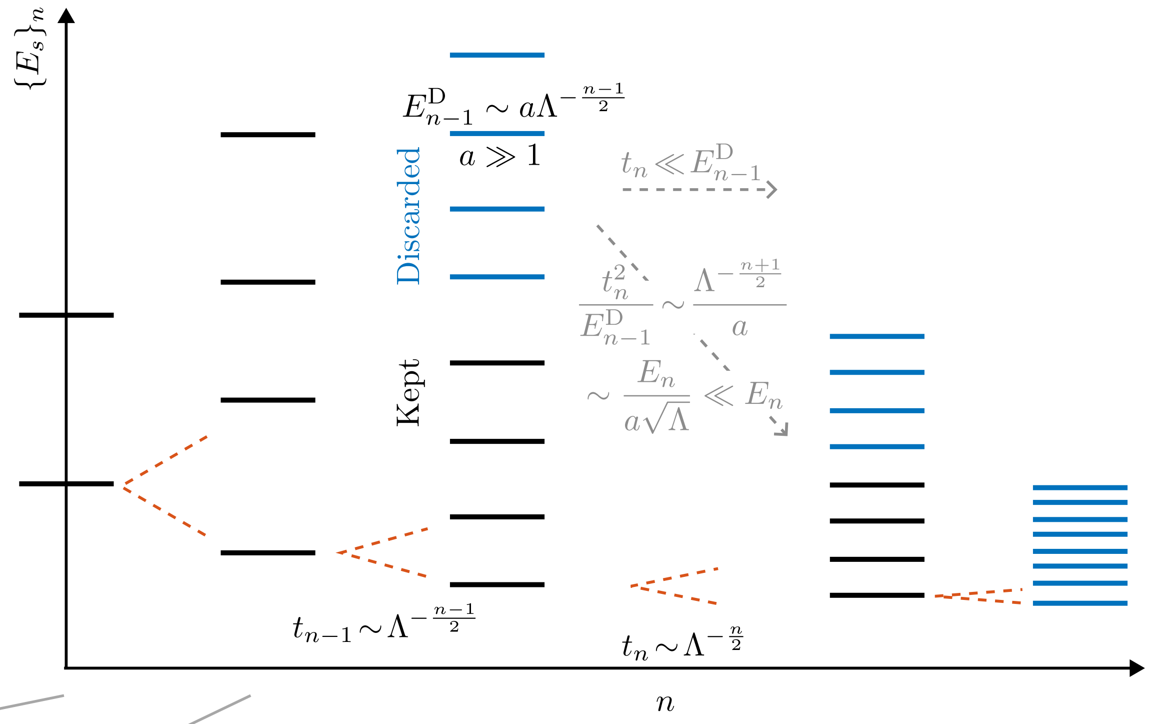

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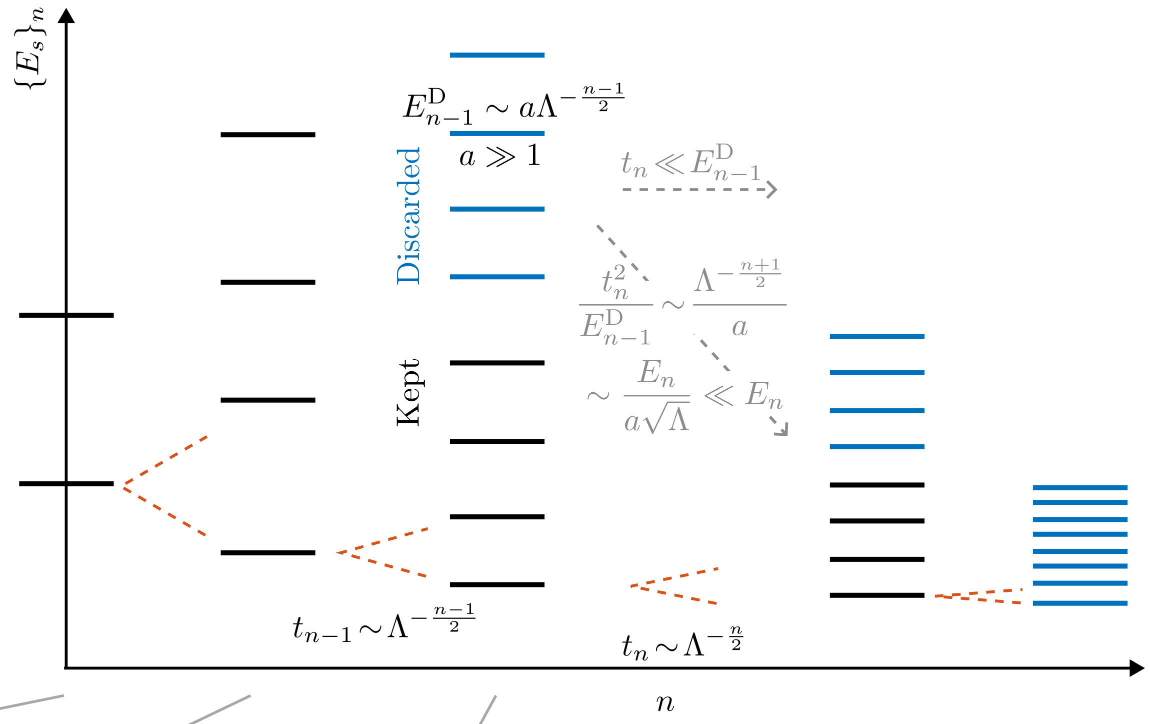

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$$\{|se\rangle^{\mathrm{D}}_{n-1}, |se\rangle^{\mathrm{K}}_{n-1}\}$$

$$\left(\frac{N_{\mathrm{D}}}{N_{\max}} + \frac{N_{\mathrm{K}}}{N_{\max}}\right) d^3 \times d^2$$

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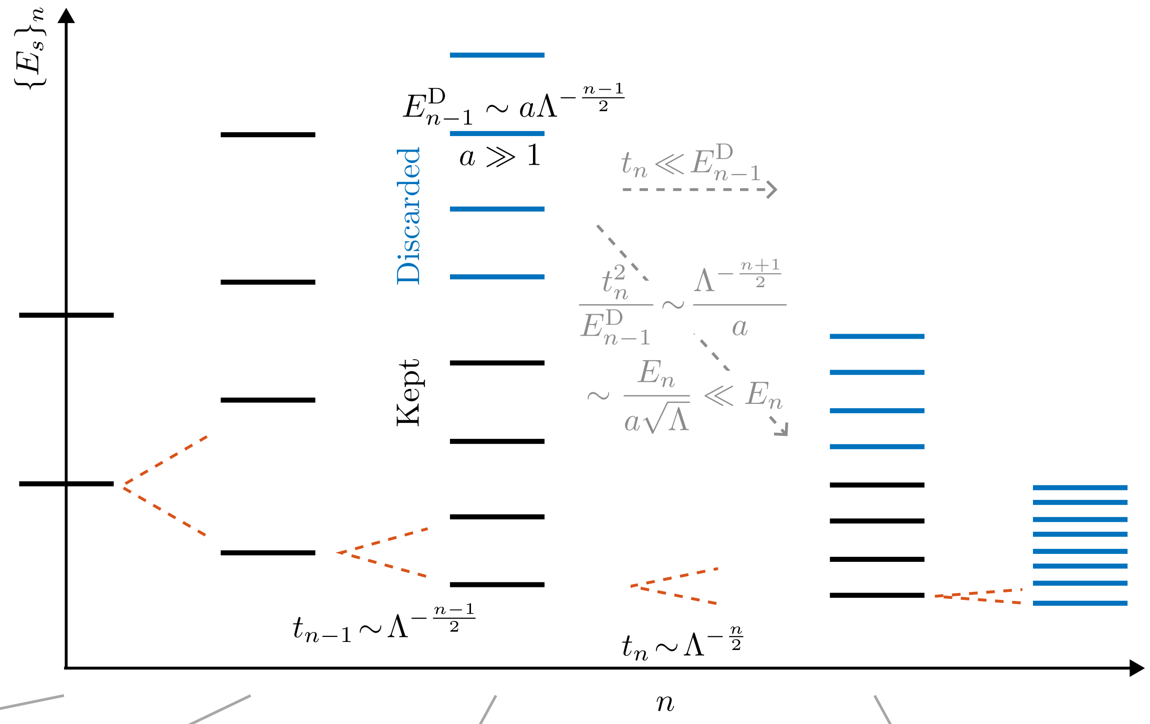

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$$\{|se\rangle^{\mathrm{D}}_{n-1}, |se\rangle^{\mathrm{D}}_{n}, |se\rangle^{\mathrm{K}}_{n}\}$$

$$\Big(\frac{N_{\mathrm{D}}}{N_{\max}} + \frac{N_{\mathrm{K}}(N_{\mathrm{D}} + N_{\mathrm{K}})}{N^2_{\max}}\Big) d^5$$

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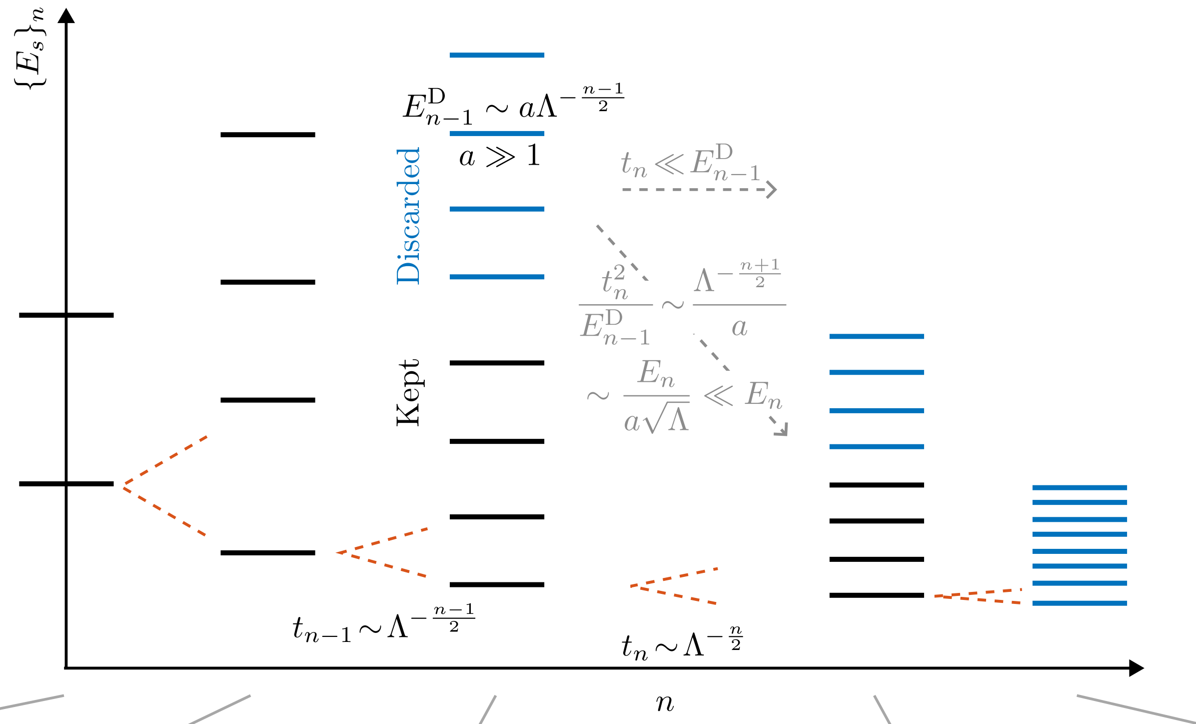

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$$\Big(\frac{N_{\mathrm{D}}}{N_{\mathrm{max}}} + \frac{N_{\mathrm{K}}(N_{\mathrm{D}} + N_{\mathrm{K}})}{N^2_{\mathrm{max}}}\Big) d^5$$

$$\{|se\rangle^{\mathrm{D}}_{n_0}, \ldots |se\rangle^{\mathrm{D}}_{N-2}, |se\rangle^{\mathrm{D}}_{N-1}\}$$

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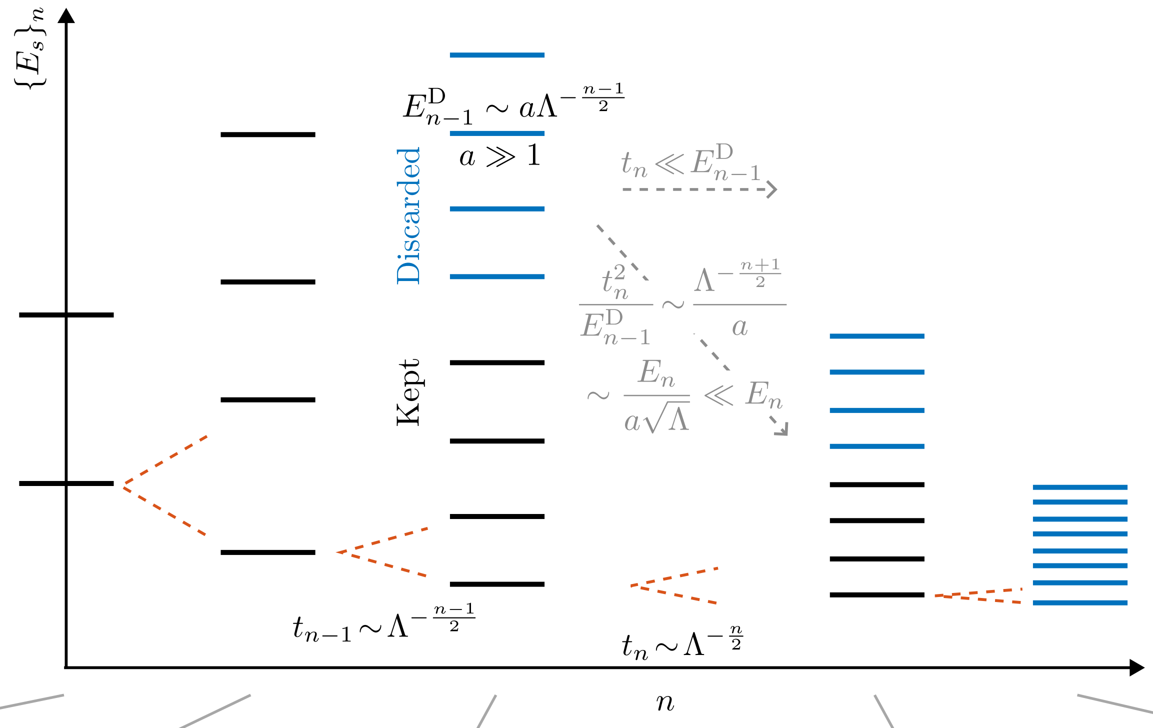

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$= \{|se\rangle_{\rm imp}\}$

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$d^2 \times d^3$

$\{|se\rangle^{\rm D}_{n-1}, |se\rangle^{\rm K}_{n-1}\}$

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$\{|se\rangle^{\rm D}_{n-1}, |se\rangle^{\rm D}_{n}, |se\rangle^{\rm K}_{n}\}$

$\left(\frac{N_{\rm D}}{N_{\rm max}} + \frac{N_{\rm K}(N_{\rm D}+N_{\rm K})}{N^2_{\rm max}}\right) d^5$

$\{|se\rangle^{\rm D}_{n_0}, \dots |se\rangle^{\rm D}_{N-2}, |se\rangle^{\rm D}_{N-1}\}$

d^5

Complete basis $\mathbf{1} = \sum_{n,s,e} |se\rangle^{\rm D}_{n}\,{}^{\rm D}_{n}\langle se|$ of approximate eigenstates $H|se\rangle^{\rm D}_n = E^{[n]}_s |se\rangle^{\rm D}_n + O\left(\Lambda^{-\frac{n+1}{2}}\right)$

Single-shell Lehmann representation

Building block of spectral function:
(Einstein summation convention for s, e)

$$\mathcal{A}_{AB}(t) = \mathrm{Tr}\,\rho\, e^{\mathrm{i}Ht} A e^{-\mathrm{i}Ht} B$$
$$= \sum_{n\tilde{n}} \mathrm{Tr}\,\rho\, e^{\mathrm{i}Ht} |se\rangle_{n}^{\mathrm{D}}\,{}_{n}^{\mathrm{D}}\langle se| A |\tilde{s}\tilde{e}\rangle_{\tilde{n}}^{\mathrm{D}}\,{}_{\tilde{n}}^{\mathrm{D}}\langle \tilde{s}\tilde{e}| e^{-\mathrm{i}Ht} B$$

Peters, Pruschke, Anders, PRB 2006
Weichselbaum, von Delft, PRL 2007

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① $n = \tilde{n}:$

$$\sum_{n} \mathrm{Tr}\, \underline{\rho\, e^{\mathrm{i}Ht} |se\rangle^{\mathrm{DD}}_{n\,n}} \langle se|A|\tilde{s}e\rangle^{\mathrm{DD}}_{n\,n} \underline{\langle \tilde{s}e| e^{-\mathrm{i}Ht} B}$$

$$= \sum_{n} e^{\mathrm{i}(E^{[n]}_{s} - E^{[n]}_{\tilde{s}})t} [A^{[n]}_{\mathrm{DD}}]_{s\tilde{s}} [B^{[n]}_{\mathrm{DD}}]_{\tilde{s}s} [\rho^{[n]}_{\mathrm{D}}]_{ss}$$

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$$= \sum_n e^{\mathrm{i}(E^{[n]}_s - E^{[n]}_{\tilde{s}})t} [A^{[n]}_{\mathrm{DD}}]_{s\tilde{s}} [B^{[n]}_{\mathrm{DD}}]_{\tilde{s}s} [\rho^{[n]}_{\mathrm{D}}]_{ss}$$

② $n < \tilde{n}$:

$$\sum_n \mathrm{Tr}\,\underline{\rho\, e^{\mathrm{i}Ht} |se\rangle^{\mathrm{DD}}_{n\,n}} \langle se|A\underline{|\tilde{s}e\rangle^{\mathrm{KK}}_{n\,n} \langle \tilde{s}e| e^{-\mathrm{i}Ht}} B$$
$$= \sum_n e^{\mathrm{i}(E^{[n]}_s - E^{[n]}_{\tilde{s}})t} [A^{[n]}_{\mathrm{DK}}]_{s\tilde{s}} [B^{[n]}_{\mathrm{KD}}]_{\tilde{s}s} [\rho^{[n]}_{\mathrm{D}}]_{ss}$$

Hilbert space partitioning: $|se\rangle^{\mathrm{KK}}_{n\,n}\langle se| = \sum_{\tilde{n}>n} |\tilde{s}\tilde{e}\rangle^{\mathrm{DD}}_{\tilde{n}\,\tilde{n}} \langle \tilde{s}\tilde{e}|$

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Peters, Pruschke, Anders, PRB 2006
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$$= \sum_n e^{\mathrm{i}(E^{[n]}_s - E^{[n]}_{\tilde{s}})t} [A^{[n]}_{\mathrm{DK}}]_{s\tilde{s}} [B^{[n]}_{\mathrm{KD}}]_{\tilde{s}s} [\rho^{[n]}_{\mathrm{D}}]_{ss}$$

③ $\tilde{n} < n:$

$$\sum_{\tilde{n}} \mathrm{Tr}\, \underline{e^{\mathrm{i}Ht} |se\rangle^{\mathrm{KK}}_{\tilde{n}\,\tilde{n}} \langle se|} A |\tilde{s}\tilde{e}\rangle^{\mathrm{DD}}_{\tilde{n}\,\tilde{n}} \underline{\langle \tilde{s}\tilde{e}| e^{-\mathrm{i}Ht}} B\rho$$
$$= \sum_{\tilde{n}} e^{\mathrm{i}(E^{[\tilde{n}]}_s - E^{[\tilde{n}]}_{\tilde{s}})t} [A^{[\tilde{n}]}_{\mathrm{KD}}]_{s\tilde{s}} \underline{{}^{\mathrm{D}}_{\tilde{n}}\langle \tilde{s}e| B\rho |se\rangle^{\mathrm{K}}_{\tilde{n}}}$$

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$$= \sum_{\tilde{n}} e^{\mathrm{i}(E^{[\tilde{n}]}_{s} - E^{[\tilde{n}]}_{\tilde{s}})t} [A^{[\tilde{n}]}_{\mathrm{KD}}]_{s\tilde{s}}\, \underline{{}^{\mathrm{D}}_{\tilde{n}}\langle \tilde{s}e|B\rho|se\rangle^{\mathrm{K}}_{\tilde{n}}}$$

$${}^{\mathrm{D}}_{\tilde{n}}\langle \tilde{s}e|B\rho|se\rangle^{\mathrm{K}}_{\tilde{n}} = \sum_{\bar{n}} {}^{\mathrm{D}}_{\tilde{n}}\langle \tilde{s}e|B|\bar{s}\bar{e}\rangle^{\mathrm{D}}_{\bar{n}} [\rho^{[\bar{n}]}_{\mathrm{D}}]_{\bar{s}\bar{s}}\, {}^{\mathrm{D}}_{\bar{n}}\langle \bar{s}\bar{e}|se\rangle^{\mathrm{K}}_{\tilde{n}}$$
$$= \underbrace{{}^{\mathrm{D}}_{\tilde{n}}\langle \tilde{s}e|B|\hat{s}e\rangle^{\mathrm{K}}_{\tilde{n}}}_{[B^{[\tilde{n}]}_{\mathrm{DK}}]_{\tilde{s}\hat{s}}} \underbrace{\sum_{\bar{n}>\tilde{n}} {}^{\mathrm{K}}_{\tilde{n}}\langle \hat{s}e|\bar{s}\bar{e}\rangle^{\mathrm{D}}_{\bar{n}} [\rho^{[\bar{n}]}_{\mathrm{D}}]_{\bar{s}\bar{s}}\, {}^{\mathrm{D}}_{\bar{n}}\langle \bar{s}\bar{e}|se\rangle^{\mathrm{K}}_{\tilde{n}}}_{[\rho^{[\tilde{n}]}_{\mathrm{K}}]_{\hat{s}s}}$$

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① $n = \tilde{n}$:
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③ $\tilde{n} < n$:
$$\sum_{\tilde{n}} \mathrm{Tr}\, \underline{e^{\mathrm{i}Ht} |se\rangle^{\mathrm{KK}}_{\tilde{n}\,\tilde{n}}\langle se|}A|\tilde{s}e\rangle^{\mathrm{DD}}_{\tilde{n}\,\tilde{n}}\underline{\langle \tilde{s}e| e^{-\mathrm{i}Ht}} B\rho$$
$$= \sum_{\tilde{n}} e^{\mathrm{i}(E^{[\tilde{n}]}_s - E^{[\tilde{n}]}_{\tilde{s}})t} [A^{[\tilde{n}]}_{\mathrm{KD}}]_{s\tilde{s}}\, \underline{{}^{\mathrm{D}}_{\tilde{n}}\langle \tilde{s}e|B\rho|se\rangle^{\mathrm{K}}_{\tilde{n}}}$$

$${}^{\mathrm{D}}_{\tilde{n}}\langle \tilde{s}e|B\rho|se\rangle^{\mathrm{K}}_{\tilde{n}} = \sum_{\bar{n}} {}^{\mathrm{D}}_{\tilde{n}}\langle \tilde{s}e|B|\bar{s}\bar{e}\rangle^{\mathrm{D}}_{\bar{n}} [\rho^{[\bar{n}]}_{\mathrm{D}}]_{\bar{s}\bar{s}}\, {}^{\mathrm{D}}_{\bar{n}}\langle \bar{s}\bar{e}|se\rangle^{\mathrm{K}}_{\tilde{n}}$$
$$= \underbrace{{}^{\mathrm{D}}_{\tilde{n}}\langle \tilde{s}e|B|\hat{s}e\rangle^{\mathrm{K}}_{\tilde{n}}}_{[B^{[\tilde{n}]}_{\mathrm{DK}}]_{\tilde{s}\hat{s}}} \underbrace{\sum_{\bar{n}>\tilde{n}} {}^{\mathrm{K}}_{\tilde{n}}\langle \hat{s}e|\bar{s}\bar{e}\rangle^{\mathrm{D}}_{\bar{n}} [\rho^{[\bar{n}]}_{\mathrm{D}}]_{\bar{s}\bar{s}}\, {}^{\mathrm{D}}_{\bar{n}}\langle \bar{s}\bar{e}|se\rangle^{\mathrm{K}}_{\tilde{n}}}_{[\rho^{[\tilde{n}]}_{\mathrm{K}}]_{\hat{s}s}}$$

Hilbert space partitioning: $|se\rangle^{\mathrm{KK}}_{n\,n}\langle se| = \sum_{\tilde{n}>n} |\tilde{s}\tilde{e}\rangle^{\mathrm{DD}}_{\tilde{n}\,\tilde{n}}\langle \tilde{s}\tilde{e}|$

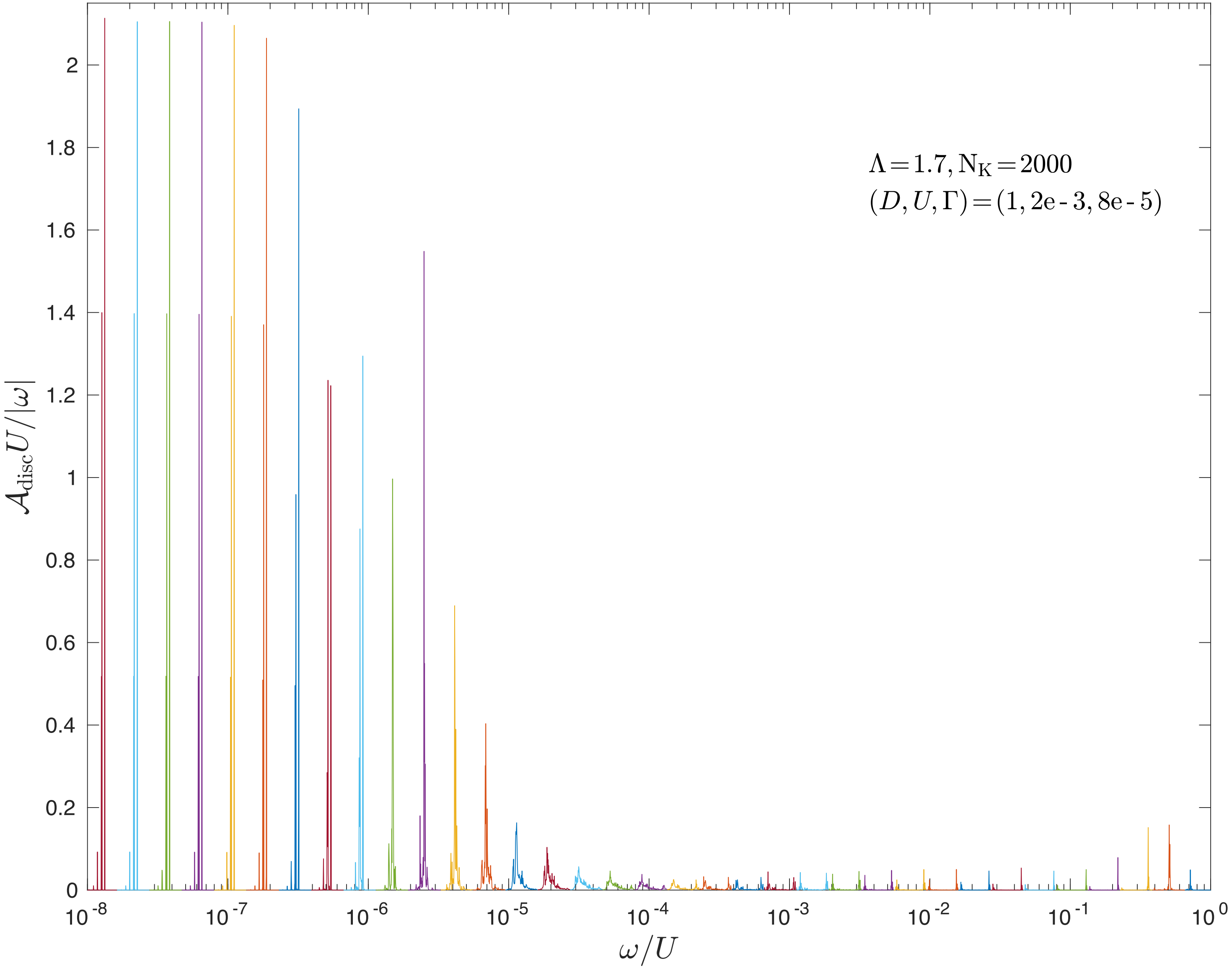
Extend eigenstate approx.
(suffices for differences) $H|se\rangle^{\mathrm{X}}_n = E^{[n]}_s |se\rangle^{\mathrm{X}}_n + O\big(\Lambda^{-\frac{n+1}{2}}\big)$

In total: $$\mathcal{A}(\omega) = \sum_n \sum_{\mathrm{X}\tilde{\mathrm{X}}}^{\neq \mathrm{KK}} [A^{[n]}_{\mathrm{X}\tilde{\mathrm{X}}}]_{s\tilde{s}} [B^{[n]}_{\tilde{\mathrm{X}}\mathrm{X}} \rho^{[n]}_{\mathrm{X}}]_{\tilde{s}s} \delta(\omega + E^{[n]}_s - E^{[n]}_{\tilde{s}})$$

Peters, Pruschke, Anders, PRB 2006
Weichselbaum, von Delft, PRL 2007

Log-Gaussian broadening

Eigenspectrum is resolved on a logarithmic scale
→ δ peaks from Lehmann representation roughly uniformly spaced on logarithmic scale



Weichselbaum, von Delft, PRL 2007

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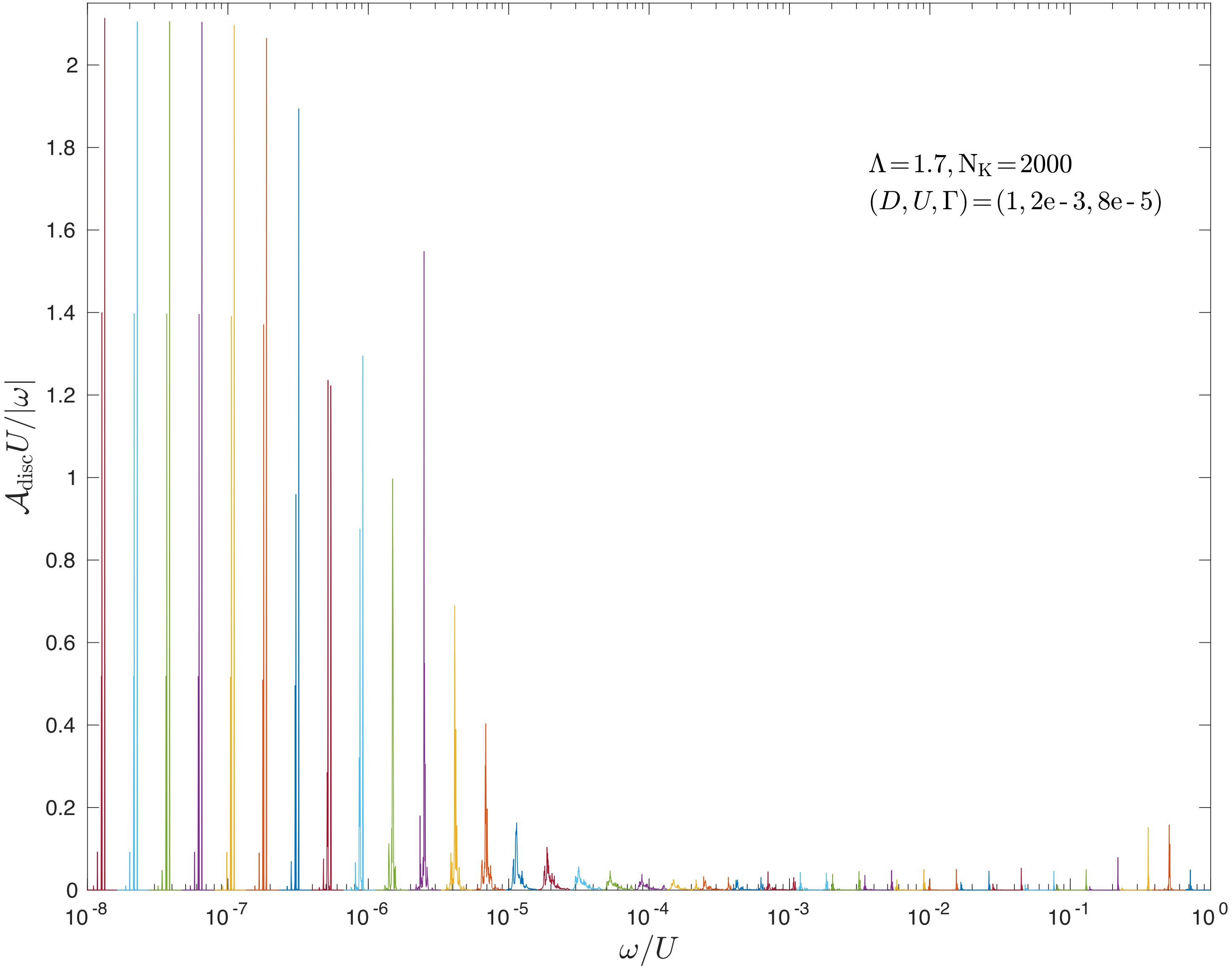
Broaden δ peaks by Gaussians of width α on log scale
→ broadening width $\propto \omega'$ on linear scale



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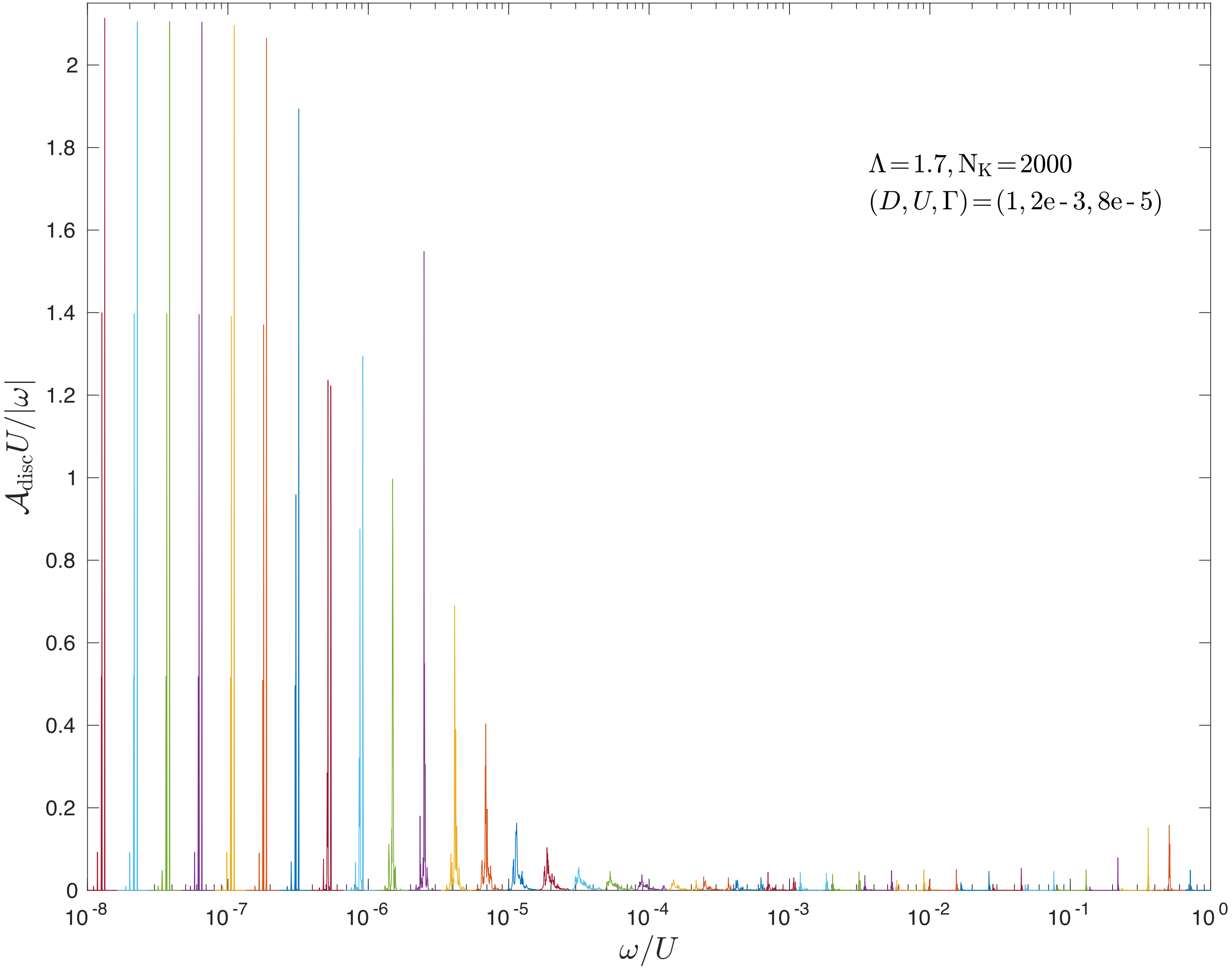
$$\mathcal{A}_{\mathrm{cont}}(\omega) = \int L(\omega,\omega')\mathcal{A}_{\mathrm{disc}}(\omega')\mathrm{d}\omega'$$

$$L(\omega,\omega') = \frac{c\,\Theta(\omega\omega')}{\sqrt{|\omega||\omega'|}}\exp\left[-\frac{(\ln|\omega| - \ln|\omega'|)^2}{\alpha^2}\right]$$

normalized: $\int L(\omega,\omega')\mathrm{d}\omega = \int L(\omega,\omega')\mathrm{d}\omega' = 1$



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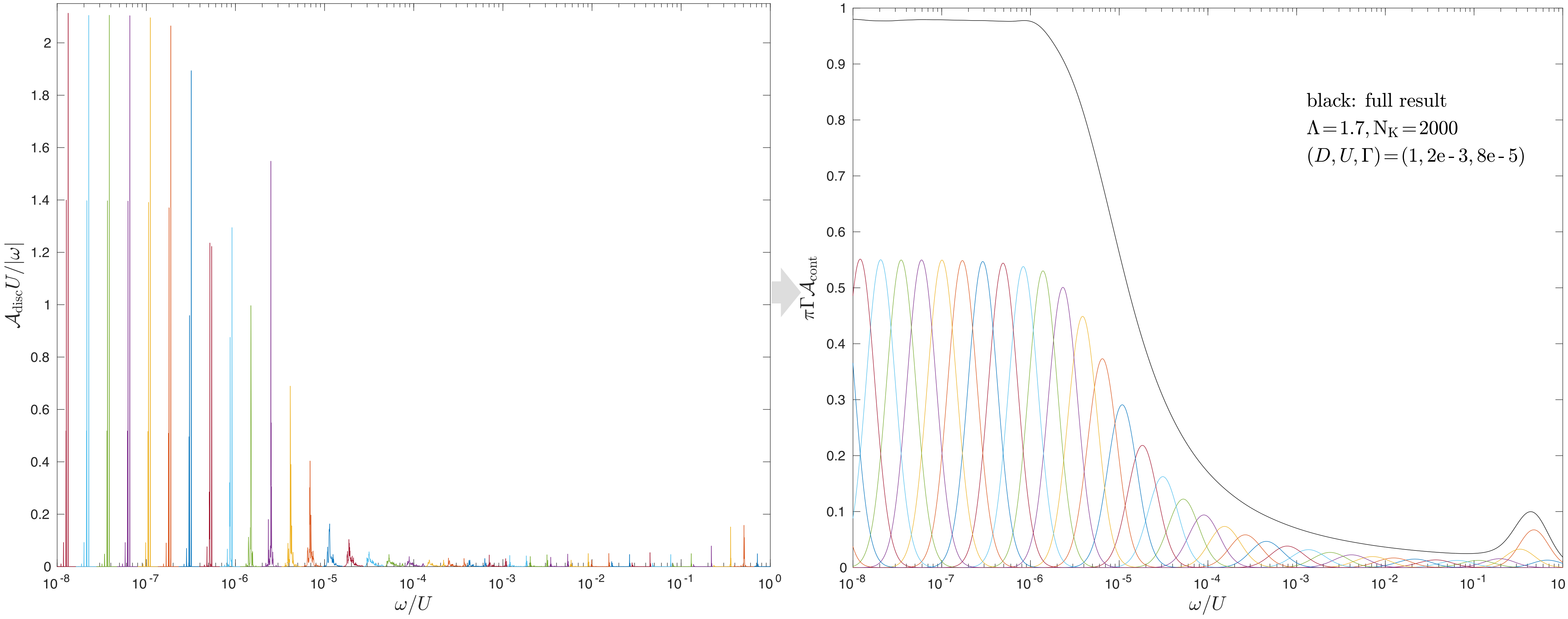

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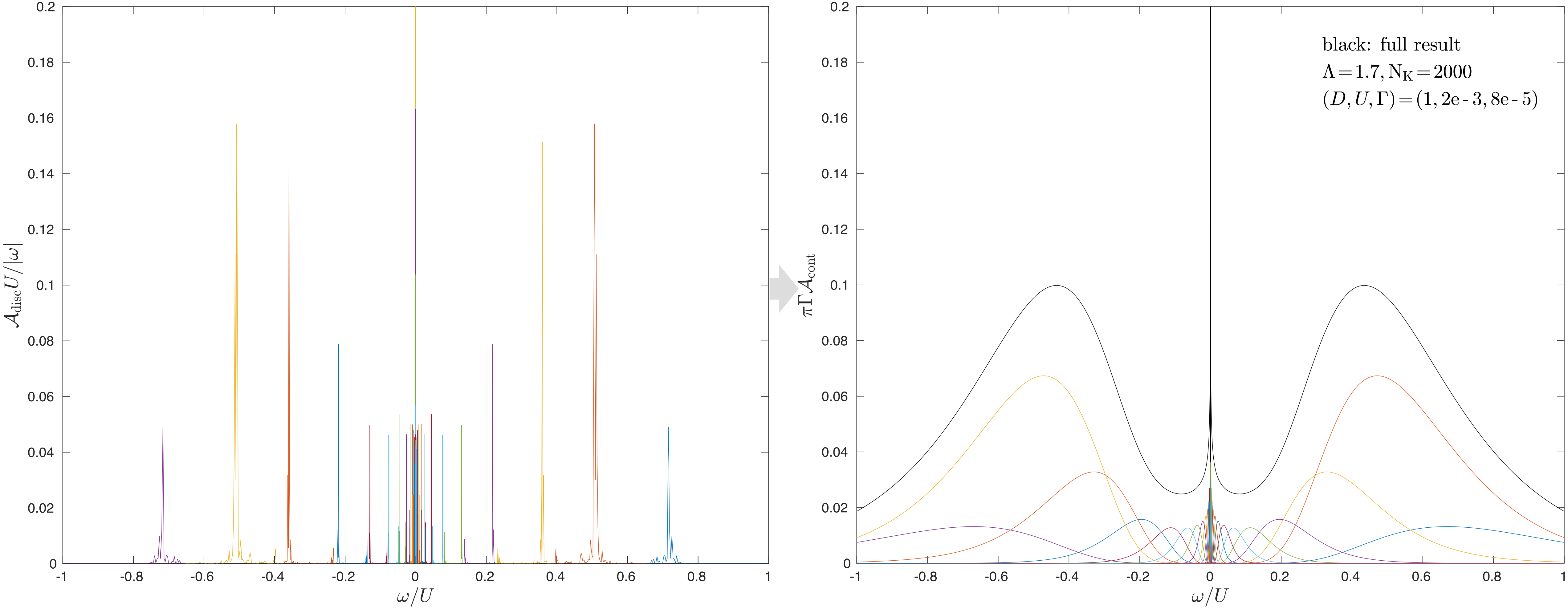

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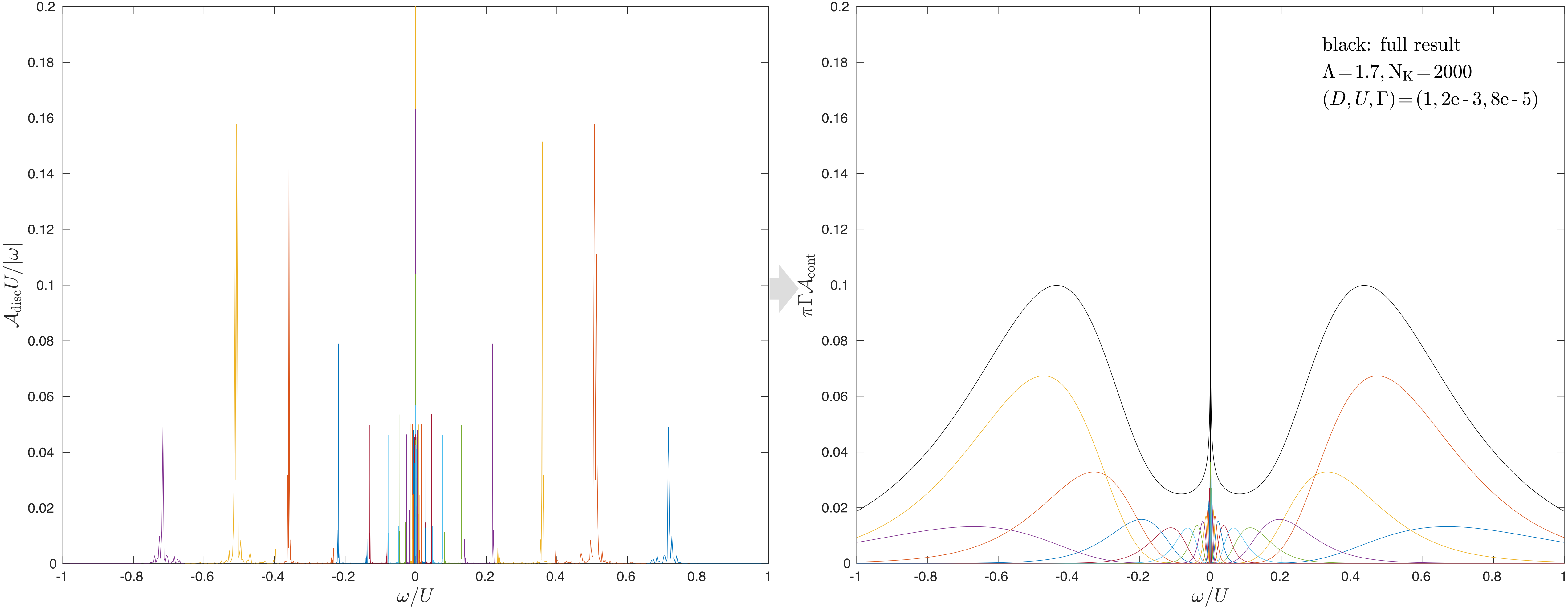

black: full result

$\Lambda = 1.7, \mathrm{N_K} = 2000$

$(D, U, \Gamma) = (1, 2\mathrm{e}\text{-}3, 8\mathrm{e}\text{-}5)$

Ways to increase high-energy resolution:

- z-averaging: average results from shifted grid $\sim\Lambda^{-n+z}$, $z \in [0,1)$
- adaptive broadening : track sensitivity of eigenstates to variations of bath parameters
- self-energy trick: obtain spectral function via self-energy + continuous hybridization

Žitko, Pruschke, PRB 2009

Lee, Weichselbaum, PRB 2016

Spectral functions at finite temperature

$(D, U, \Gamma) = (1, 2\times 10^{-3}, 3\times 10^{-5})$

Lowest relevant energy scale: Kondo temperature,
can be deduced from Bethe-ansatz formula $T_\mathrm{K} = \sqrt{U\Gamma/2}\, \mathrm{e}^{-\pi U/8\Gamma + \pi\Gamma/2U} \sim 10^{-8}$
or $T_\mathrm{K} \sim 1/[4\chi(0)]$ or maximum of $\chi''_{T=0}(\omega)$ or ...

vD22

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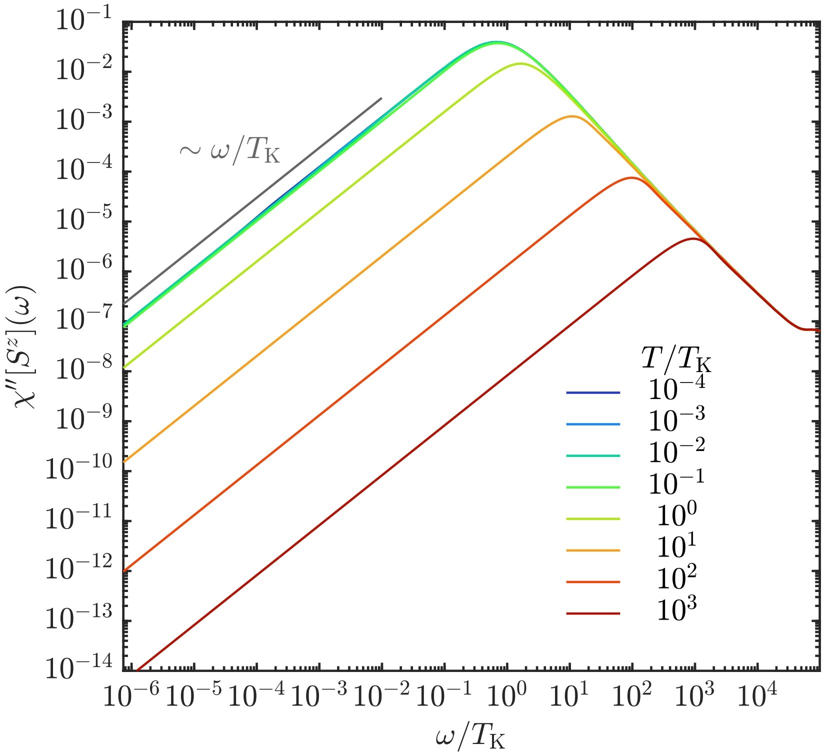

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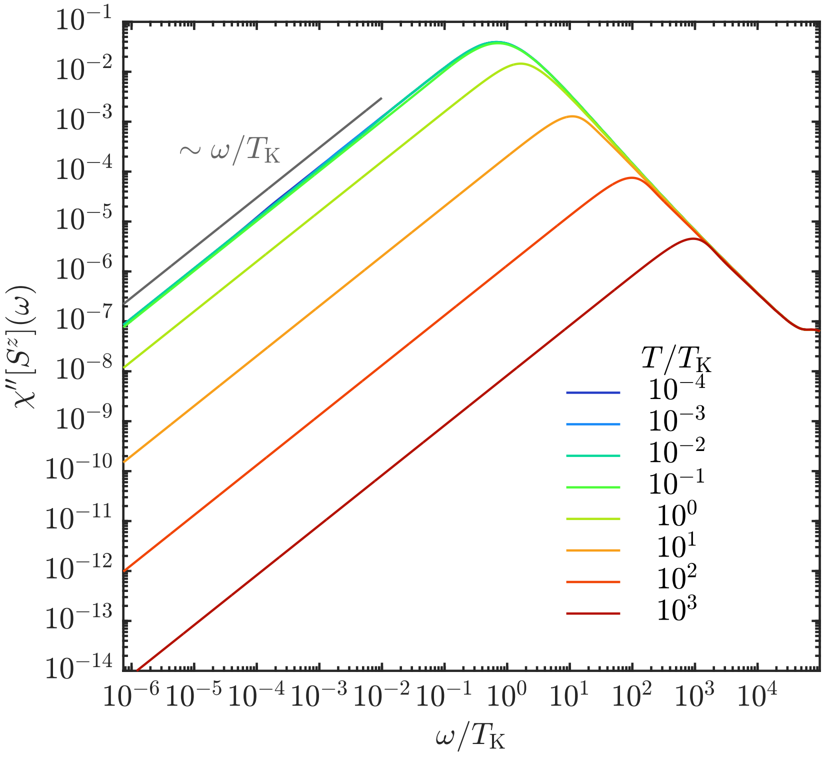

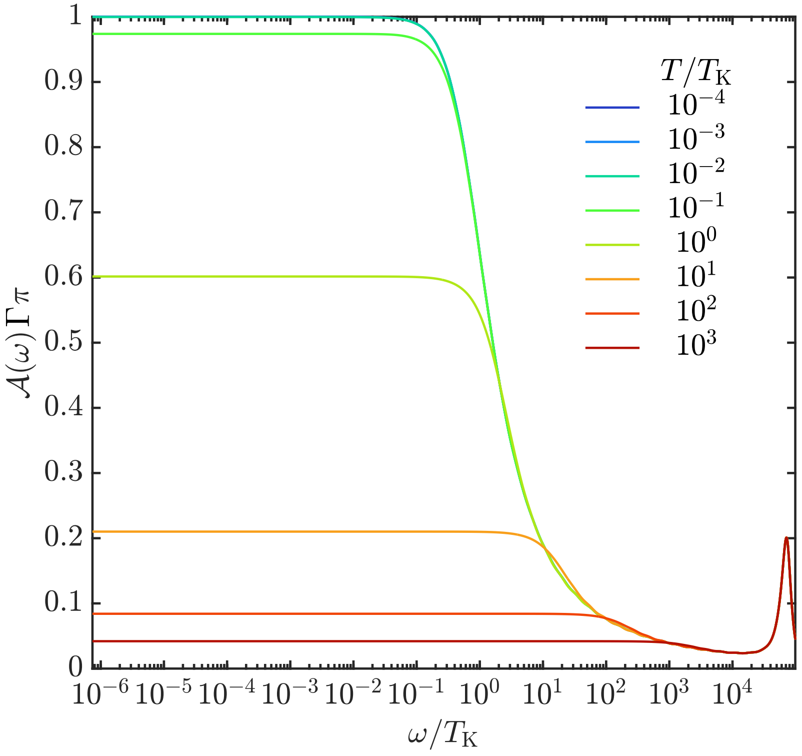

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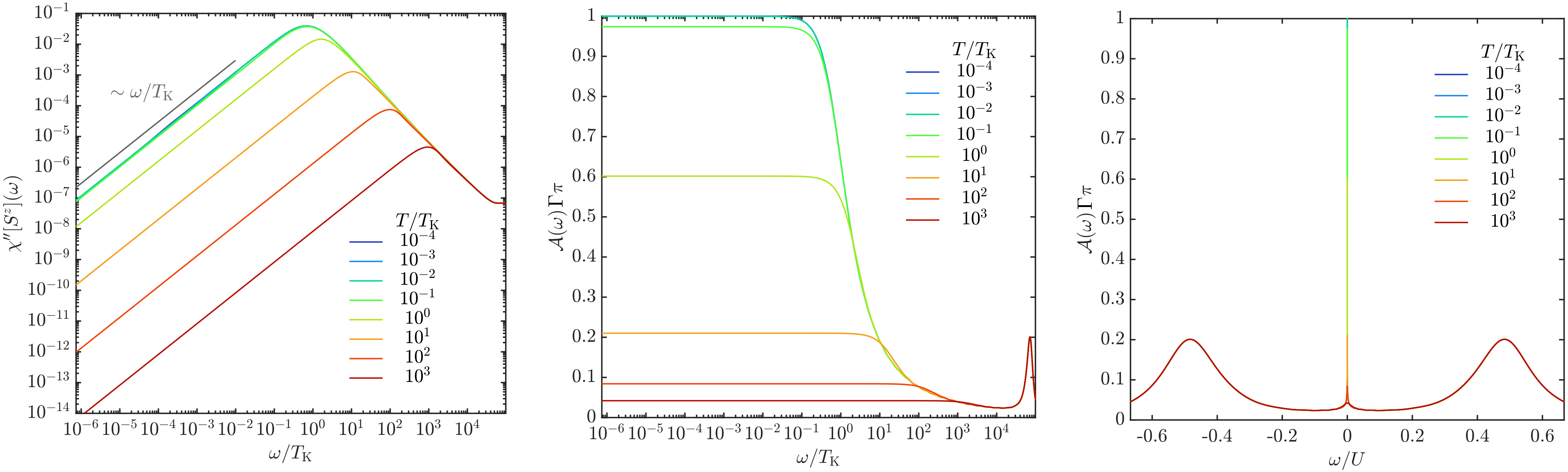

Self-energy

Straightforward from spectral function via Dyson equation?

$$\mathcal{A}(\omega) = -\frac{1}{\pi}\operatorname{Im} G(\omega), \quad \operatorname{Re} G(\omega) = \mathrm{P}\int \frac{\mathcal{A}(\omega')}{\omega-\omega'}\mathrm{d}\omega', \quad \Sigma(\omega) = \frac{1}{G_0(\omega)} - \frac{1}{G(\omega)}$$

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No, because (i) G stems from discretized and G_0 from continuum model and (ii) accurate $\operatorname{Im}\Sigma(\omega \to 0) \to 0$ hard to extract from difference

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→ "equations of motion"
(relating different correlation functions)

$$-\partial_\tau \langle \mathcal{T} d(\tau) d^\dagger \rangle = -\partial_\tau \langle \Theta(\tau) d(\tau) d^\dagger - \Theta(-\tau) d^\dagger d(\tau) \rangle = \delta(\tau) \langle \underbrace{\{d, d^\dagger\}}_{1} \rangle - \langle \mathcal{T} \partial_\tau d(\tau) d^\dagger \rangle$$

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Bulla, Hewson, Pruschke, J. Phys. Cond. Mat. 1998

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Kugler, PRB 2022

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🙁

Bulla, Hewson, Pruschke, J. Phys. Cond. Mat. 1998

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Kugler, PRB 2022

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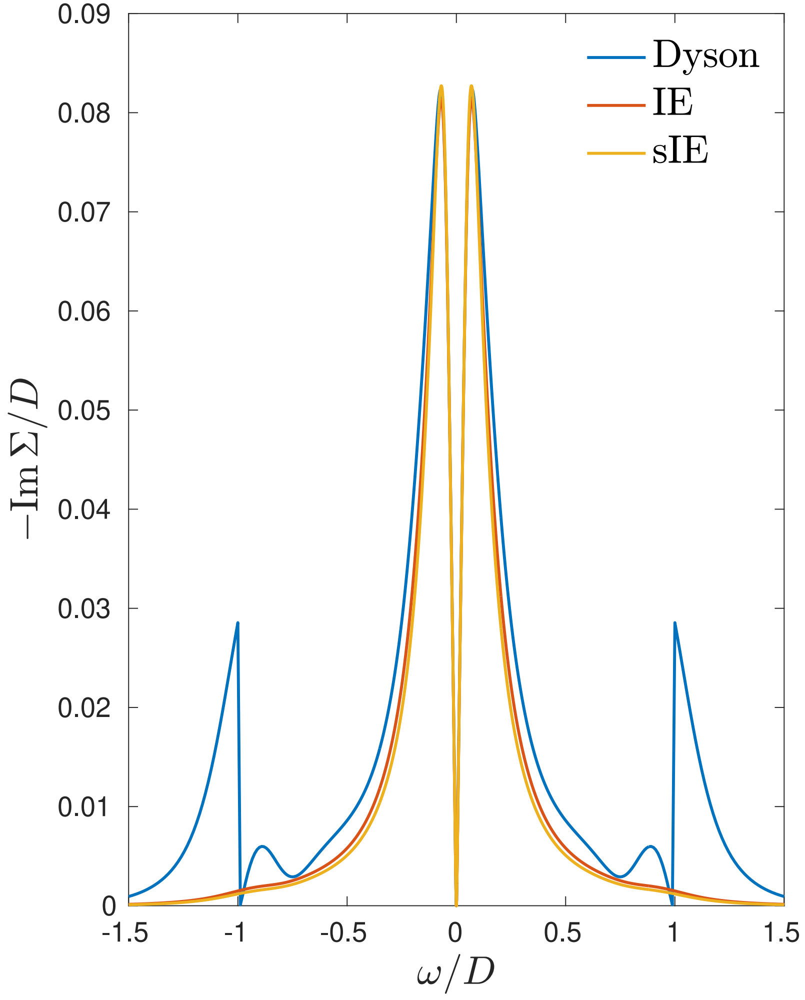
🙂

Kugler, PRB 2022

Self-energy results at zero temperature

Dyson $\Sigma(\omega) = \frac{1}{G_0(\omega)} - \frac{1}{G(\omega)}$, improved estimator (IE) $\Sigma = \frac{\langle\langle q, d^\dagger \rangle\rangle_z}{\langle\langle d, d^\dagger \rangle\rangle_z}$, symmetric IE (sIE) $\Sigma = \Sigma_{\text{Hartree}} + \langle\langle q, q^\dagger \rangle\rangle_z - \frac{\langle\langle q, d^\dagger \rangle\rangle_z \langle\langle d, q^\dagger \rangle\rangle_z}{\langle\langle d, d^\dagger \rangle\rangle_z}$



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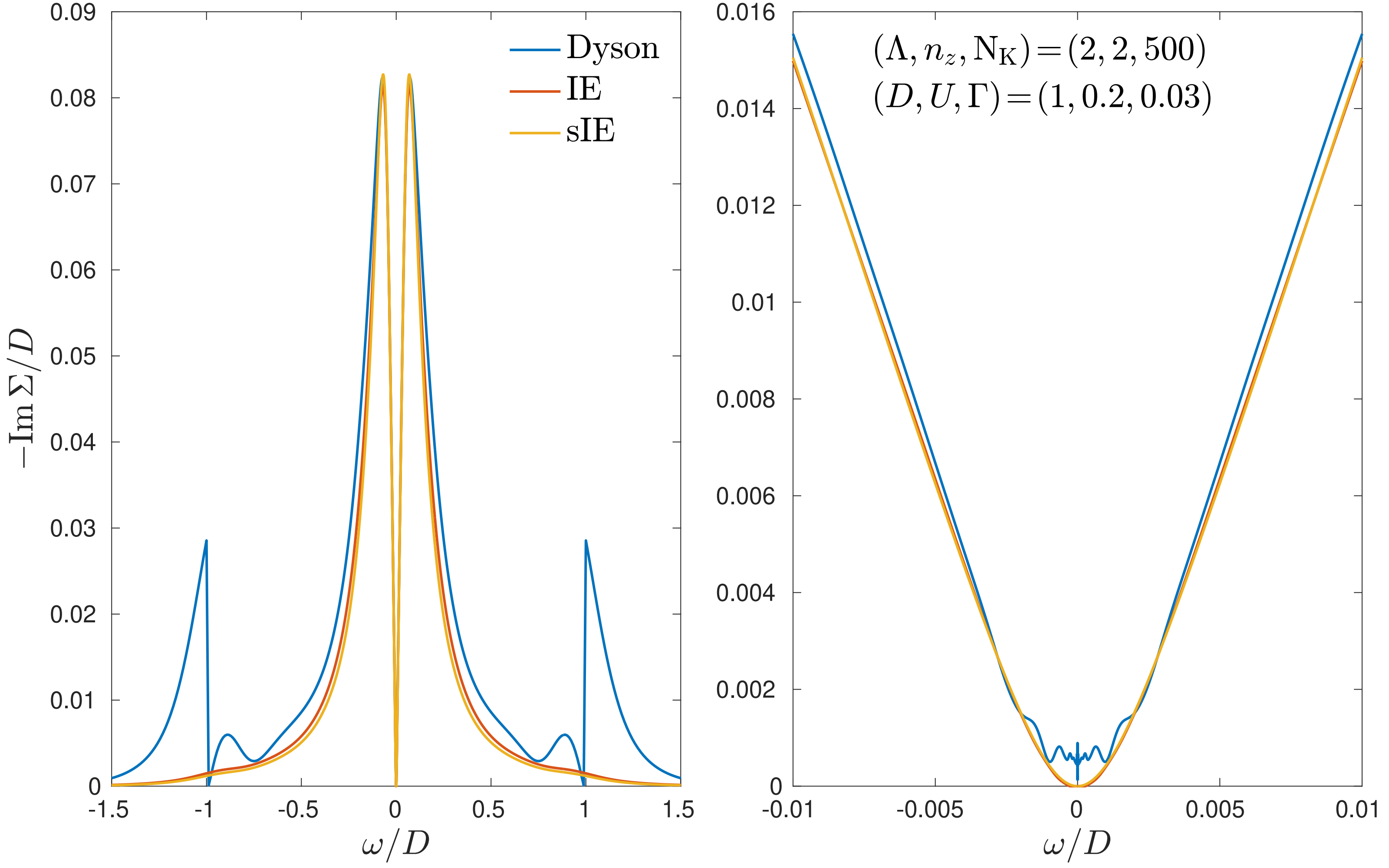

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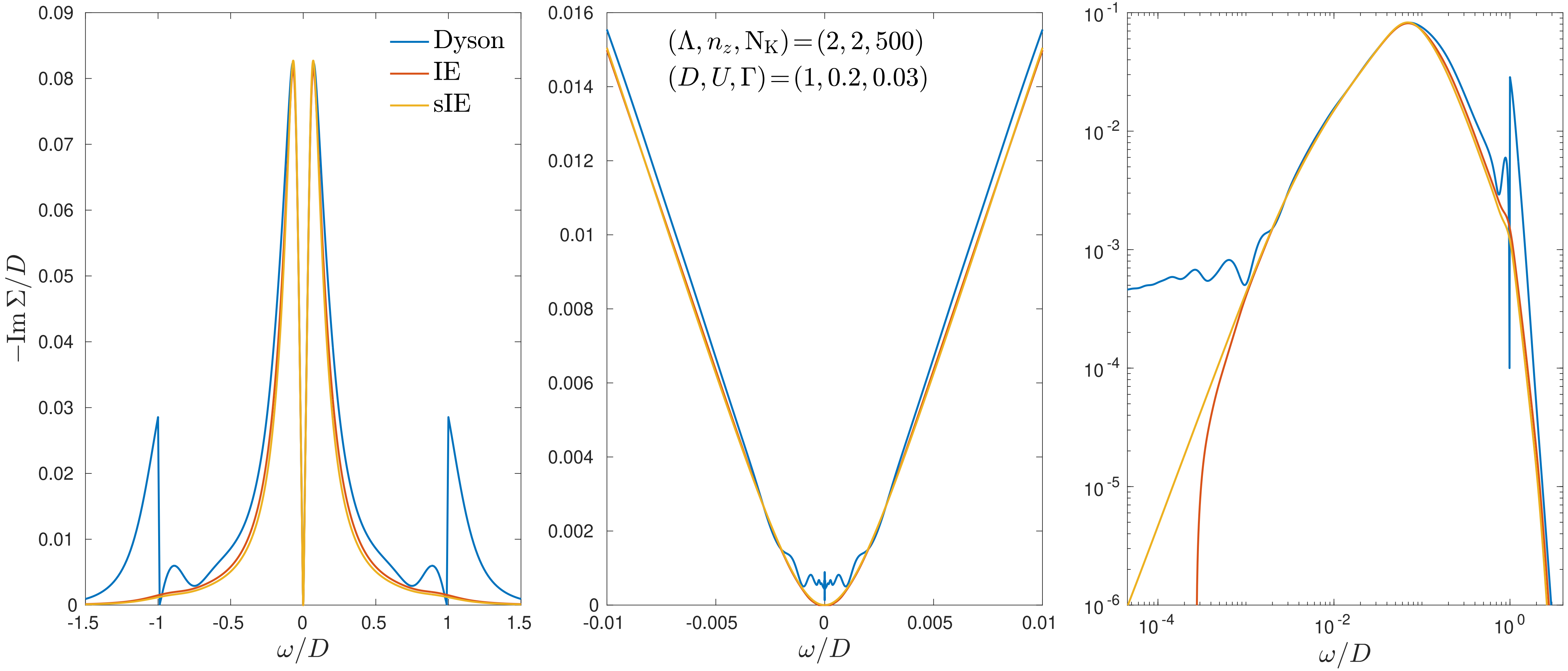

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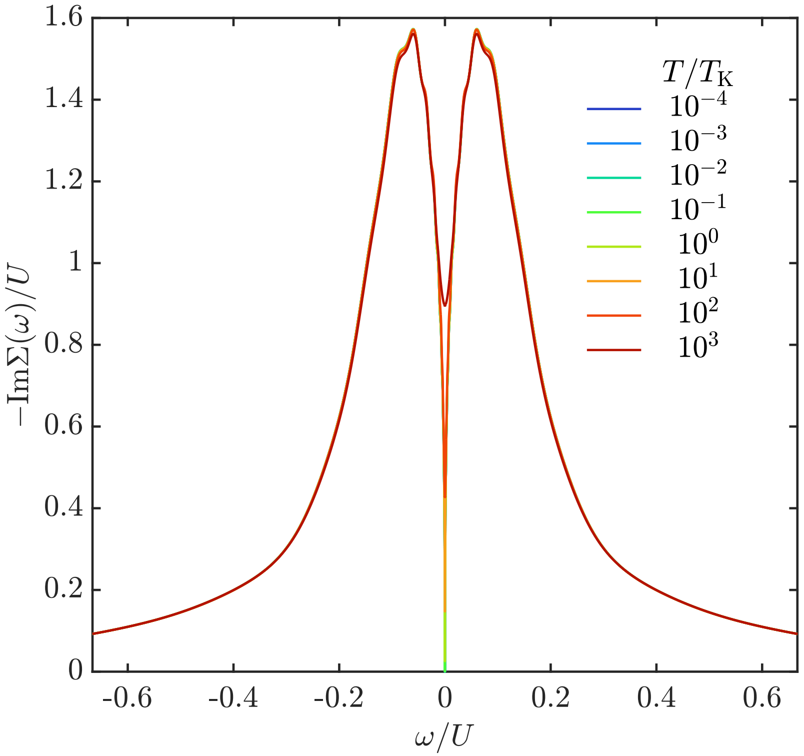

vD22

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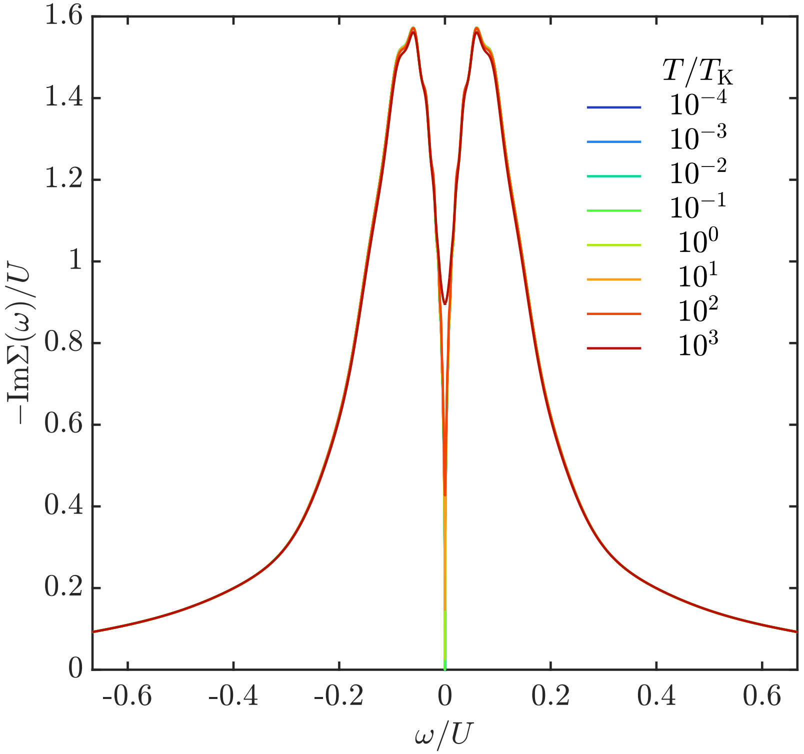

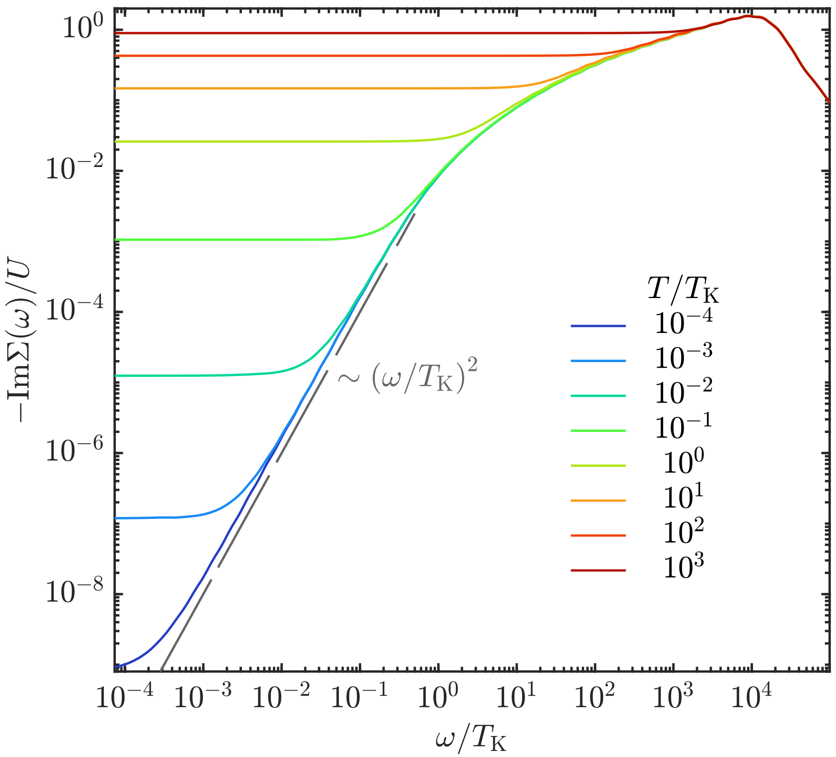

Symmetric estimator crucial
for such high resolution!

Kugler, PRB 2022

vD22

Self-energy results at finite temperature

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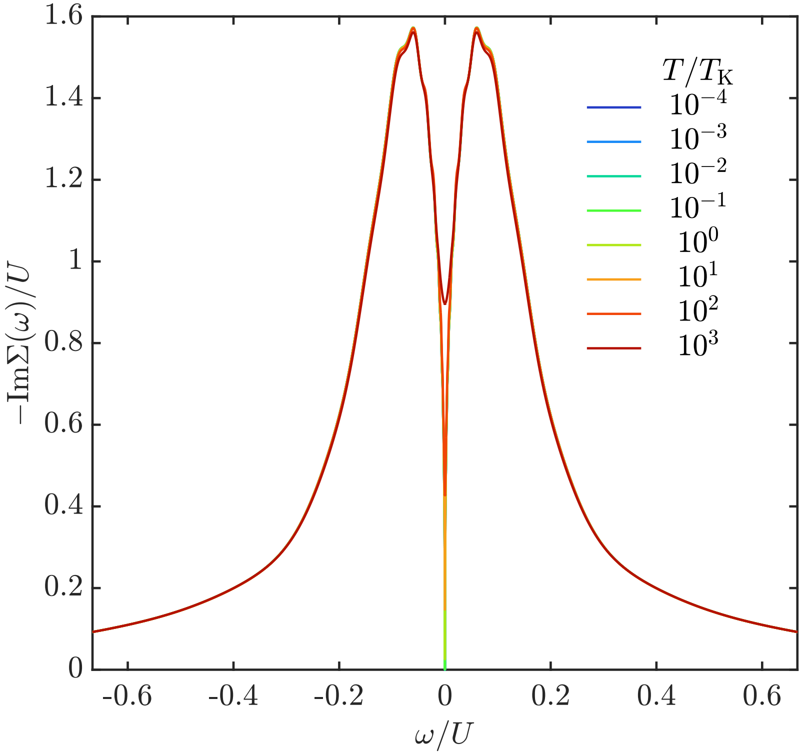

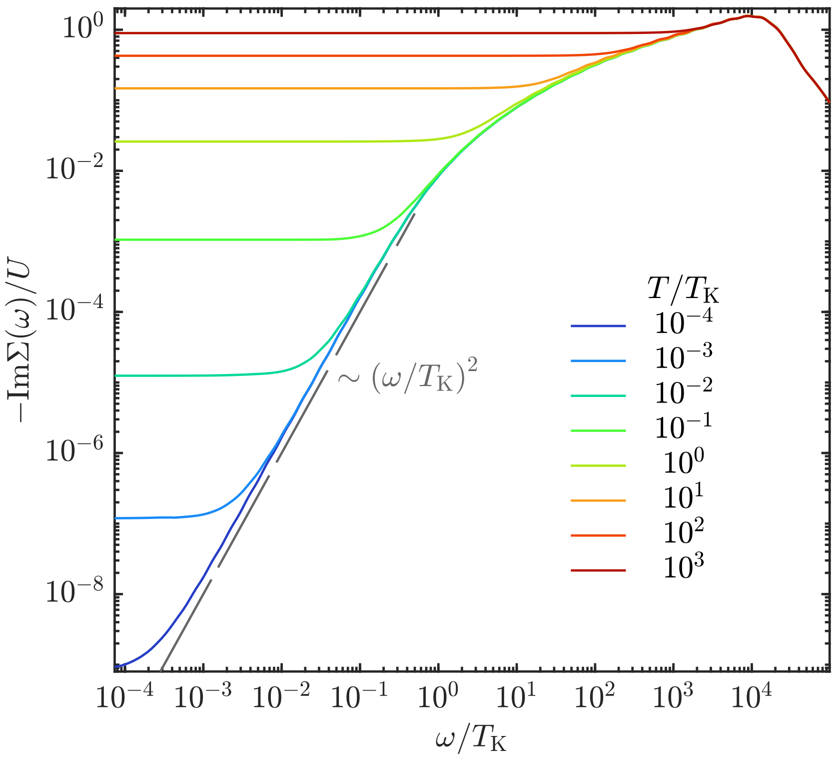

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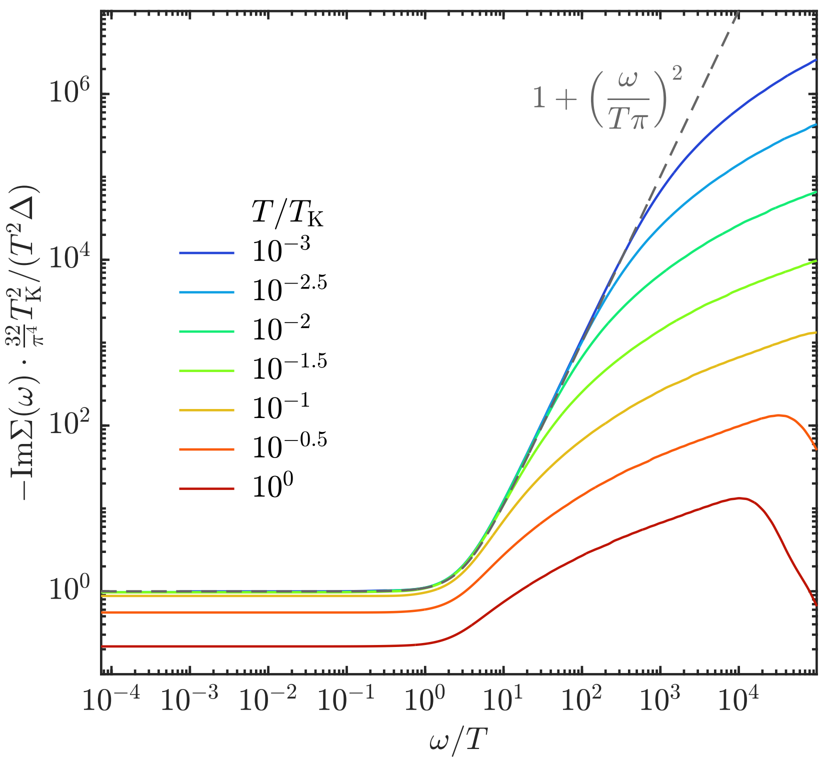


Scaling collapse (Fermi-liquid form)
(T_{K} only relevant low-energy scale)

Kugler, PRB 2022

vD22

Orbital-selective Mott phase ($T = 0$)

Consider multi-orbital Hubbard model with some orbital(s) more correlated than other(s)

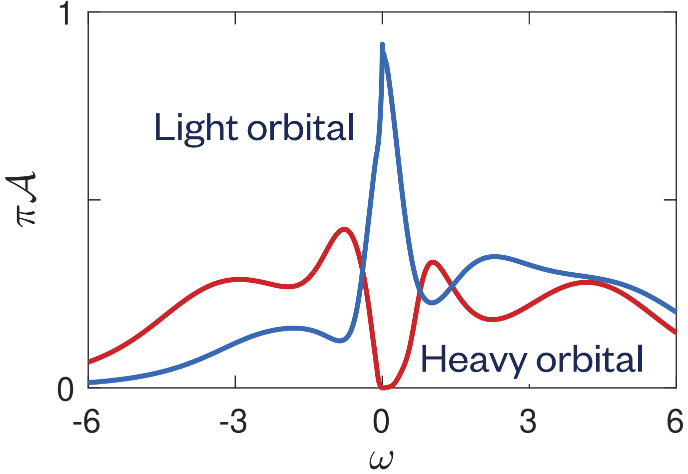
→ Coexistent Mott-insulating + metallic orbitals

$$\frac{|\uparrow;\uparrow\rangle|\downarrow;\emptyset\rangle_{\mathrm{bath}} - |\downarrow;\downarrow\rangle|\uparrow;\emptyset\rangle_{\mathrm{bath}}}{\sqrt{2}} \otimes |N-1\rangle_{\mathrm{bath}}$$

Hund's coupling

No low-energy modes in insulating orbital

e.g. different occupations



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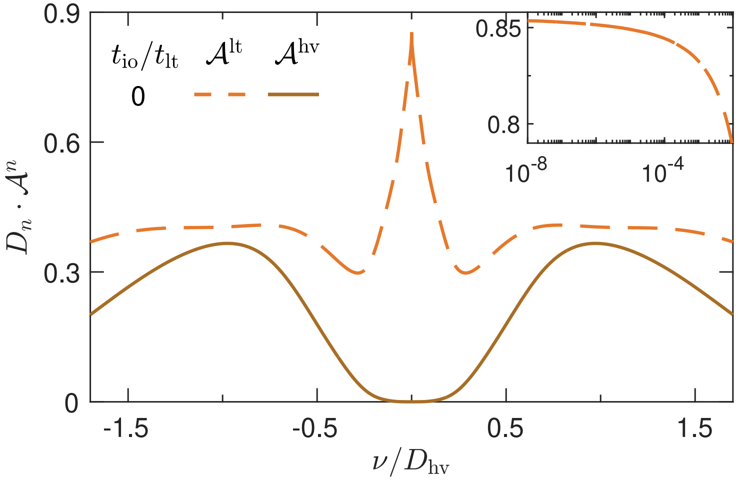

Kugler et al.,
PRB 2019

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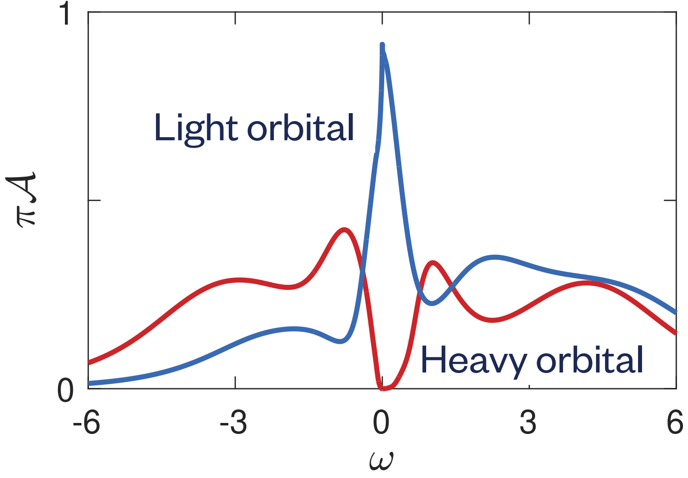

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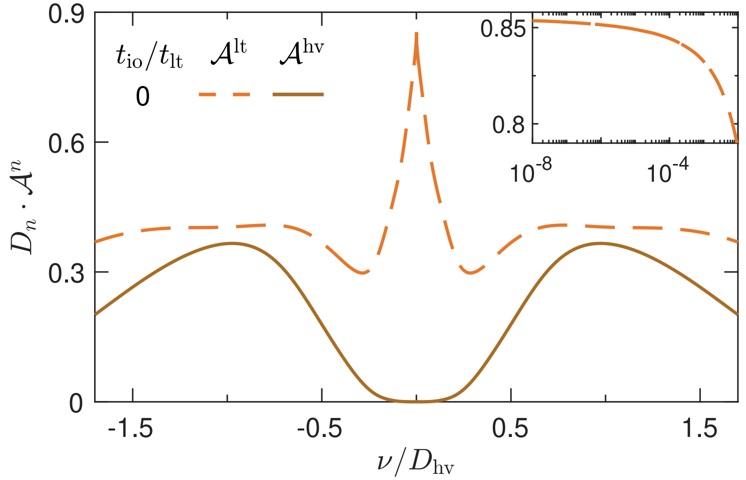
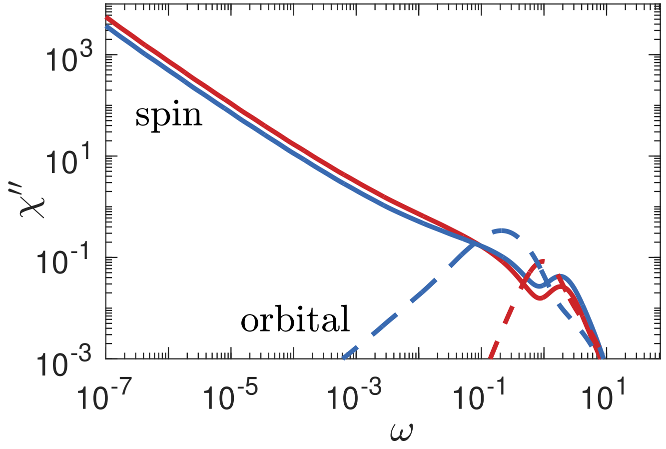


Kugler et al., PRB 2019



Light orbital insulating

→ underscreened Kondo effect

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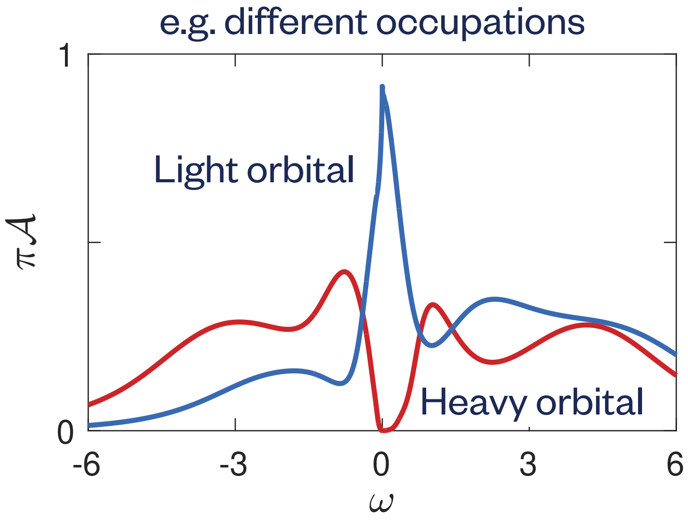
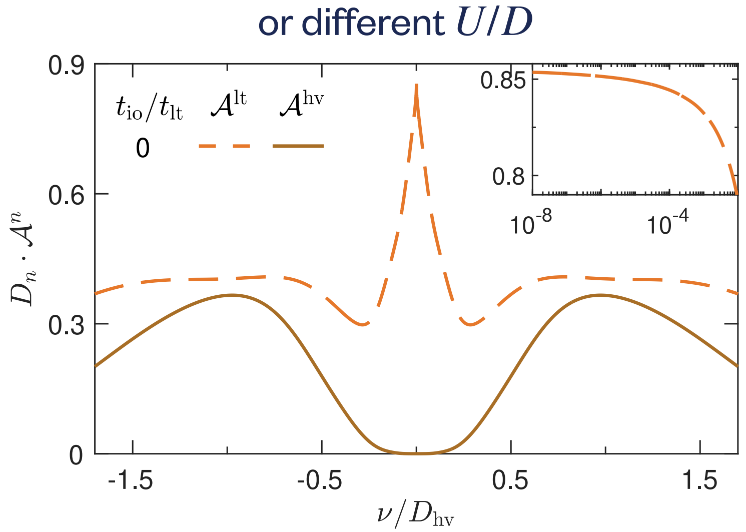
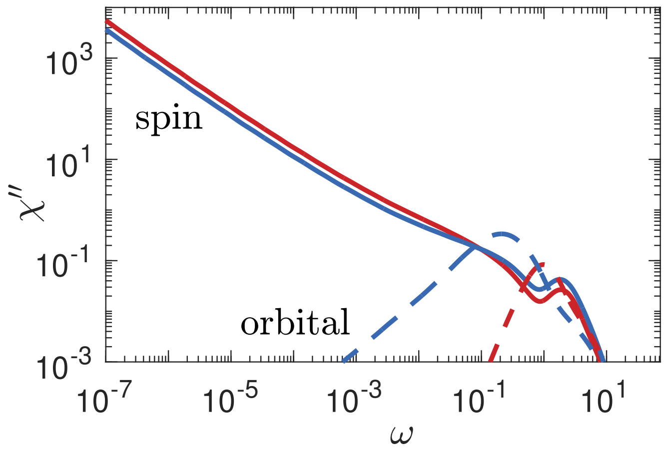




Kugler et al., PRB 2019



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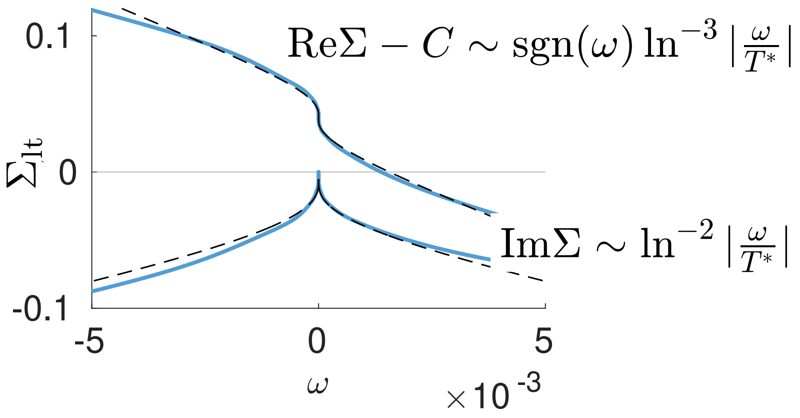

Heavy orbital metallic but
$Z=0$ → singular Fermi liquid

Orbital-selective Mott phase ($T\!=\!0$)

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Hund's coupling

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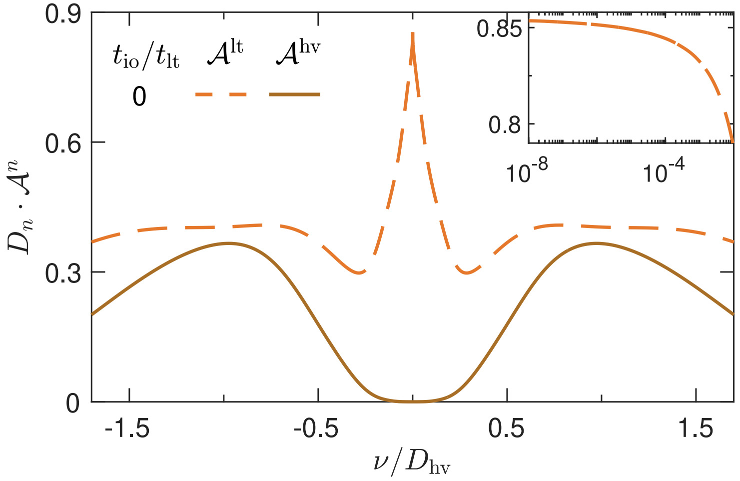
different U/D



Kugler, Kotliar, PRL 2022

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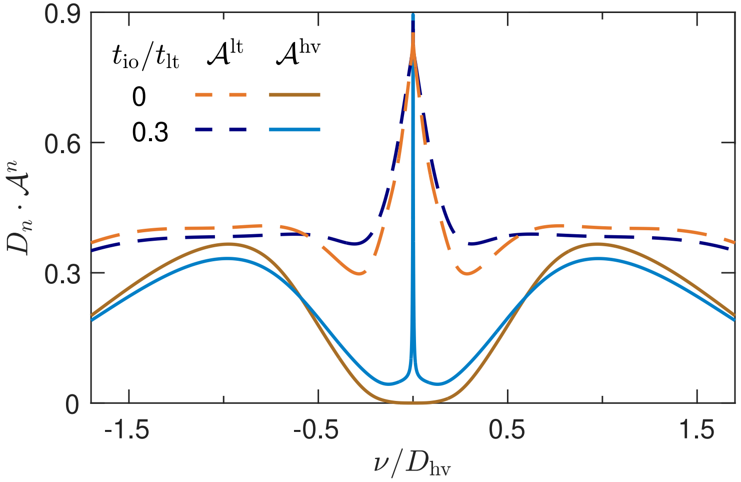

Kugler, Kotliar, PRL 2022

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Kugler, Kotliar, PRL 2022

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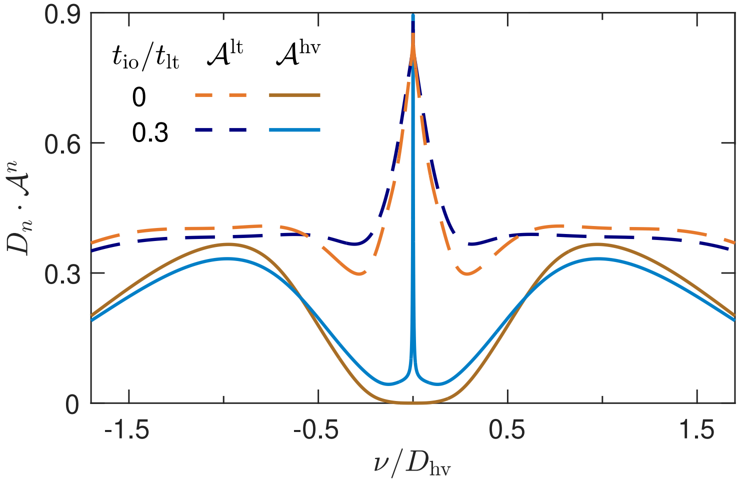

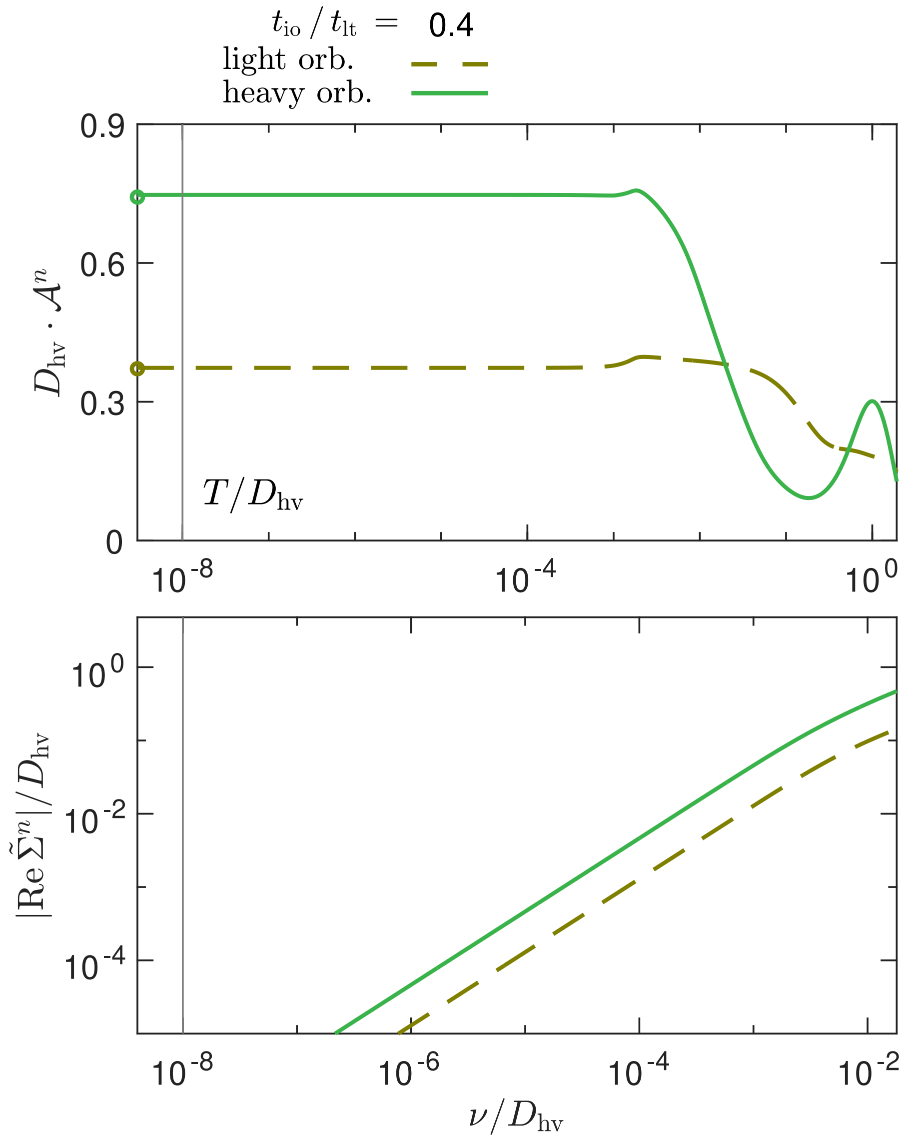

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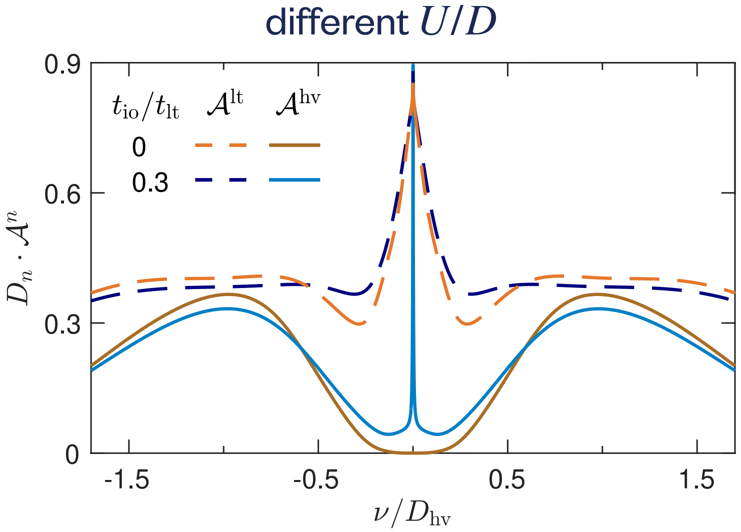
Kugler, Kotliar, PRL 2022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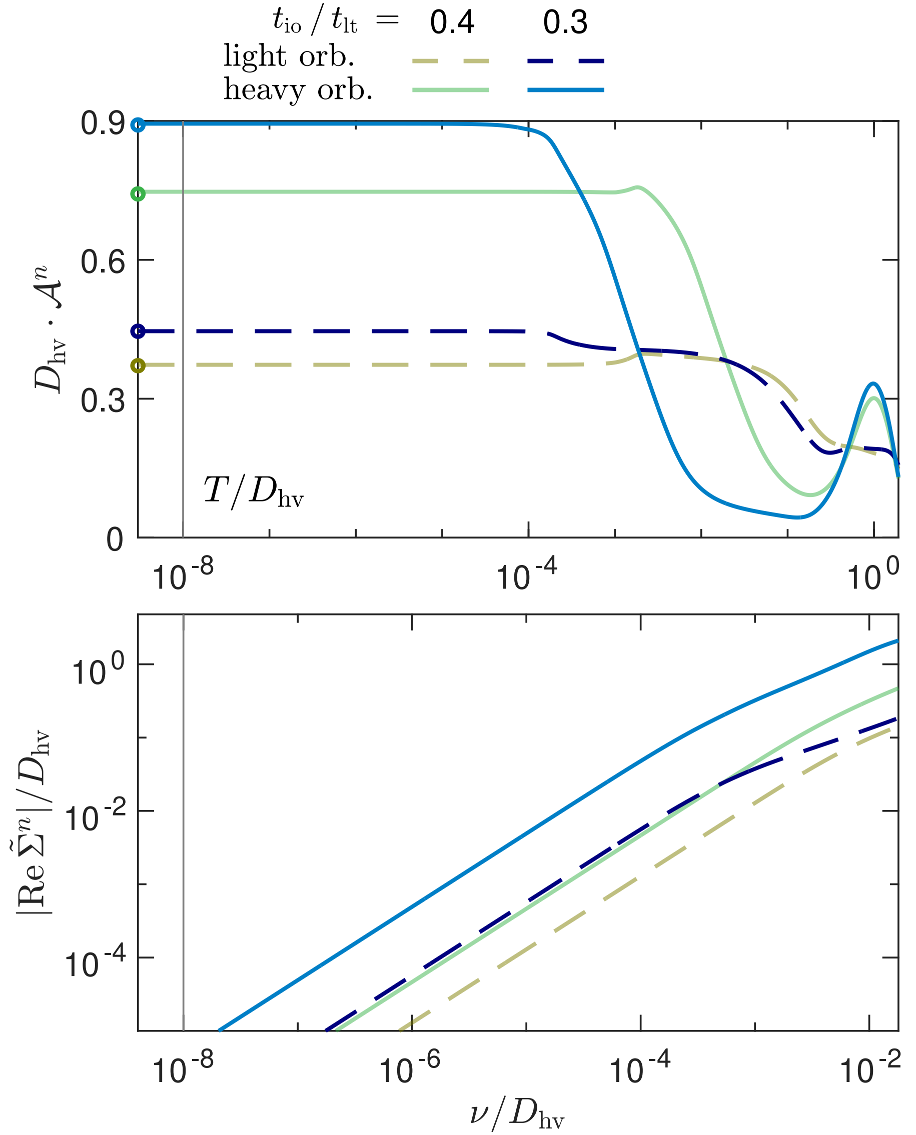

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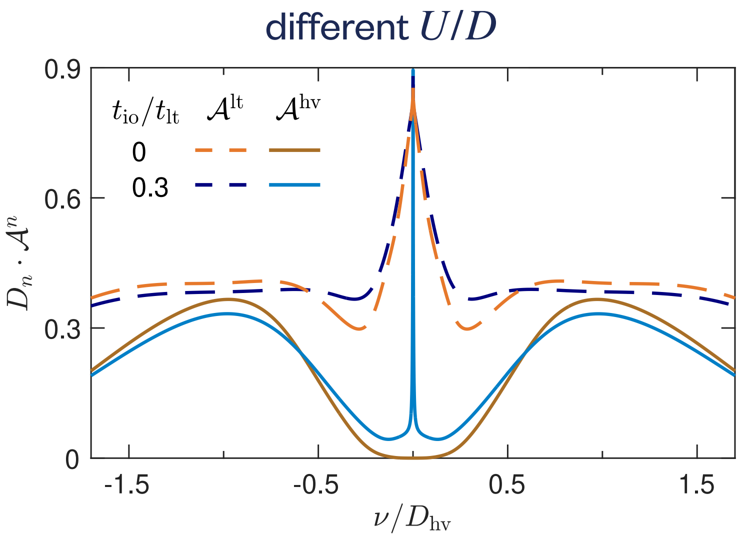
Kugler, Kotliar, PRL 2022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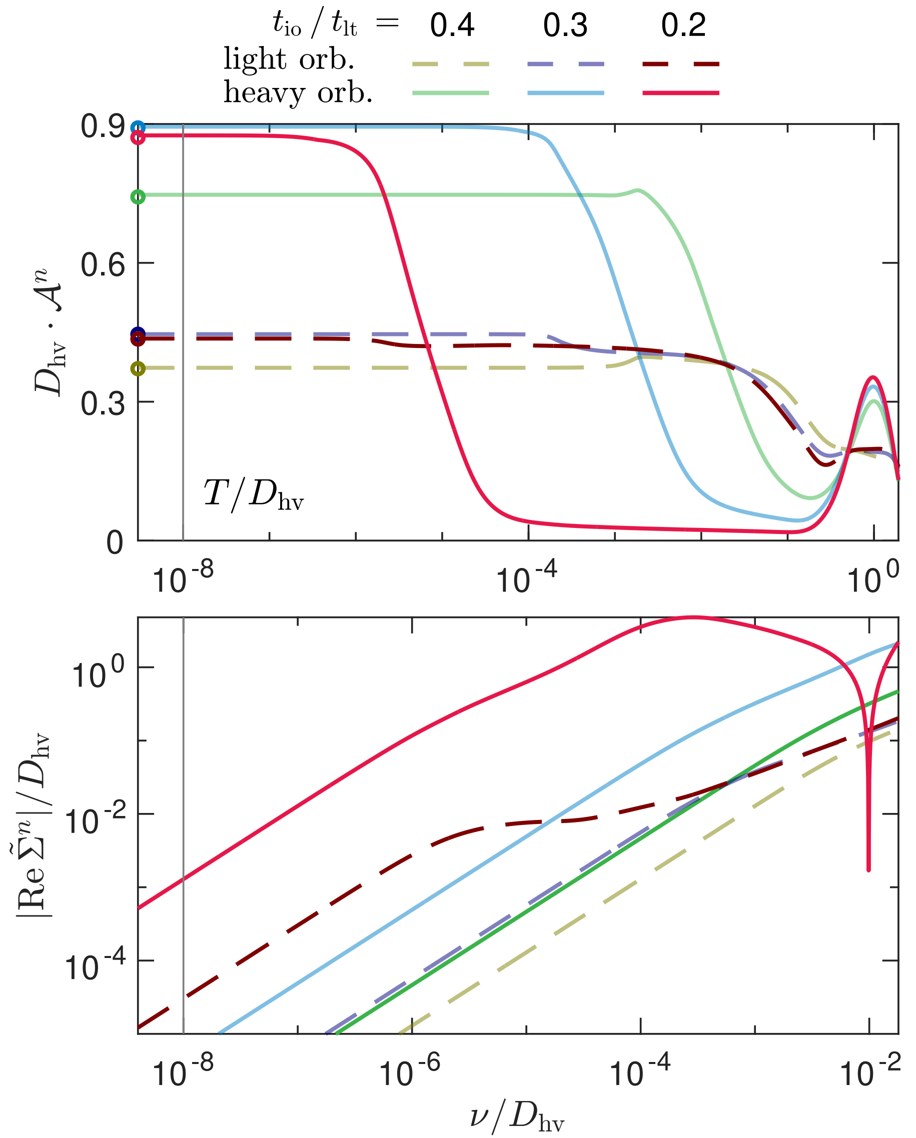

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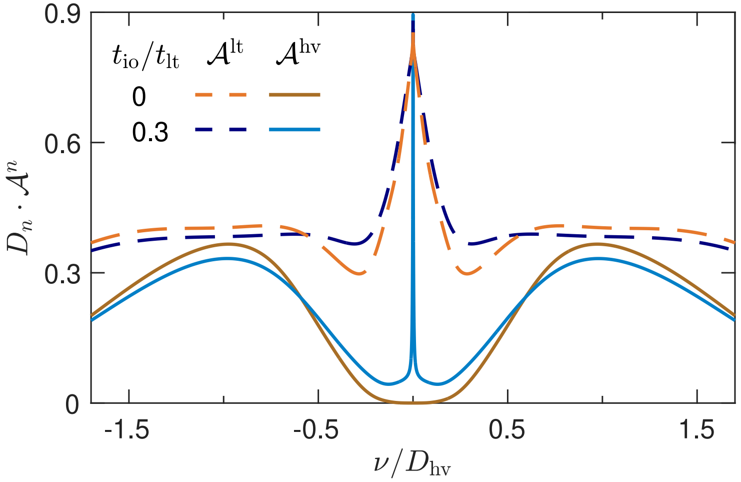
Kugler, Kotliar, PRL 2022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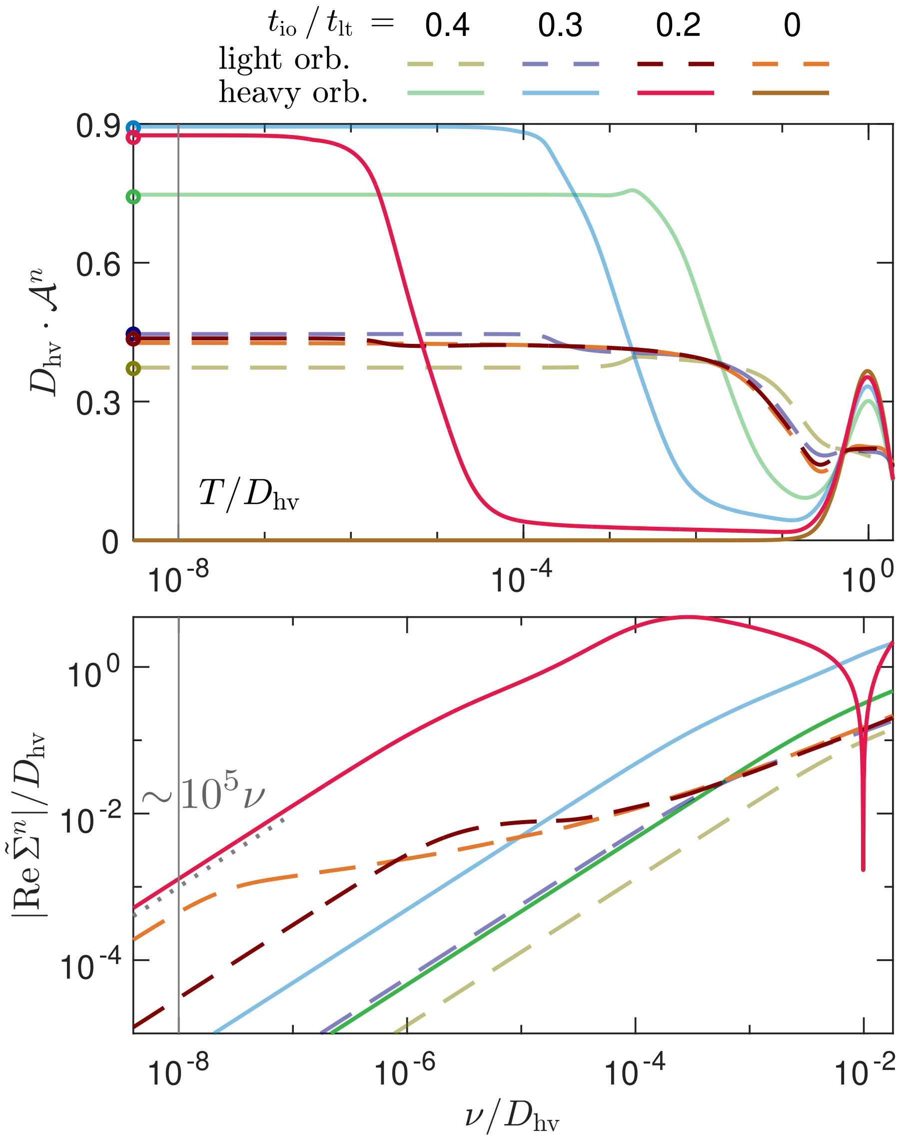

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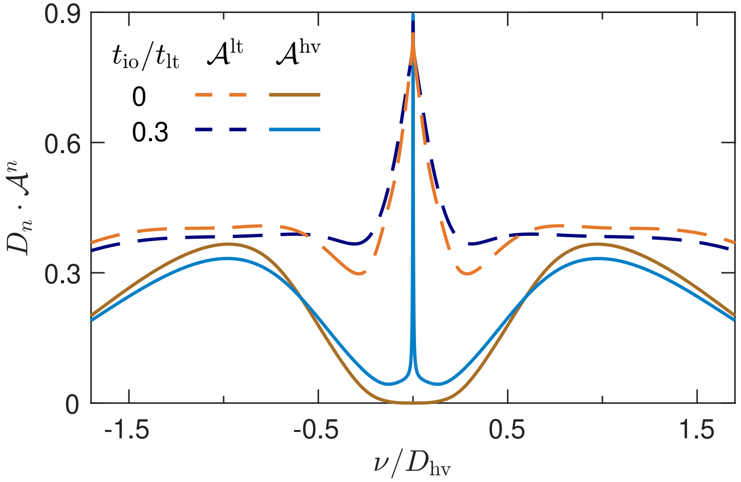

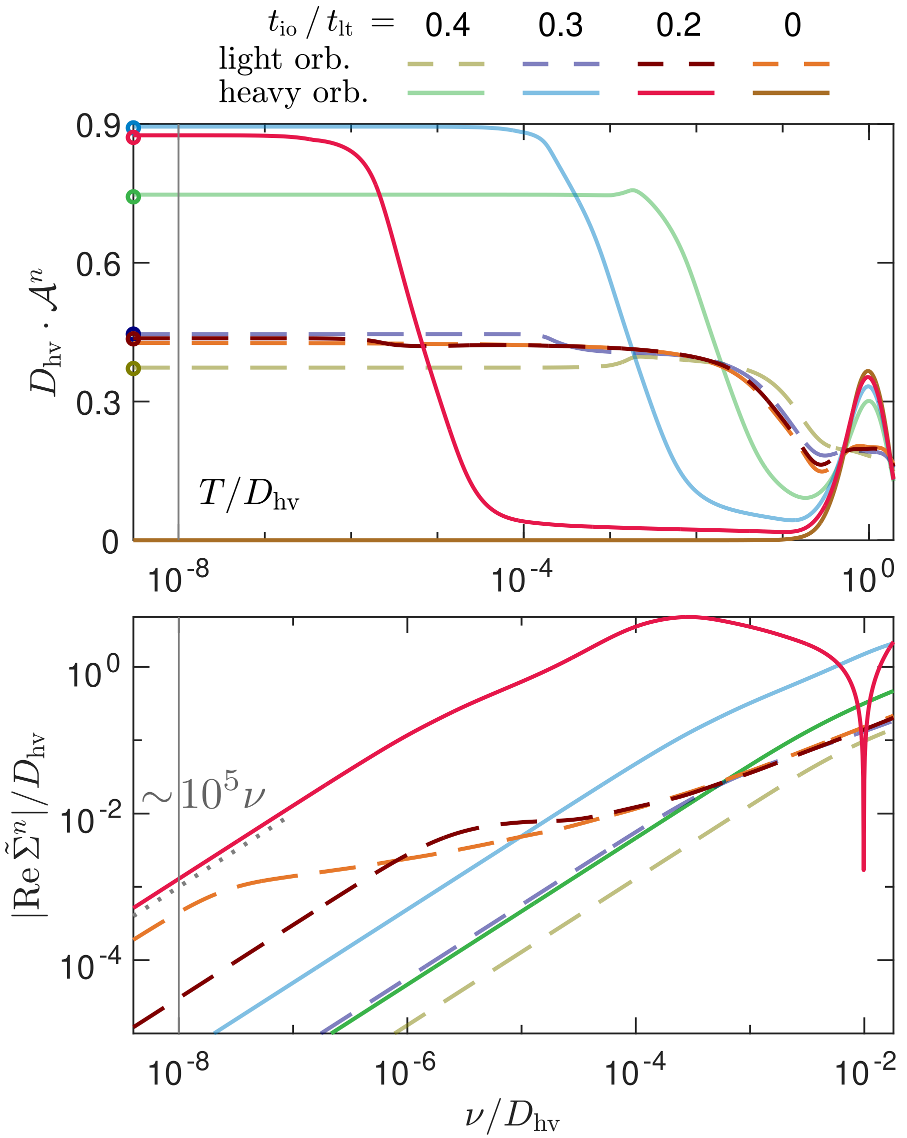

Kugler, Kotliar, PRL 2022

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(relevant to recent ARPES in FeTe$_{1\text{-x}}$Se$_{\text{x}}$, group of Ming Yi @ Rice U.)

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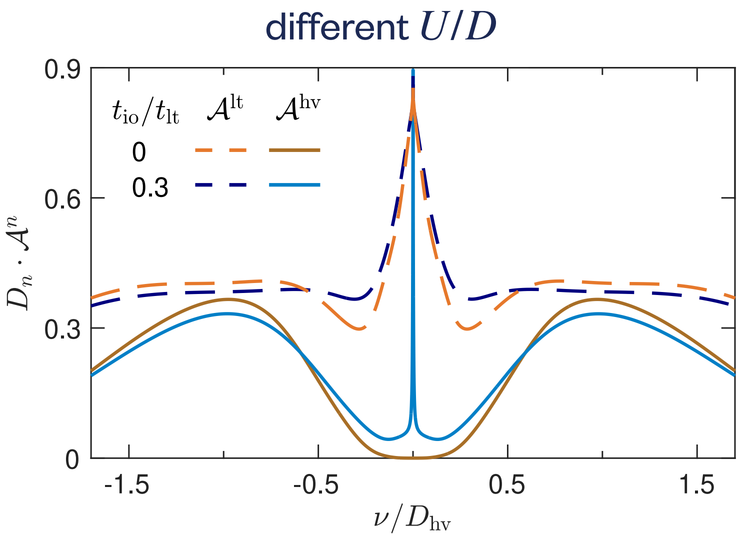

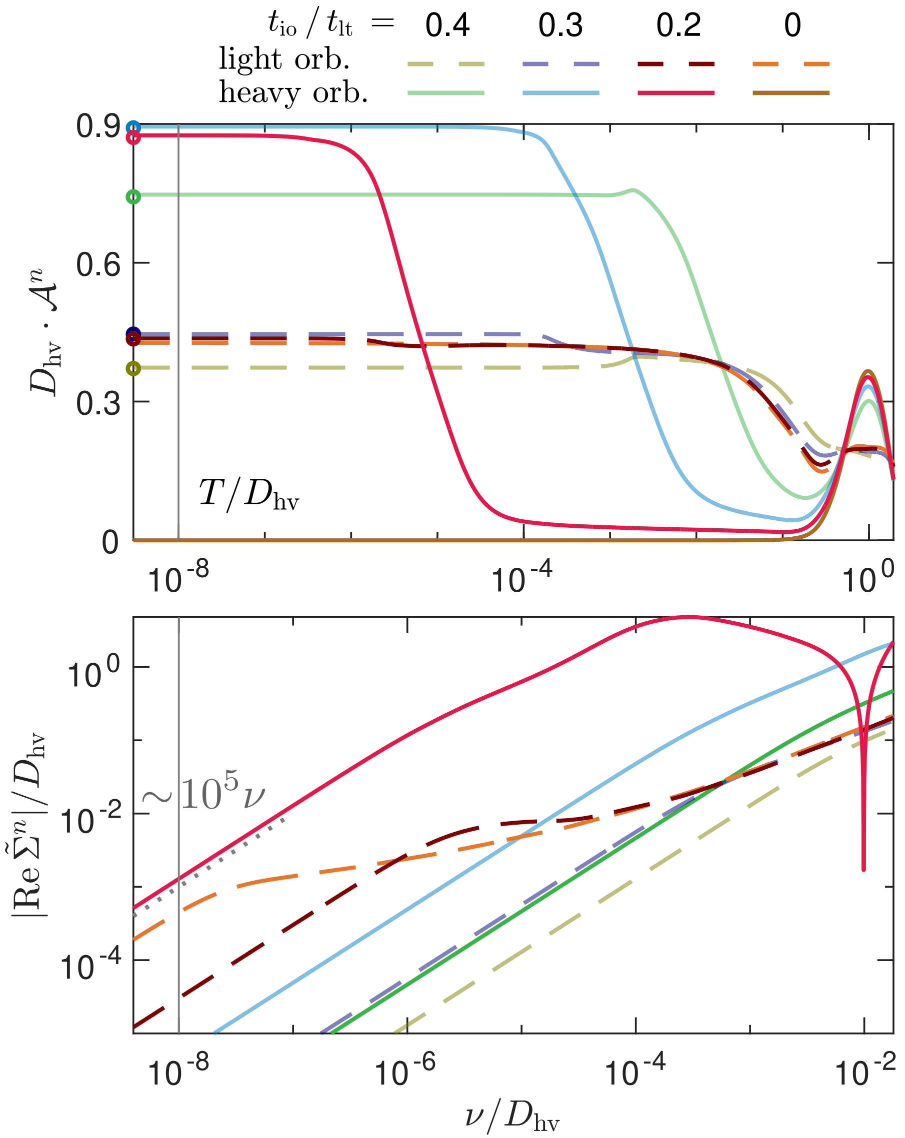

Kugler, Kotliar, PRL 2022

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Huang et al., Comm. Phys. 2022

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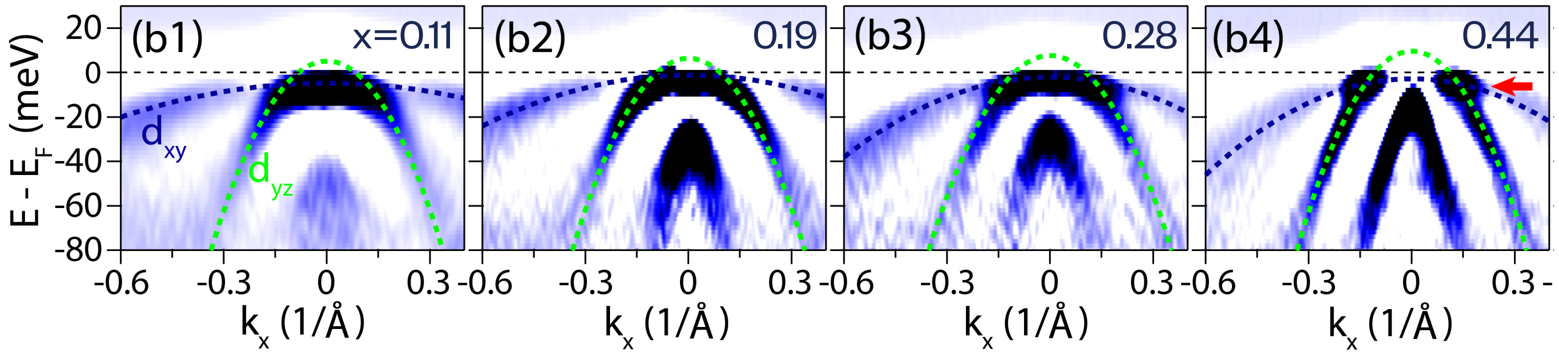
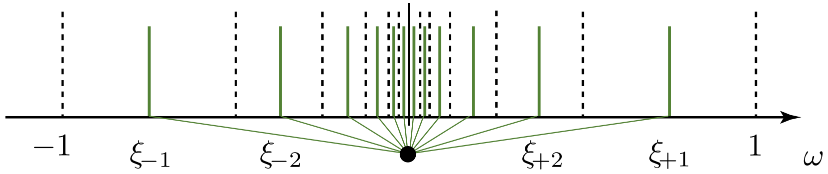


Conclusion

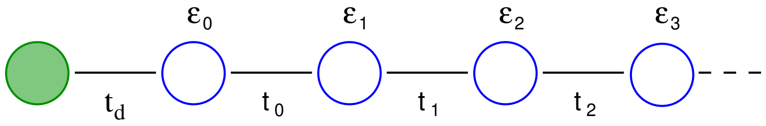
3 steps of Wilson's NRG: Wilson, RMP 1975

① logarithmic discretization



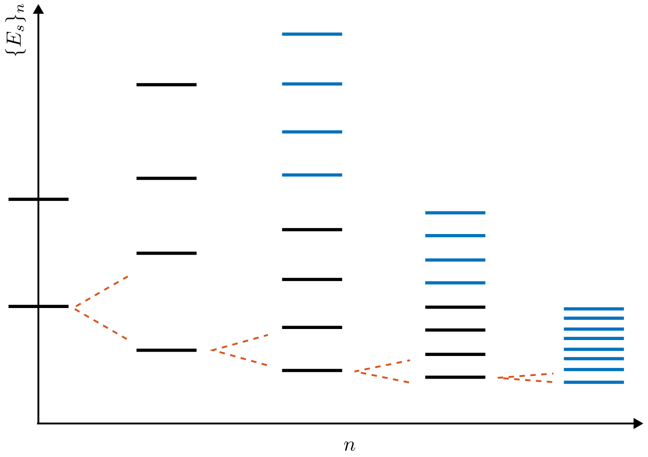
vD22

② mapping to Wilson chain



BCP08

③ iterative diagonalization



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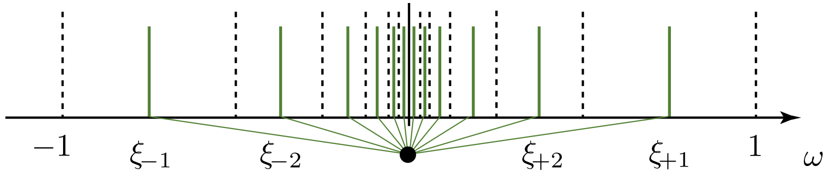

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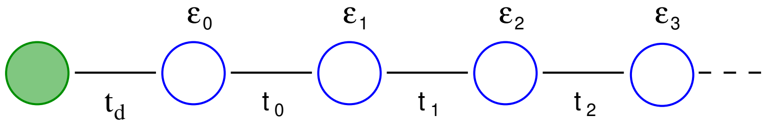

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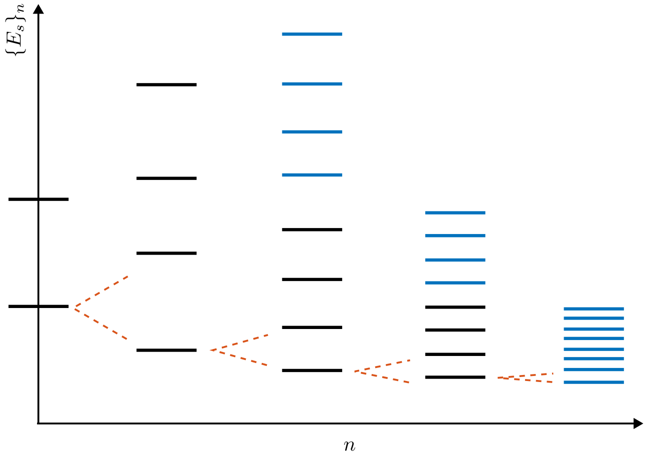

Modern developments:

- Complete basis of approximate eigenstates for sum-rule conversing spectral functions
- Increased resolution through z-averaging, adaptive broadening, improved estimators

Weichselbaum, von Delft, PRL 2008
Žitko, Pruschke, PRB 2009
Lee, Weichselbaum, PRB 2016
Kugler, PRB 2022

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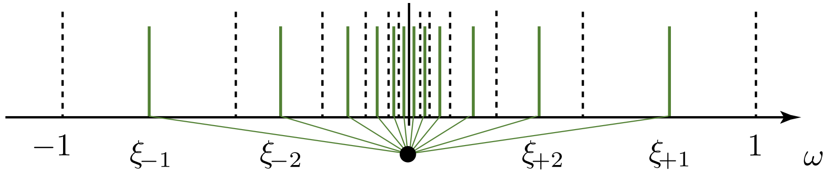

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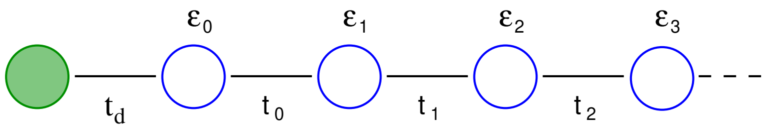

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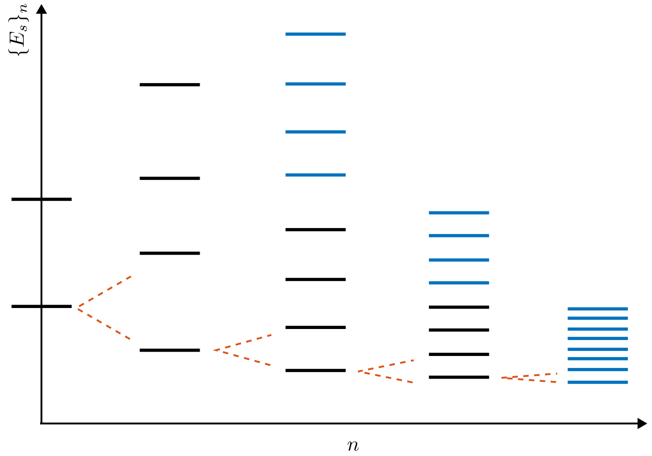

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⊕ Real-frequency, any temperature

⊕ Fine low-energy resolution

⊖ Coarse high-energy resolution

⊖ Full diagonalization requires symmetries
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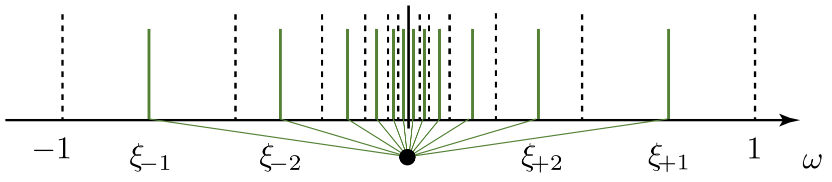

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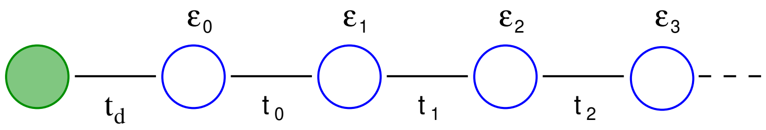

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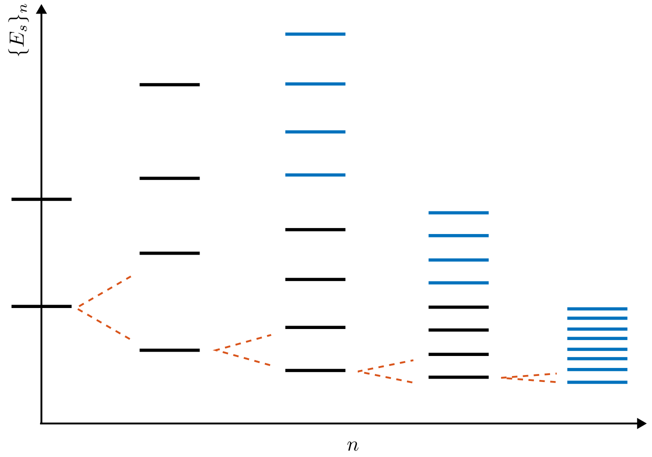

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Current frontiers:

- Ab-initio multi-orbital systems
- Multi-point correlation functions
  → real-freq. two-particle vertex

Kugler, Lee, von Delft, PRX 2021, Lee, Kugler, von Delft, PRX 2021, Lihm, ..., Kugler, Lee, PRB 2024