The Physics of Quantum Impurity Models

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Introduction

Single-impurity Anderson model: local moment formation

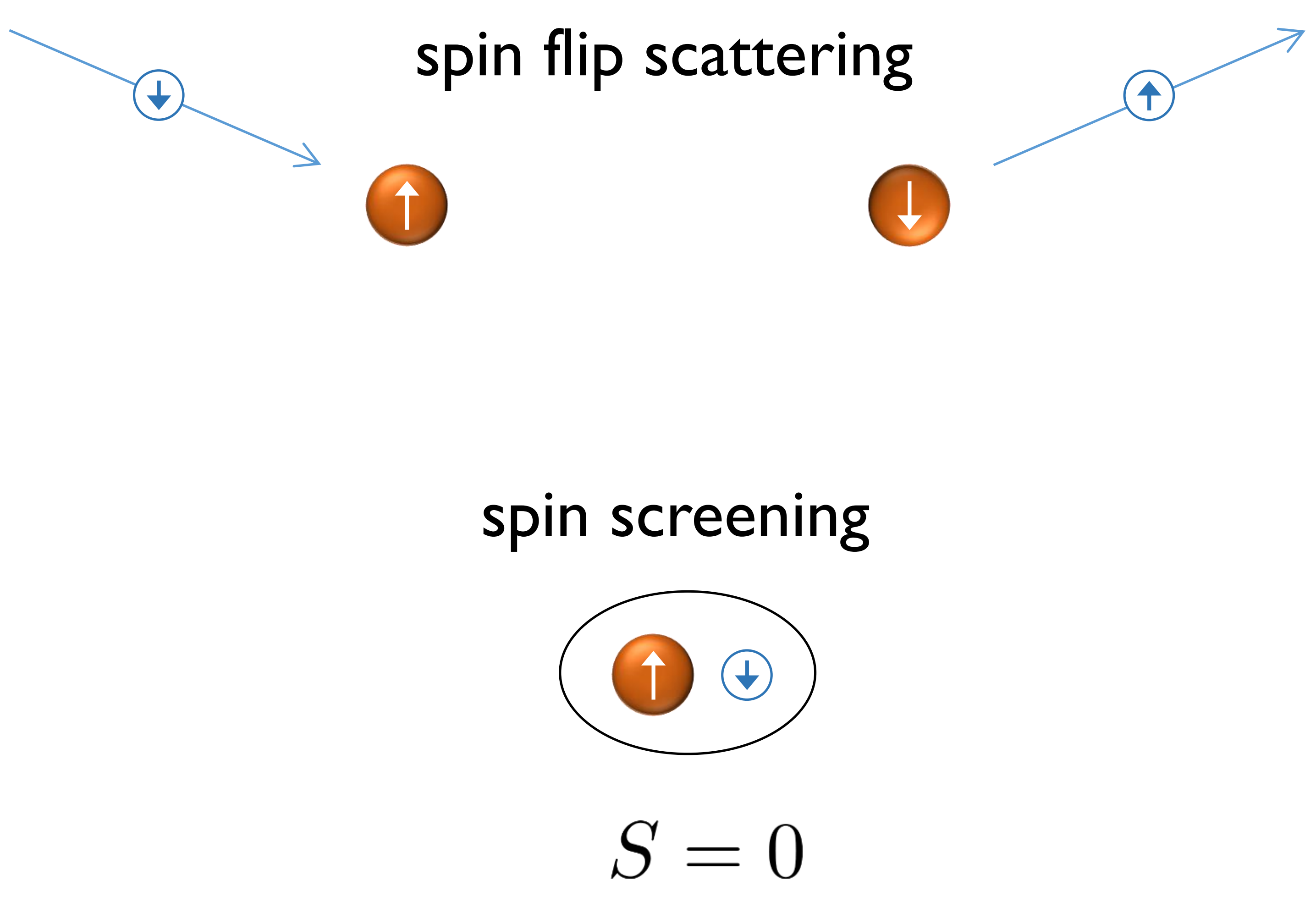
Kondo model: spin exchange interaction

Numerical renormalization group

NRG results for the single-impurity Anderson model

Two-channel Kondo model

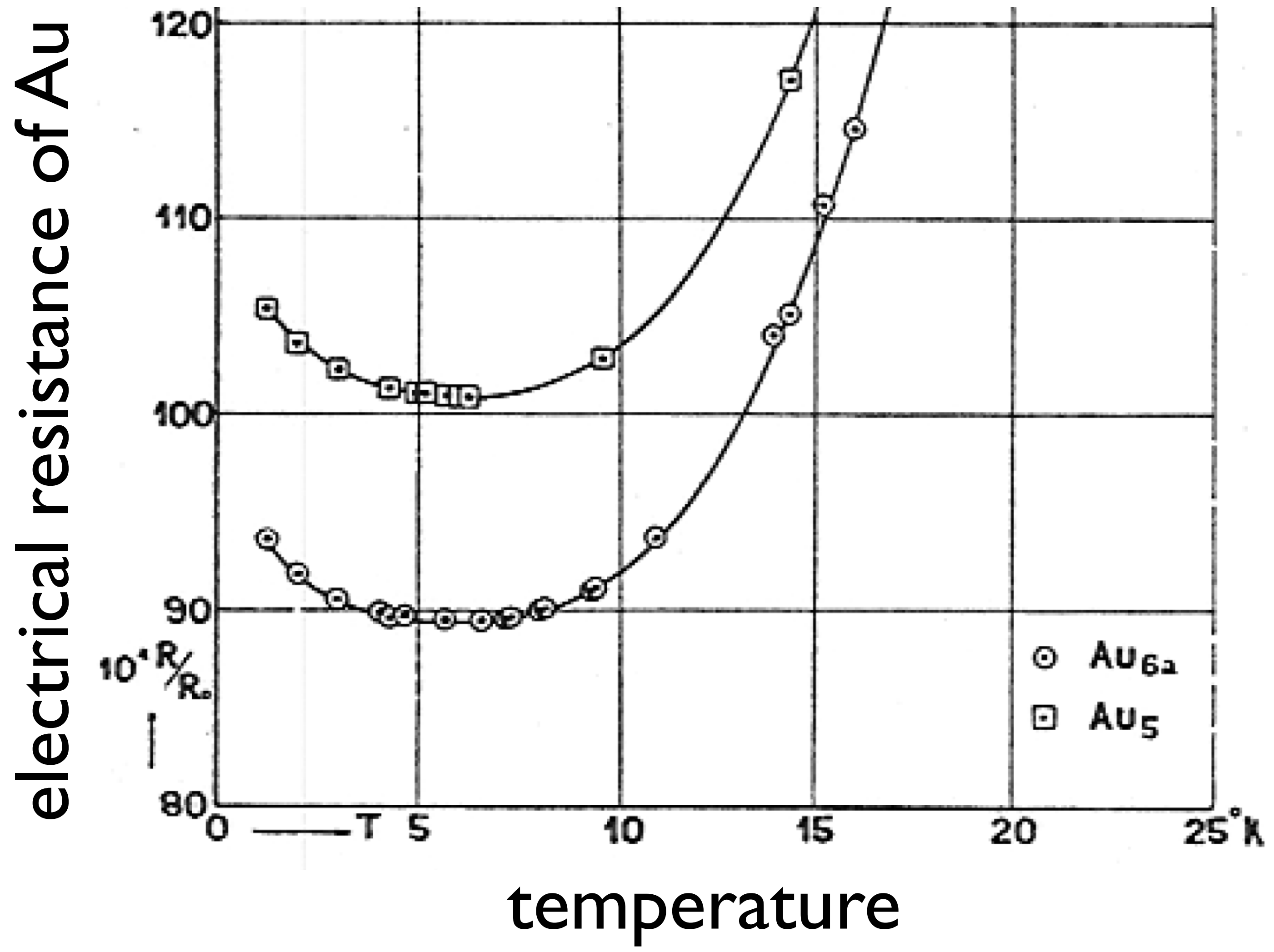
(DMFT+NRG application: Hund metals)



Introduction

1934: Resistance of magnetic alloys shows a minimum at low temperatures

de Haas, de Boer, van den Berg, Physica (1934)



1964: Kondo explains resistance anomaly:

Kondo, *Prog. Th. Phys.* (1964)

Kondo model: $H_{\text{Kondo}} = \sum_{ks} \varepsilon_k c^\dagger_{ks} c_{ks} + J \mathbf{S}_d \cdot \mathbf{s}_c,$ $\quad \mathbf{s}_c = \sum_{ks,k's'} c^\dagger_{ks} \tfrac{1}{2} \boldsymbol{\sigma}_{ss'} c_{k's'}$

spin flip scattering

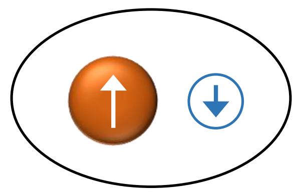
spin-flip scattering leads to scattering rate which increases with decreasing temperature

$$T \searrow: \quad \gamma(T) \nearrow, \quad \rho(T) \nearrow$$

Kondo problem: perturbative result for scattering rate diverges logarithmically $\gamma(T) \sim J + \underbrace{\nu}_{\text{density of states per spin}} J^2 \log(\underbrace{D}_{\text{high-energy cutoff}}/T)$

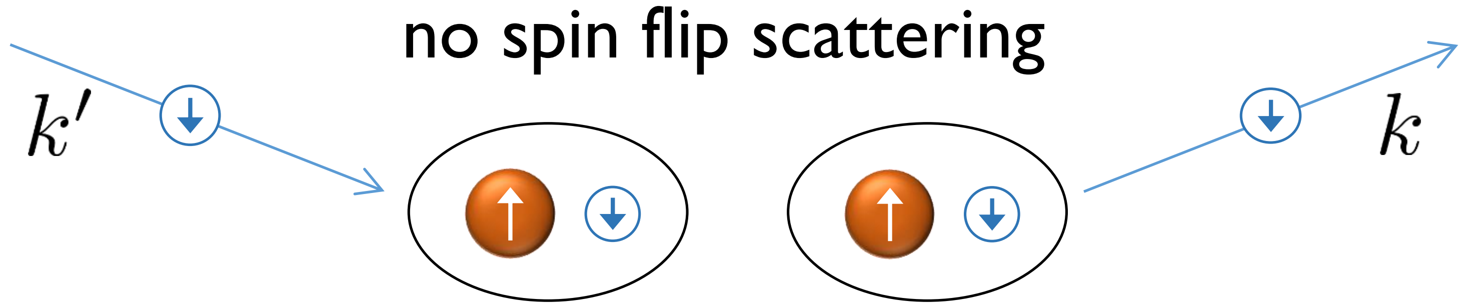
Kondo effect: for $T \to 0$, local spin is screened into spin singlet:

spin screening



$S = 0$

no spin flip scattering



1975: Wilson develops RG treatment of flow from weak to strong coupling

Wilson, *RMP* (1975)

Single-impurity Anderson model (SIAM): local moment formation

Anderson, *Phys. Rev.* (1961)

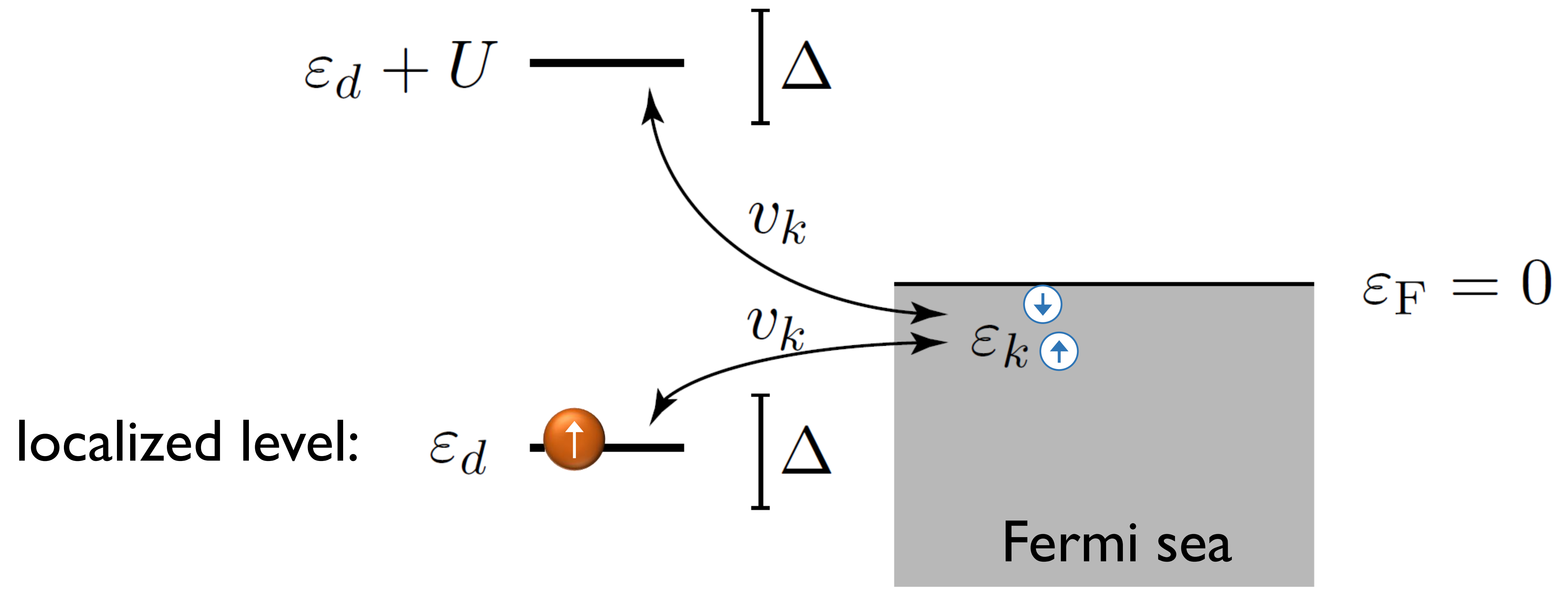
How can a stable local moment arise in a metal?

$$H_{\mathrm{SIAM}} = H_{\mathrm{bath}} + H_{\mathrm{loc}} + H_{\mathrm{hyb}}$$

$$H_{\mathrm{bath}} = \sum_{ks} \varepsilon_k \hat{n}_{ks} \,, \qquad \hat{n}_{ks} = c^\dagger_{ks} c_{ks}$$

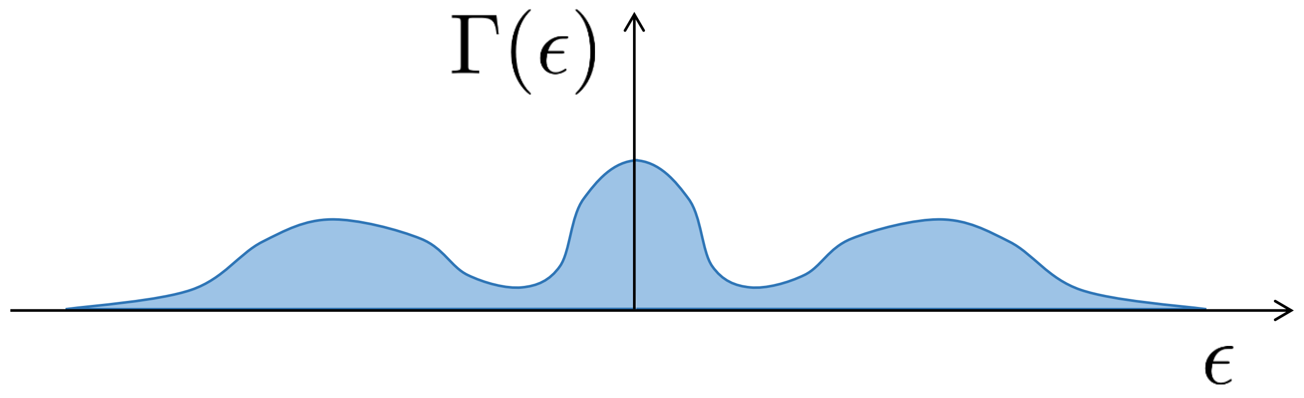
$$H_{\mathrm{loc}} = \sum_{s} (\varepsilon_d - \tfrac{1}{2} h s) \hat{n}_{ds} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \,, \qquad \hat{n}_{ds} = d^\dagger_s d_s$$

$$H_{\mathrm{hyb}} = \sum_{ks} v_k (c^\dagger_{ks} d_s + d^\dagger_s c_{ks})$$



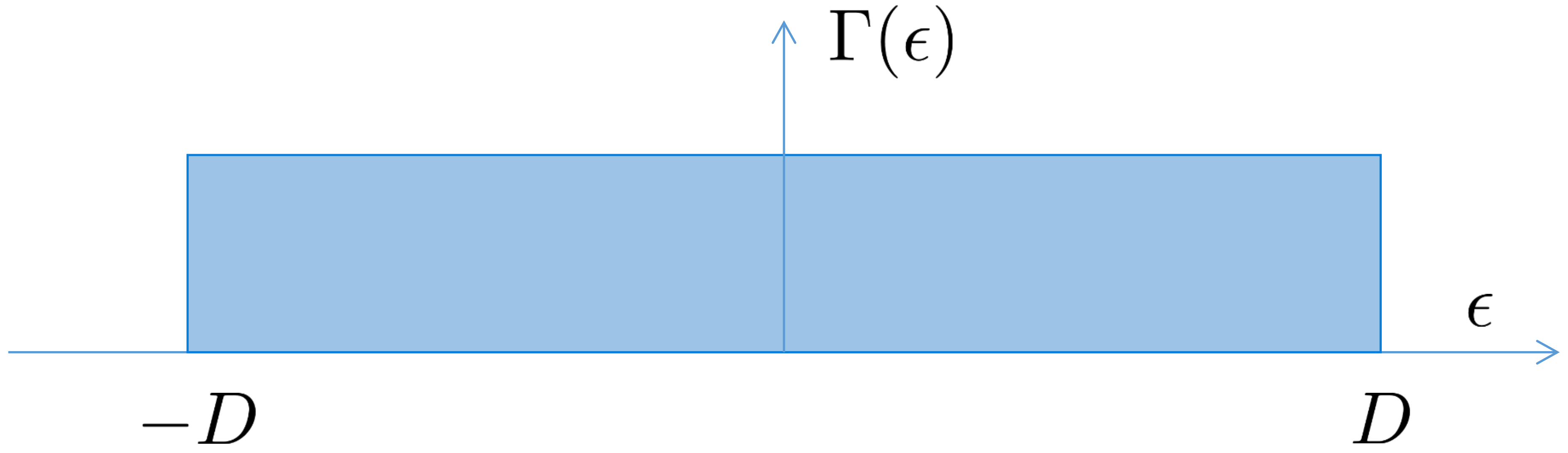
Hybridization function: $\Delta(\omega) = \sum_k \frac{v_k^2}{\omega - \varepsilon_k + \mathrm{i}0^+}$ (fully describes effect of bath parameters on *d*-level dynamics)

Spectral representation: $= \int \mathrm{d}\epsilon \frac{\Gamma(\epsilon)}{\omega - \epsilon + \mathrm{i}0^+}$



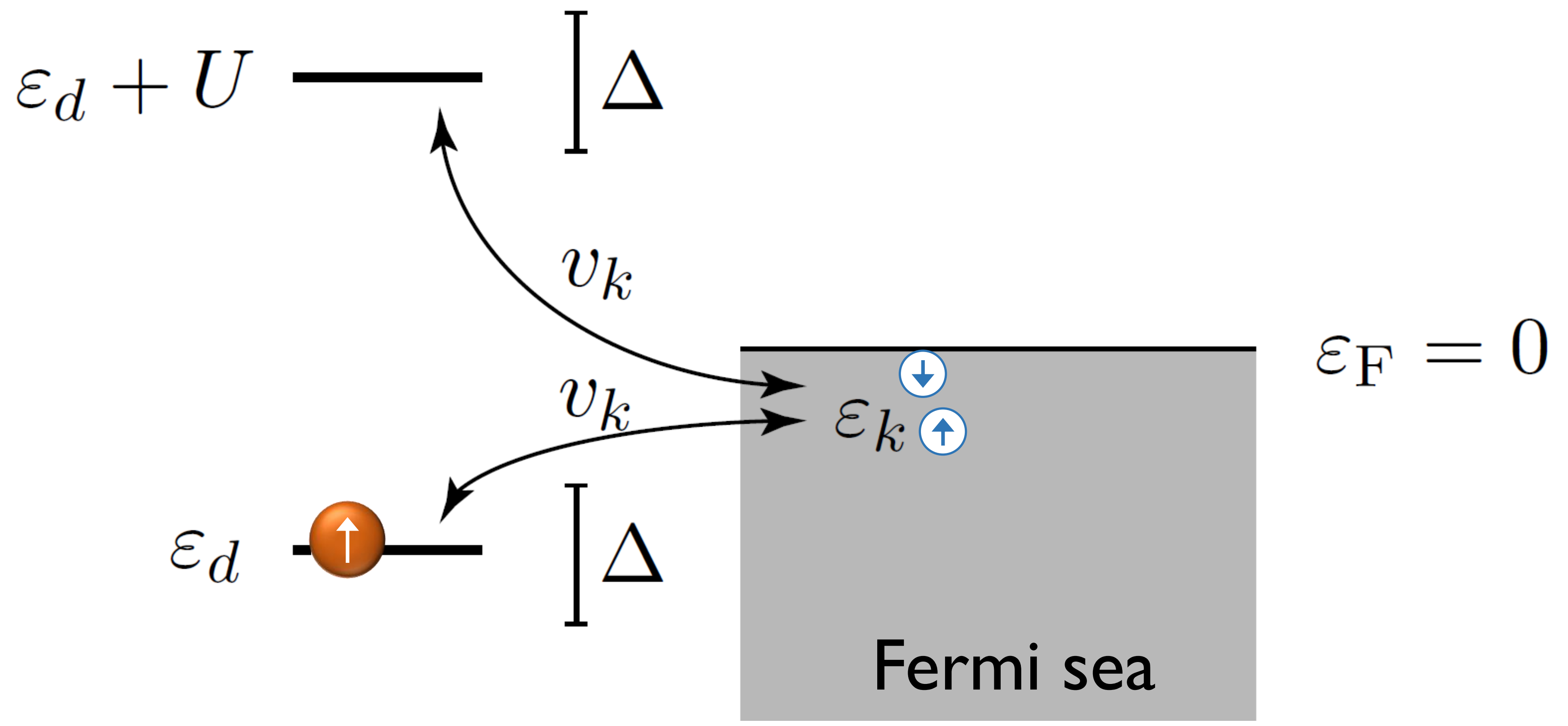
Hybridization spectrum: $\Gamma(\epsilon) = \sum_k |v_k|^2 \delta(\epsilon - \varepsilon_k)$

For simplicity, assume box-shaped spectrum: $\Gamma(\epsilon) = (\Delta/\pi)\, \Theta(D - |\epsilon|) \,, \qquad \Delta/\pi = v^2 \nu$



Single-impurity Anderson model (SIAM): local moment formation

Anderson, *Phys. Rev.* (1961)



Local state space:		Energy:
empty:	$\|0\rangle$	$E_0 = 0$
singly-occupied:	$\|\uparrow\rangle, \|\downarrow\rangle$	$E_s: \quad E_\uparrow = \varepsilon_d - \frac{1}{2}h, \quad E_\downarrow = \varepsilon_d + \frac{1}{2}h,$
doubly occupied:	$\|\uparrow\downarrow\rangle$	$E_{\uparrow\downarrow} = 2\varepsilon_d + U$

Condition for single occupancy: $\quad E_0 - E_s > \Delta, \qquad E_{\uparrow\downarrow} - E_s > \Delta$

$$\varepsilon_d + \Delta < 0, \qquad \varepsilon_d + U > \Delta$$

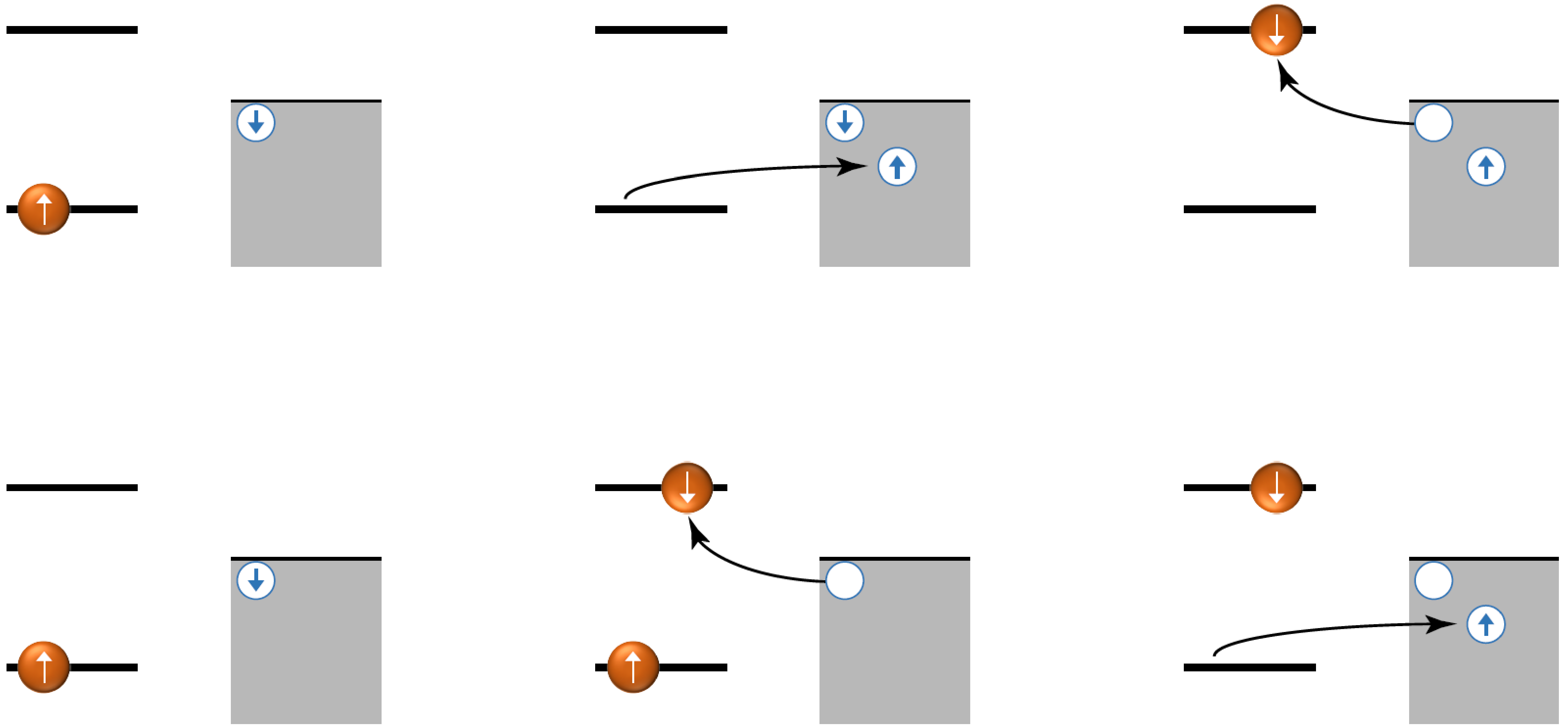
local moment regime

Spin-flip transitions occur via second-order hopping:

$$J = -\frac{v^2}{\varepsilon_d} + \frac{v^2}{\varepsilon_d + U}$$

$$= -\frac{Uv^2}{\varepsilon_d(\varepsilon_d + U)} = -\frac{2U\Delta}{\pi\varepsilon_d(\varepsilon_d + U)} \qquad > 0 \quad \text{if} \quad \varepsilon_d < 0$$

= effective exchange coupling constant of Kondo model



From Anderson to Kondo model: Schrieffer-Wolff transformation

Schrieffer, Wolff, *Phys. Rev.* (1966)

Project to subspace with $n_d = 1$ $\quad \cancel{|0\rangle}, |\uparrow\rangle, |\downarrow\rangle, \cancel{|\uparrow\downarrow\rangle}$

Starting point: $$H_{\rm SIAM} = \underbrace{H_{\rm bath} + H_{\rm loc}}_{H_0 \sim \mathcal{O}(v^0)} + \underbrace{H_{\rm hyb}}_{H_1 \sim \mathcal{O}(v^1)}$$

Goal: find unitary transformation, such that $\widetilde{H} = e^{A} H_{\rm SIAM} e^{-A}$, with $A = -A^\dagger \sim \mathcal{O}(v^1) + \mathcal{O}(v^2) + \ldots$

contains no terms $\mathcal{O}(v^1)$

should cancel

Expanding $\widetilde{H}$ in powers of v, one obtains $$\widetilde{H} = (H_0 + H_1) + [A, H_0 + H_1] + \tfrac{1}{2}[A, [A, H_0 + \cancel{H_1}]] + \mathcal{O}(v^3)$$

Choose A such that $H_1 = -[A, H_0]$, then $\widetilde{H} = H_0 + \tfrac{1}{2}[A, H_1] + \mathcal{O}(v^3)$

$$A = \sum_{ks} v \left[\frac{1}{\varepsilon_k - \varepsilon_d} c^\dagger_{ks} d_s + \frac{U}{(\varepsilon_d - \varepsilon_k)(\varepsilon_d + U - \varepsilon_k)} d^\dagger_{-s} d_{-s} c^\dagger_{ks} d_s \right] - \text{h.c.}$$

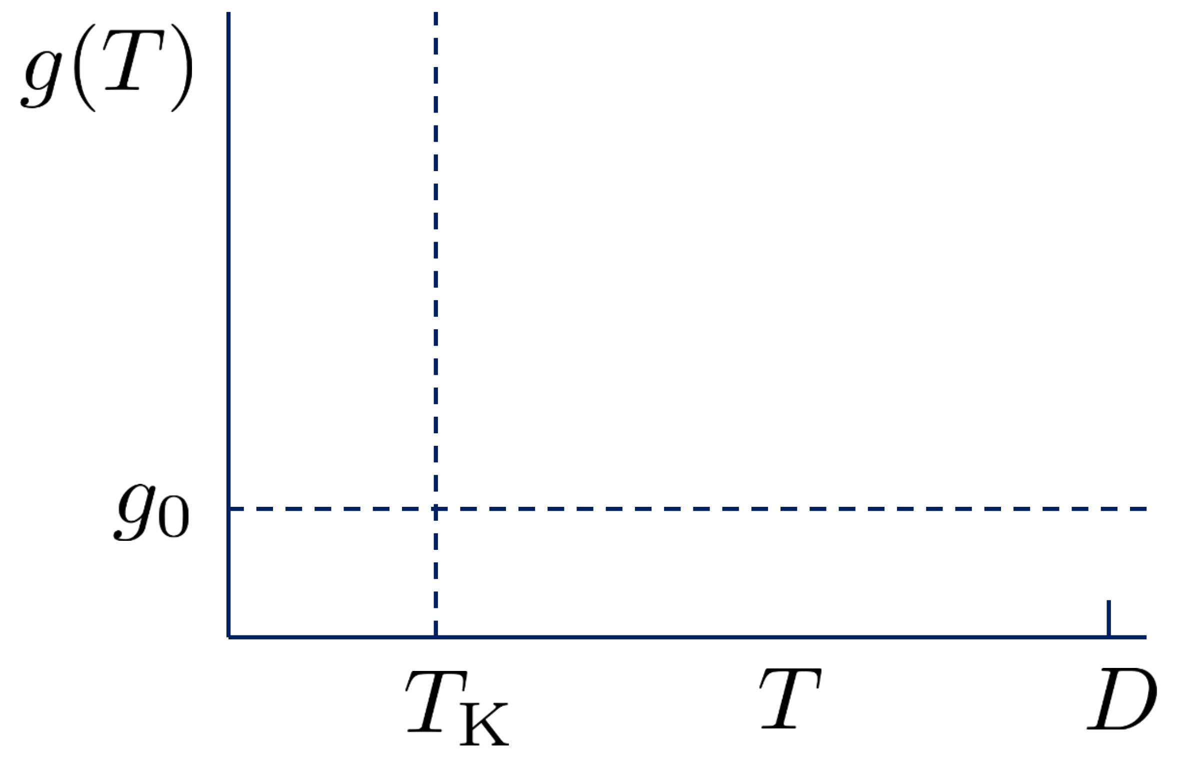
$$\widetilde{H}_{n_d=1} = \sum_{ks} \varepsilon_k \hat{n}_{ks} + \sum_{kk'} \widetilde{v}_{kk'} \mathbf{S}_d \cdot c^\dagger_{ks} \tfrac{1}{2} \boldsymbol{\sigma}_{ss'} c_{k's'} + \ldots, \qquad \widetilde{v}_{kk'} = \frac{-\frac{1}{2} v^2 U}{(\varepsilon_d - \varepsilon_k)(\varepsilon_d + U - \varepsilon_k)} + (k \leftrightarrow k')$$

Low-energy limit: $\simeq H_{\rm Kondo}$ $$\simeq -\frac{v^2 U}{\varepsilon_d(\varepsilon_d + U)} = J, \qquad \forall\, |\varepsilon_k|, |\varepsilon_{k'}| \ll |\varepsilon_d|, |\varepsilon_d + U|$$

Kondo model: effective coupling constant

$$H_{\text{Kondo}} = \sum_{ks} \varepsilon_k c^\dagger_{ks} c_{ks} + J\mathbf{S}_d \cdot \mathbf{s}_c, \qquad \mathbf{s}_c = \sum_{ks,k's'} c^\dagger_{ks} \tfrac{1}{2} \boldsymbol{\sigma}_{ss'} c_{k's'}$$

Anderson, *J. Phys. C* (1970)



Perturbative result for scattering rate: $\gamma(T) \sim J + \nu J^2 \log(D/T)$

Effective dimensionless coupling: $g(T) = \dfrac{1}{1/g_0 - \ln(D/T)}, \qquad g_0 = \nu J$

Kondo temperature: $g(T_{\text{K}}) = \infty \quad \Rightarrow \quad 1/g_0 = \ln(D/T_{\text{K}})$

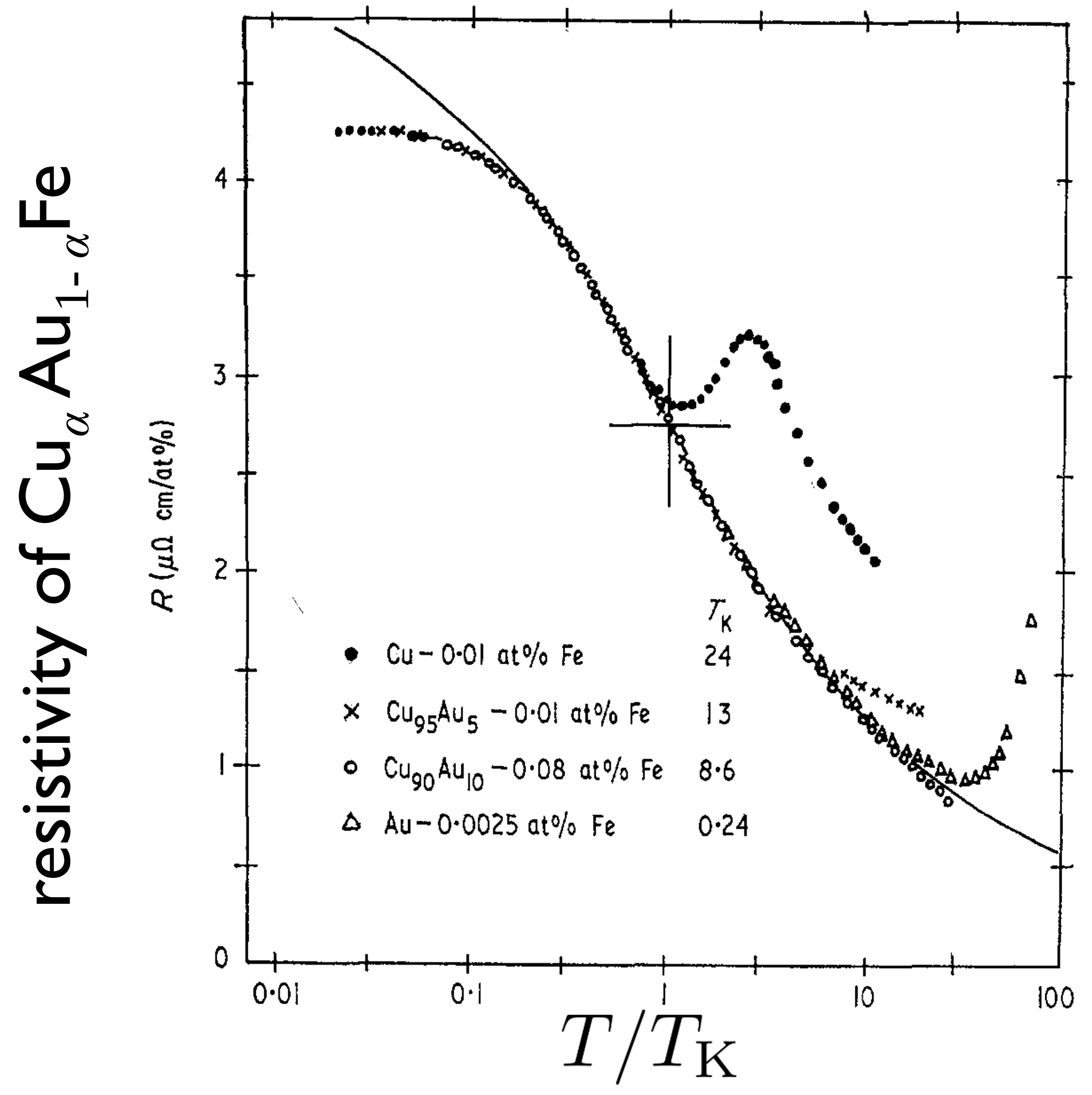
$\Rightarrow \quad T_{\text{K}} = De^{-1/(J\nu)}$ exponentially small

Universality: $g(T) = \dfrac{1}{\ln(D/T_{\text{K}}) - \ln(D/T)} = \dfrac{1}{\ln(T/T_{\text{K}})}$

Physical quantities depend on temperature only via the ratio T/T_{K}

For example, resistivity $\rho = \rho(T/T_{\text{K}})$, spin susceptibility $\chi = \chi(T/T_{\text{K}})$

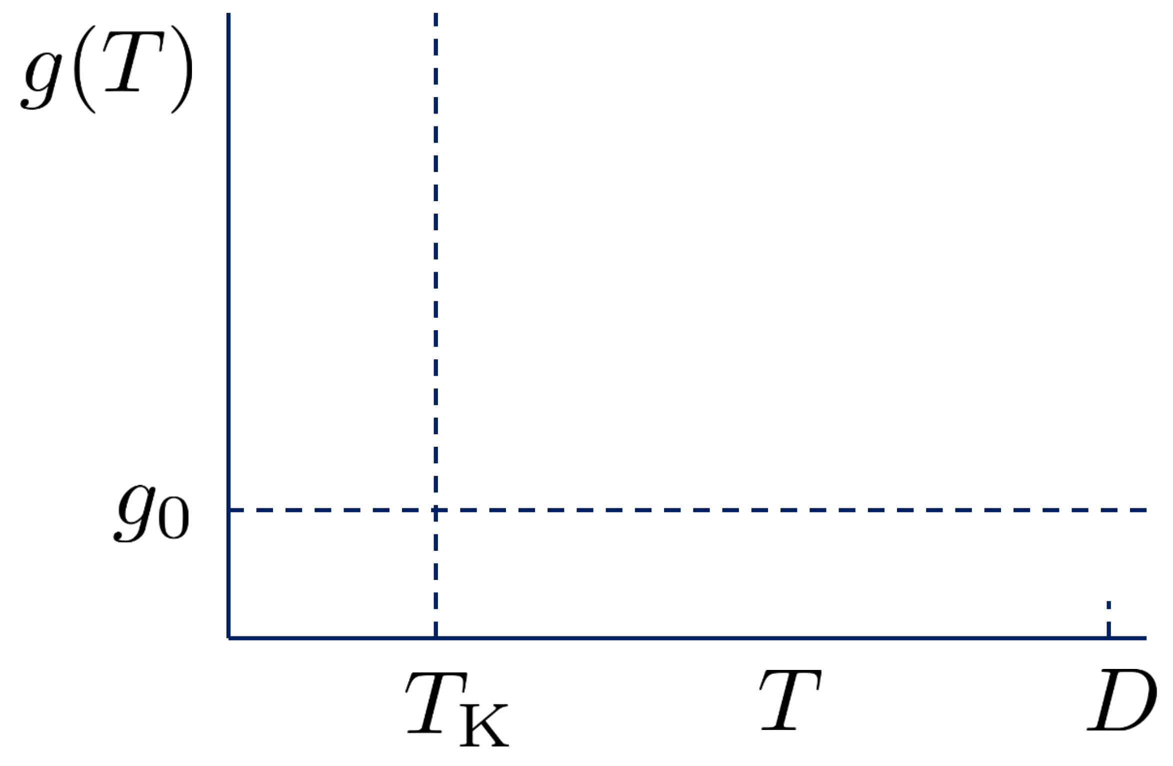
Grüner, Zawadowski, *Rep. Prog. Phys* (1974)



Kondo model: spin screening

Anderson, *J. Phys. C* (1970)

Effective dimensionless coupling: $g(T) = \dfrac{1}{1/g_0 - \ln(D/T)}$, $\quad g_0 = \nu J$

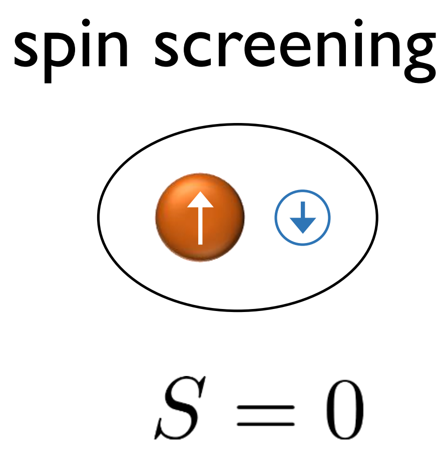


Perturbative treatment breaks down for $T < T_{\mathrm{K}}$. What really happens for $T \to 0$?

Ground state is a spin singlet, with total spin $S_{\mathrm{tot}} = 0$

Spin screening: cloud of conduction electrons with a net spin $s_c = \frac{1}{2}$, the so-called Kondo cloud, screens local spin to form singlet.

Cartoons depictions of singlet:



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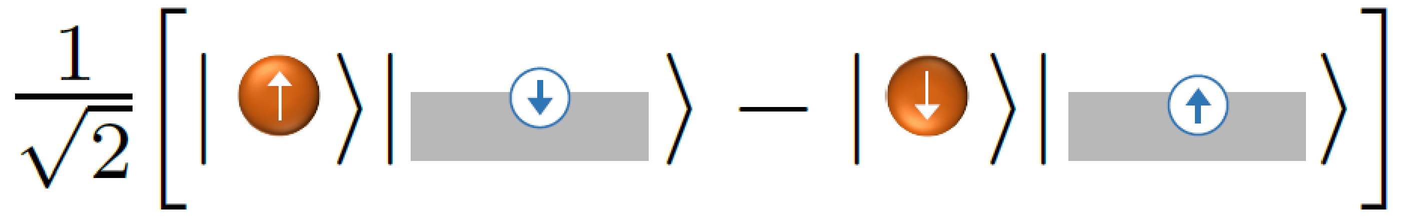

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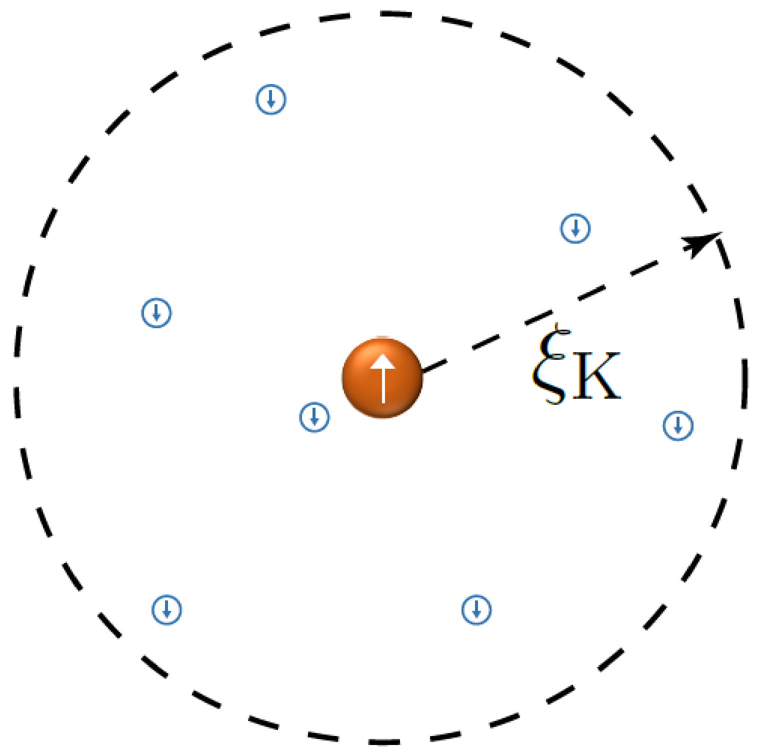
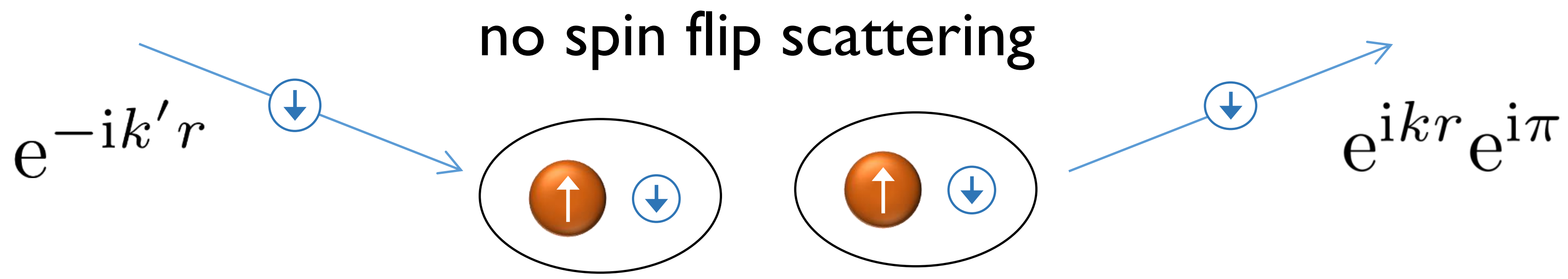


$\xi \sim 1/T_{\mathrm{K}}$

local moment regime: $T \gg T_{\mathrm{K}}$



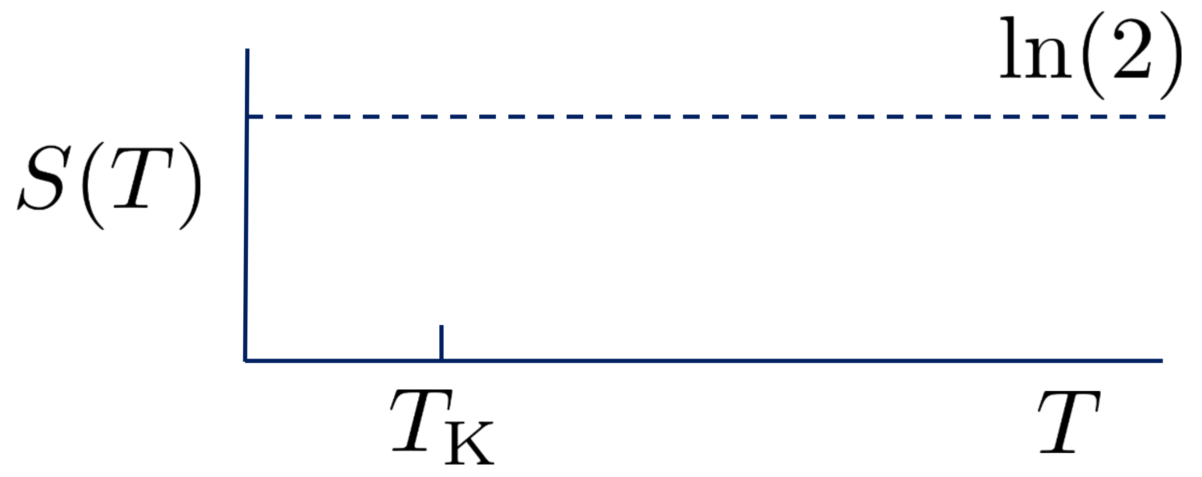
phase shift of π

strong-coupling regime: $T \ll T_{\mathrm{K}}$

Physical consequences of spin screening

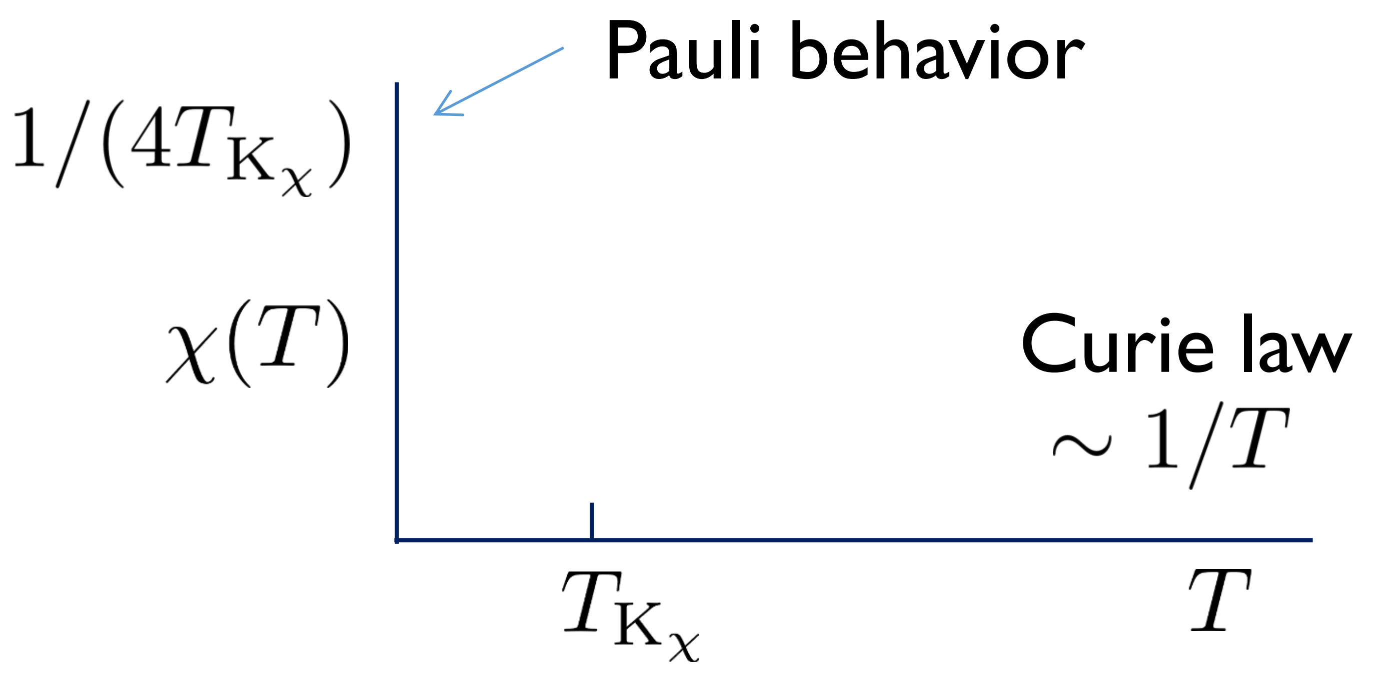
Wilson, *RMP* (1975)

Impurity entropy: $S(T) \simeq \begin{cases} \ln(2)\,, & T \gg T_{\rm K} \quad \text{degenerate doublet} \\ \ln(1) = 0\,, & T \ll T_{\rm K} \quad \text{non-degenerate singlet} \end{cases}$



Static impurity spin susceptibility: $\chi(T) = \left.\dfrac{d\langle S_d^z(h)\rangle_T}{dh}\right|_{h=0} \simeq \dfrac{1}{4\,(T + T_{\mathrm{K}_\chi})}$ Curie-Weiss law

alternative definition of Kondo temperature $T_{\mathrm{K}_\chi} = \dfrac{1}{4\chi(0)}$

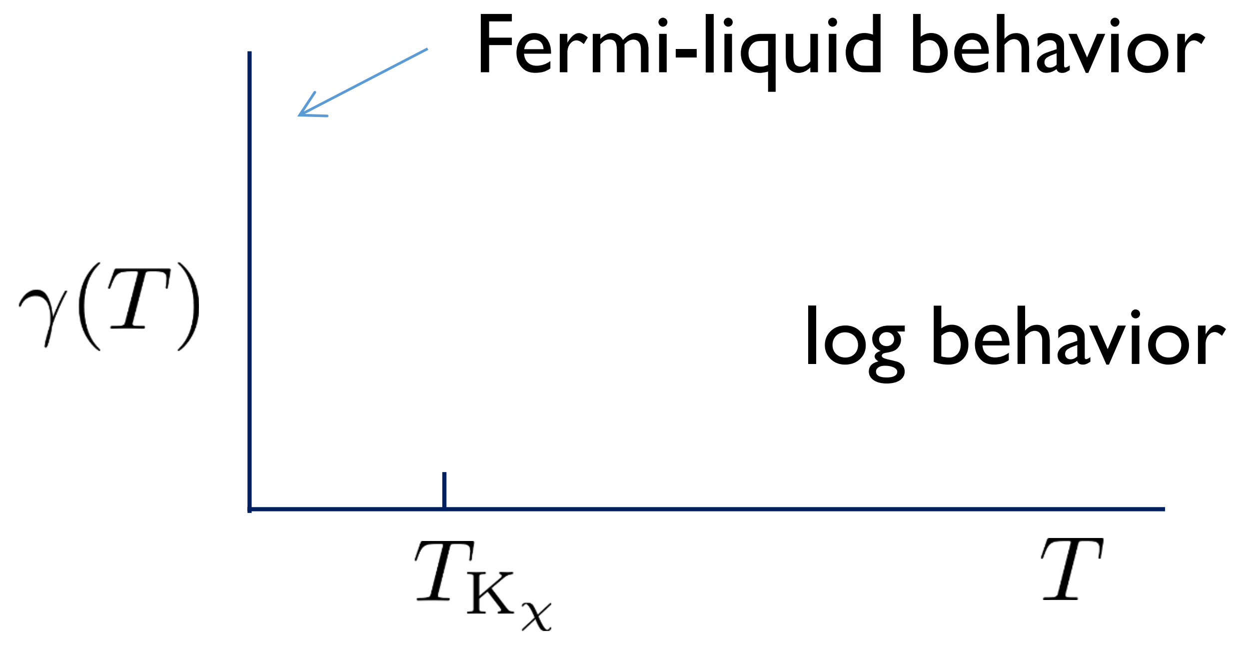


asymptotic behavior: $\chi(T) = \left.\dfrac{d\langle S_d^z(h)\rangle_T}{dh}\right|_{h=0} \simeq \begin{cases} \dfrac{1}{4T}\left[1 - \mathcal{O}[\ln(T/T_{\rm K})]\right], & T \gg T_{\rm K} \\ \chi(0)[1 - \mathcal{O}(T^2/T_{\rm K}^2)]\,, & T \ll T_{\rm K} \end{cases}$

Electron scattering rate:

$\gamma(T) \sim \dfrac{1}{\ln(T/T_{\rm K})}\,, \qquad T \gg T_{\rm K}$

$\gamma(T) = \gamma(0)\left[1 - \mathcal{O}(T/T_{\rm K})^2\right], \qquad T/T_{\rm K} \ll 1$

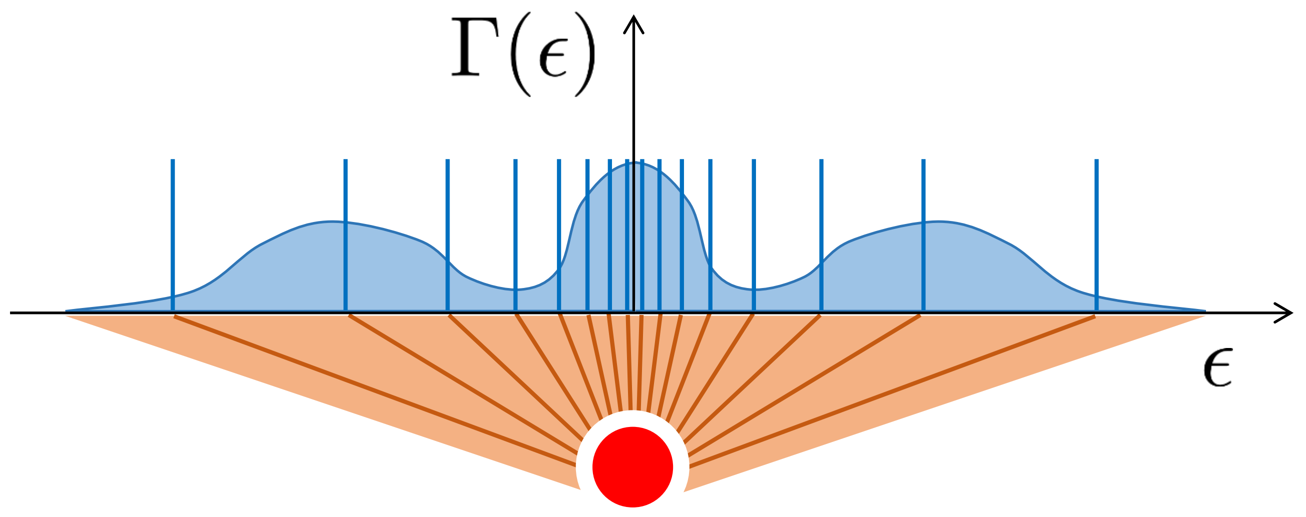


Universal prefactors in strong-coupling regime: $\dfrac{\chi(T)}{\chi(0)} - 1 = -0.821\dfrac{T^2}{T_{\mathrm{K}_\chi}^2}, \qquad \dfrac{\gamma(T)}{\gamma(0)} - 1 = -\dfrac{\pi^4}{16}\dfrac{T^2}{T_{\mathrm{K}_\chi}^2}, \qquad T/T_{\mathrm{K}_\chi} \ll 1$

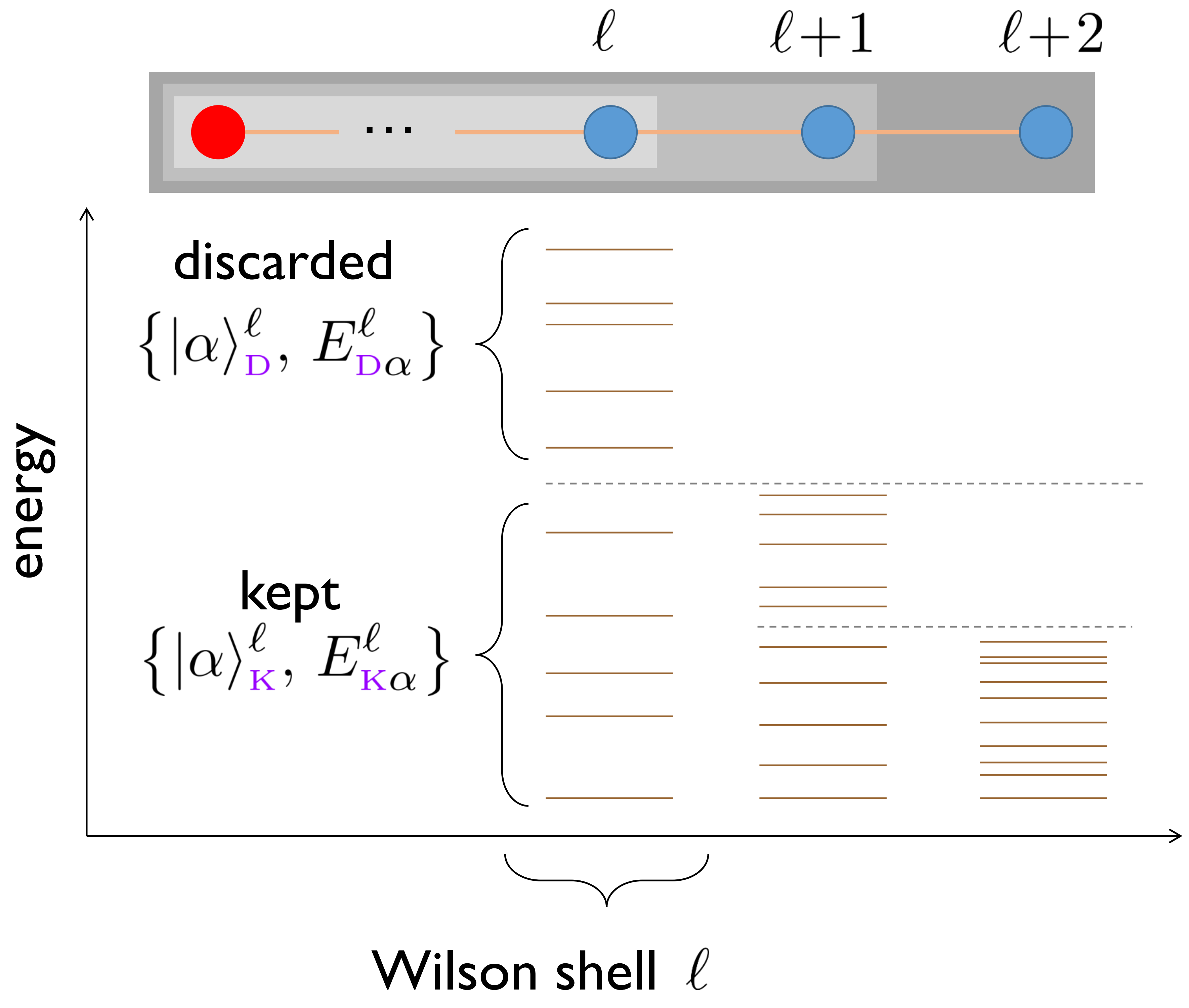
Numerical renormalization group (NRG): low-energy spectrum

Logarithmic discretization

Discretization grid
$\sim \Lambda^{-n} \quad (\Lambda > 1)$



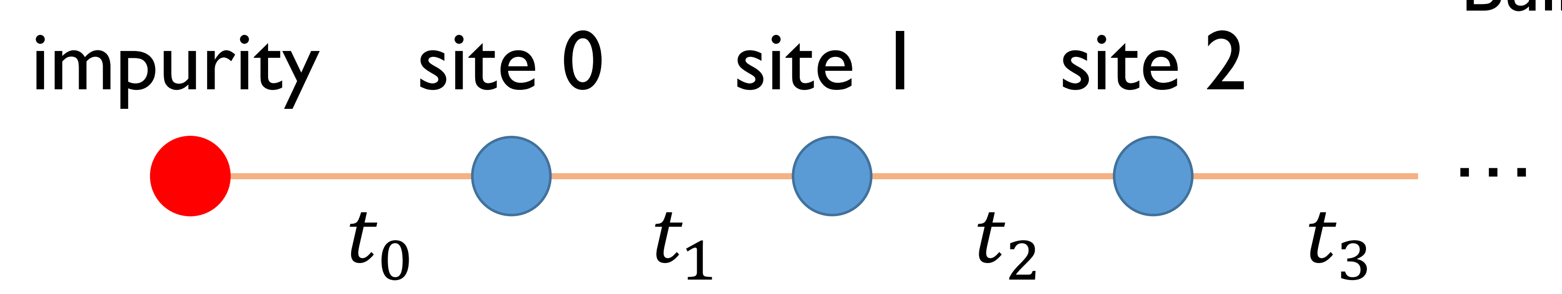
Iterative diagonalization



Iterative refinement of energy spectrum

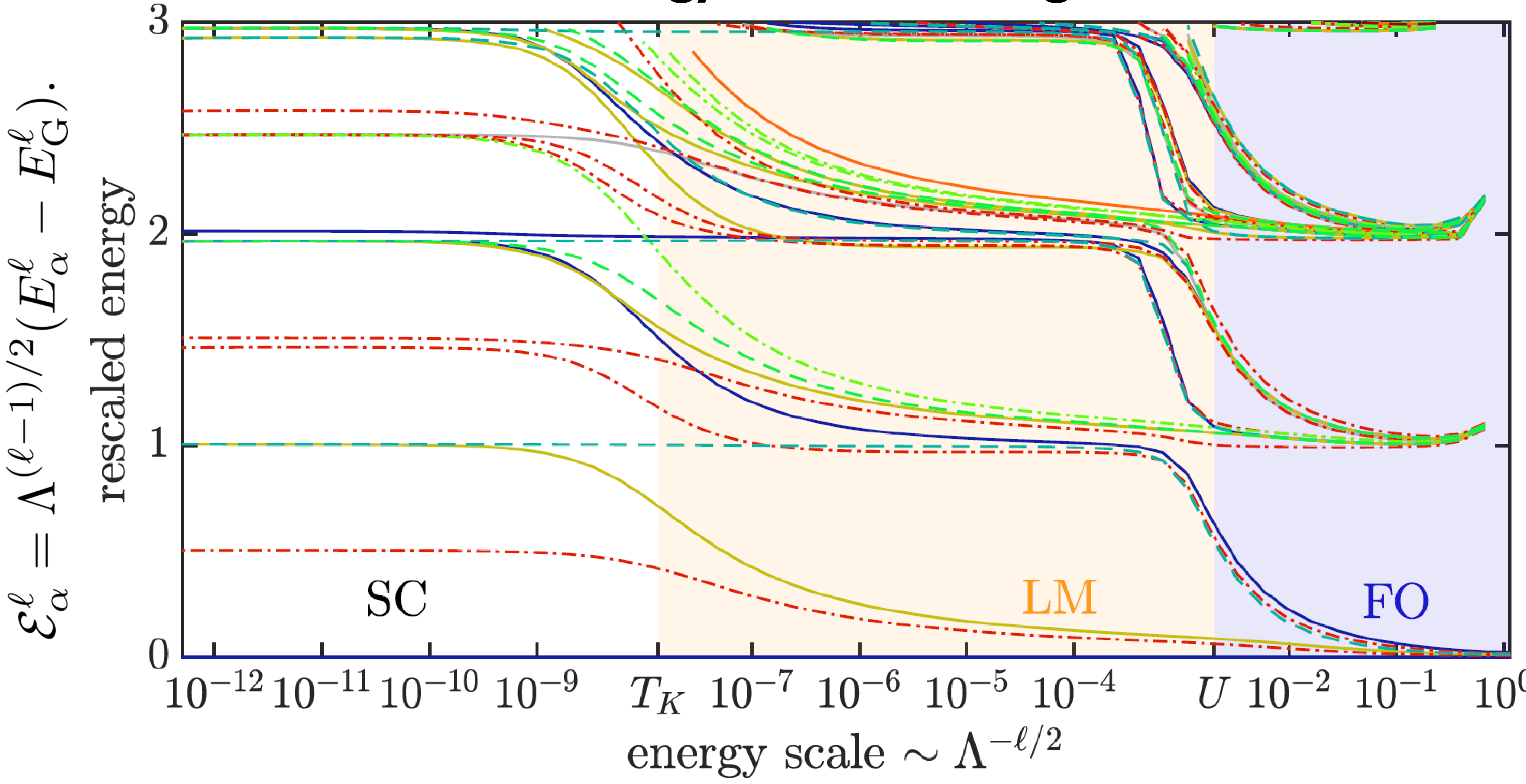
Wilson chain

Wilson, *RMP* (1975)
Bulla, Costi, Pruschke, *RMP* (2008)



energy scale separation
$t_\ell \sim \Lambda^{-\ell/2}$

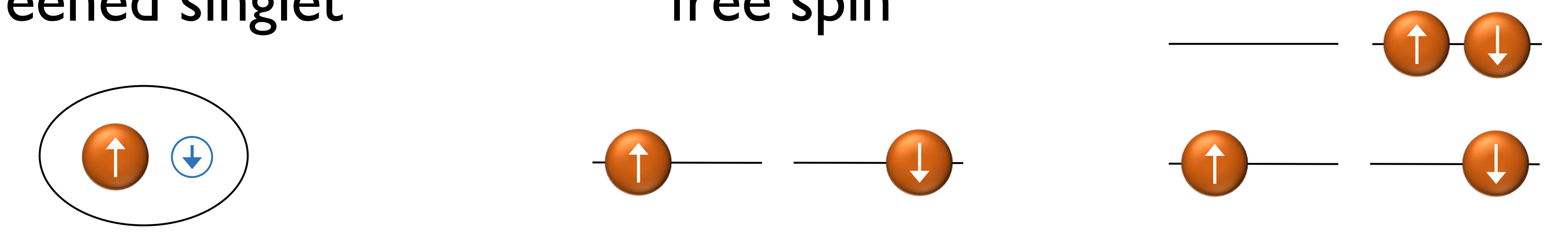
NRG energy-level flow diagram



Fermi liquid regime:
screened singlet

local moment regime:
free spin

free orbital
regime:

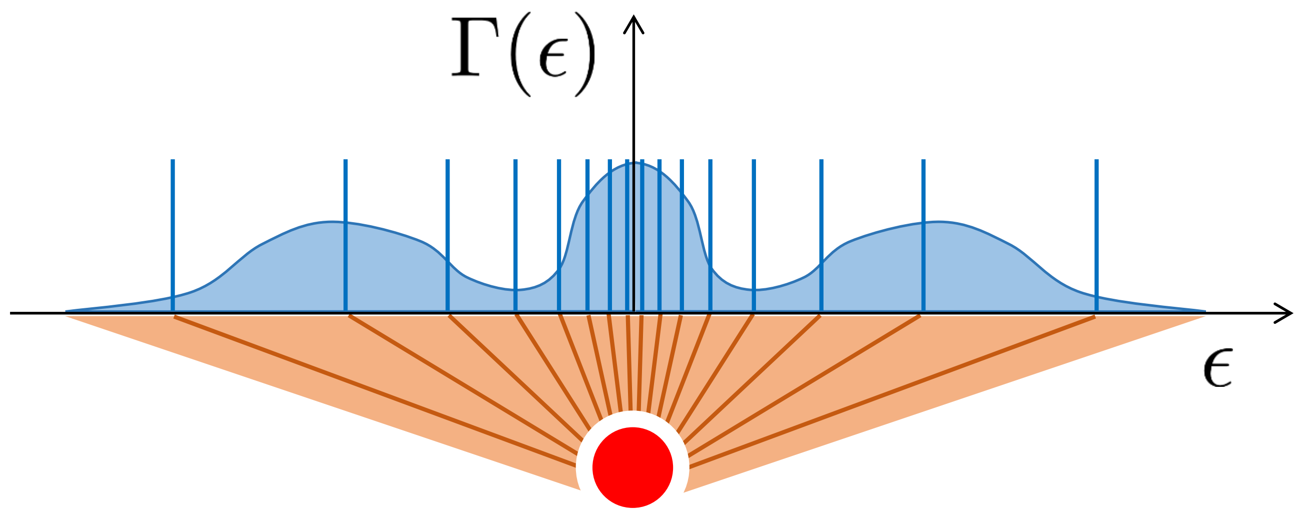


Detailed description of crossovers between fixed points

NRG: complete basis

Logarithmic discretization

Discretization grid
$\sim \Lambda^{-n} \quad (\Lambda > 1)$



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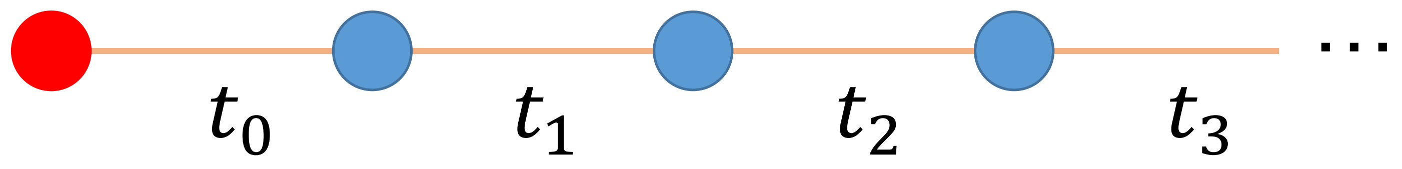

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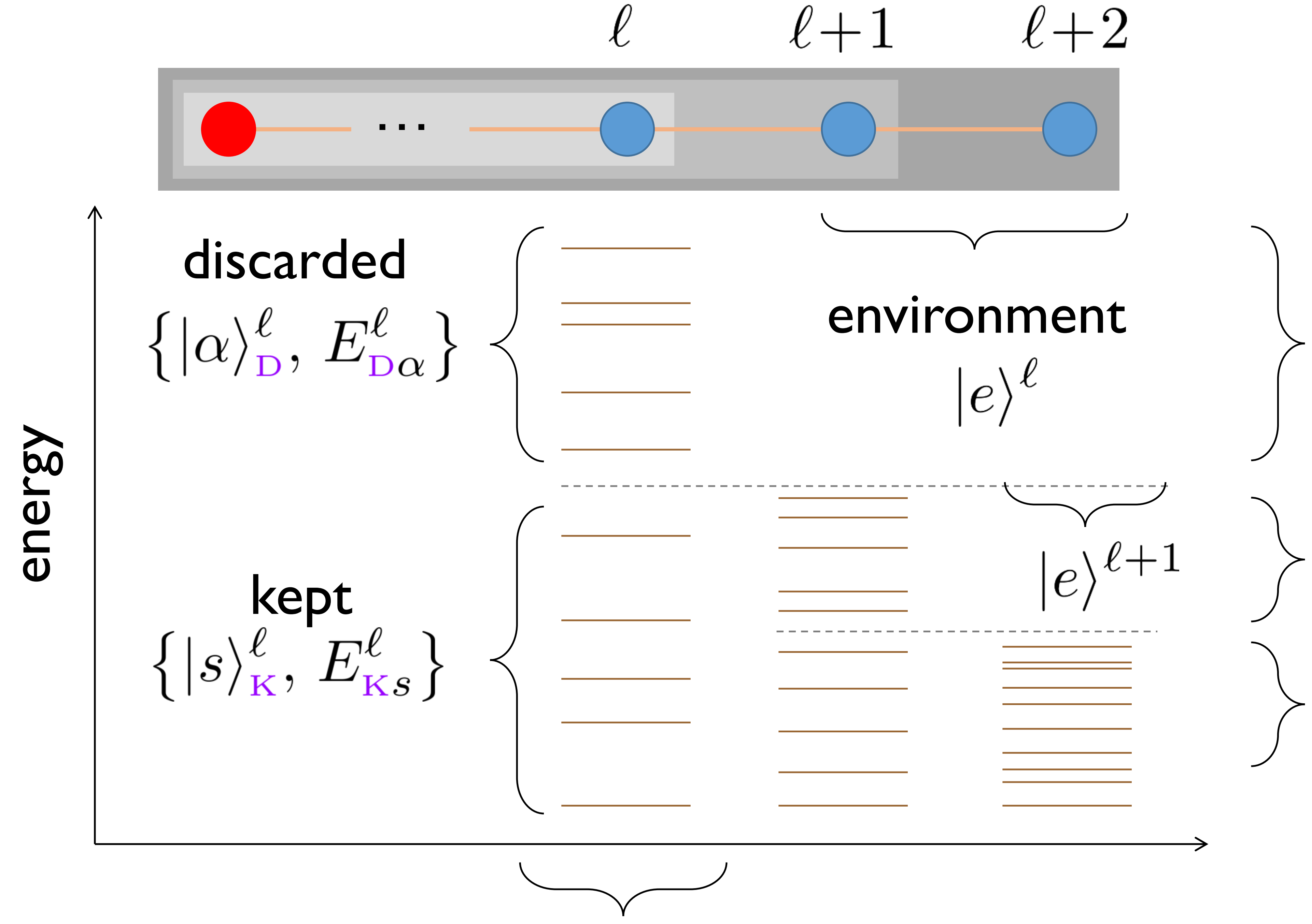
Iterative diagonalization



NRG approximation

$$\mathcal{H}|\alpha e\rangle^\ell_{\mathrm{X}} \approx E^\ell_{\mathrm{X}\alpha}|\alpha e\rangle^\ell_{\mathrm{X}},$$

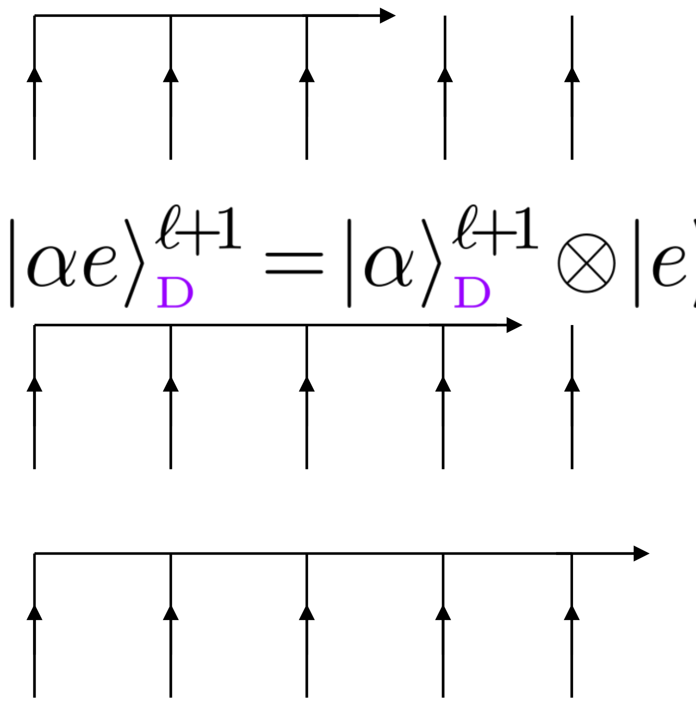
$$|\alpha e\rangle^\ell_{\mathrm{X}} = |\alpha\rangle^\ell_{\mathrm{X}} \otimes |e\rangle^\ell, \qquad \mathrm{X} = \mathrm{K}, \mathrm{D}$$

Anders, Schiller, *PRL* (2005)

Anders-Schiller basis

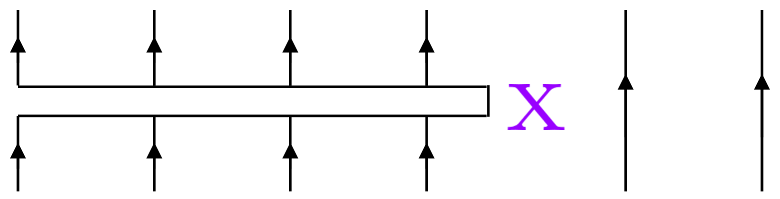
$|\alpha e\rangle^\ell_{\mathrm{D}} = |\alpha\rangle^\ell_{\mathrm{D}} \otimes |e\rangle^\ell$

$|\alpha e\rangle^{\ell+1}_{\mathrm{D}} = |\alpha\rangle^{\ell+1}_{\mathrm{D}} \otimes |e\rangle^{\ell+1}$



Projector onto sector X of shell ℓ,
resolving part of spectrum with energy $\sim \Lambda^{-\ell/2}$:

$$\mathcal{P}^\ell_{\mathrm{X}} = \sum_{\alpha e} |\alpha e\rangle^{\ell}_{\mathrm{X}}\, {}^{\ell}_{\mathrm{X}}\langle \alpha e| =$$



Iterative refinement: $\quad \mathcal{P}^\ell_{\mathrm{K}} = \mathcal{P}^{\ell+1}_{\mathrm{D}} + \mathcal{P}^{\ell+1}_{\mathrm{K}}$

Discarded states form $\boxed{\text{complete basis}}$ for full Hilbert space: $\quad 1 = \sum_\ell \mathcal{P}^\ell_{\mathrm{D}}$

Spectral representations of dynamical correlators:

$$S[\mathcal{A},\mathcal{B}](\omega) = \mathrm{Tr}\big[(\varrho\mathcal{A})\delta(\omega-\mathcal{H})\mathcal{B}\big] \mapsto \sum_\ell \sum_{\mathrm{XX}'}^{\neq \mathrm{KK}} \mathrm{Tr}\big[\mathcal{P}^\ell_{\mathrm{X}}(\varrho\mathcal{A})\mathcal{P}^\ell_{\mathrm{X}'}\delta(\omega-\mathcal{H})\mathcal{B}\big]$$

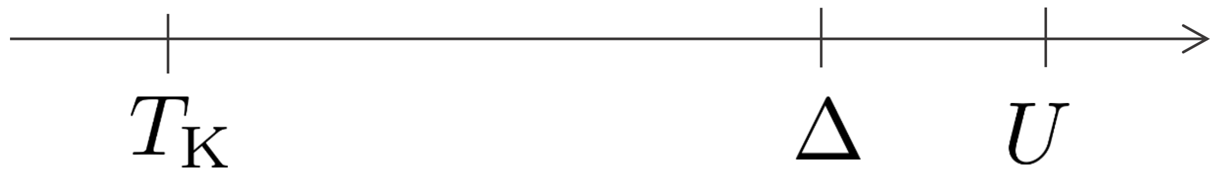
Iterative refinement of energy spectrum

NRG resolves real-frequency dynamics on all energy scales

NRG for SIAM: thermodynamic quantities

[numerical results for SIAM computed by Andreas Gleis]

Symmetric Anderson model: $\varepsilon_d = -U/2, \quad U = 2 \cdot 10^{-3}, \quad \Delta = 0.04U, \quad h = 0$



Haldane's definition of Kondo temperature:

$$T_{\mathrm{K}} = \frac{1}{4\chi(0)} \simeq \sqrt{U\Delta/2}\, \mathrm{e}^{-\frac{\pi U}{8\Delta} + \frac{\pi\Delta}{2U}}$$

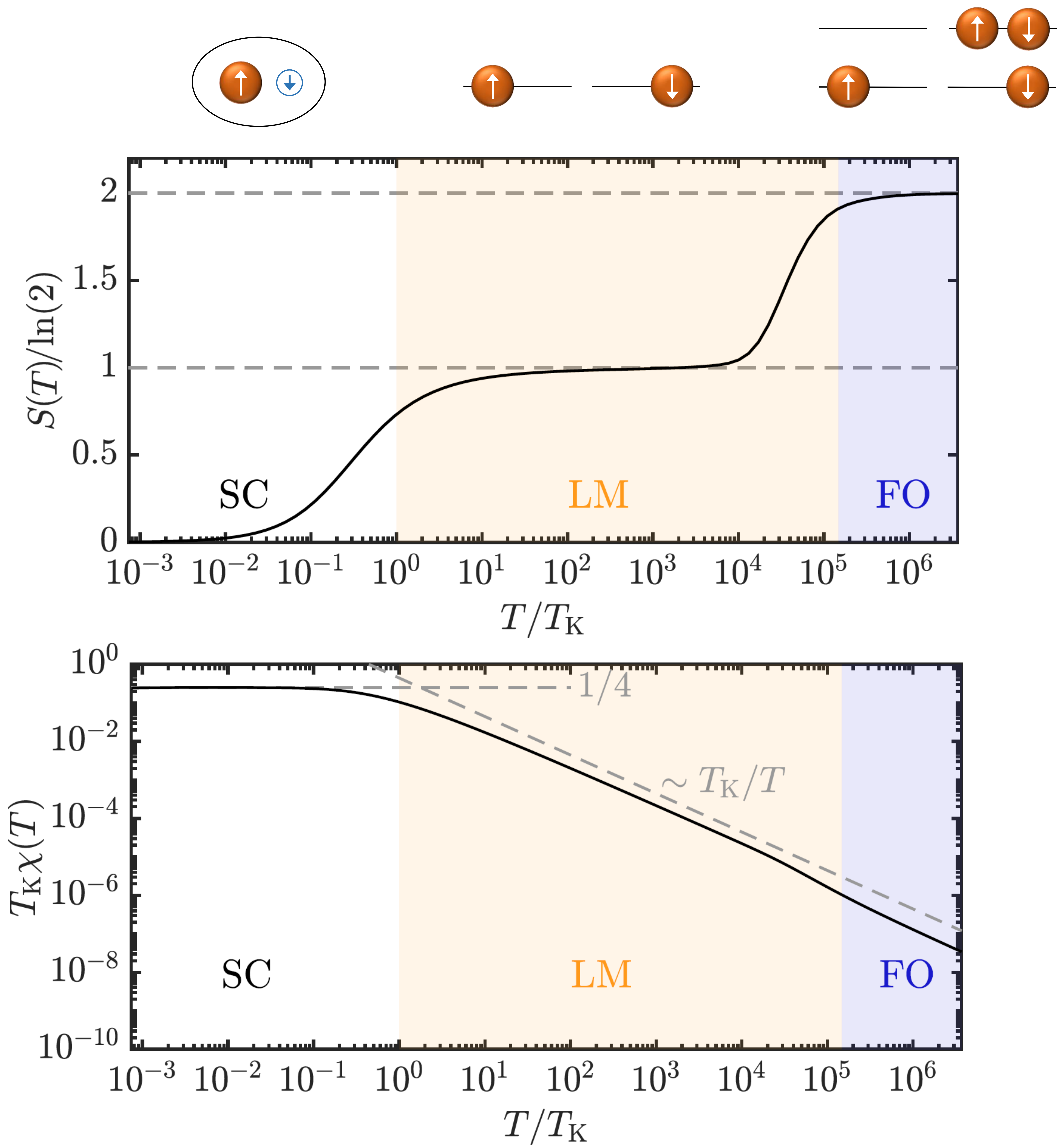
Haldane, J. Phys. C (1978)

Impurity entropy:

$$S(T) \simeq \begin{cases} \ln(4) = 2\ln(2)\,, & U \ll T \quad \text{“degenerate” quartet} \\ \ln(2)\,, & T_{\mathrm{K}} \ll T \ll U \quad \text{degenerate doublet} \\ \ln(1) = 0\,, & T \ll T_{\mathrm{K}} \quad \text{non-degenerate singlet} \end{cases}$$

Static impurity spin susceptibility:

$$T_{\mathrm{K}}\chi(T) \simeq \begin{cases} \frac{1}{4}\frac{T_{\mathrm{K}}}{T}\,, & T_{\mathrm{K}} \ll T \ll U \quad \text{Curie law} \\ \frac{1}{4}\,, & T \ll T_{\mathrm{K}} \quad \text{Pauli behavior} \end{cases}$$

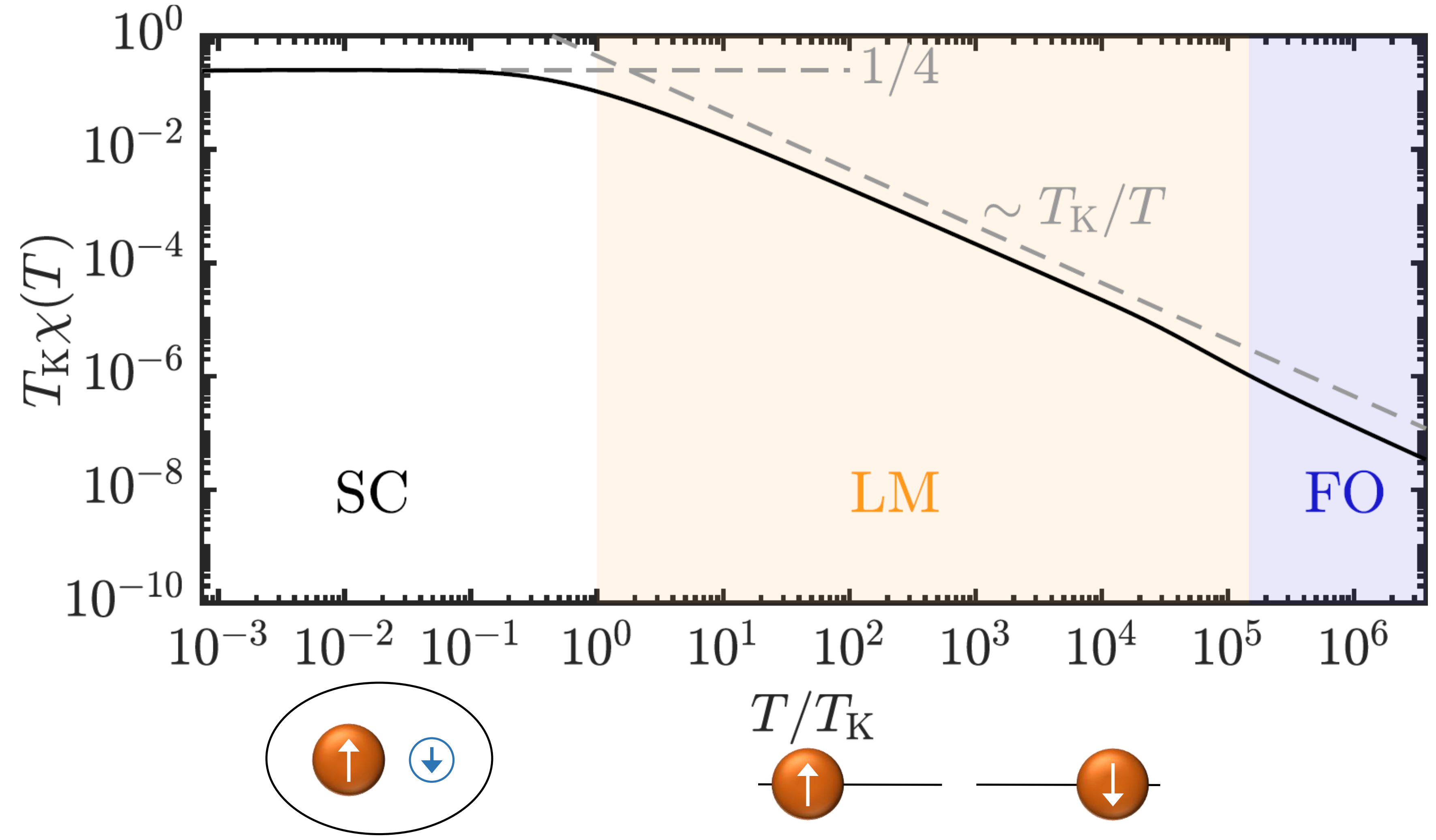


NRG for SIAM: dynamical spin susceptibility

Static impurity spin susceptibility:

$$T_\mathrm{K}\chi(T) \simeq \begin{cases} \dfrac{1}{4}\dfrac{T_\mathrm{K}}{T}\,, & T_\mathrm{K} \ll T \ll U \\ \dfrac{1}{4}\,, & T \ll T_\mathrm{K} \end{cases}$$

Curie law (first case); Pauli behavior (second case)

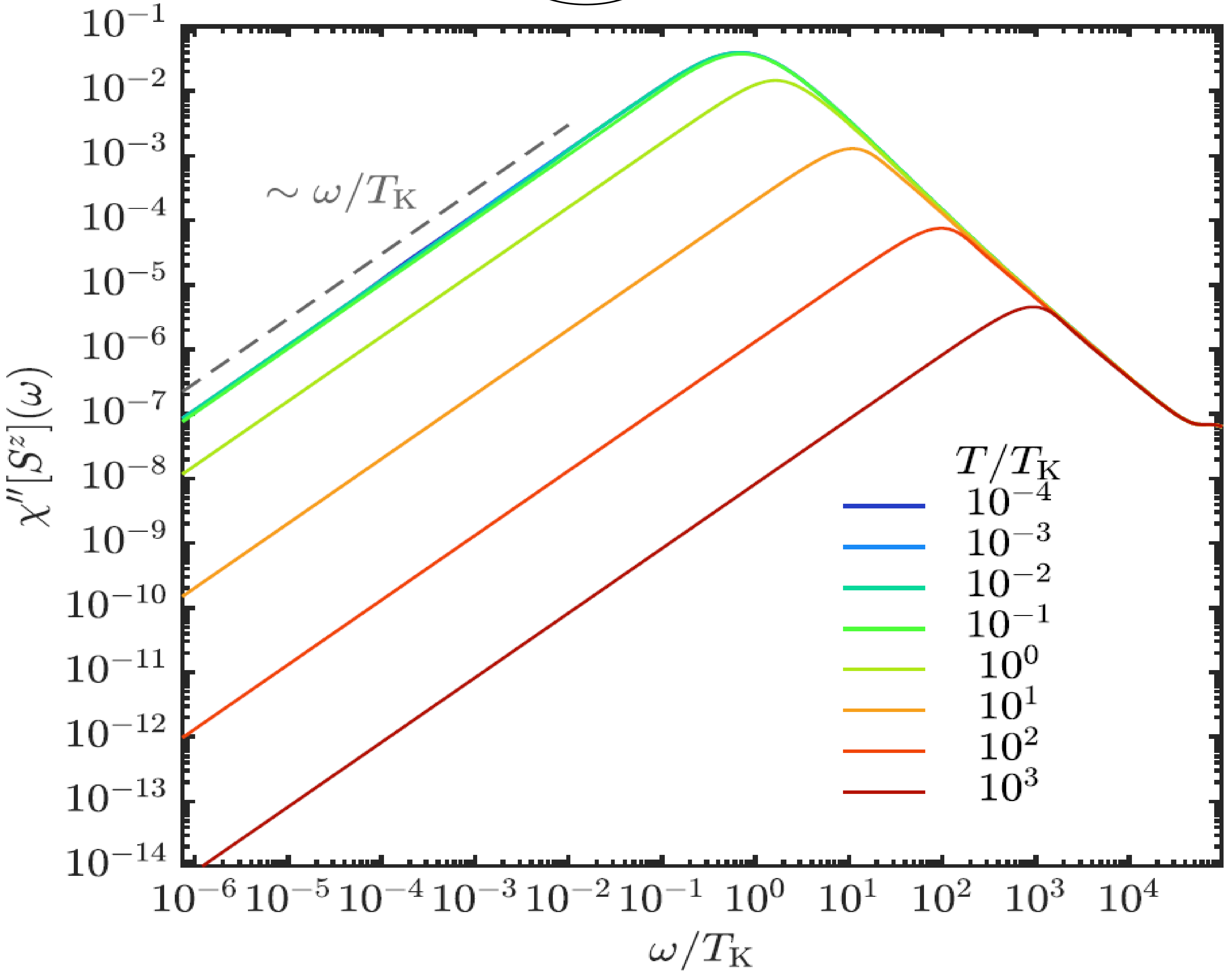


Dynamical impurity spin susceptibility:

$$\chi(\omega) = \chi'(\omega) + \mathrm{i}\chi''(\omega) = \int_{-\infty}^{\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t}(-\mathrm{i})\theta(t)\langle[\mathrm{S}^z(t), \mathrm{S}^z(0)\rangle_T$$

$$\chi''(\omega) \sim \begin{cases} \dfrac{1}{\omega}, & \max\{T_\mathrm{K}, T\} \ll \omega \ll U \\ \omega\,, & \omega \ll \max\{T_\mathrm{K}, T\} \end{cases}$$

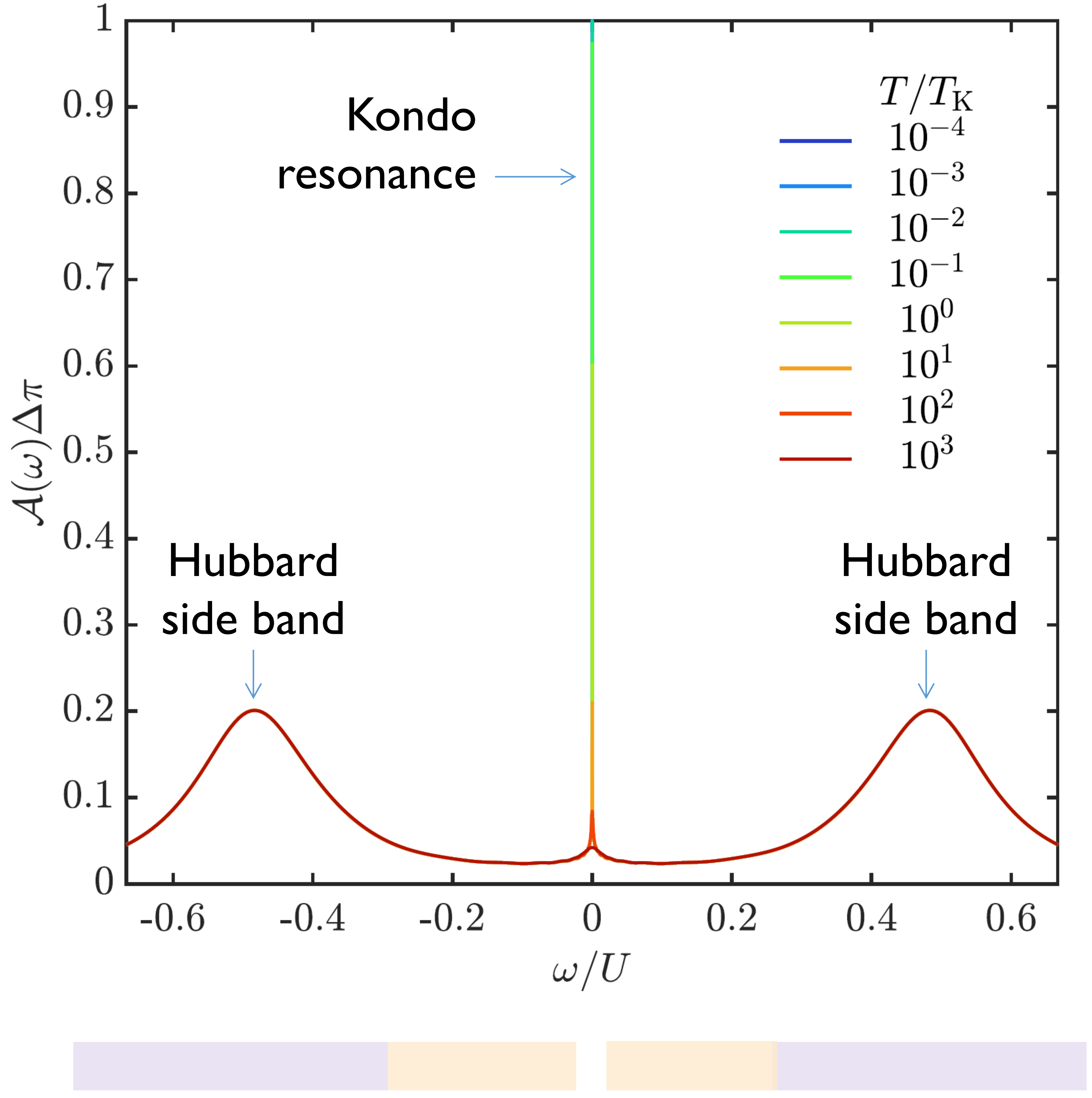
similar to Curie law (first case); Fermi-liquid behavior (second case)

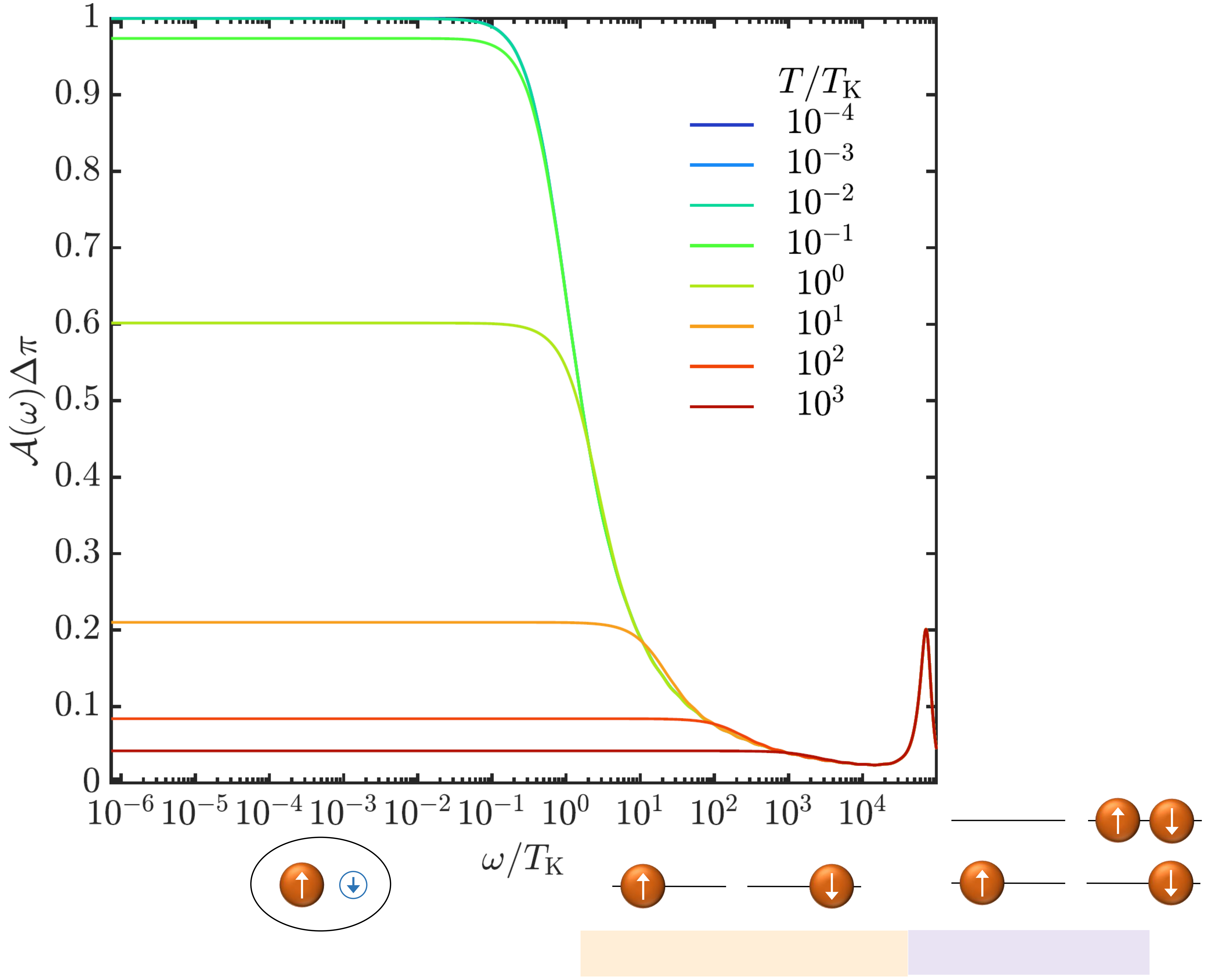


NRG for SIAM: local spectral function

Local d-level spectral function:

$$G_s(\omega) = \int_{-\infty}^{\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t}(-\mathrm{i})\theta(t)\langle\{d_s(t), d_s(0)\}\rangle_T = \int \mathrm{d}\omega' \frac{\mathcal{A}_s(\omega')}{\omega - \omega' + \mathrm{i}0^+}$$

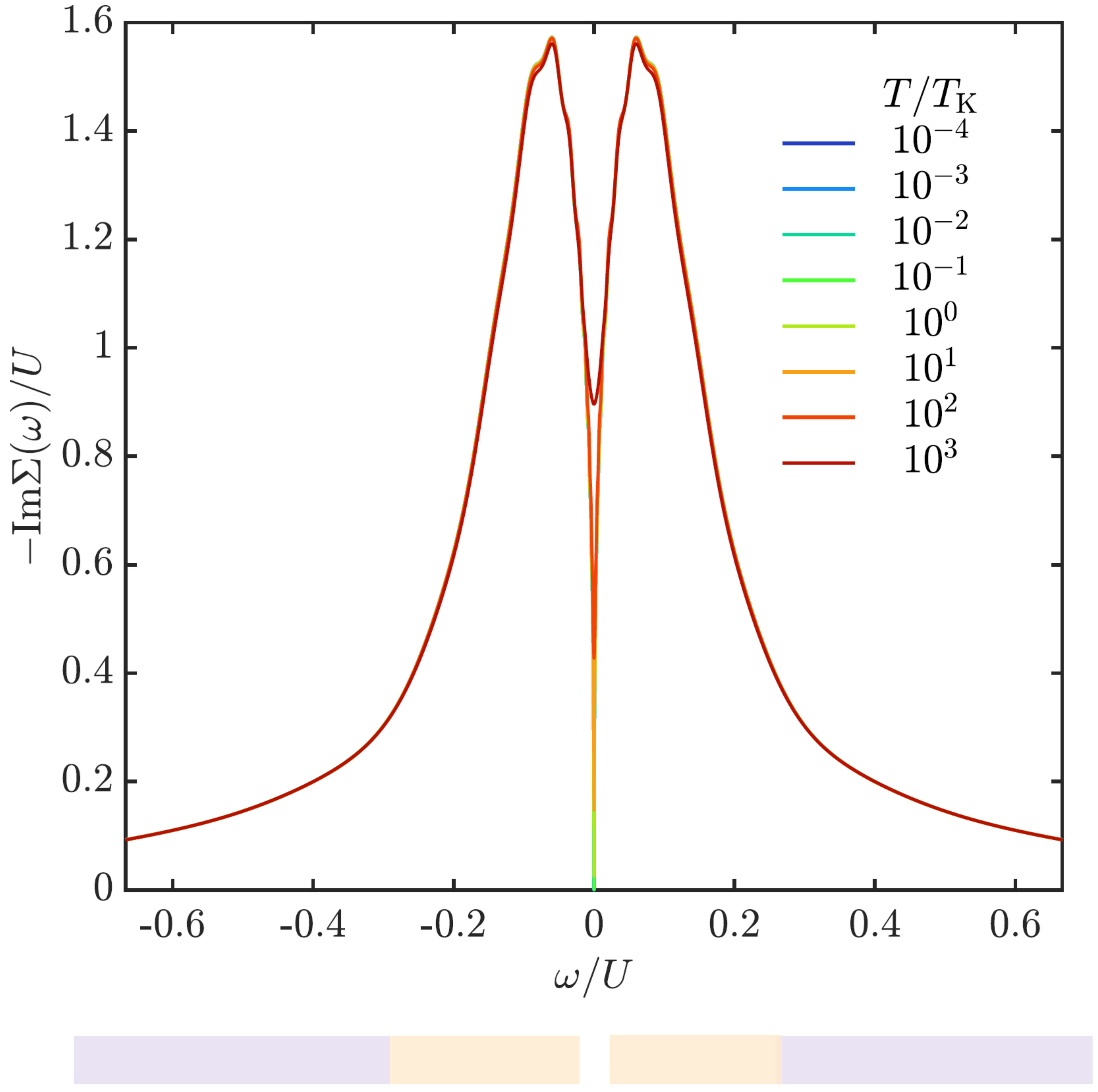


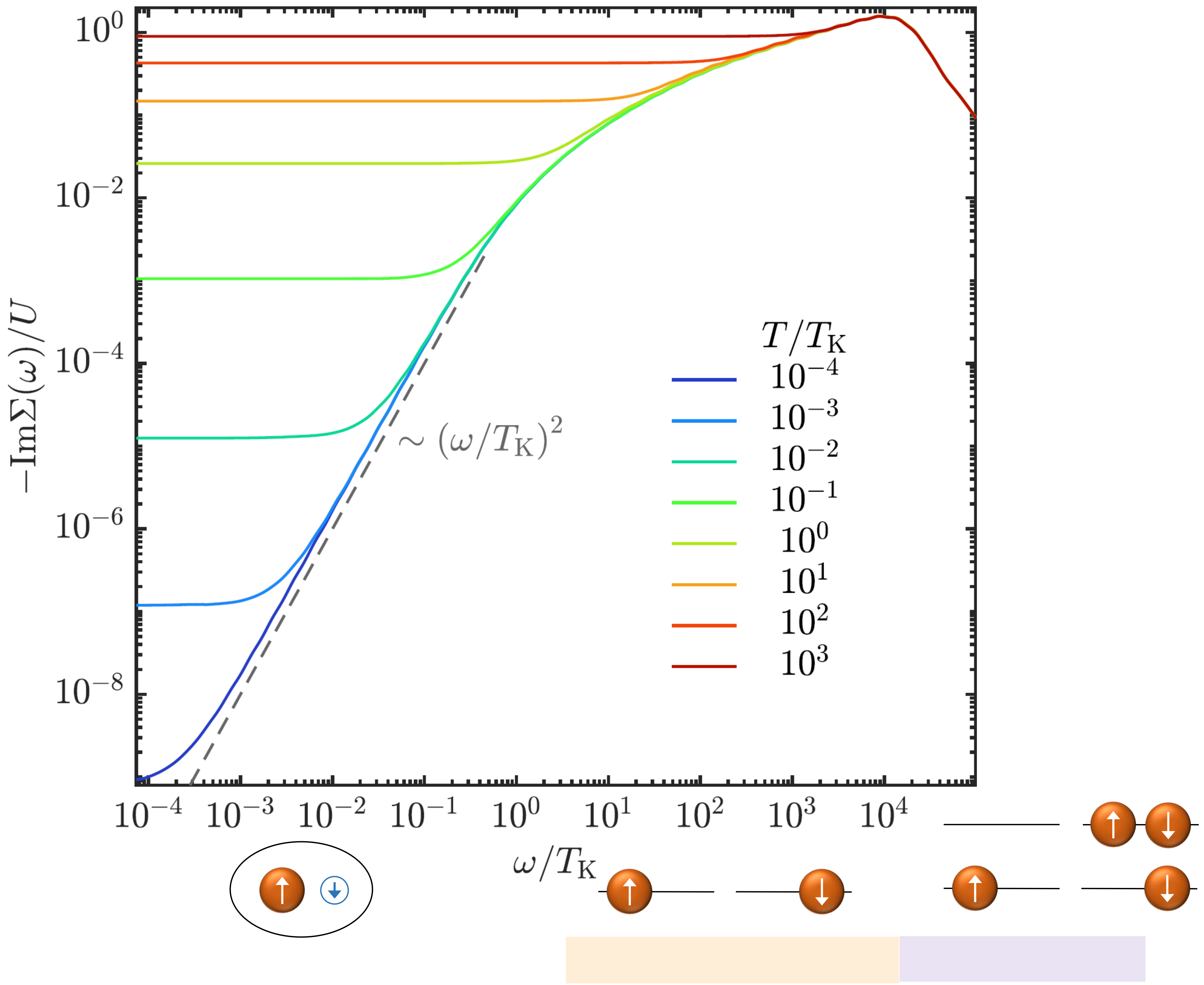


NRG for SIAM: local self-energy

Local self-energy:

$$G_s(\omega) = \frac{1}{\omega - \varepsilon_d - \Delta(\omega) - \Sigma_s(\omega)}$$

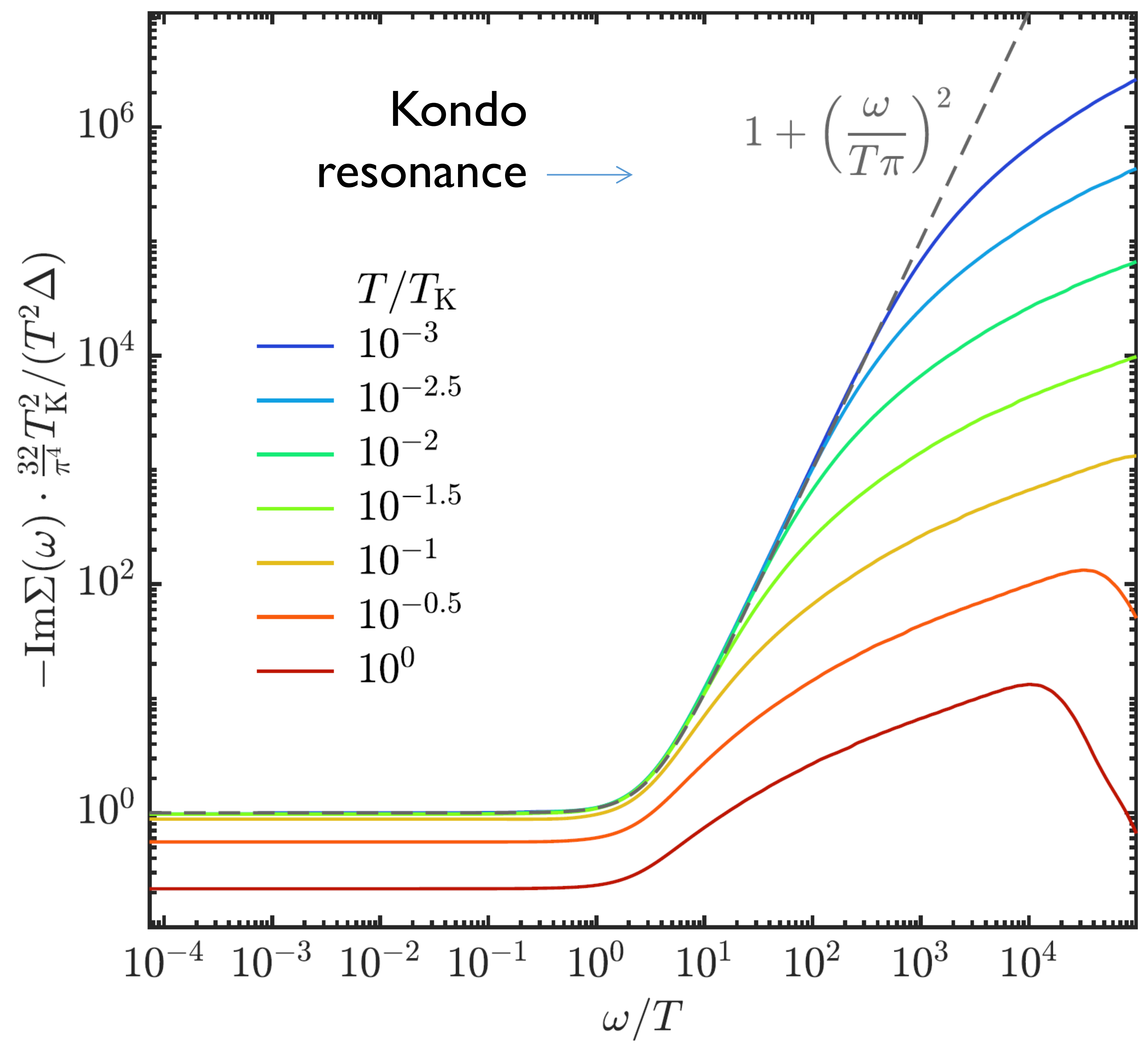


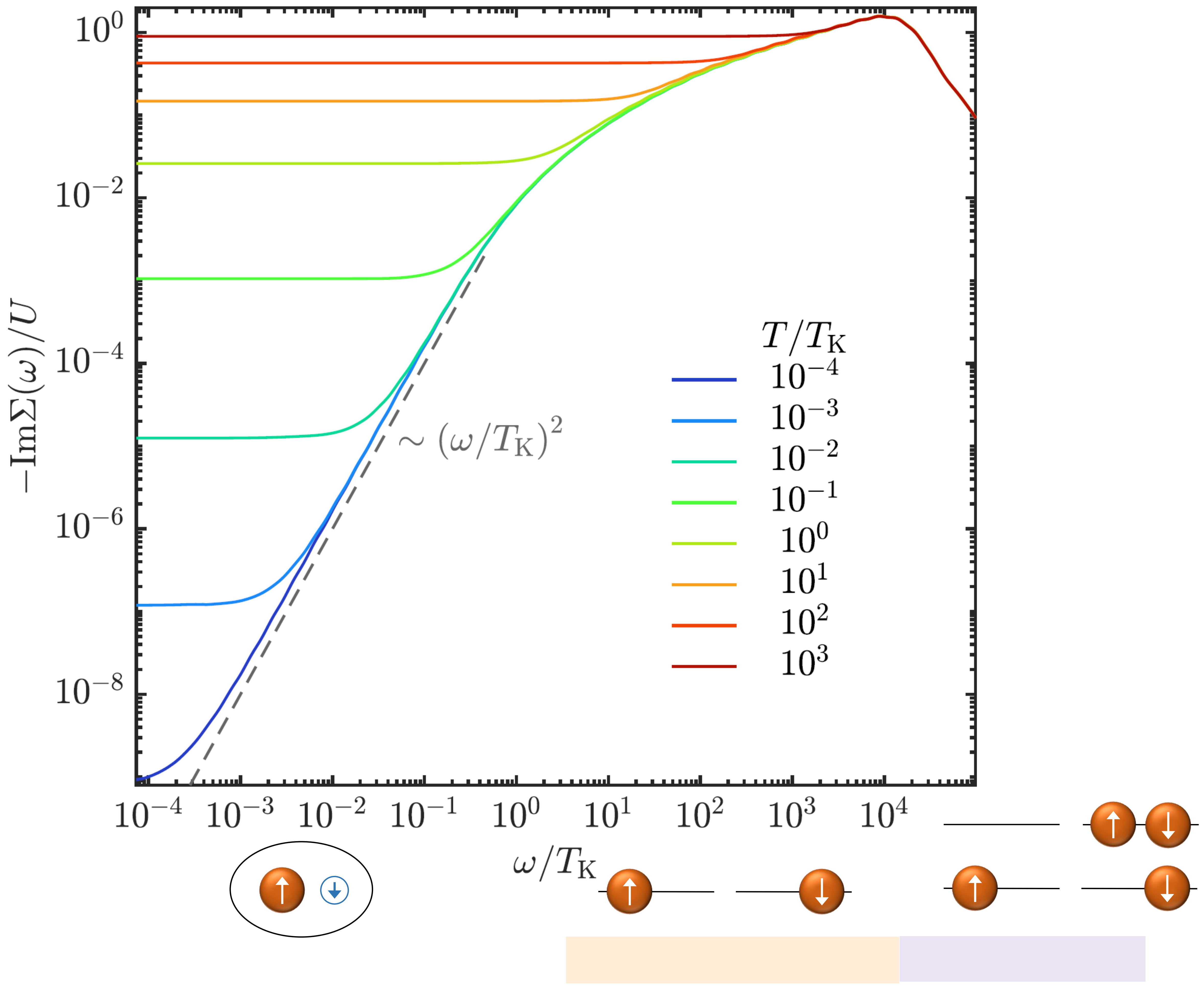


NRG for SIAM: $\omega\,/\,T$ scaling of local self-energy

Andreas Gleis, *unpublished* (2022)

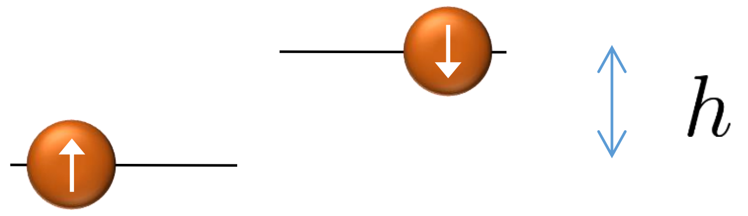
In Fermi-liquid regime: $$-\mathrm{Im}\Sigma(\omega,T) = \frac{\pi^2}{32}\frac{\Delta(\omega^2+\pi^2T^2)}{T_\mathrm{K}^2}\,, \qquad \omega, T \ll T_\mathrm{K}$$



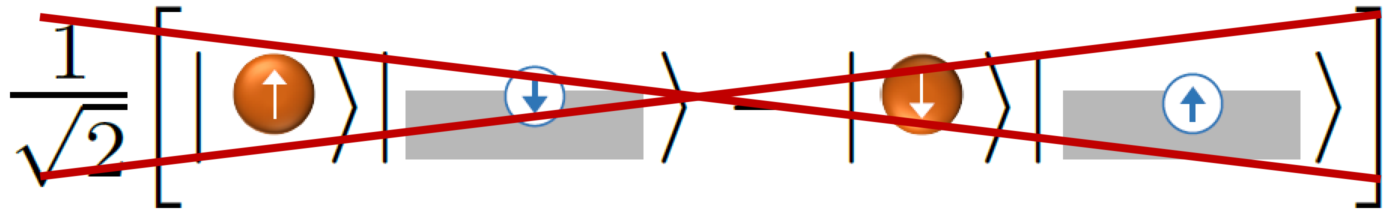


NRG for SIAM: magnetic field

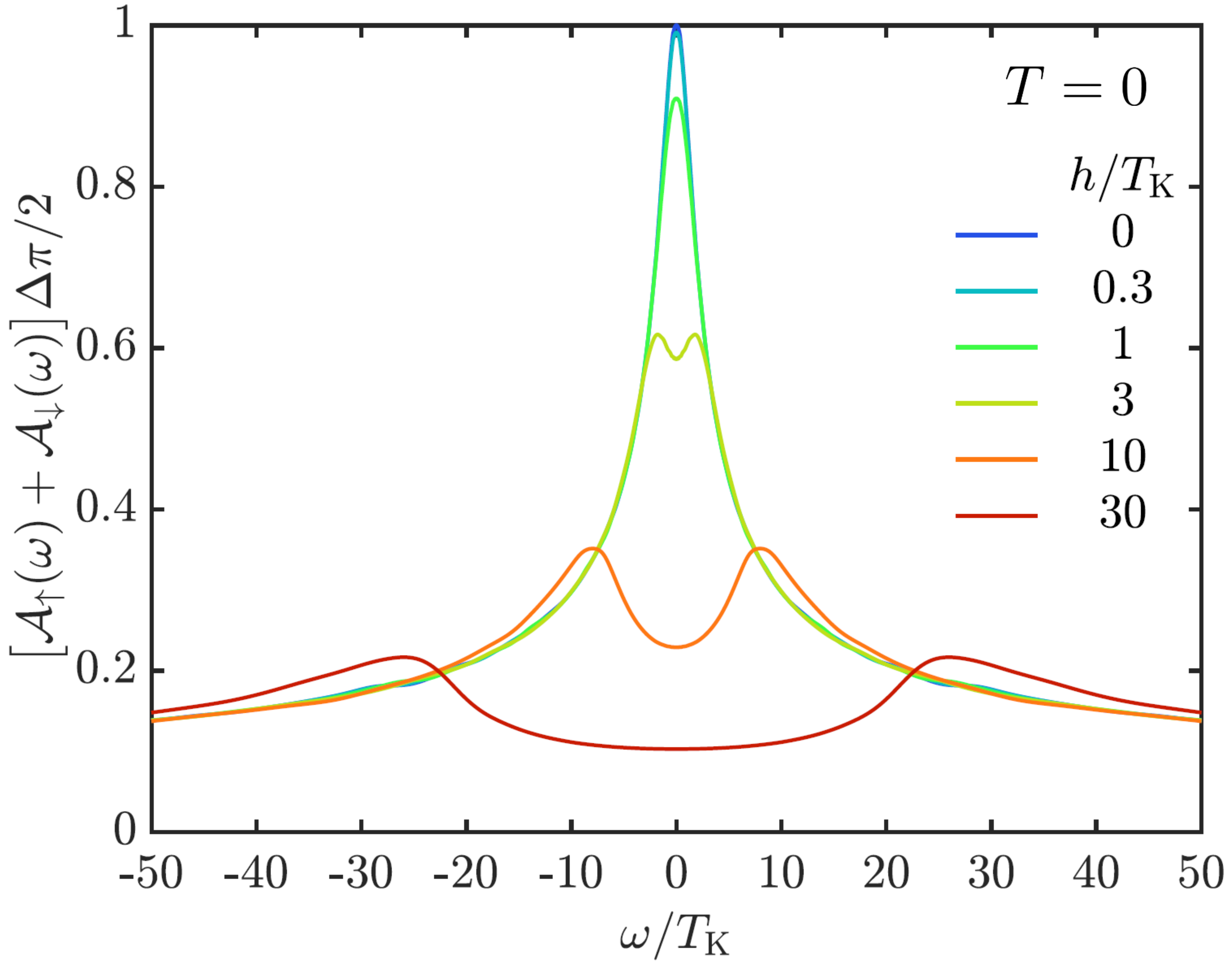
Magnetic field splits the local levels:

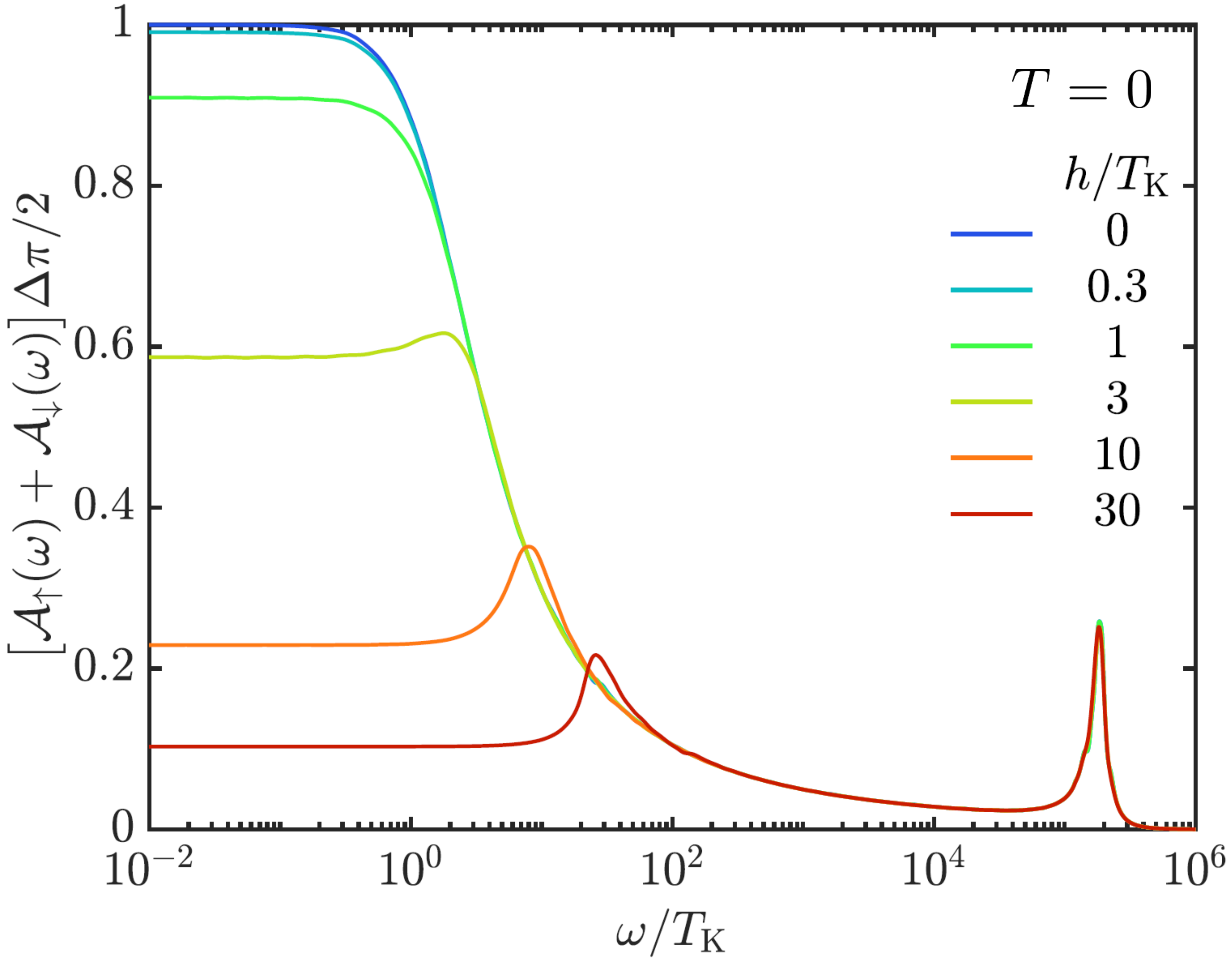


It breaks up the Kondo singlet if $h \gtrsim T_{\mathrm{K}}$



It shifts apart spin- $\uparrow$ and spin- $\downarrow$ contributions to $\mathcal{A}(\omega) = \mathcal{A}_{\uparrow}(\omega) + \mathcal{A}_{\downarrow}(\omega)$, causing the Kondo resonance to split:





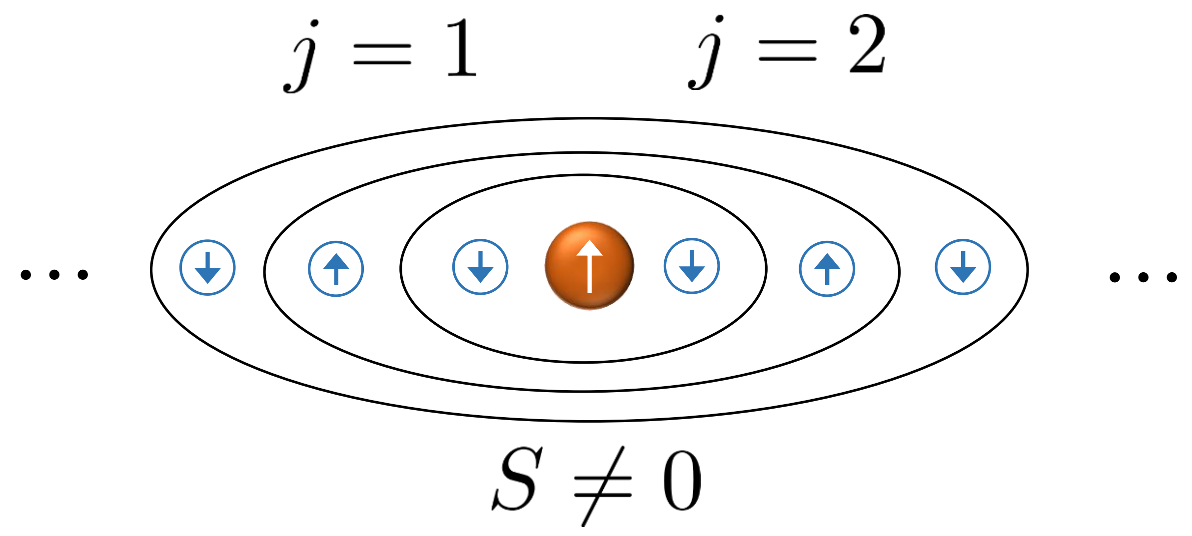
Two-channel Kondo model

Nozières, Blandin, *J. Phys.* (1980)

[numerical results for SIAM computed by Jeongmin Shim]

Local spin coupled to two separate but identical conduction band:

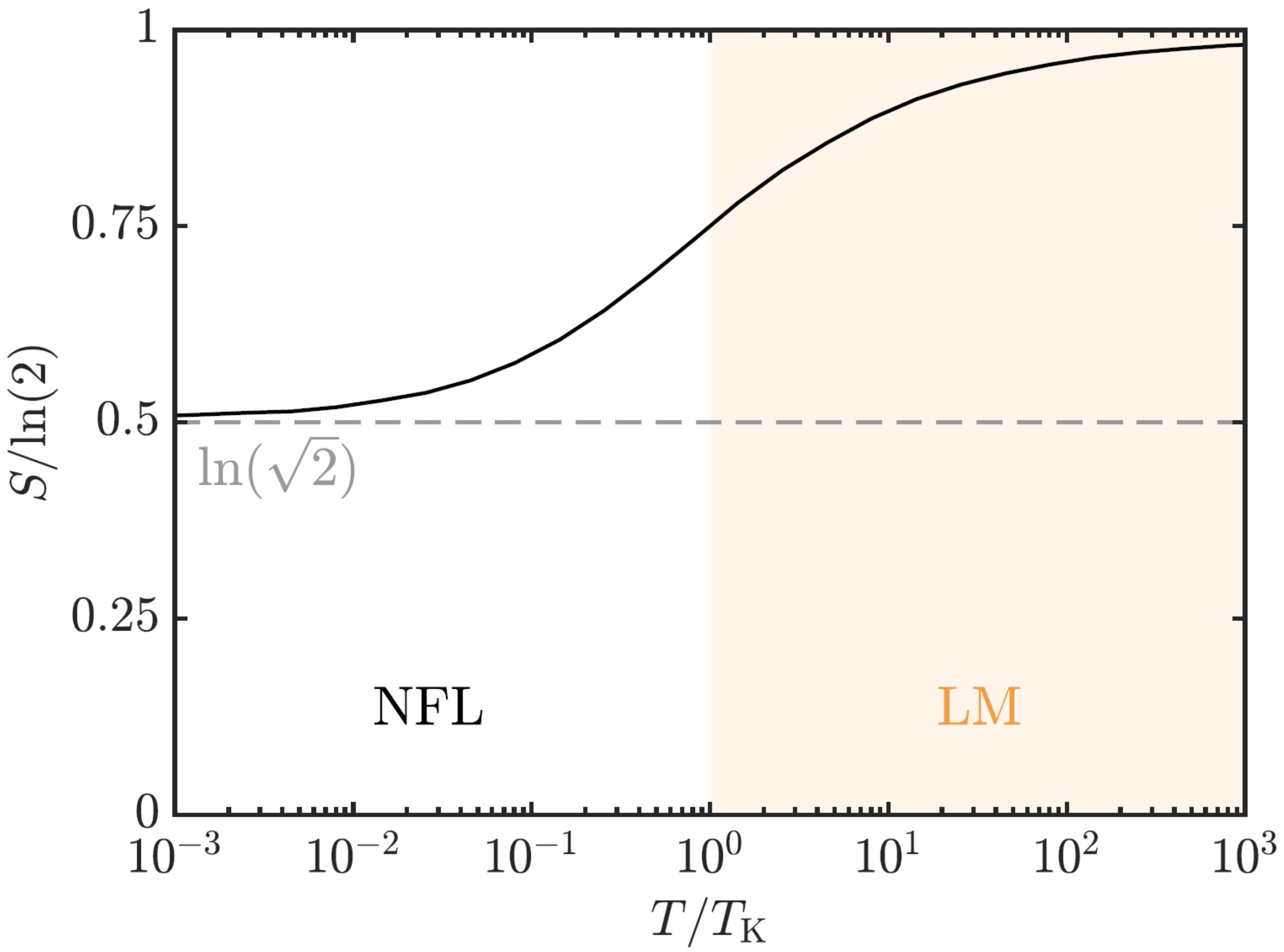
$$H_{2\mathrm{CK}} = \sum_{ks}\sum_{j=1,2} \varepsilon_k \hat{n}_{kjs} + J\mathbf{S}_d \cdot \mathbf{s}_c, \qquad \mathbf{s}_c = \sum_{ks,k's'}\sum_{j=1,2} c^\dagger_{kjs}\tfrac{1}{2}\boldsymbol{\sigma}_{ss'}c_{k'js'}$$



Due to channel symmetry, both channels contribute *equally* to screening.

Spin singlet can not be formed – local spin is "overscreened", causing non-Fermi-liquid behavior.

Impurity entropy:
$$S(T) \simeq \begin{cases} \ln(2)\,, & T_\mathrm{K} \ll T \\ \ln(\sqrt{2}) = \frac{1}{2}\ln(2)\,, & T \ll T_\mathrm{K} \end{cases}$$



Dynamical spin susceptibility:
$$\chi''(\omega) \sim \begin{cases} \dfrac{1}{\omega}, & \max\{T_\mathrm{K}, T\} \ll \omega \\ \mathrm{const.}\,, & \omega \ll \max\{T_\mathrm{K}, T\} \end{cases}$$