Thermodynamics of a Quantum Impurity in interacting environments

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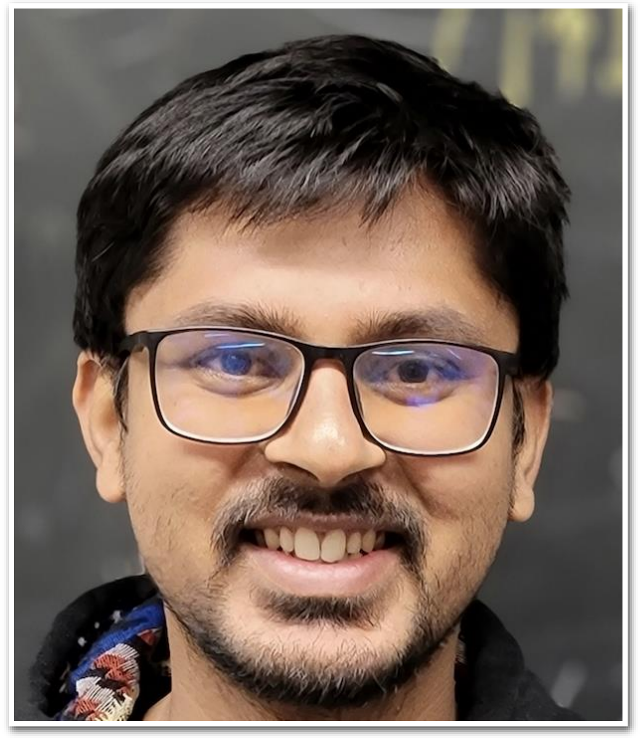

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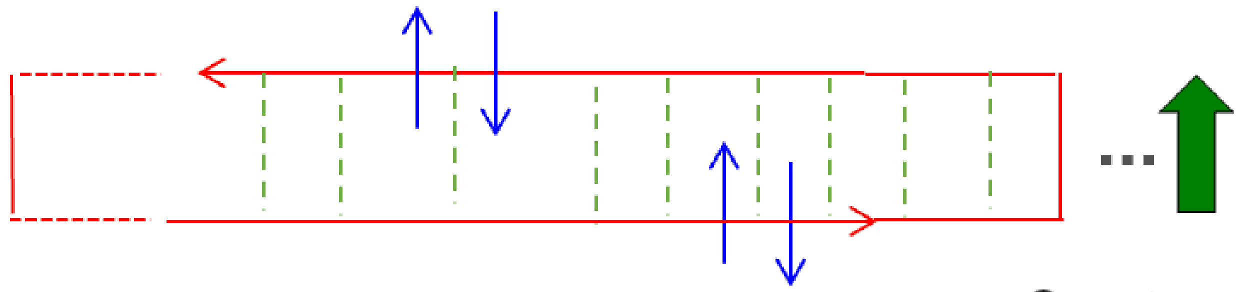
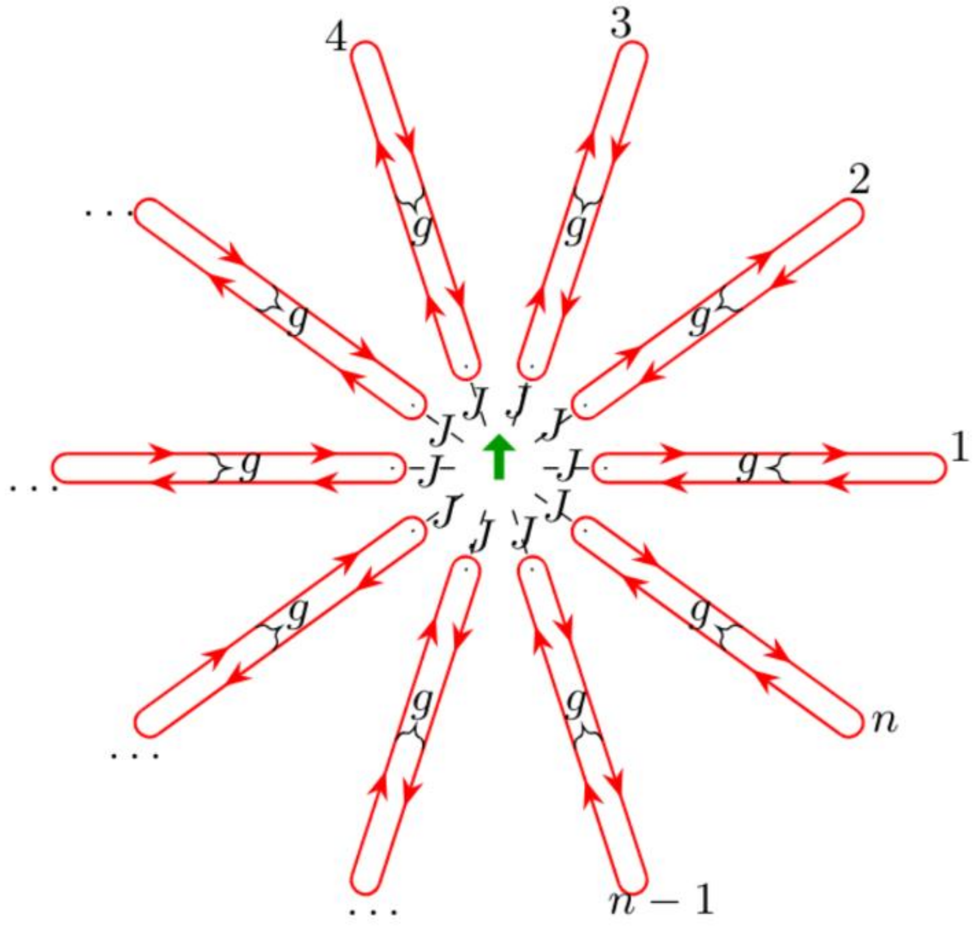
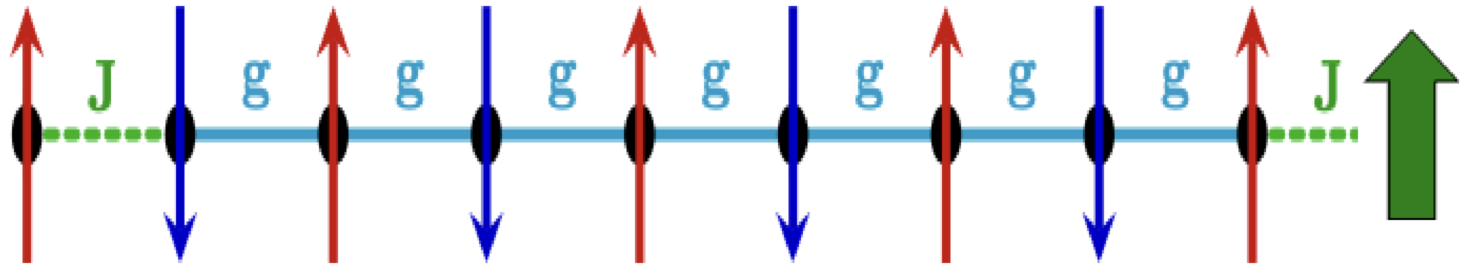


Quantum spin 1/2

Kondo impurity attached to one superconducting wire

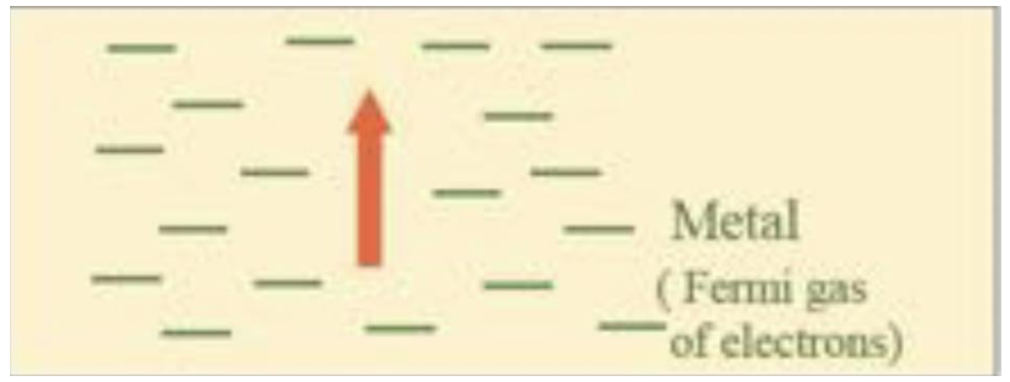


Kondo impurity attached to many superconducting wires



Kondo impurity at the edge of a spin chain

Non-interacting electrons coupled to a local spin impurity - The Kondo Model



The standard Kondo effect: electrons are non-interacting (Landau Ferm-liquid)

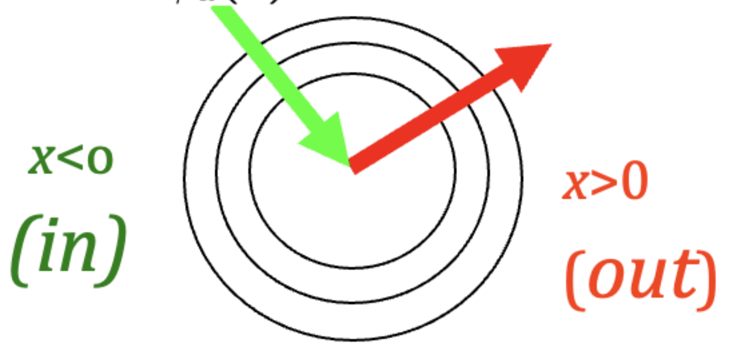
$$H = -i\int_{-L}^{0} \mathrm{dx}\,(\psi^\dagger_{+,\mathrm{a}}\partial_\mathrm{x}\psi_{+,\mathrm{a}} - \psi^\dagger_{-,\mathrm{a}}\partial_\mathrm{x}\psi_{-,\mathrm{a}}) + \mathrm{J}\psi^\dagger_{-,\mathrm{a}}(0)\tilde{\sigma}_{\mathrm{a,b}}\psi_{+,\mathrm{a}}(0)\cdot\tilde{\mathrm{S}}$$

$c_{\vec{k},a} \to c_{k,l,m,a}$ spherical modes

$\to c_{k,o,o,a}$ s-waves

$\to c_{k_F+q,a}$ linearize around k_F

$\to \psi_a(x)$ Fourier transform



- The effective coupling flows to strong coupling $\dfrac{dJ}{dl} \sim J^2$

Anderson: Poor man's scaling

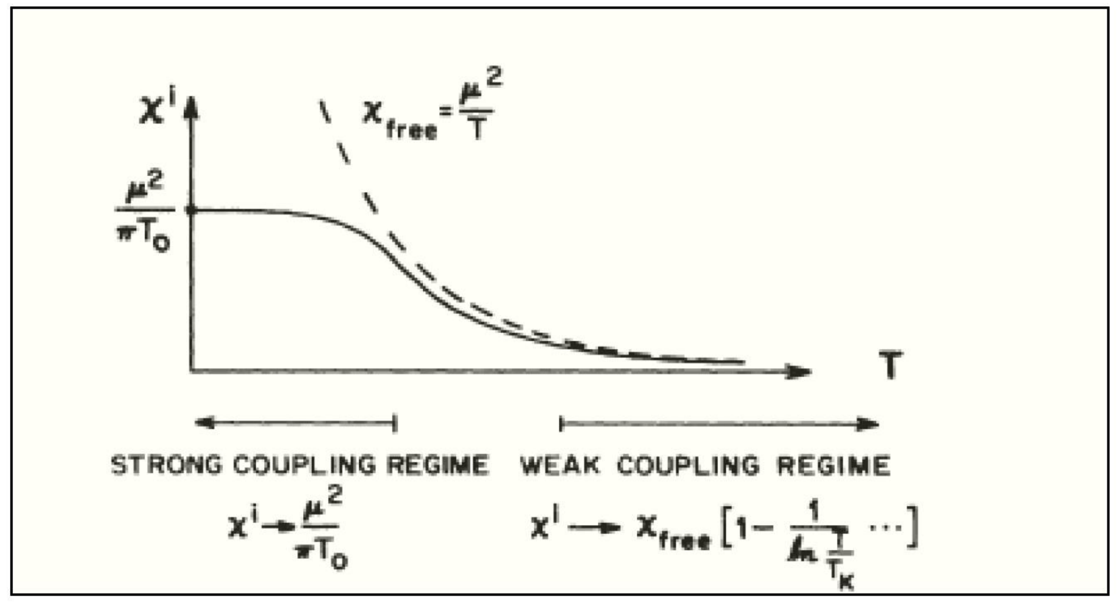
Wilson: NRG

- Critical behavior at low –T determined by fixed point: impurity screened

- Bethe Ansatz Solution

  Andrei 1980

  Wiegmann 1980



$$\mathcal{S}_{\mathrm{imp}}(T) : \ln 2 \to 0$$

$$C = \frac{\pi}{6T_0}$$

$$\chi = \frac{\mu^2}{\pi T_0}$$

- Conformal field theory approach: fusion rules change at criticality

Impurity absorbed

$$H = \int_{-L}^{0} dx\,(\mathcal{J}^2(x) + \bar{\mathcal{J}}^2(x)) + J(\mathcal{J}(0) + \bar{\mathcal{J}}(0))\cdot S \xrightarrow{\text{At criticality}} H^* = \int_{-L}^{0} dx\left(\mathfrak{J}^2(x) + \bar{\mathfrak{J}}^2(x)\right)$$

Affleck, Ludwig 1991-1994

Conformal currents $\mathcal{J}^a(z)\mathcal{J}^b(w) \sim \dfrac{\frac{1}{2}\delta^{ab}}{(z-w)^2} + \dfrac{i\epsilon^{abc}\mathcal{J}^c}{z-w}$ $\bar{\mathcal{J}}^a(z)\bar{\mathcal{J}}^b(w) \sim \dfrac{\frac{1}{2}\delta^{ab}}{(z-w)^2} + \dfrac{i\epsilon^{abc}\bar{\mathcal{J}}^c}{z-w}$ $\mathfrak{J}^a(x) = \mathcal{J}^a(x) + S^a\delta(x)$

Multichannel *Non-interacting* Electrons coupled to a local spin impurity

The multichannel Kondo effect: electrons are non-interacting, carry channel quantum number $m = 1 \cdots f$

$$H = -i \int_{-L}^{0} \mathrm{dx} \left(\sum_{\mathrm{m=1}}^{\mathrm{f}} \psi^{\dagger}_{+,\mathrm{a,m}} \partial_{\mathrm{x}} \psi_{+,\mathrm{a,m}} - \psi^{\dagger}_{-,\mathrm{a,m}} \partial_{\mathrm{x}} \psi_{-,\mathrm{a,m}} \right) + \mathrm{J} \sum_{\mathrm{m=1}}^{\mathrm{f}} \psi^{\dagger}_{-,\mathrm{a,m}}(0) \tilde{\sigma}_{\mathrm{a,b}} \psi_{+,\mathrm{a,m}}(0) \cdot \tilde{\mathrm{S}}$$

- The effective coupling flows to ***intermediate*** fixed point $\frac{\mathrm{d}J}{\mathrm{d}l} \sim J^2 - \frac{f}{2} J^3$ Nozieres, Blandin1980

  - determines the critical behavior at low –T

- Bethe Ansatz Solution: impurity overscreened

$$\mathcal{S}_{\mathrm{imp}}(T) : \ln 2 \to \ln\, 2 \cos\left(\frac{\pi}{f+2}\right)$$

Andrei, Destri 1984

Tsvelik, Wiegmann 1985

$$C \sim \left(\frac{T}{T_0}\right)^{\frac{4}{f+2}}$$

$$\chi \sim \frac{1}{T} \left(\frac{T}{T_0}\right)^{\frac{4}{f+2}}$$

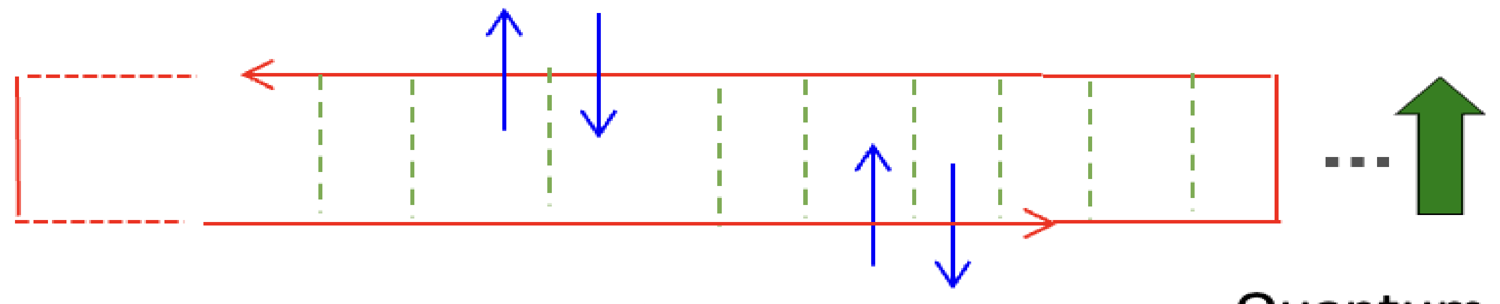
- Conformal field theory approach

$$H = \int_{-L}^{0} dx \left(\mathcal{J}^2(x) + \bar{\mathcal{J}}^2(x) + \mathcal{F}^2(x) + \bar{\mathcal{F}}^2(x)\right) + J(\mathcal{J}(0) + \bar{\mathcal{J}}(0)) \cdot S$$

Affleck, Ludwig 1991-1994

Interacting electrons coupled to a local spin impurity

SC wire coupled to a spin ½ impurity



$$\underbrace{H = -i\int_{-L}^{0} \mathrm{dx}\,(\psi_+^\dagger\partial_x\psi_+ - \psi_-^\dagger\partial_x\psi_-) + 2\mathrm{g}\int_{-\mathrm{L}}^{0}\mathrm{dx}\,\psi_+^\dagger\tilde{\sigma}\psi_+\cdot\psi_-^\dagger\tilde{\sigma}\psi_-}_{\text{1D spin-singlet superconductor}} + \underbrace{\mathrm{J}\psi_-^\dagger(0)\tilde{\sigma}\psi_+(0)\cdot\tilde{\mathrm{S}}}_{\text{Quantum spin 1/2}}$$

1D **spin-singlet superconductor** $\mathcal{O}_{\mathrm{SSS}}(x) = \psi_-^\dagger(x)\sigma^y\psi_+^\dagger(x)$ **Quantum spin 1/2**

- Both couplings g, J run under RG: *competing effects*

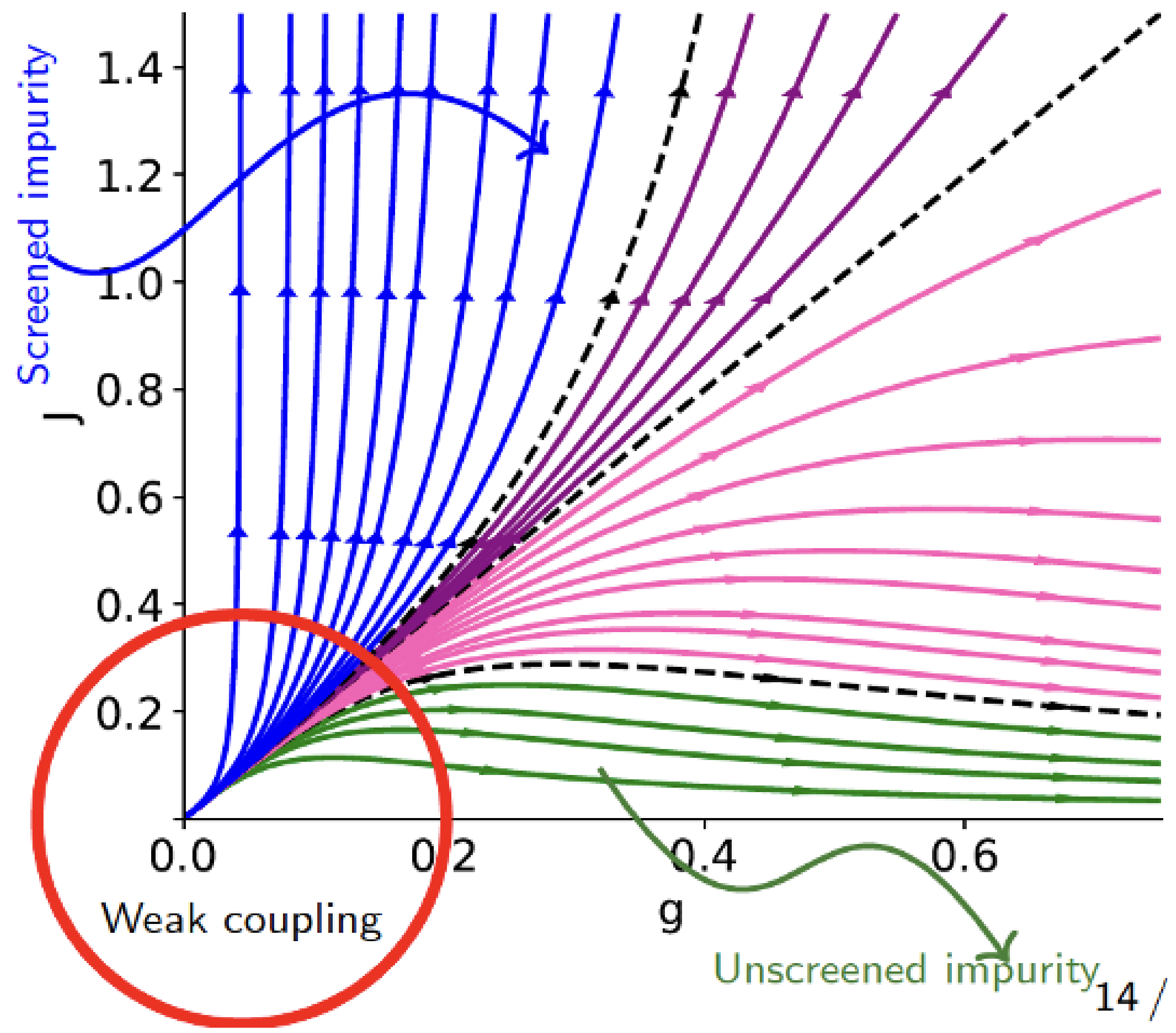
$$\frac{\mathrm{d}g}{\mathrm{d}l} \sim g^2 \qquad \frac{\mathrm{d}J}{\mathrm{d}l} \sim J^2 - Jg$$

- Different phases arise, depending on relative strengths of g, J

- RG invariant $d(J,g) = \sqrt{b^2 - 2b/c - 1}$ labels the phases

  here: $b = \frac{4-g^2}{8g}$ effective bulk constant, $c = \frac{2J}{1-\frac{3}{4}J^2}$ effective impurity constant

- Conformal field theory not applicable (electrons gapful)



- **Bethe Ansatz solution provides full description of the phases and their thermodynamics**

Pasnoori, Andrei Rylands, Azaria 2022

The Thermodynamics (open BC)

- The partition function of a given phase is obtained by summing over all energies of the phase, and from it the total free energy $F(T)$

$$Z = \sum_n e^{-\beta E_n} = e^{-\beta F(T)}$$

- The total free energy of system with open BC $F(T) = F_{\text{bulk}}(T) + F_{\text{boundary}}(T) + F_{\text{imp}}(T)$

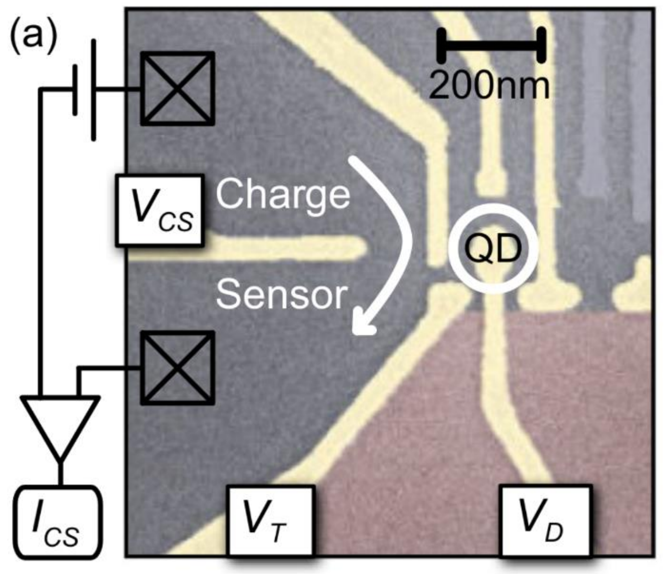
- Calculate the free energy using Yang-Yang's TBA approach *(YY 1969)* Another approach: *QTM* *(Klumper 2007)*

Comment: Calculating the free energy from TBA for open BC often misses $F_{\text{boundary}}(T)$ which arises from the Jacobian of the Yang-Yang change of variables (equal to 1 for PBC) . ***Pozsgay 2010 He, Jiang 2024***

- Not part of the *impurity free energy* *(Obtained by subtracting the bulk and boundary terms from F(T))*

- Compute the ***impurity entropy***: $S_{\text{imp}}(T) = -\partial_T F_{\text{imp}}(T)$

 - It is experimentally measurable (*Folk et al 2018, Ensslin et al 2025)*



Outline: *Interacting electrons* coupled to a local impurity

i. **Solve the models using the Bethe Ansatz approach**

ii. **Identify the phases:** They depend on relative strengths of the interactions: g, J RG invariant measure $d(J,g) \sim \sqrt{(\frac{1}{2g})^2 - 2\frac{J}{g} - 1}$

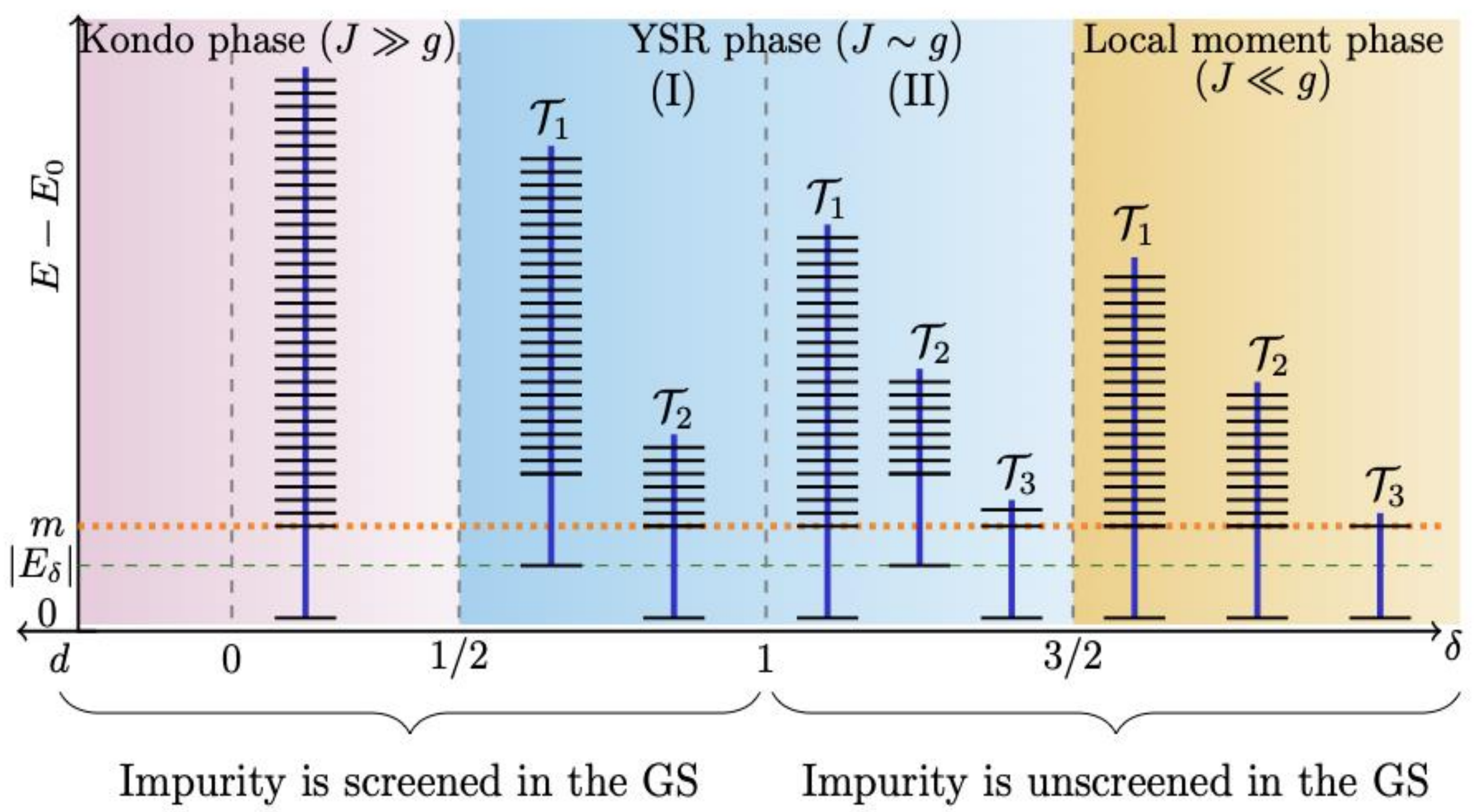
- Kondo Phase *(many body screening of impurity)* *the only phase for non interacting electrons*
- Zero mode phase (in the case of multichannel electrons)
- Bound mode phase (YSR) *(Local screening by bound state)* ***(Yu 1965, Shiba 1968, Rusinov) 1969)***
- Local moment phase *(impurity not screened at any energy)*

iii. **Each phase consists of several *__towers__ of excitations* (split Hilbert space)**

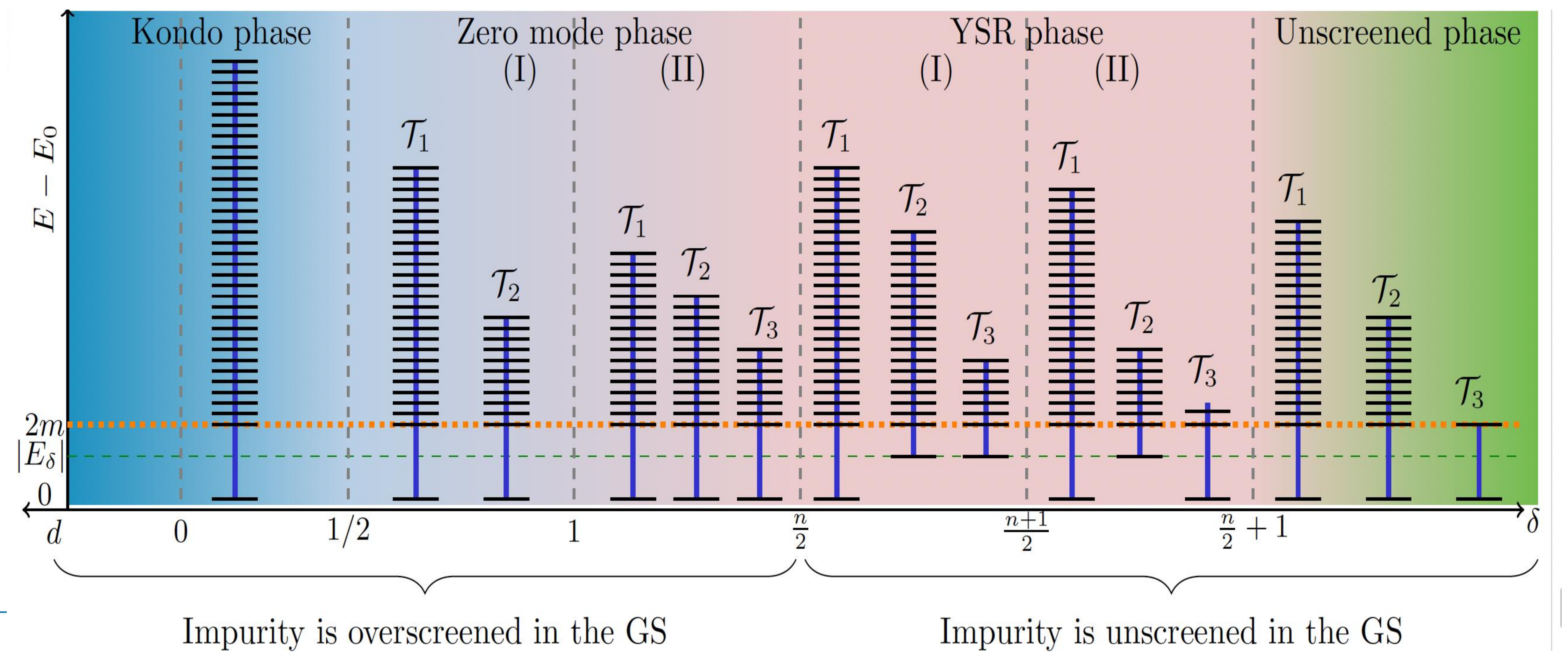
iv. **Free energy of each phase : Carry out the multi-tower summation**

v. **Compute the Impurity entropy**

Phase diagram of the impurity attached to a superconducting wire

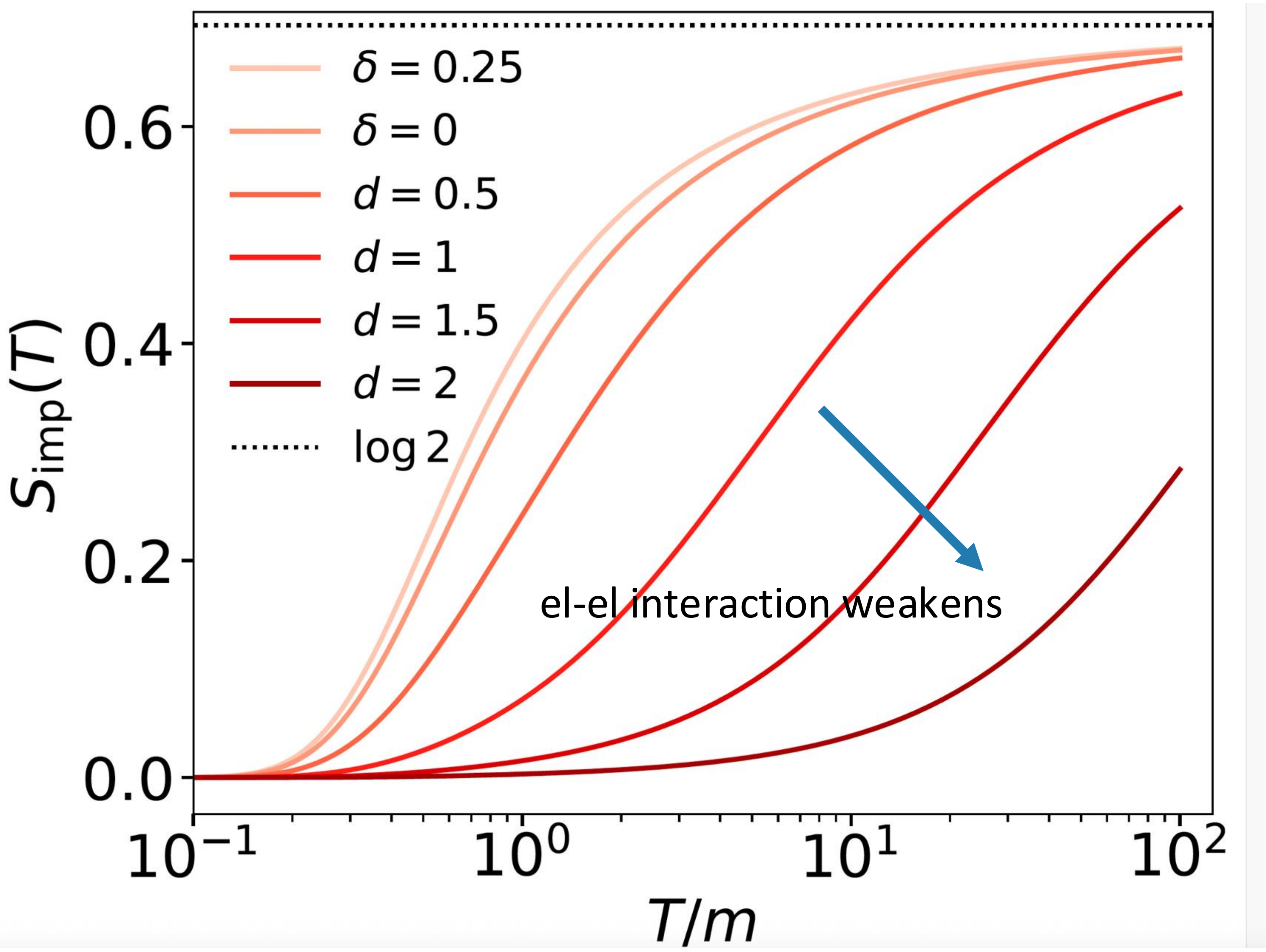


Phase diagram of the impurity attached to *f* superconducting wires



$S_{\mathrm{imp}}(T)$: The impurity entropy as function of the temperature in the Kondo phase

Entropy of the impurity attached to one superconductor

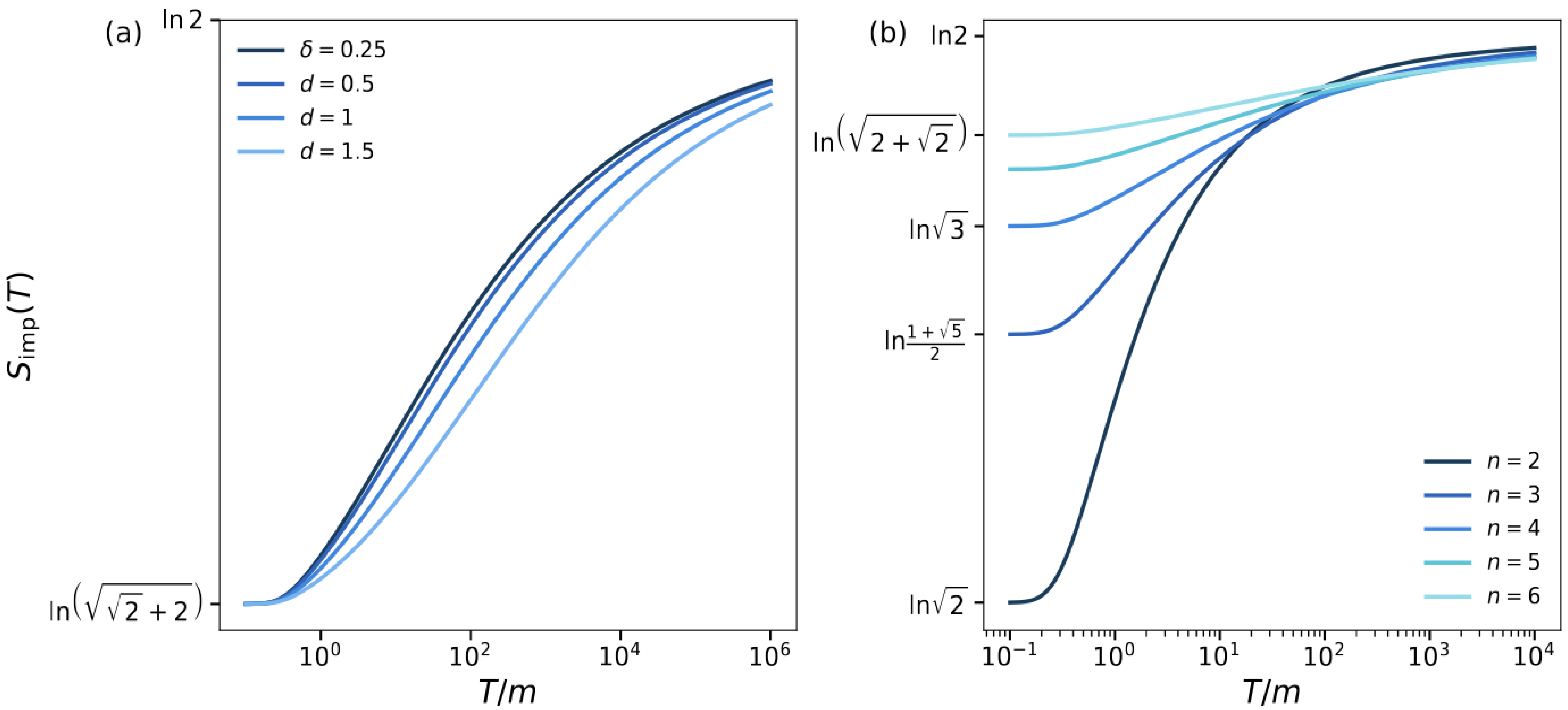


$$S_{\mathrm{imp}}(T) : \ln 2 \to 0$$

Entropy of the impurity attached to f-superconductors

Kondo phase (6 channels, vary *d)*

Kondo phase (d=0.25, vary *f)*

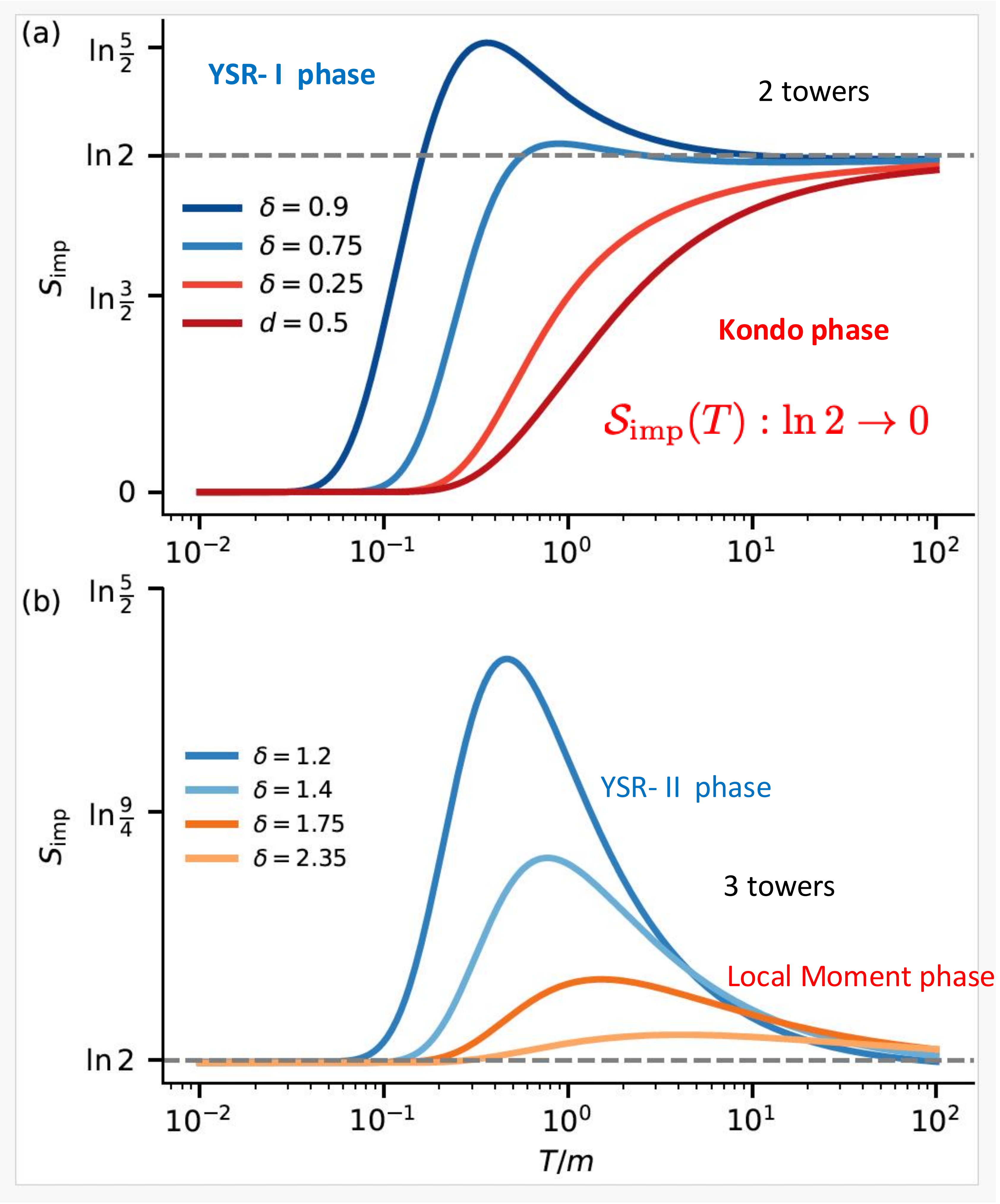


$$S_{\mathrm{imp}}(T) : \ln 2 \to \ln 2 \cos\left(\frac{\pi}{f+2}\right)$$

Remarkable: In the Kondo and Zero mode phase the zero-T entropy is the same as for the conformal electrons

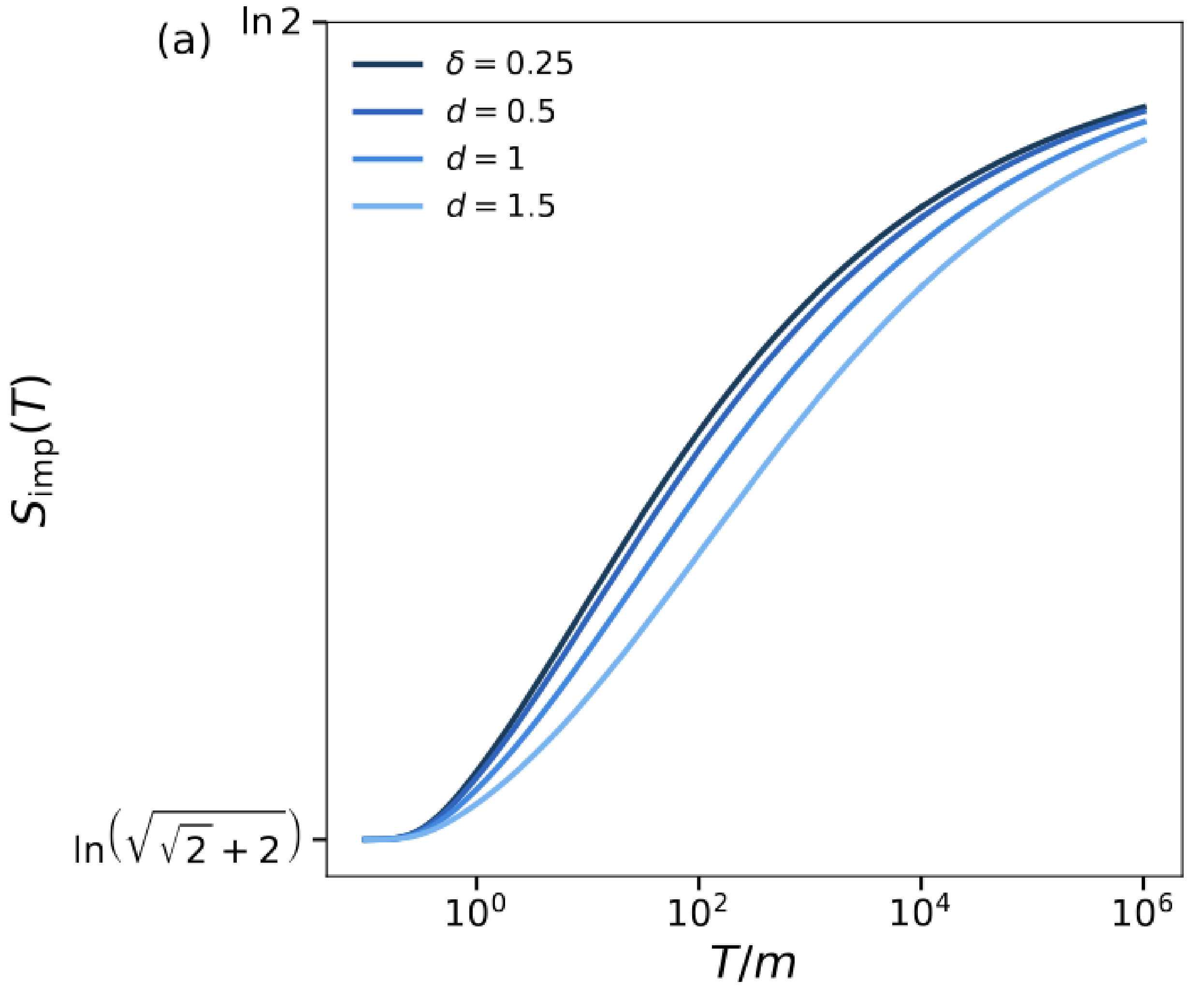
$S_{\mathrm{imp}}(T)$: The impurity entropy as function of the temperature in the various phases

Entropy of the impurity attached to one superconductor

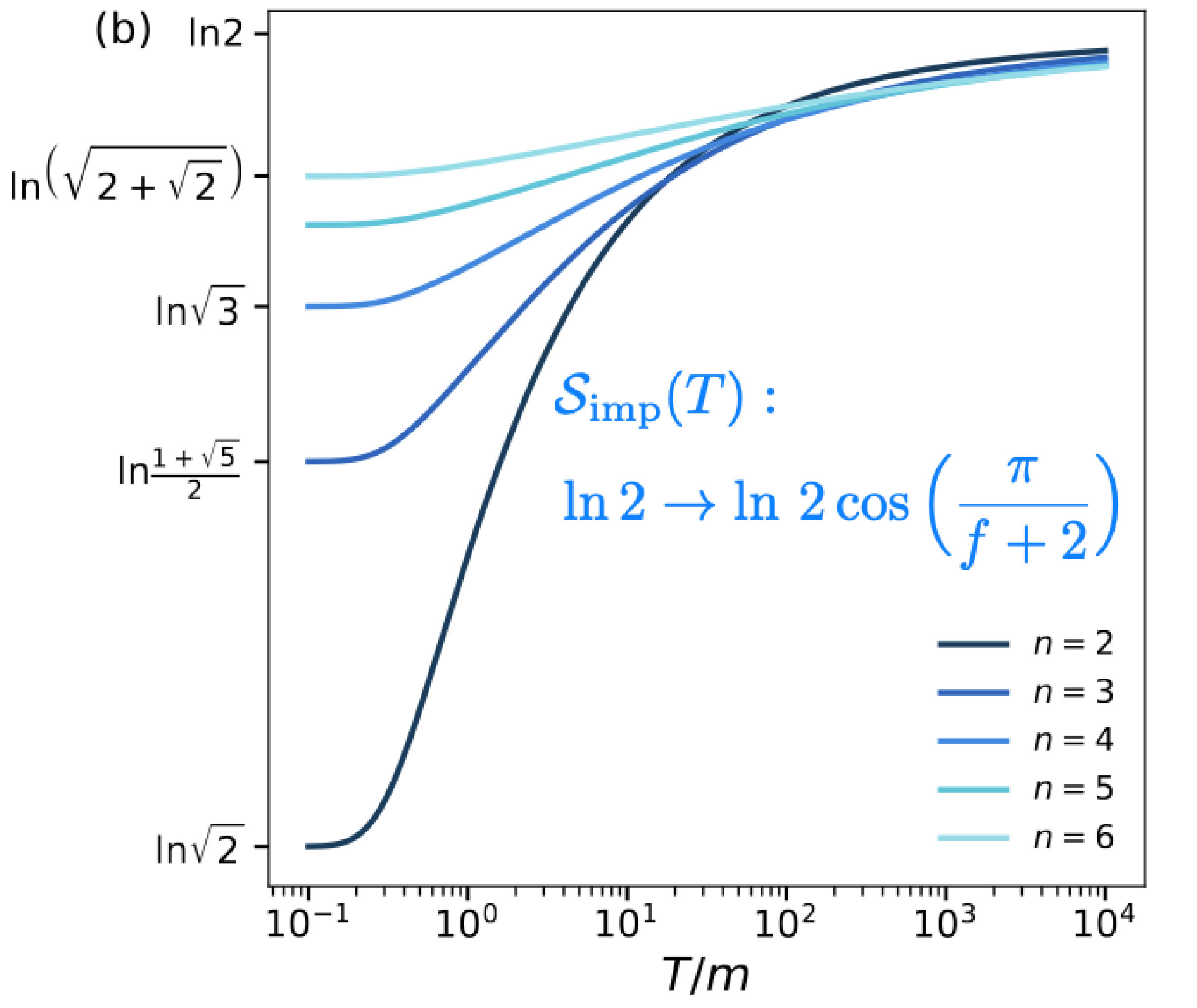


Entropy of the impurity attached to f-superconductors

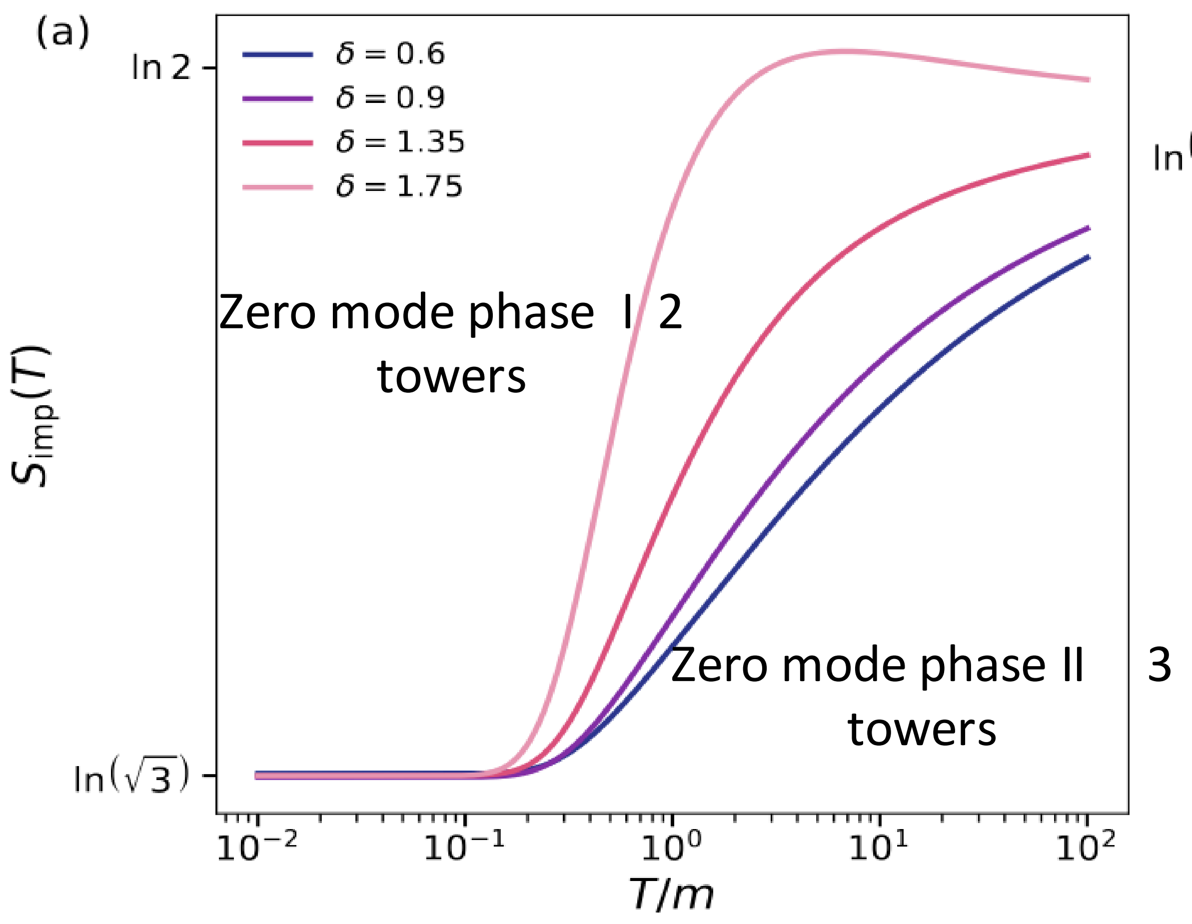
Kondo phase (6 channels, vary *d*)



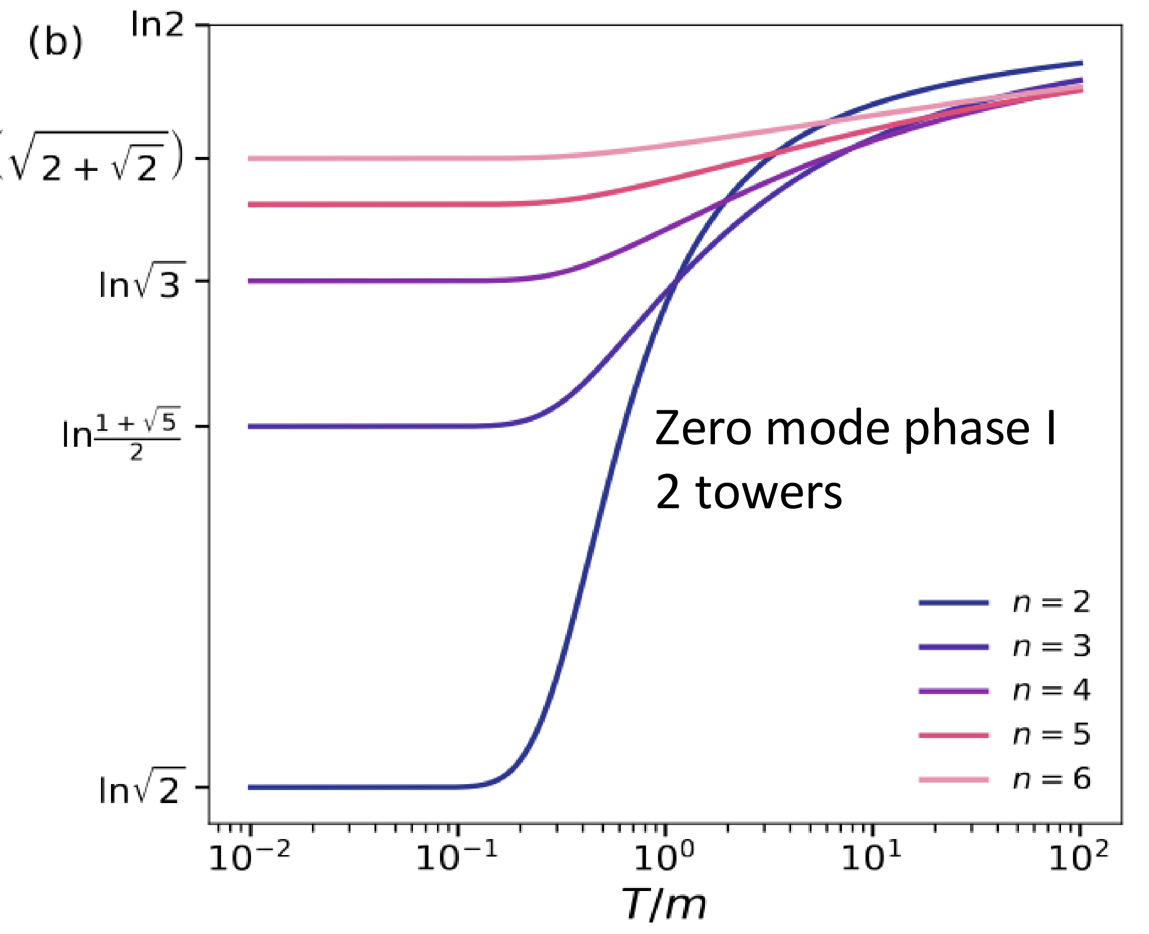
Kondo phase (d=0.25, vary *f*)



Zero mode phase I/II (4 channels, vary *d*)

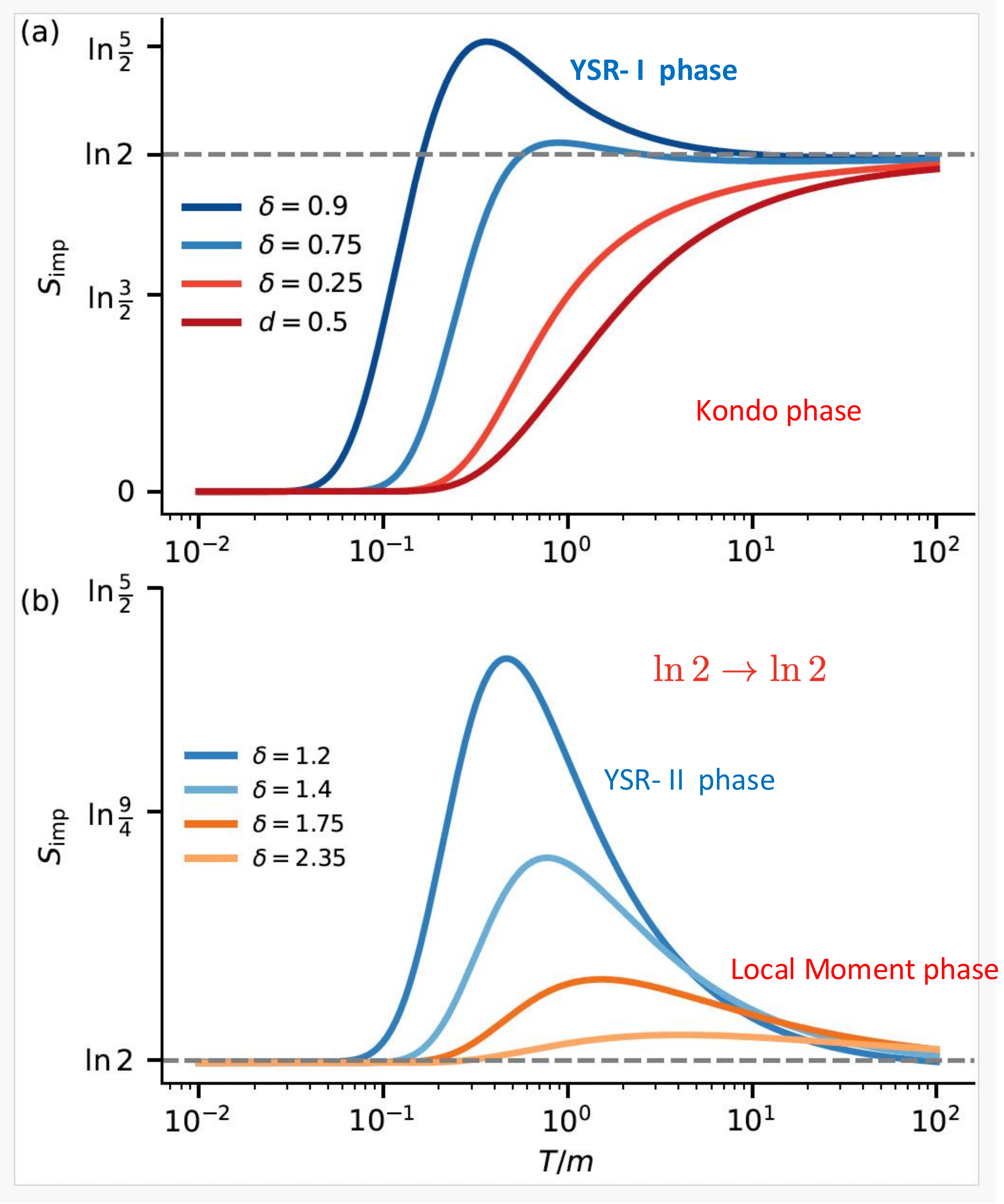


Zero mode phase I (d=0.75, vary *f*)



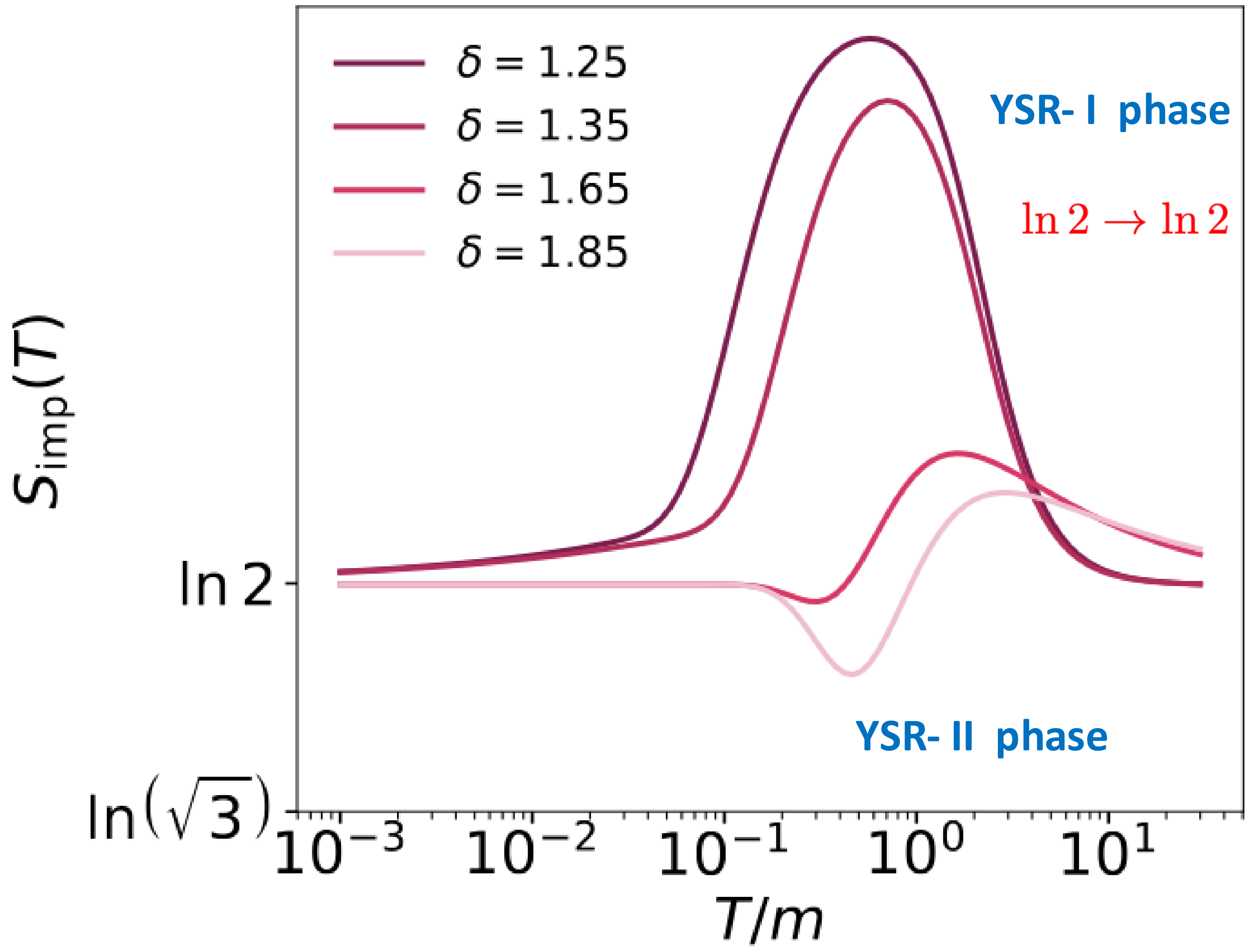
$S_{\mathrm{imp}}(T)$: The impurity entropy as function of the temperature in the various phases

Entropy of the impurity attached to one superconductor

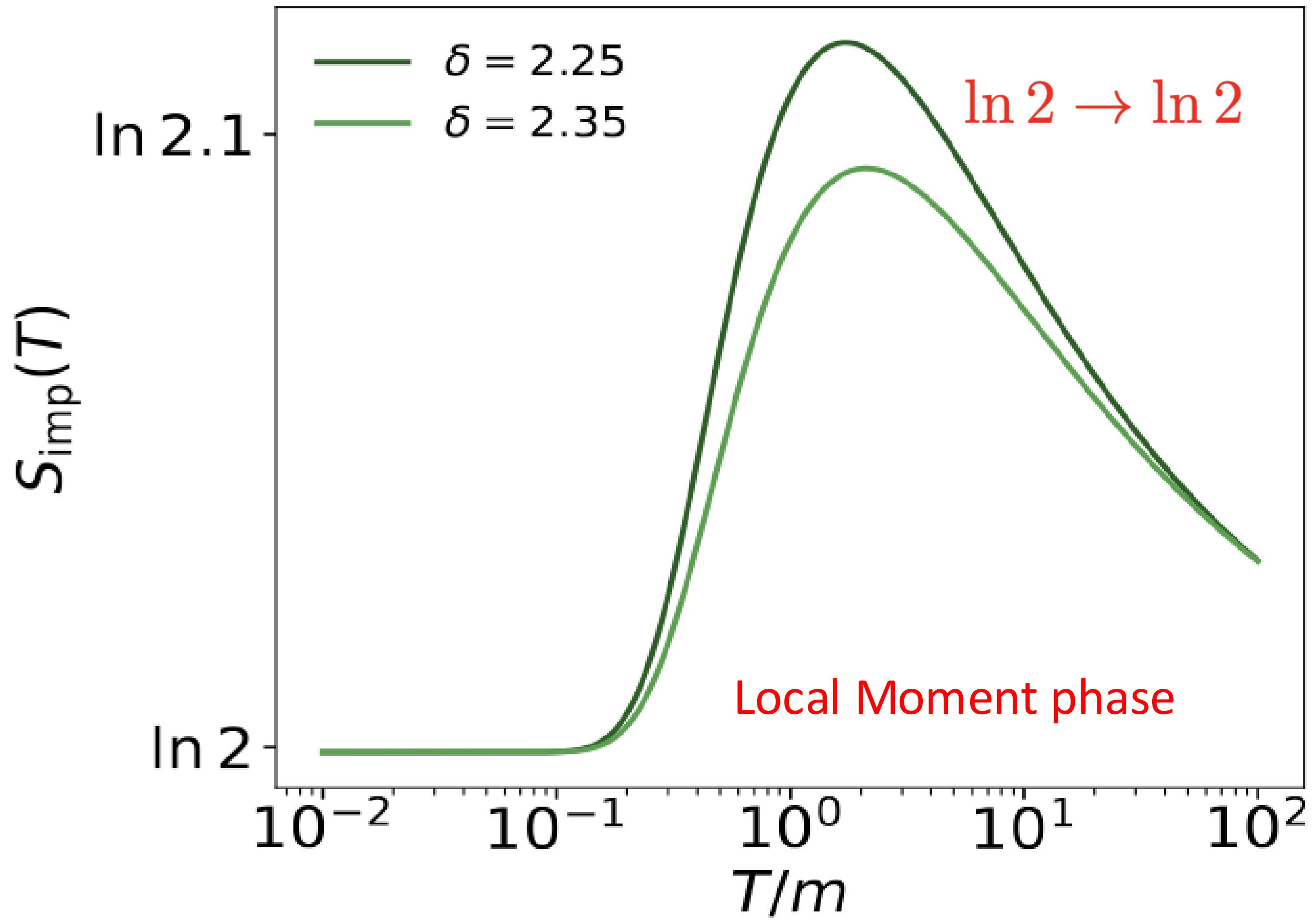


Entropy of the impurity attached to f-superconductors

YSR phase (2 channels, vary *d)*



Local moment (2 channels, vary *d)*



overshoots at

intermediate temperatures due to the presence of

boundary states, which become thermally activated

only when

$$T \sim E_\delta$$

Boundary state energy

$$E_\delta = -m\cos\left(\frac{\pi}{2}(f - 2\delta)\right).$$

The Impurity at the edge of f SC wires – The Bethe Ansatz equations

- The BA wave functions of *N*- electrons moving on the open line interacting with the impurity at the edge

-- Energy $E = \sum_j k_j$ (requires a *cut-off* - D; the coupling constants g, J depend on D, carry out renormalization)

-- Spin component $S^z = \frac{N+1}{2} - M$ *M* down spins, *N+1* up spins

- The quasi-momenta k_j are obtained from the open BC Bethe Ansatz equations (Sklyanin) where the spin momenta $\lambda_\alpha, \alpha = 1, \cdots, M$ describe the spin dynamics

$$e^{-2ik_jL} = \prod_{\upsilon=\pm} \frac{b + \upsilon\lambda_\alpha + \frac{fi}{2}}{b + \upsilon\lambda_\alpha - \frac{fi}{2}},$$

(f=1, Pasnoori, Andrei, Rylands , Azaria 2022)

$$\prod_{\upsilon=\pm} \left(\frac{\lambda_\alpha + \upsilon b + \frac{fi}{2}}{\lambda_\alpha + \upsilon b - \frac{fi}{2}} \right)^N \left(\frac{\lambda_\alpha + \upsilon d + \frac{i}{2}}{\lambda_\alpha + \upsilon d - \frac{i}{2}} \right) = \prod_{\upsilon=\pm} \prod_{\substack{\beta=1 \\ \beta\neq\alpha}}^{M} \left(\frac{\lambda_\alpha + \upsilon\lambda_\beta + i}{\lambda_\alpha + \upsilon\lambda_\beta - i} \right)$$

where $d(J,g) = \sqrt{b^2 - 2b/c - 1}$ $c = \frac{2J}{1 - 3J^2/4} \sim 2J$ $b = \frac{4 - g^2}{8g} \sim \frac{1}{2g}$

Relative strength of *J* and *g* Impurity variable bulk variable

- The combination $d(J,g) = \sqrt{b^2 - 2b/c - 1}$ is RG invariant, independent of D

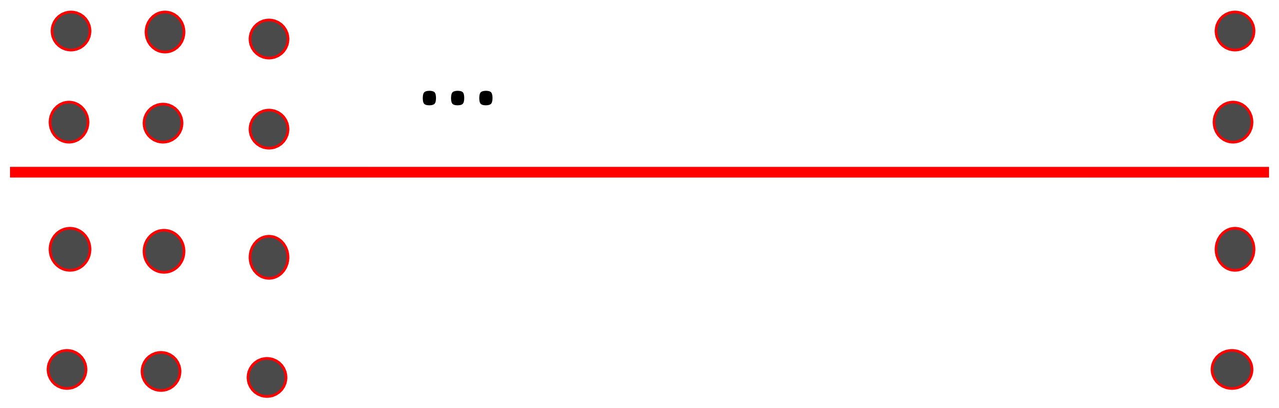
- Use to label phases

Solutions of the BA equations – Phases and towers, splitting of Hilbert space

- The solutions of the BA equations are *f*-strings

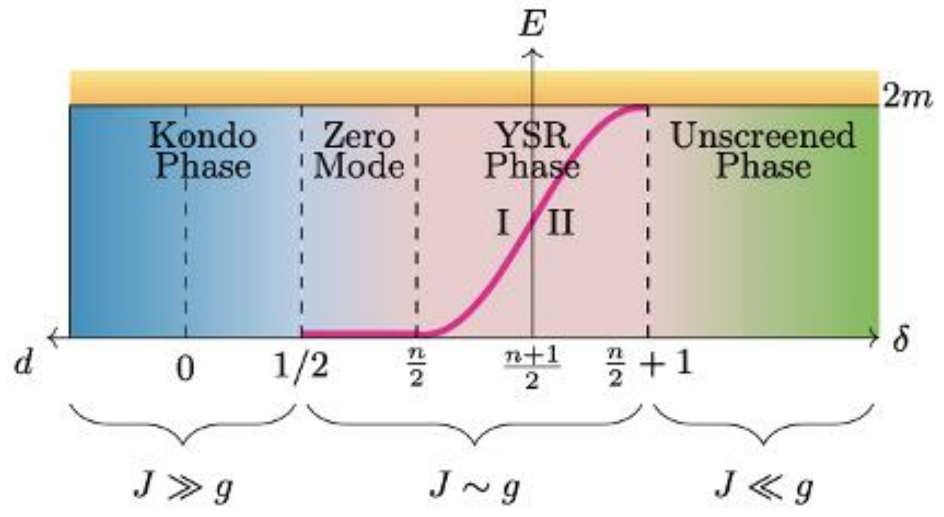
$$\left\{\lambda^{(f)}_{\alpha,j}\right\}_{j=1}^{f} = \left\{\Lambda_\alpha + \frac{i}{2}(f+1-2j)\Big| j=1,\dots,f\right\},$$

ground state of f=4 channels model



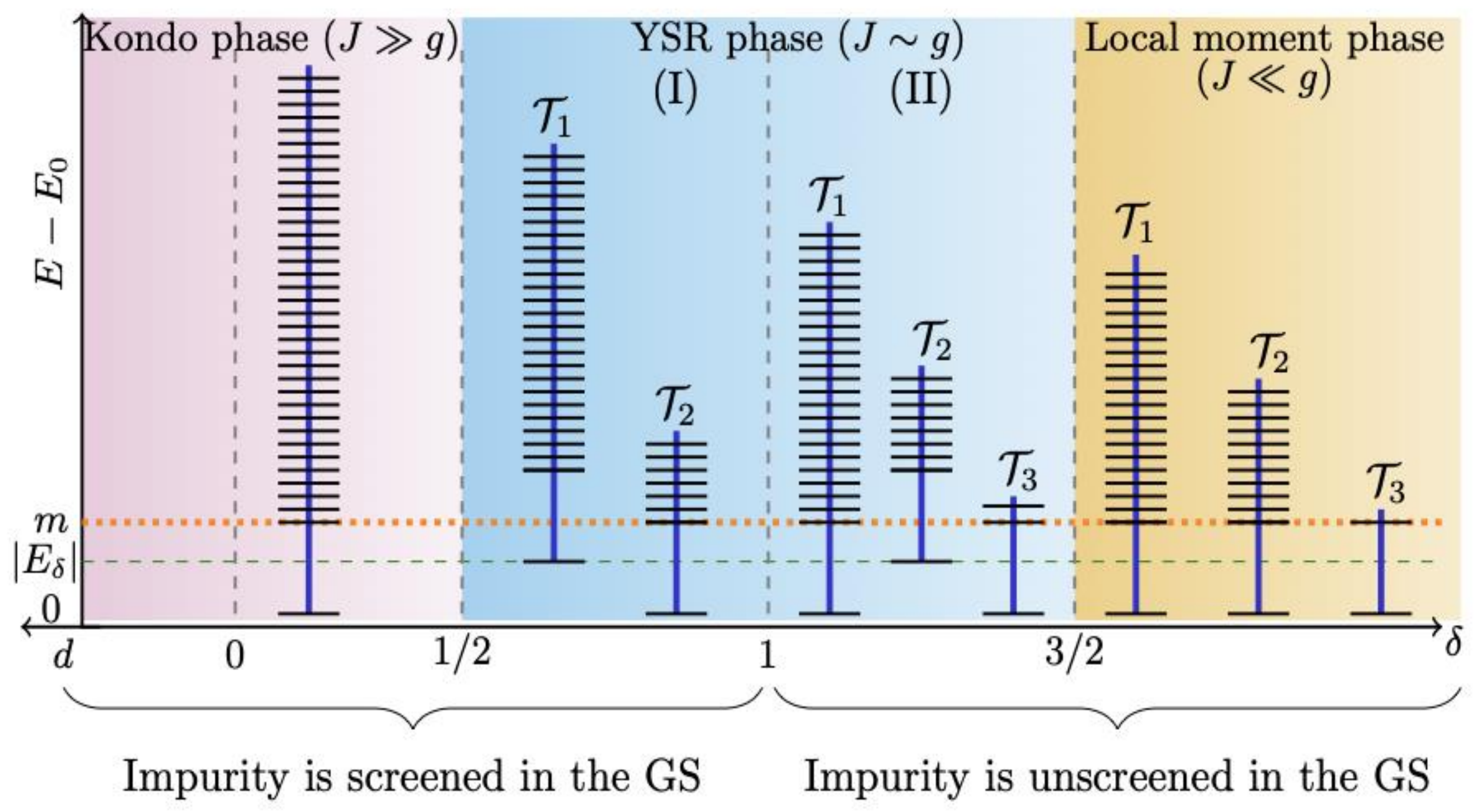
- As $d(J,g)=\sqrt{b^2-2b/c-1}$ increases beyond ½ the equations admit a new solution $\lambda_\delta = i\left(\delta - \frac{1}{2}\right)$ (boundary string solution) with midgap energy :

$$E_\delta = -m\cos\left(\frac{\pi}{2}(f-2\delta)\right).$$

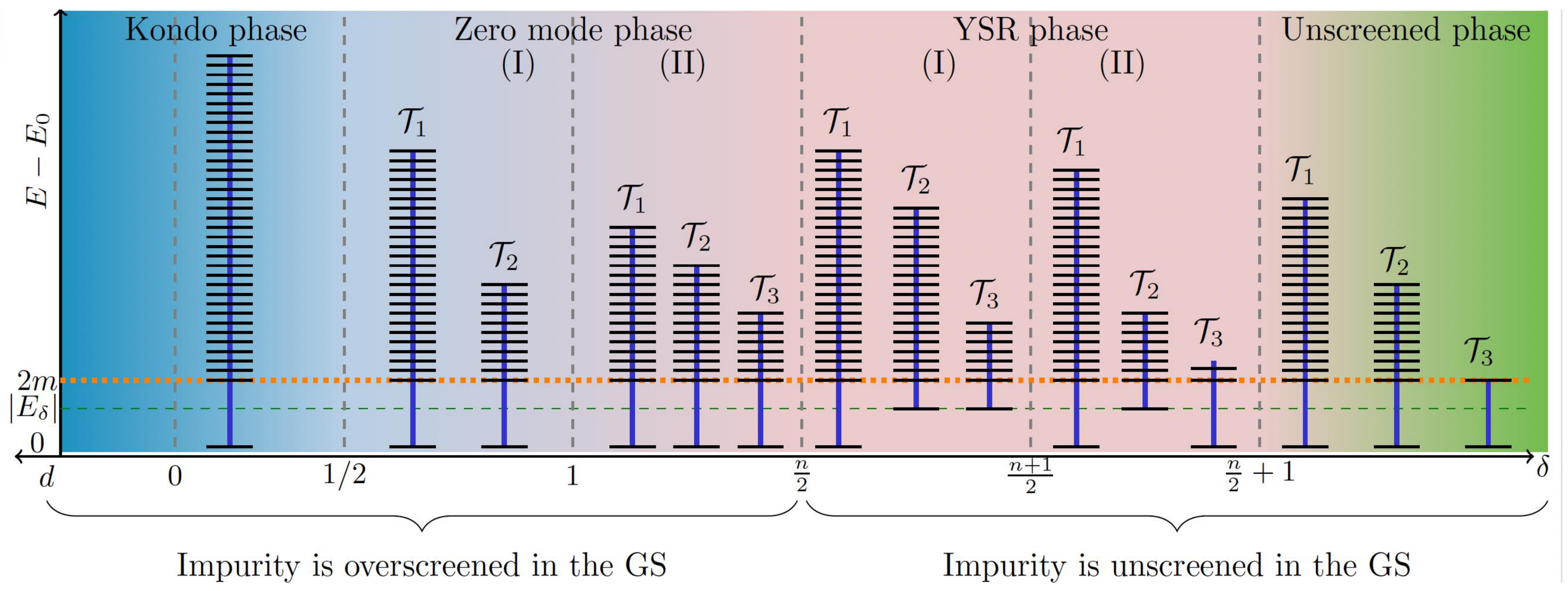


- As δ increases also higher boundary string solutions appear with $\lambda^{(p)}_{\delta,\ell} = \lambda_\delta + i\ell$ $\quad \ell = 1,\dots,p$ and $p = \lfloor \delta + \frac{1}{2} \rfloor$

Phase diagram of the single channel model



Phase diagram of the multichannel channel model



The energies of all higher boundary string solutions vanish in the thermodynamic limit, except p=1 string

- **These boundary solutions induce towers and restructure the Hilbert space**

The Thermodynamics (multichannel)

- From the solutions of the Bethe Ansatz equation one obtains the Free Energy summing over the solutions in each tower

e.g. for two towers:

$$Z = e^{-\beta F(T)} = \sum_{i=1}^{2} e^{-\beta F^{(\mathcal{T}_i)}} = e^{-\beta F_0(T)} \sum_{i=1}^{2} e^{-\beta F^{(\mathcal{T}_i)}_{\text{imp}}(T)} = e^{-\beta F_0(T)} e^{-\beta F_{\text{imp}}(T)}$$

$$\longrightarrow \quad \boxed{e^{\beta F_{\text{imp}}} = e^{\beta F^{(\mathcal{T}_1)}_{\text{imp}}} + e^{\beta F^{(\mathcal{T}_2)}_{\text{imp}}}}$$

- To carry out the summation we use the Thermodynamic Bethe Ansatz approach *(Yang and Yang 1969, Takahashi book 1999)*

- The TBA equations for $\eta_n(\lambda) = \dfrac{\sigma_n^h(\lambda)}{\sigma_n(\lambda)}$ which give the probability for an *n-string* at temperature *T*

$$\ln \eta_n(\lambda) = -\frac{m}{T} \cosh(\pi\lambda)\delta_{n,f} + \sum_{\upsilon=\pm 1} G \ln(1+\eta_{n+\upsilon})$$

BC $$\lim_{n\to\infty} \{[n+1]\ln(1+\eta_n) - [n]\ln(1+\eta_{n+1})\} = -\frac{\mu h}{T}$$

Limit values:

$$\eta_{n(T\to\infty)} = \frac{\sinh^2\left((n+1)\frac{\mu h}{T}\right)}{\sinh^2 \frac{\mu h}{T}} - 1, \quad n = 1, 2, \ldots$$

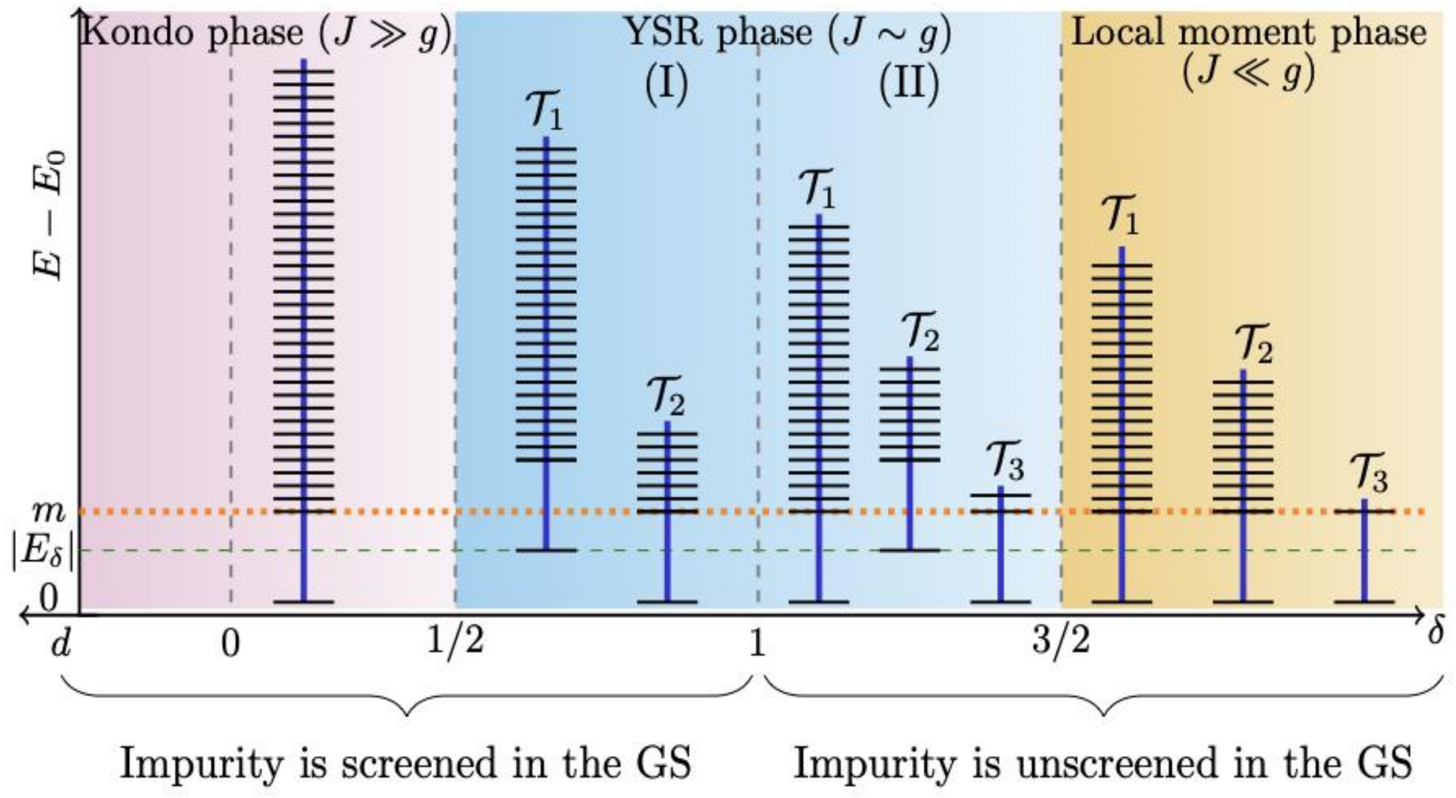
$$\eta_{n(T\to 0)} = \begin{cases} \dfrac{\sin^2[(n+1)\pi/(f+2)]}{\sin^2[\pi/(f+2)]} - 1, & \text{for } n < f \\ \dfrac{\sinh^2[(n+1-f)\mu h/T]}{\sinh^2(\mu h/T)} - 1, & \text{for } n \geq f \end{cases}$$

with $$[n]f(\nu) = \int d\lambda \frac{1}{\pi} \frac{\mathrm{n}/2}{(\mathrm{n}/2)^2 + (\nu-\lambda)^2} \mathrm{f}(\lambda) \qquad Gf(\lambda) = \int d\nu \frac{1}{2\cosh \pi(\lambda-\nu)} \mathrm{f}(\nu)$$

The Impurity Thermodynamics (*one*-channel)

- The TBA equation are the same in all phases, but the expression for the free energy in terms of η_n depends on the phase

$$e^{-\beta F_{\mathrm{imp}}(T)} = \sum_i e^{-\beta F^{(\mathcal{T}_i)}_{\mathrm{imp}}(T)}$$



Kondo phase - one tower

$$F_{\mathrm{imp}}(T) = -\frac{T}{4}\sum_{\upsilon=\pm}\int \frac{\ln(1+\eta_1)}{\cosh\left(\pi(\lambda+\upsilon d)\right)}d\lambda.$$

YSR I phase - two towers

$$F^{(\mathcal{T}_1)}_{\mathrm{imp}}(T) = |E_\delta| - \frac{T}{4}\int \mathrm{d}\lambda \sum_{\upsilon=\pm}\frac{\ln\left[1+\eta_1(\lambda)\right]}{\cosh(\pi(\lambda+\mathrm{i}\upsilon\delta))} - \frac{\mathrm{T}}{4}\int \mathrm{d}\lambda \sum_{\upsilon=\pm}\frac{\ln\left[1+\eta_2(\lambda)\right]}{\cosh(\pi(\lambda+\mathrm{i}\upsilon(\delta-\frac{1}{2})))}$$

$$F^{(\mathcal{T}_2)}_{\mathrm{imp}}(T) = -\frac{T}{4}\int \mathrm{d}\lambda \sum_{\upsilon=\pm}\frac{\ln\left[1+\eta_1(\lambda)\right]}{\cosh(\pi(\lambda+\mathrm{i}\upsilon\delta))}$$

$$F^{(\mathcal{T}_1)}_{\mathrm{imp}} = -\frac{T}{4}\sum_{\upsilon=\pm}\int \mathrm{d}\lambda\left[\frac{\ln\left(1+\eta_{\lfloor 2\delta\rfloor+1}(\lambda)\right)}{\cosh\left(\pi\left(\lambda+\frac{i\upsilon}{2}(2\delta-\lfloor 2\delta\rfloor)\right)\right)} - \frac{\ln\left(1+\eta_{\lfloor 2\delta\rfloor}(\lambda)\right)}{\cosh\left(\pi\left(\lambda+\frac{i\upsilon}{2}(\lfloor 2\delta\rfloor+1-2\delta)\right)\right)}\right]$$

YSR II phase - three towers

$$F^{(\mathcal{T}_2)}_{\mathrm{imp}} = \frac{T}{4}\sum_{\upsilon=\pm}\int \mathrm{d}\lambda\left[\frac{\ln\left(1+\eta_{\lfloor 2\delta\rfloor-1}(\lambda)\right)}{\cosh\left(\pi\left(\lambda+\frac{i\upsilon}{2}(2\delta-\lfloor 2\delta\rfloor)\right)\right)} - \frac{\ln\left(1+\eta_{\lfloor 2\delta\rfloor-2}(\lambda)\right)}{\cosh\left(\pi\left(\lambda+\frac{i\upsilon}{2}(\lfloor 2\delta\rfloor+1-2\delta)\right)\right)}\right] + E_\delta$$

$$F^{(\mathcal{T}_3)}_{\mathrm{imp}} = \frac{T}{4}\sum_{\upsilon=\pm}\int \mathrm{d}\lambda\left[\frac{\ln\left(1+\eta_{\lfloor 2\delta\rfloor}(\lambda)\right)}{\cosh\left(\pi\left(\lambda+\frac{i\upsilon}{2}(\lfloor 2\delta\rfloor+1-2\delta)\right)\right)} + \frac{\ln\left(1+\eta_{\lfloor 2\delta\rfloor-1}(\lambda)\right)}{\cosh\left(\pi\left(\lambda+\frac{i\upsilon}{2}(2\delta-\lfloor 2\delta\rfloor)\right)\right)}\right]$$

Local moment phase– three towers

Phases and Excitation Towers : Kondo phase (one channel)

- **Impurity physics** falls into various phases labeled by the RG invariant $d(J,g) = \sqrt{b^2 - 2b/c - 1}$

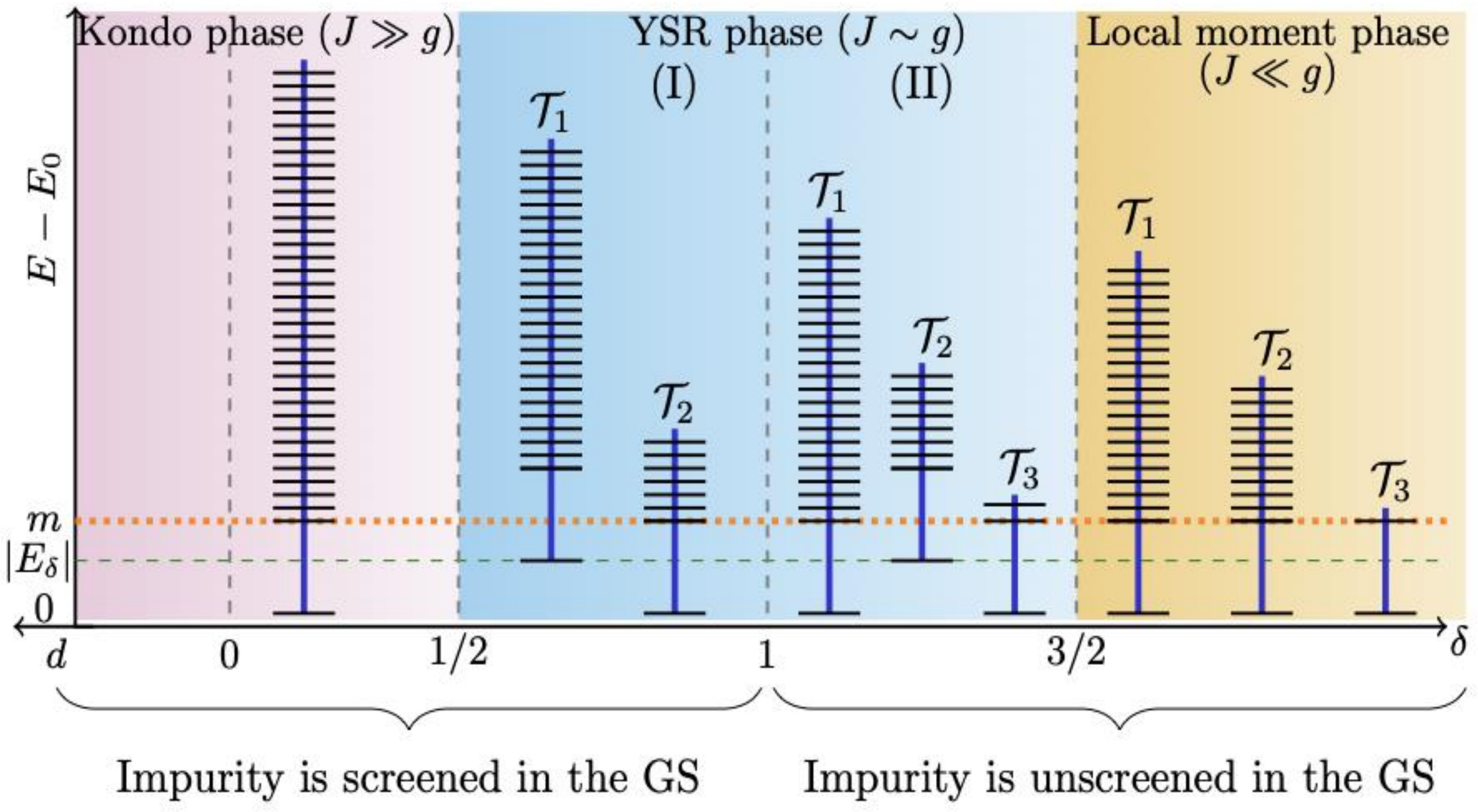
  It can be real or imaginary $d = i\delta$ It determines relative strength of *g* and *J*

The Kondo phase: d is real or $\delta \in [0, 1/2)$

The ground state $|K\rangle$ consisting of $(N+1)/2$ real roots

The Hilbert space of excitations is spanned by ***spinons*** - ***gapped*** spin ½ excitations (holes and strings) over the ground state $m = D \sinh[1/\sinh(\pi b)] \to De^{-\pi b}$

The impurity in the ground state is screened by the cloud of spinons (many body effect)

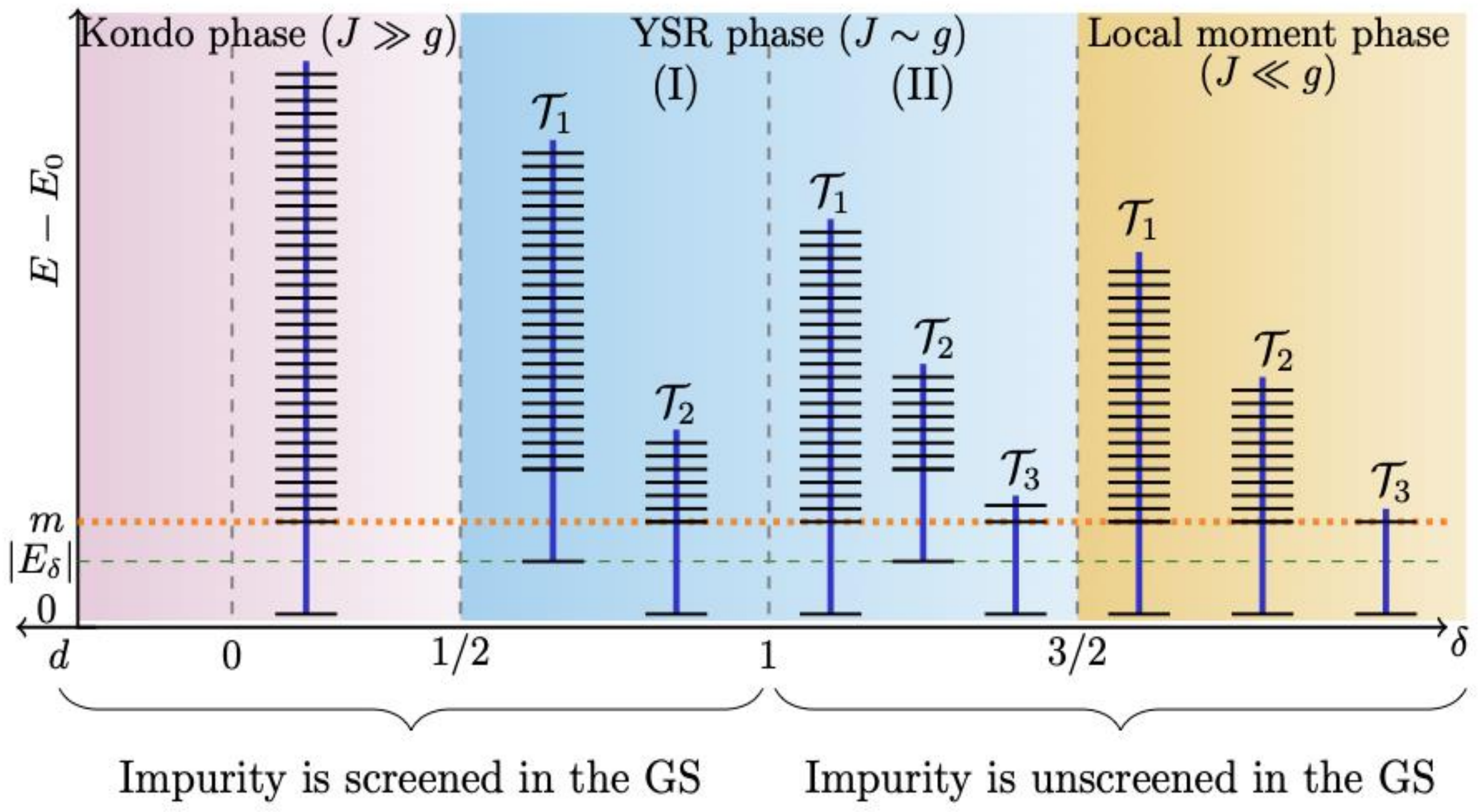


-- The description of the crossover between the asymptotically free impurity at the UV and the screened impurity requires the solution of the thermodynamic Bethe Ansatz equations

Impurity Entropy: Kondo phase (one channel)

The kondo phase:

All eigenstates are organized into a single tower of excitations made by adding of holes and bulk string solutions on top of the ground state.



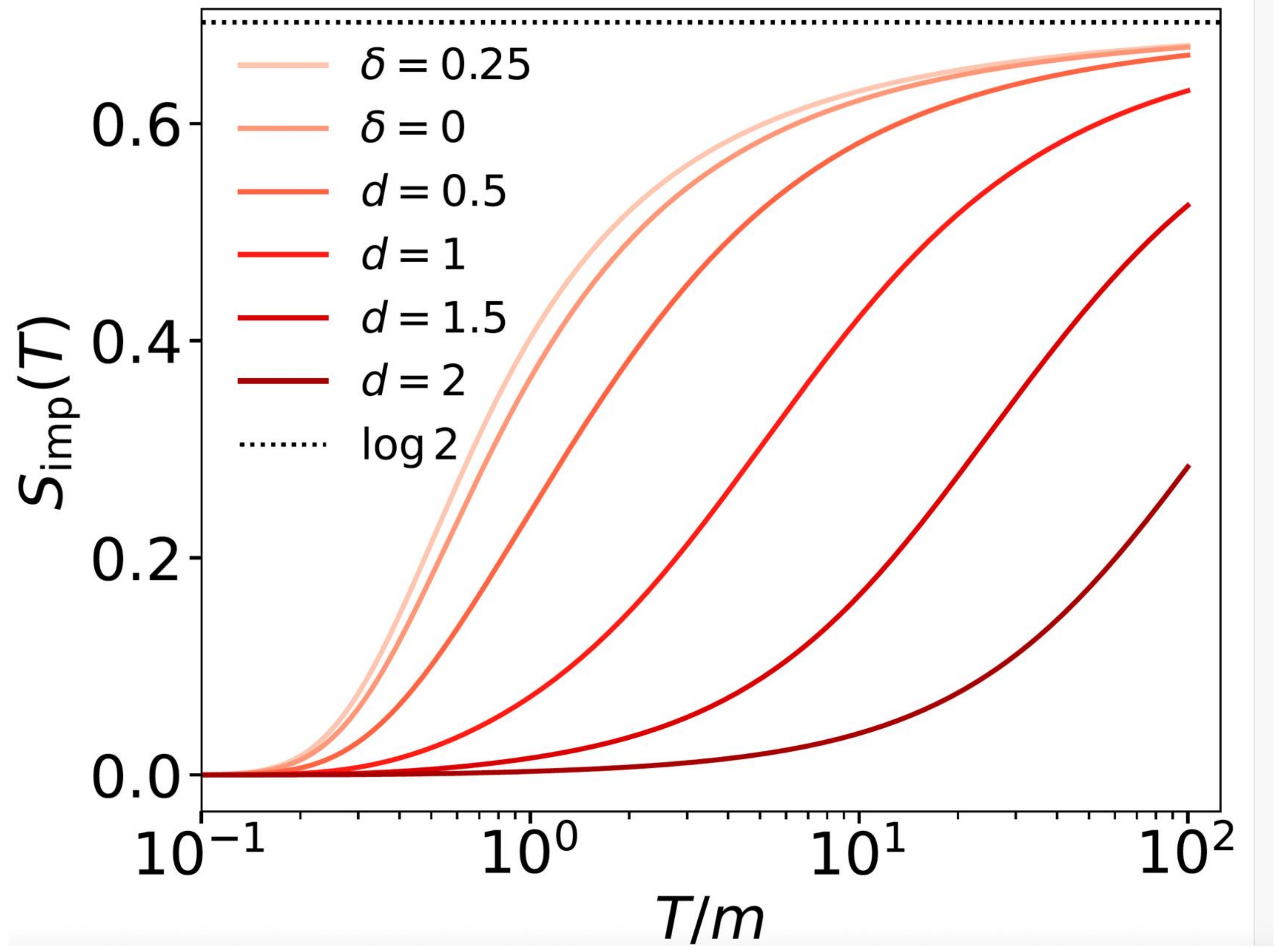
$$F_{\mathrm{imp}}(T) = -\frac{T}{4}\sum_{v=\pm}\int \frac{\ln(1+\eta_1)}{\cosh\left(\pi(\lambda+vd)\right)}d\lambda.$$

$$S_{\mathrm{imp}}(T) = -\partial_T F_{\mathrm{imp}}(T)$$

-- A new scale emerges $T_K = f(d)m$, with $f(d) = \sqrt{1+\cosh\pi d}$

For $d \gg 1$ (i.e. $J \gg g$ deep in the Kondo regime) $f(d) = \longrightarrow e^{-\pi/2J}$

-- As temperature is lowered S_{imp} decreases monotonically from $\ln 2$ (weak coupling) to 0 (strong coupling).

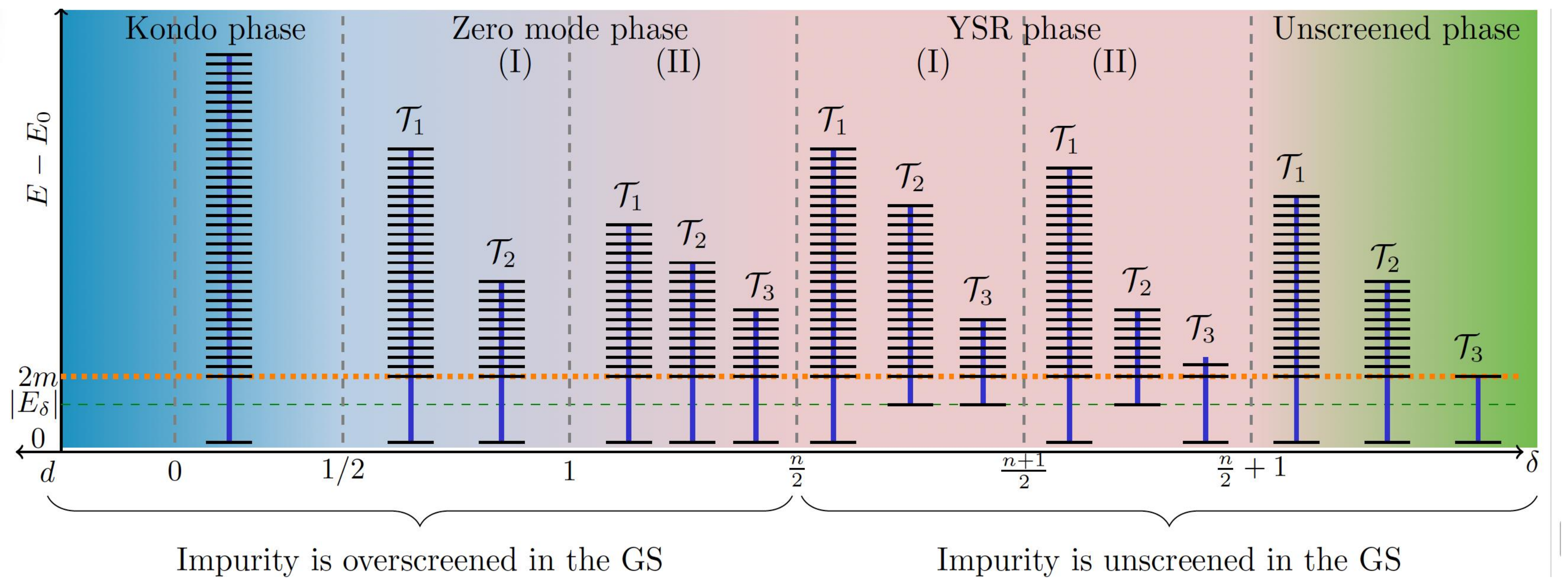


-- The same low-T critical behavior as the conventional Kondo problem

-- This monotonic behavior persists even though the ***g***-theorem does not apply in a gapped bulk

Scale of crossover $T_K = m\sqrt{1+\cosh^2\pi d} \underset{J\gg g}{\rightarrow} De^{-\pi/2J}$

Impurity Entropy: Kondo phase (Multichannel)



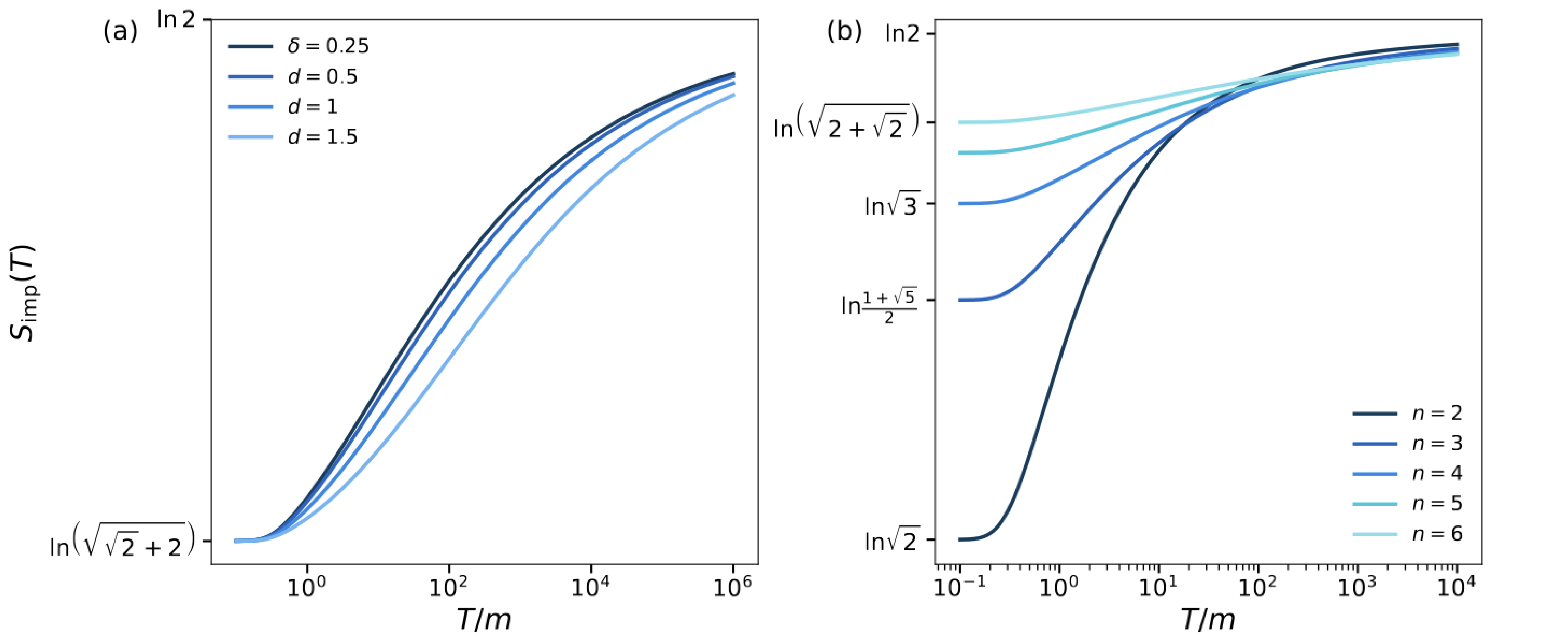
The multichannel kondo phase:

All eigenstates are organized into a single tower of excitations made by adding of holes and bulk string solutions on top of the ground state.

$$F_{\text{imp}}(T) = -\frac{T}{4}\sum_{\upsilon=\pm}\int \frac{\ln(1+\eta_1)}{\cosh\left(\pi(\lambda+\upsilon d)\right)}d\lambda.$$

$$S_{\text{imp}}(T) = -\partial_T F_{\text{imp}}(T)$$

Kondo phase (6 channels, vary *d*) Kondo phase (d=0.25, vary *f*)



-- As temperature is lowered S_{imp} decreases monotonically from $\ln 2$ (weak coupling) to *f*-dependent value $\ln\, 2\cos\left(\frac{\pi}{f+2}\right)$

--The same low-*T* critical behavior as the conformal multichannel Kondo problem

-- This monotonic behavior persists even though the ***g***-theorem does not apply in a gapped bulk

Scale of crossover $T_K = m\sqrt{1+\cosh^2 \pi d} \underset{J \gg g}{\rightarrow} De^{-\pi/2J}$

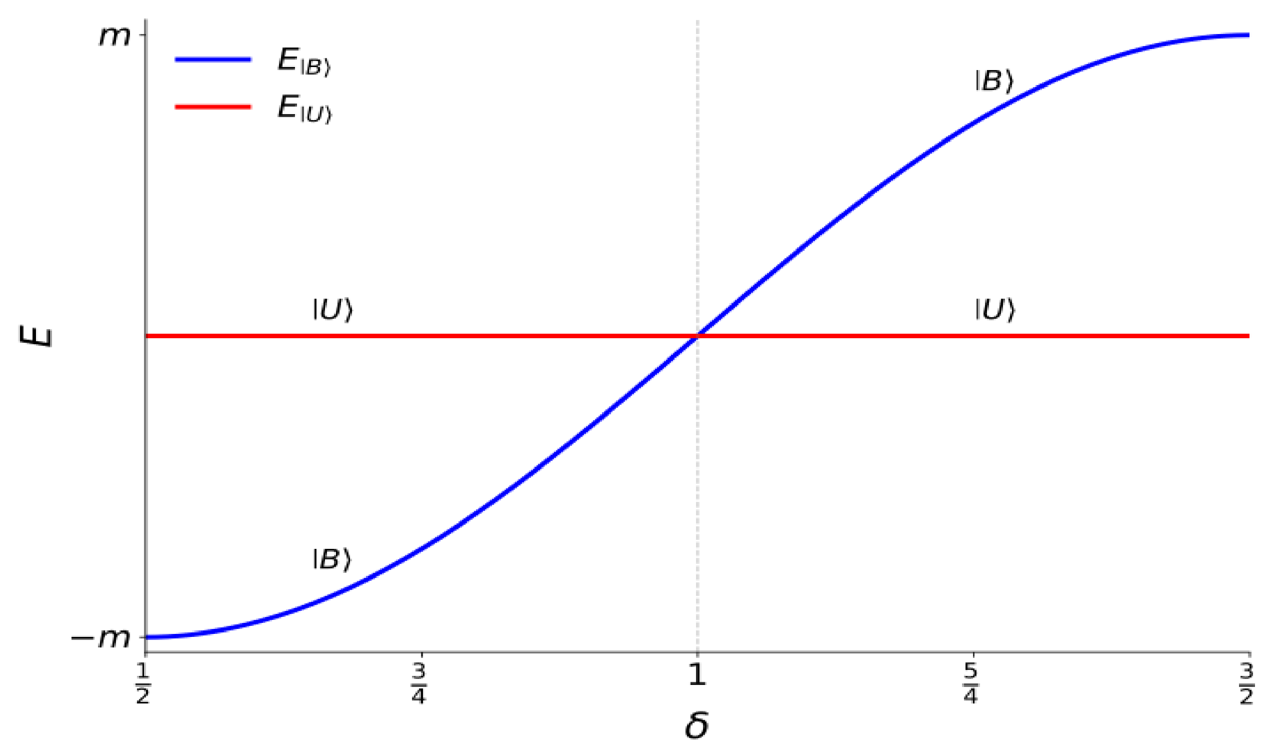
Phases and Excitation Towers (one channel)

ii. <u>The YSR-I Phase</u> $\delta \in [1/2, 1]$ — δ determines relative strength of *g* and *J*

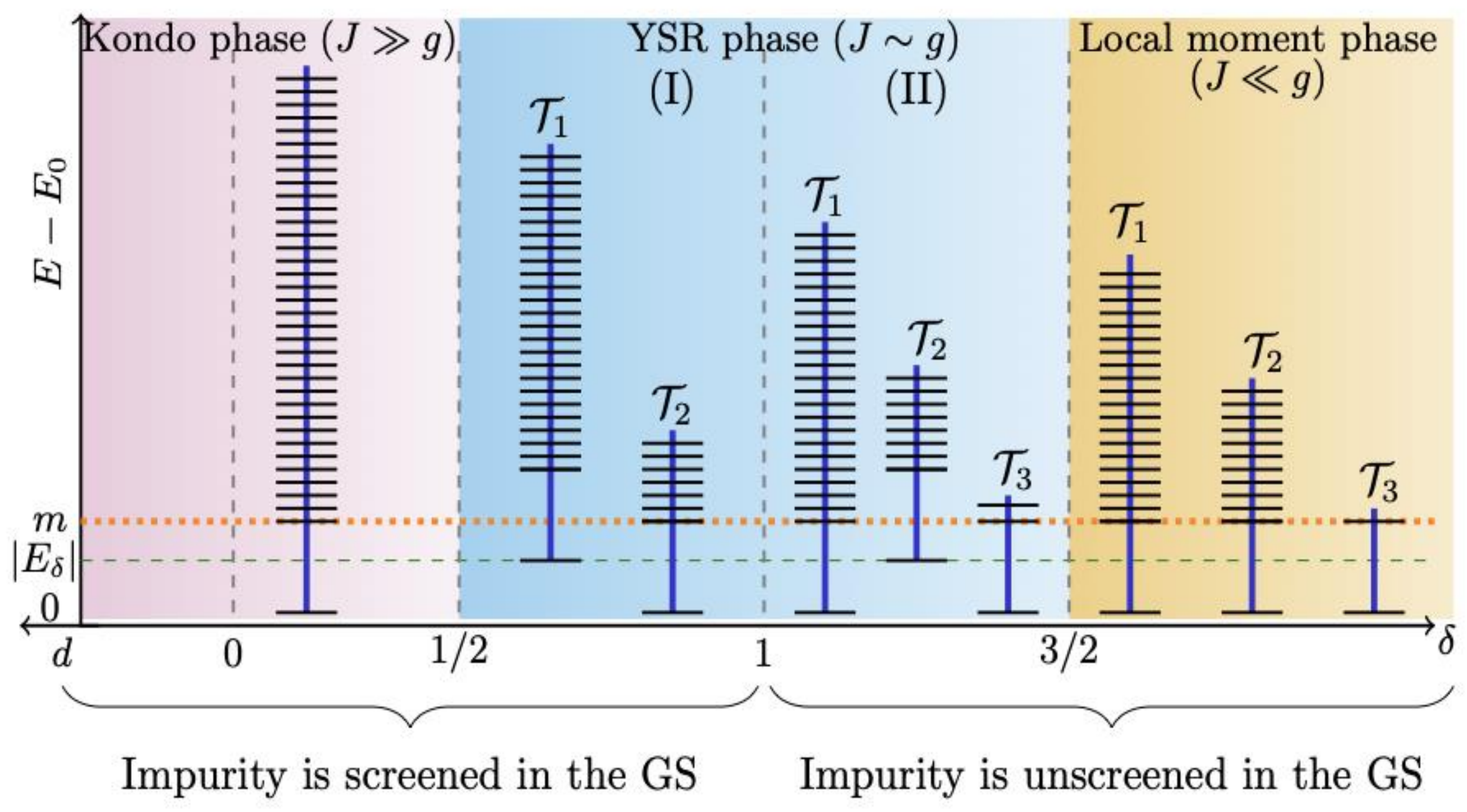
A purely imaginary boundary root appears $\lambda_\delta = i(\delta - \frac{1}{2})$

The *bound state* lies inside the gap with energy $E_\delta = -m\sin(\pi\delta)$

This BS can be filled or unfilled



δ



Tower $\mathcal{T}_1$ built of excitations over ground state $|U\rangle$ (all real roots, bound state unfilled). Tower $\mathcal{T}_1$ contains ¾ of all states

Tower $\mathcal{T}_2$ built of excitations over ground state $|B\rangle$ (all real roots, bound state filled). Tower $\mathcal{T}_2$ contains ¼ of all states

- Tower $\mathcal{T}_1$ is lifted by E_δ w.r.t tower $\mathcal{T}_2$

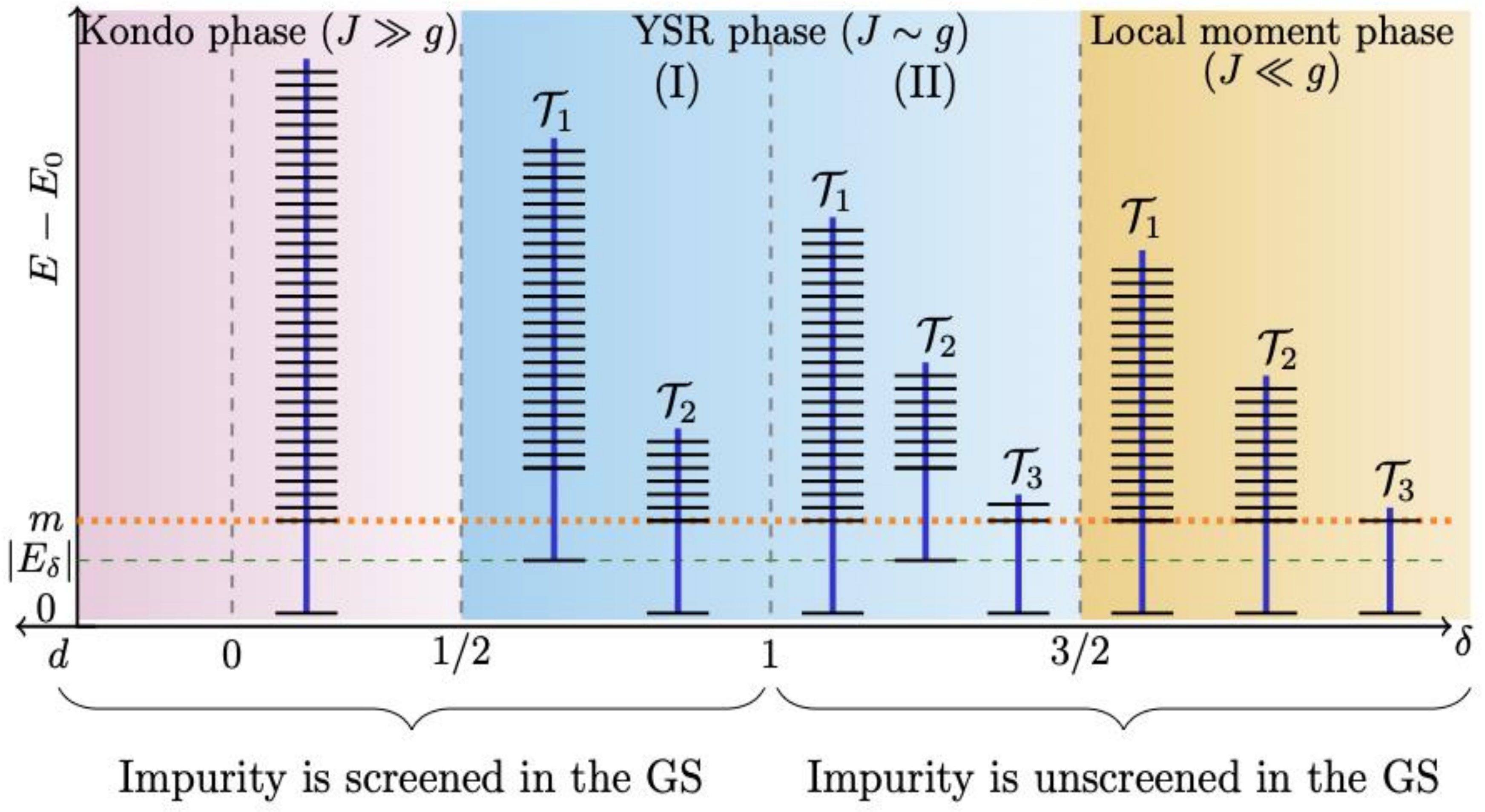
Free Energy: YSR-I phase (one channel)

The YSR-I phase:

- A boundary bound-state appears, it can be filled or not.
- The spectrum divides into two distinct excitation towers built over and $|U\rangle$ $|B\rangle$

$$Z = e^{-\beta F(T)} = \sum_{i=1}^{2} e^{-\beta F^{(\mathcal{T}_i)}} = e^{-\beta F_0(T)} \sum_{i=1}^{2} e^{-\beta F^{(\mathcal{T}_i)}_{\text{imp}}(T)} = e^{-\beta F_0(T)} e^{-\beta F_{\text{imp}}(T)}$$

$$\longrightarrow \quad \boxed{e^{\beta F_{\text{imp}}} = e^{\beta F^{(\mathcal{T}_1)}_{\text{imp}}} + e^{\beta F^{(\mathcal{T}_2)}_{\text{imp}}}}$$



with

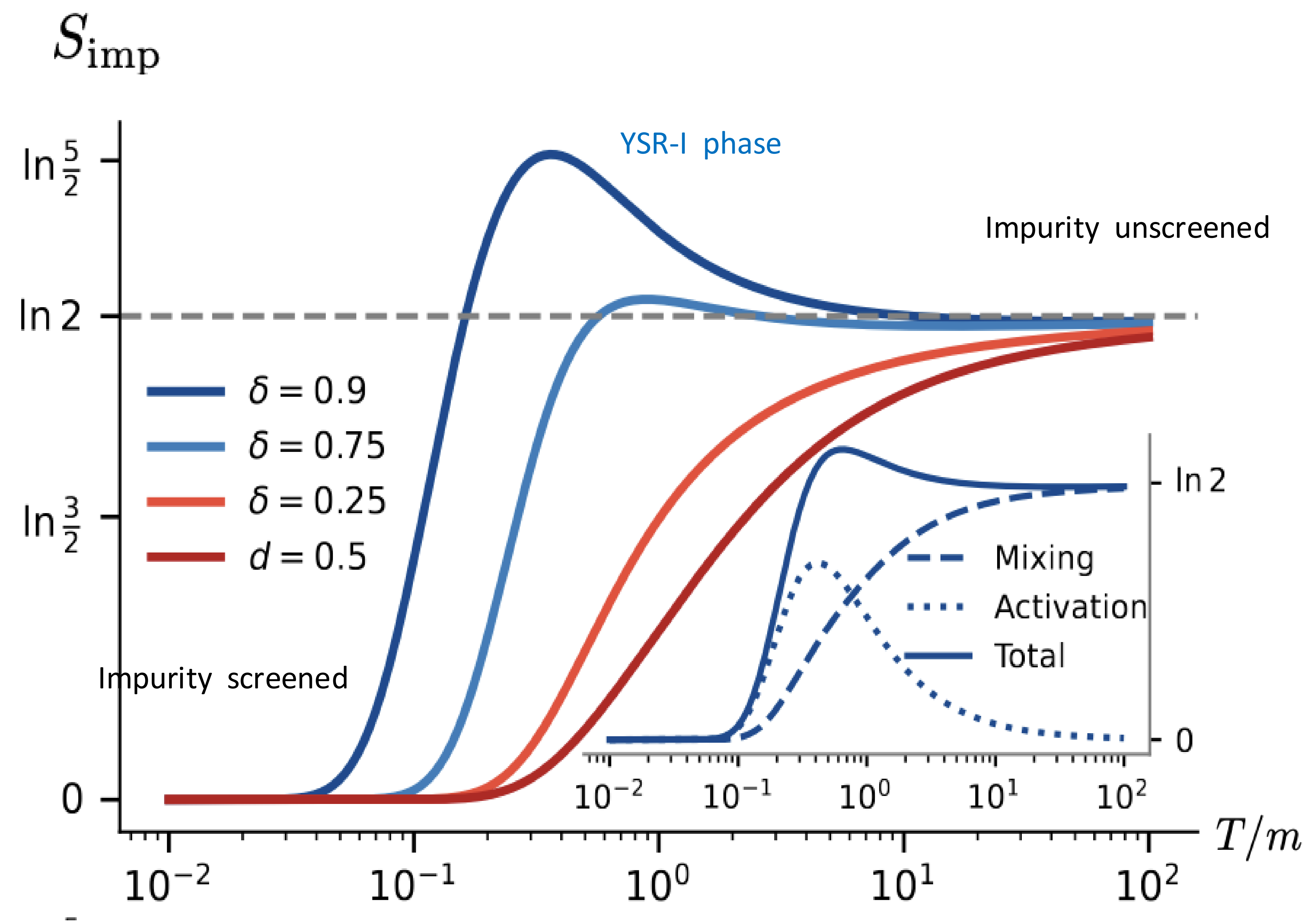
$$F^{(\mathcal{T}_1)}_{\text{imp}} = |E_\delta| - \frac{T}{4}\int \mathrm{d}\lambda \sum_{\upsilon=\pm} \frac{\ln\left[1+\eta_1(\lambda)\right]}{\cosh(\pi(\lambda + \mathrm{i}\upsilon\delta))} - \frac{\mathrm{T}}{4}\int \mathrm{d}\lambda \sum_{\upsilon=\pm} \frac{\ln\left[1+\eta_2(\lambda)\right]}{\cosh(\pi(\lambda + \mathrm{i}\upsilon(\delta - \frac{1}{2})))}$$

$$F^{(\mathcal{T}_2)}_{\text{imp}} = -\frac{T}{4}\int \mathrm{d}\lambda \sum_{\upsilon=\pm} \frac{\ln\left[1+\eta_1(\lambda)\right]}{\cosh(\pi(\lambda + \mathrm{i}\upsilon\delta))}$$

Impurity Entropy: *YSR-I* phase (one channel)

- Impurity entropy $S_{\mathrm{imp}}(T) = -\partial_T F_{\mathrm{imp}}(T)$ in the YSR-I phase phase (blue shades) $\delta = 0.75, 0.9$

$S_{\mathrm{imp}}(T)$ is non-monotonic with a bump at $T \sim E_\delta$



- Where is the bump coming from?

Impurity free energy $e^{\beta F_{\mathrm{imp}}} = e^{\beta F^{(\mathcal{T}_1)}_{\mathrm{imp}}} + e^{\beta F^{(\mathcal{T}_2)}_{\mathrm{imp}}}$

Impurity Entropy $S_{\mathrm{imp}}(T) = -\partial_T F_{\mathrm{imp}} = \ln(\mathcal{Z}) + \dfrac{|E_\delta|}{T}\,\dfrac{e^{S^{(\mathcal{T}_1)}_{\mathrm{imp}} - \beta|E_\delta|}}{\mathcal{Z}}$

mixing term

activation term

with $\mathcal{Z} = e^{S^{(\mathcal{T}_1)}_{\mathrm{imp}} - \beta|E_\delta|} + e^{S^{(\mathcal{T}_2)}_{\mathrm{imp}}}$

- *Mixing term* increases smoothly from 0 to ln 2 as follows from limits

$$S^{(\mathcal{T}_2)}_{\mathrm{imp}}(0) = 0, \quad S^{(\mathcal{T}_2)}_{\mathrm{imp}}(\infty) = -\ln 2, \quad S^{(\mathcal{T}_1)}_{\mathrm{imp}}(0) = \ln 2, \quad S^{(\mathcal{T}_1)}_{\mathrm{imp}}(\infty) = \ln\frac{3}{2}$$

- *Activation term* vanishes for $T \ll E_\delta$ and $T \gg E_\delta$ but peaks at $T \sim E_\delta$ when the YSR bound state becomes thermally accessible.

- The impurity induces a midgap bound state whose thermal population produces a transient entropy bump near its energy scale

Phases and Excitation Towers: *YSR II* Phase (one channel)

The YSR-II phase: $\delta \in [1, 3/2]$

Higher boundary strings appear

$$\lambda^{(p)}_{\delta,\ell} = \lambda_\delta + i\ell,\ \ell = 1,\dots,p \ \text{ and } \ p = \lfloor \delta + \frac{1}{2} \rfloor$$

$\lambda^{(p=1)}_{\delta,\ell}$ energy $E_\delta = m\sin(\pi\delta)$ for $\delta \in [1, 3/2]$

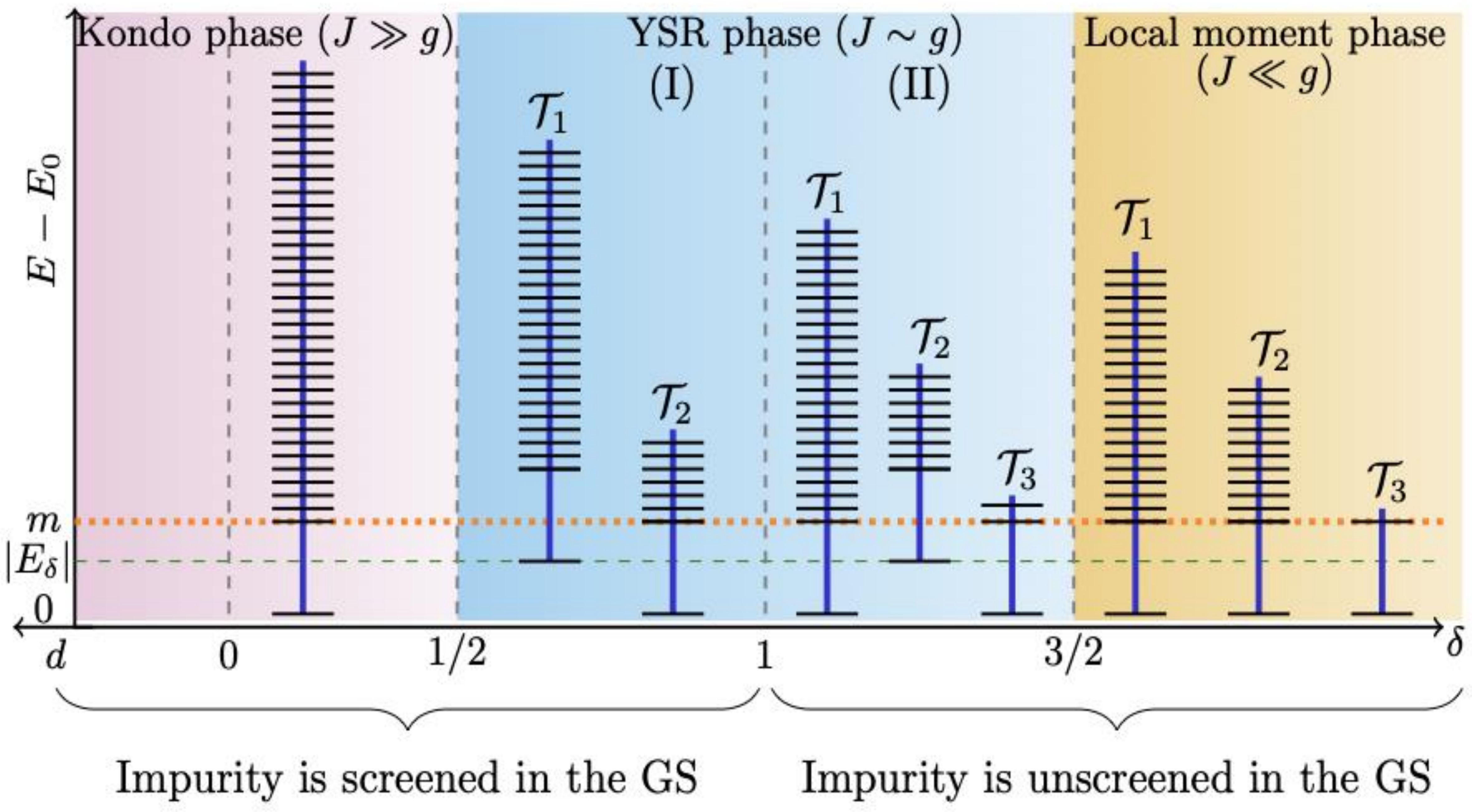
$\lambda^{(p)}_{\delta,\ell}$ energy vanishes $\delta > 3/2$

- Hilbert Space splits into three towers:

$\mathcal{T}_1$ built on $|U\rangle$(real roots) contains 2/3 of the states

$\mathcal{T}_2$ built on $|B\rangle$(real roots, λ_δ) contains 1/4 of the states

$\mathcal{T}_3$ built on $|\tilde{B}\rangle$(real roots, λ_δ and the boundary string $\lambda^{(p=1)}_{\delta,\ell}$) contains 1/12 of the states



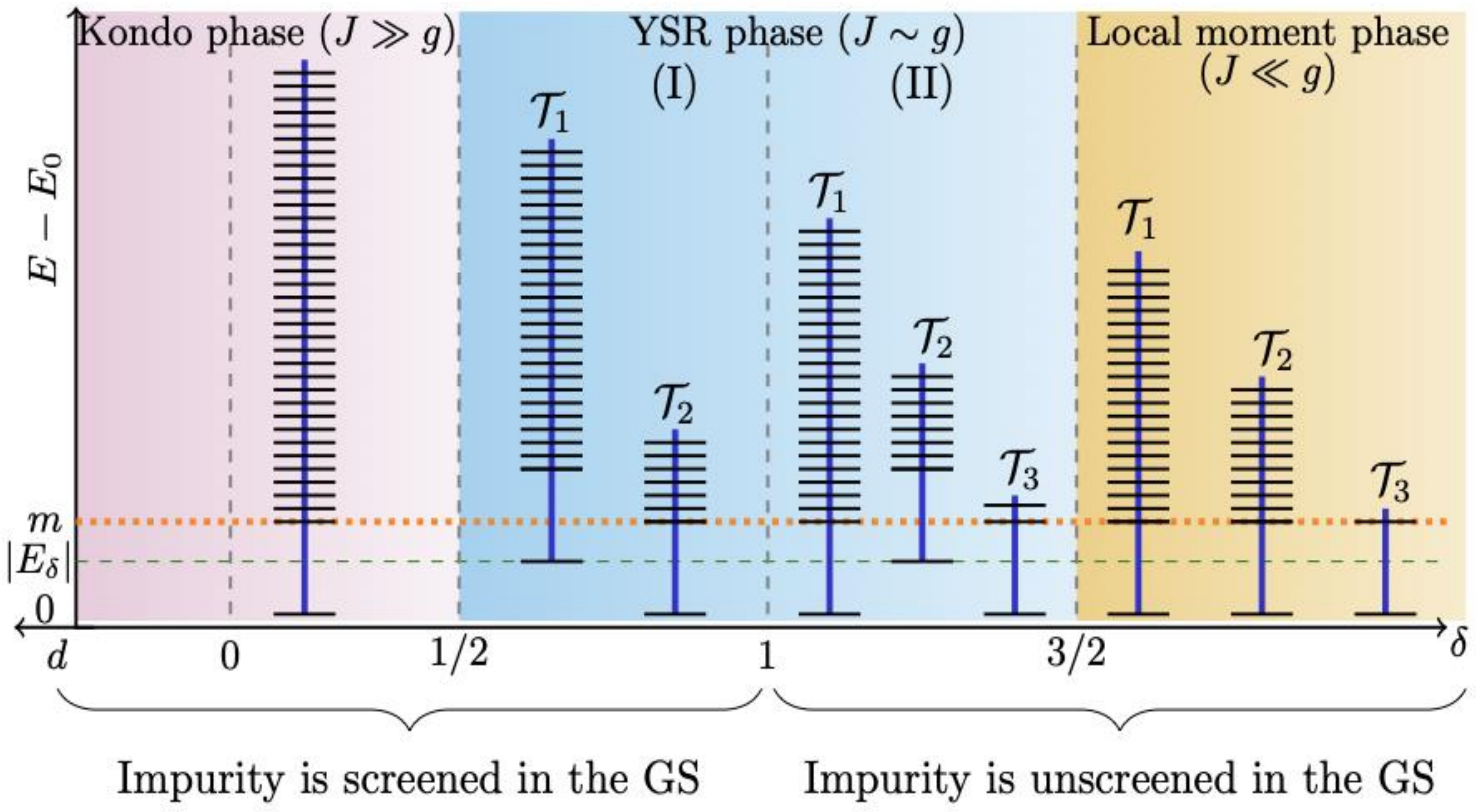
Note: the sign of the energy of the boundary string changes at delta=1.

- The fundamental boundary root $\lambda_\delta = i(\delta - \frac{1}{2})$ carries positive energy $E_\delta = -m\sin(\pi\delta)$, the higher–order boundary string $\lambda^{(p=1)}_{\delta,\ell}$ has energy $E_\delta = m\sin(\pi\delta)$ so tower $\mathcal{T}_1$ is lifted and $\mathcal{T}_3$ is not

Free Energy: **The *YSR-II* phase (one channel)**

The YSR-II phase

The eigenstates fall into three distinct towers of excitations built over $|U\rangle$, $|B\rangle$, $|\tilde{B}\rangle$



$$e^{-\beta F_{\mathrm{imp}}(T)} = \sum_{i=1}^{3} e^{-\beta F_{\mathrm{imp}}^{(\mathcal{T}_i)}(T)}$$

with

$$F_{\mathrm{imp}}^{(\mathcal{T}_1)} = -\frac{T}{4}\sum_{\upsilon=\pm}\int \mathrm{d}\lambda \left[\frac{\ln\left(1+\eta_{\lfloor 2\delta\rfloor+1}(\lambda)\right)}{\cosh\left(\pi\left(\lambda+\frac{i\upsilon}{2}(2\delta-\lfloor 2\delta\rfloor)\right)\right)} - \frac{\ln\left(1+\eta_{\lfloor 2\delta\rfloor}(\lambda)\right)}{\cosh\left(\pi\left(\lambda+\frac{i\upsilon}{2}(\lfloor 2\delta\rfloor+1-2\delta)\right)\right)}\right]$$

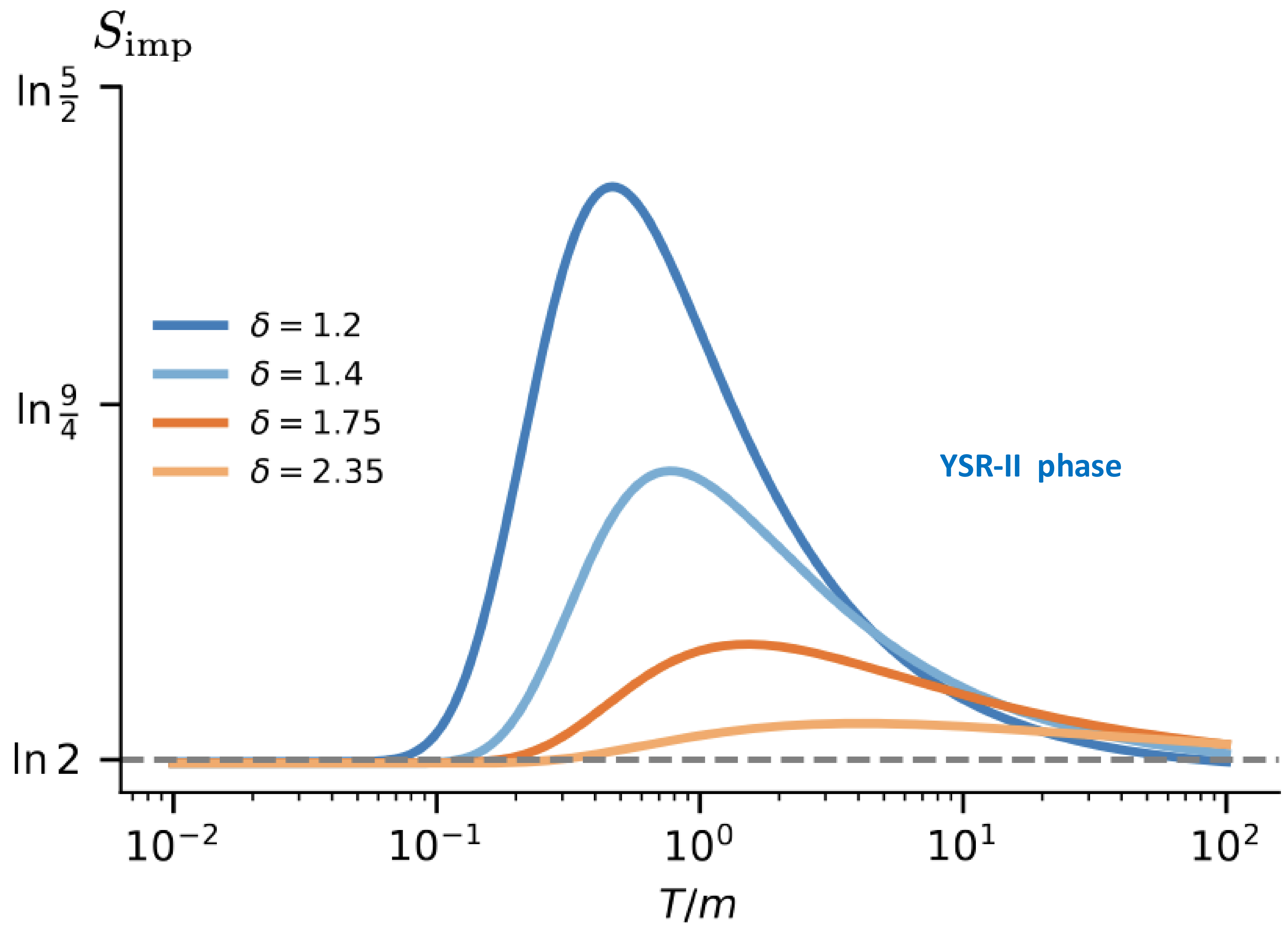
$$F_{\mathrm{imp}}^{(\mathcal{T}_2)} = \frac{T}{4}\sum_{\upsilon=\pm}\int \mathrm{d}\lambda \left[\frac{\ln\left(1+\eta_{\lfloor 2\delta\rfloor-1}(\lambda)\right)}{\cosh\left(\pi\left(\lambda+\frac{i\upsilon}{2}(2\delta-\lfloor 2\delta\rfloor)\right)\right)} - \frac{\ln\left(1+\eta_{\lfloor 2\delta\rfloor-2}(\lambda)\right)}{\cosh\left(\pi\left(\lambda+\frac{i\upsilon}{2}(\lfloor 2\delta\rfloor+1-2\delta)\right)\right)}\right] + E_\delta$$

$$F_{\mathrm{imp}}^{(\mathcal{T}_3)} = \frac{T}{4}\sum_{\upsilon=\pm}\int \mathrm{d}\lambda \left[\frac{\ln\left(1+\eta_{\lfloor 2\delta\rfloor}(\lambda)\right)}{\cosh\left(\pi\left(\lambda+\frac{i\upsilon}{2}(\lfloor 2\delta\rfloor+1-2\delta)\right)\right)} + \frac{\ln\left(1+\eta_{\lfloor 2\delta\rfloor-1}(\lambda)\right)}{\cosh\left(\pi\left(\lambda+\frac{i\upsilon}{2}(2\delta-\lfloor 2\delta\rfloor)\right)\right)}\right]$$

Impurity Entropy: **The *YSR-II* phase** (one **channel**)

-- The YSR-II
eigenstates fall into three distinct towers of excitations

$$e^{-\beta F_{\text{imp}}(T)} = \sum_{i=1}^{3} e^{-\beta F_{\text{imp}}^{(\mathcal{T}_i)}(T)}$$

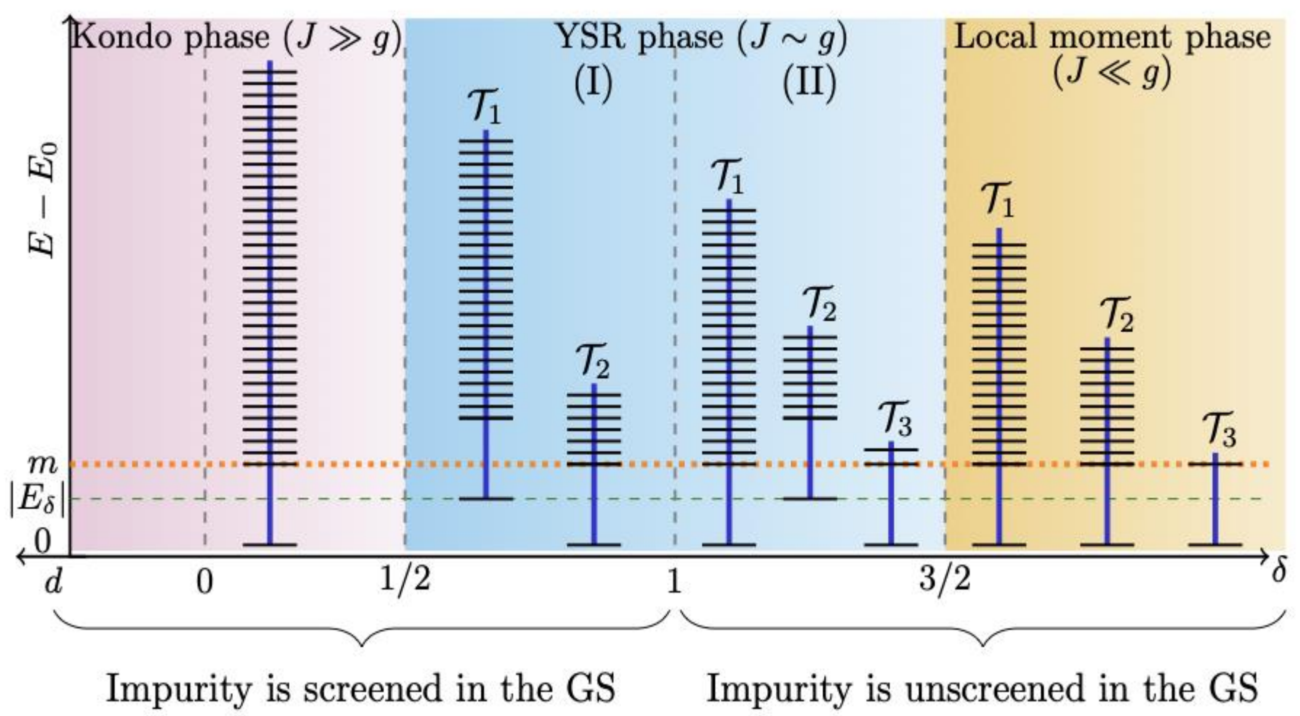


Using the limit values of $\eta_n(0), \eta_n(\infty)$ we have:

$$S_{\text{imp}}^{(\mathcal{T}_1)}(0) = \ln\left(\frac{3}{2}\right), S_{\text{imp}}^{(\mathcal{T}_2)}(0) = 0, S_{\text{imp}}^{(\mathcal{T}_3)}(0) = -\ln 2$$

$$S_{\text{imp}}^{(\mathcal{T}_1)}(\infty) = \ln\left(\frac{4}{3}\right), S_{\text{imp}}^{(\mathcal{T}_2)}(\infty) = -\ln 2 S_{\text{imp}}^{(\mathcal{T}_3)}(\infty) = -\ln 6$$

- At $T = 0$ only towers $\mathcal{T}_1, \mathcal{T}_3$ contribute: $S_{\text{imp}}(0) = \ln\left(e^{S_{\text{imp}}^{(\mathcal{T}_1)}(0)} + e^{S_{\text{imp}}^{(\mathcal{T}_3)}(0)}\right) = \ln 2$
- At $T \to \infty$ all towers contribute so: $S_{\text{imp}}(\infty) = \ln\left(e^{S_{\text{imp}}^{(\mathcal{T}_1)}(\infty)} + e^{S_{\text{imp}}^{(\mathcal{T}_2)}(\infty)} + e^{S_{\text{imp}}^{(\mathcal{T}_3)}(\infty)}\right) = \ln 2$



The impurity entropy exceeds $\ln 2$ at intermediate temperatures $T \sim E_\delta$ when the midgap states $\mathcal{T}_2$ become thermally accessible

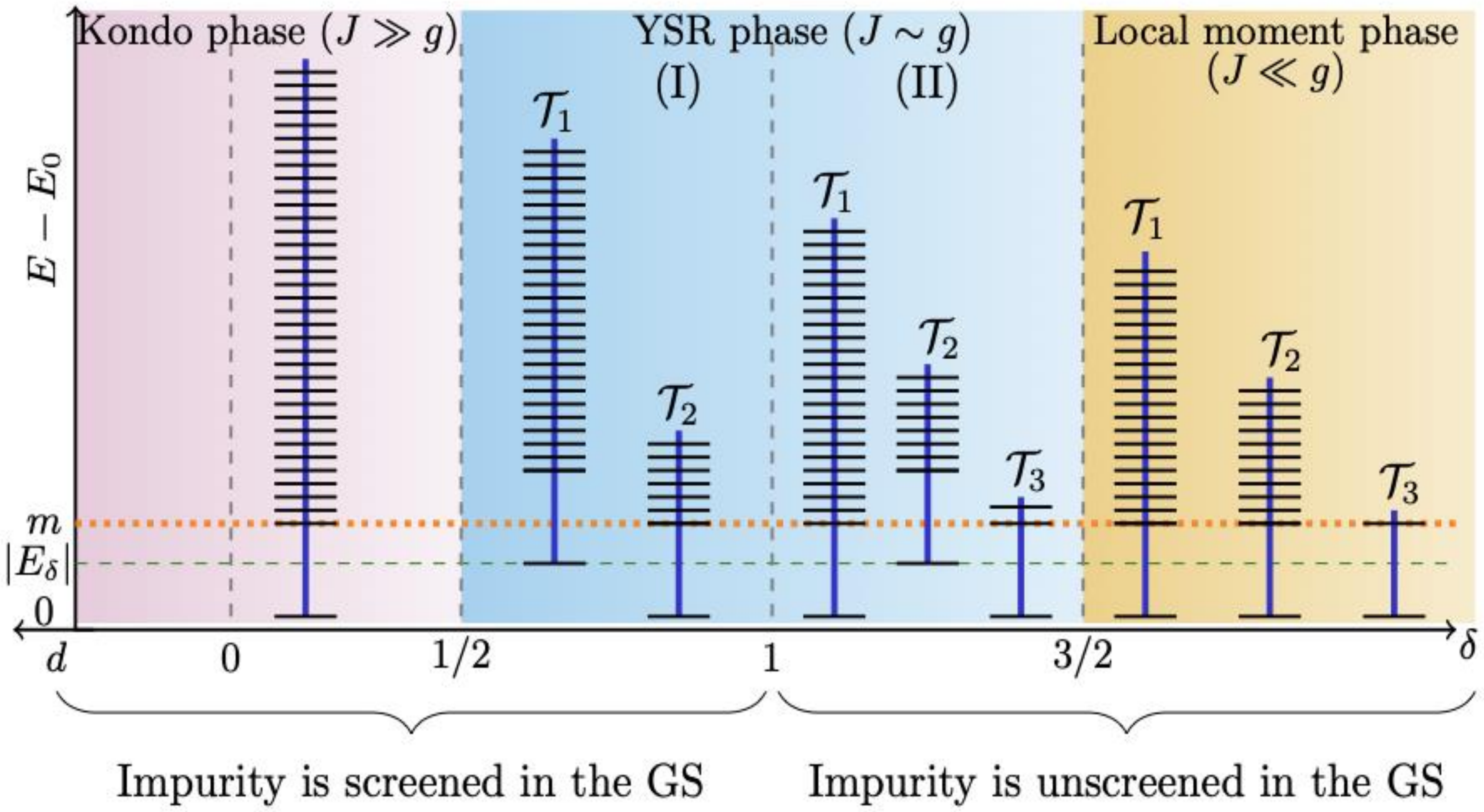
Phases and Excitation Towers: The *Local Moment* phase (one channel)

iv. ***The Local Moment phase:*** $\delta > 3/2$

Higher boundary strings appear

$$\lambda^{(p)}_{\delta,\ell} = \lambda_\delta + i\ell,\ \ell = 1,\ldots,p \ \text{ and } \ p = \lfloor \delta + \frac{1}{2} \rfloor$$

Energy of strings vanishes in this phase



- Hilbert Space splits into three towers:

$\mathcal{T}_1$ built on $|U\rangle$ (real roots) contains $(\lfloor 2\delta\rfloor + 2)/2(\lfloor 2\delta\rfloor + 1)$ of the states

$\mathcal{T}_2$ built on $|B\rangle$ (real roots, λ_δ) contains $(\lfloor 2\delta\rfloor - 1)/(2\lfloor 2\delta\rfloor)$ of the states

$\mathcal{T}_3$ built on $|\tilde{B}\rangle$ (real roots, λ_δ and the boundary strings) contains $1/(2\lfloor 2\delta\rfloor(\lfloor 2\delta\rfloor + 1))$ of the states

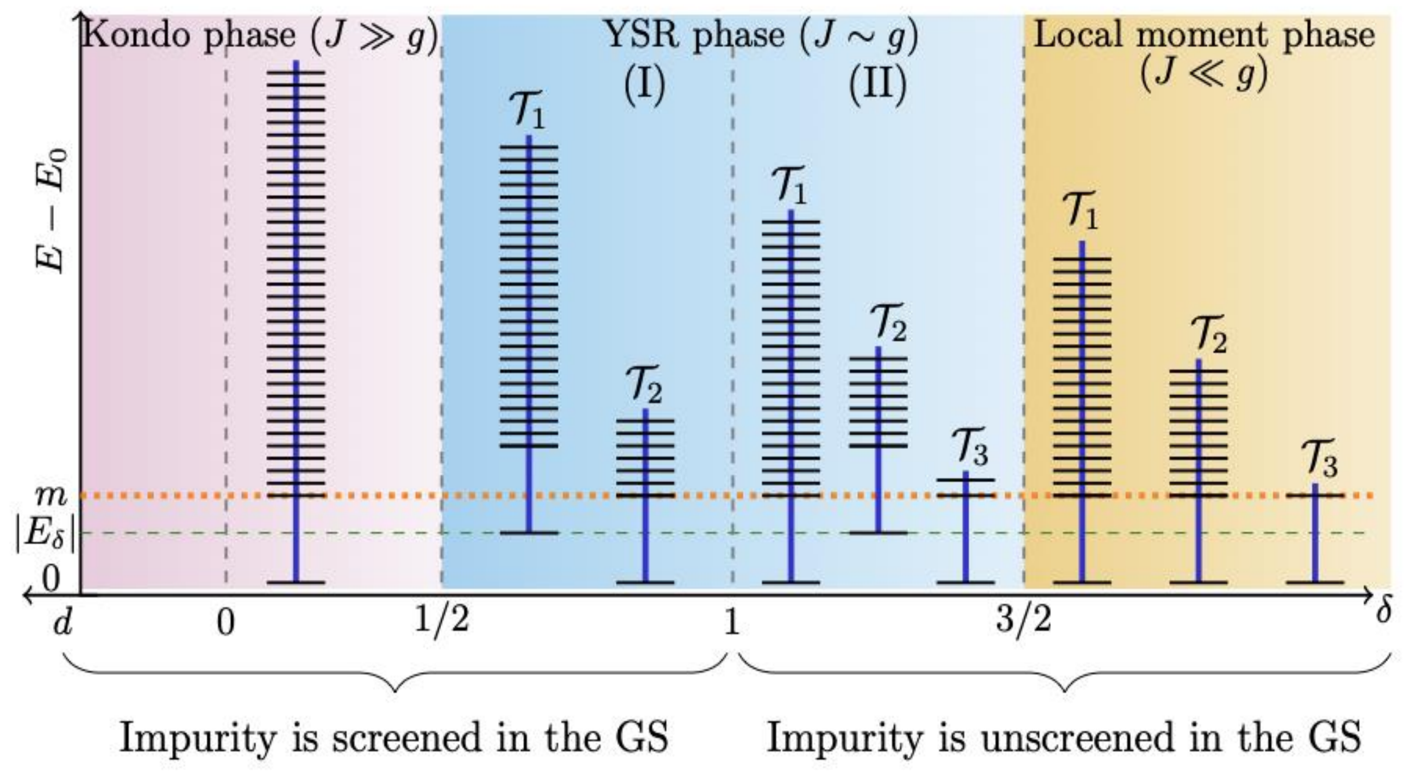
- In the local moment phase $\delta > 3/2$ the energies of both fundamental boundary root $\lambda_\delta = i(\delta + \frac{1}{2})$ and higher-order boundary strings $\lambda^{(p)}_{\delta,\ell}$ vanish. No tower is lifted

Impurity entropy: **the Local Moment phase (one channel)**

Local Moment phase -

The eigenstates fall into three distinct towers of excitations built over , $|U\rangle$ $|B\rangle$ $|\tilde{B}\rangle$

$$e^{-\beta F_{\text{imp}}(T)} = \sum_{i=1}^{3} e^{-\beta F_{\text{imp}}^{(\mathcal{T}_i)}(T)}$$



- At $T = 0$ all towers available at since the energies of all boundary string solutions vanish in the thermodynamic limit

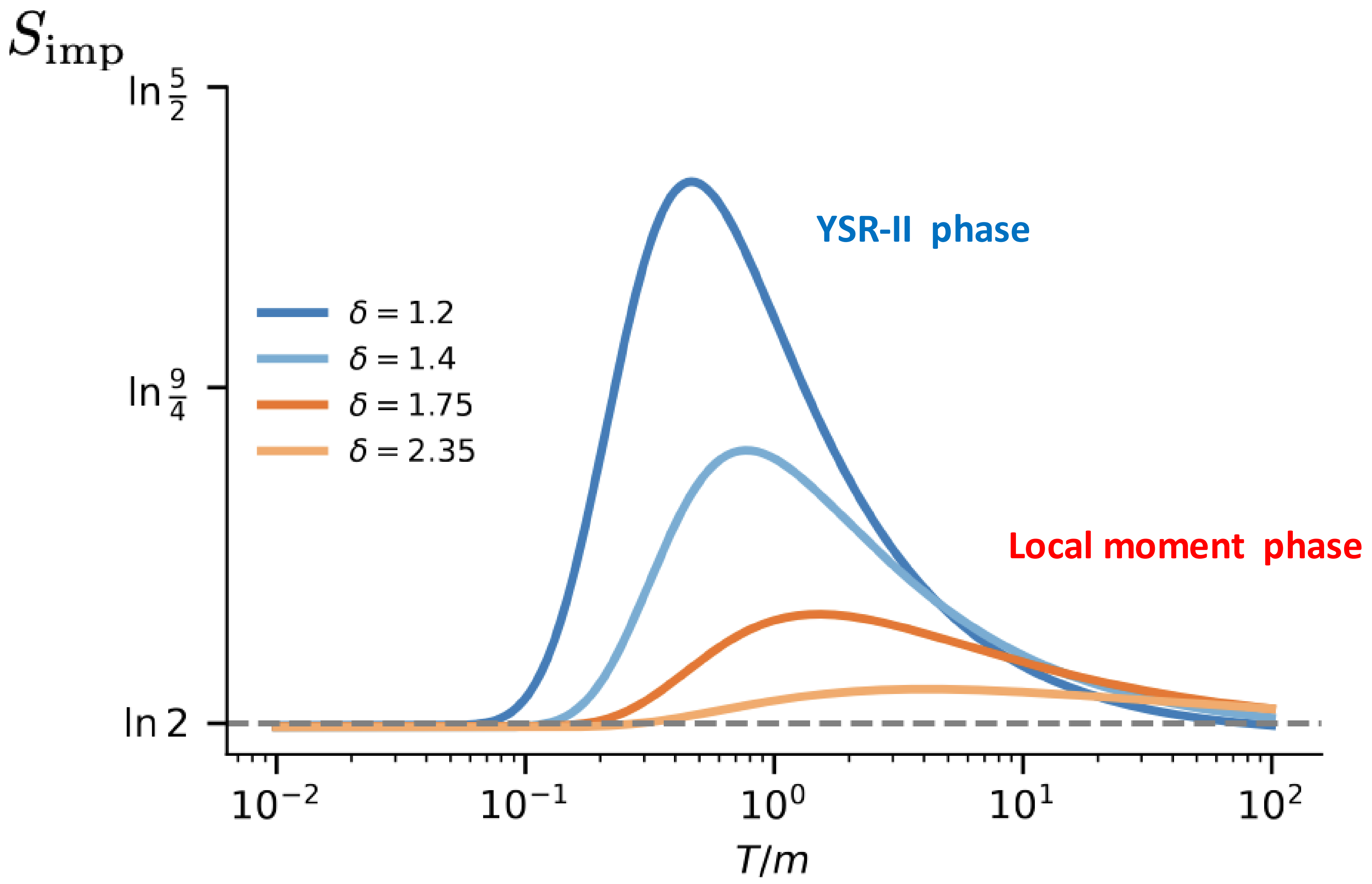
- Using the limit values of $\eta_n(0), \eta_n(\infty)$ we have:

$$S_{\text{imp}}^{(\mathcal{T}_1)}(0) = \ln\left(\frac{\lfloor 2\delta \rfloor + 1}{\lfloor 2\delta \rfloor}\right), S_{\text{imp}}^{(\mathcal{T}_2)}(0) = \ln\left(\frac{\lfloor 2\delta \rfloor - 2}{\lfloor 2\delta \rfloor - 1}\right), S_{\text{imp}}^{(\mathcal{T}_3)}(0) = \ln\left(\frac{1}{(\lfloor 2\delta \rfloor - 1)\lfloor 2\delta \rfloor}\right)$$

$$S_{\text{imp}}^{(\mathcal{T}_1)}(\infty) = \ln\left(\frac{\lfloor 2\delta \rfloor + 2}{\lfloor 2\delta \rfloor + 1}\right), S_{\text{imp}}^{(\mathcal{T}_2)}(\infty) = \ln\left(\frac{\lfloor 2\delta \rfloor - 1}{\lfloor 2\delta \rfloor}\right), S_{\text{imp}}^{(\mathcal{T}_3)}(\infty) = \ln\left(\frac{1}{(\lfloor 2\delta \rfloor)(\lfloor 2\delta \rfloor + 1)}\right)$$

- **The impurity entropy** $S_{\text{imp}}(0) = S_{\text{imp}}(\infty) = \ln 2$

Intermediate-*T* shows non-monotone overshoots $S_{\text{imp}} \gtrsim \ln 2$ (vanishing as $\delta \to \infty$)



Impurity Entropy: ***Zero mode* phase (multichannel)**

***Zero mode* phase** $\quad \frac{1}{2} < \delta < \frac{f}{2} \quad (i.e.\ g \lesssim J)$

A boundary string solution $\lambda_\delta = i(\delta - \frac{1}{2})$ appears, it has exactly vanishing energy

$(\frac{1}{2} < \delta < 1)$ Zero mode phase I : Two towers, depending on whether the mode is occupied or not

$\mathcal{T}_1$ spanned by the usual bulk string solutions, contains ¾ of the solutions

$\mathcal{T}_2$ Includes the boundary string solution λ_δ together with the associated bulk string configuration, contains ¼ of the solutions

$$F_{\rm imp}^{(\mathcal{T}_1)} = F_{\rm imp}^{(\mathcal{T}_2)} - \int \mathrm{d}\lambda \sum_{v=\pm} \frac{\frac{T}{4}\ln\left[1+\eta_2(\lambda)\right]}{\cosh(\pi(\lambda + \mathrm{i}v(\delta - \frac{1}{2})))}$$

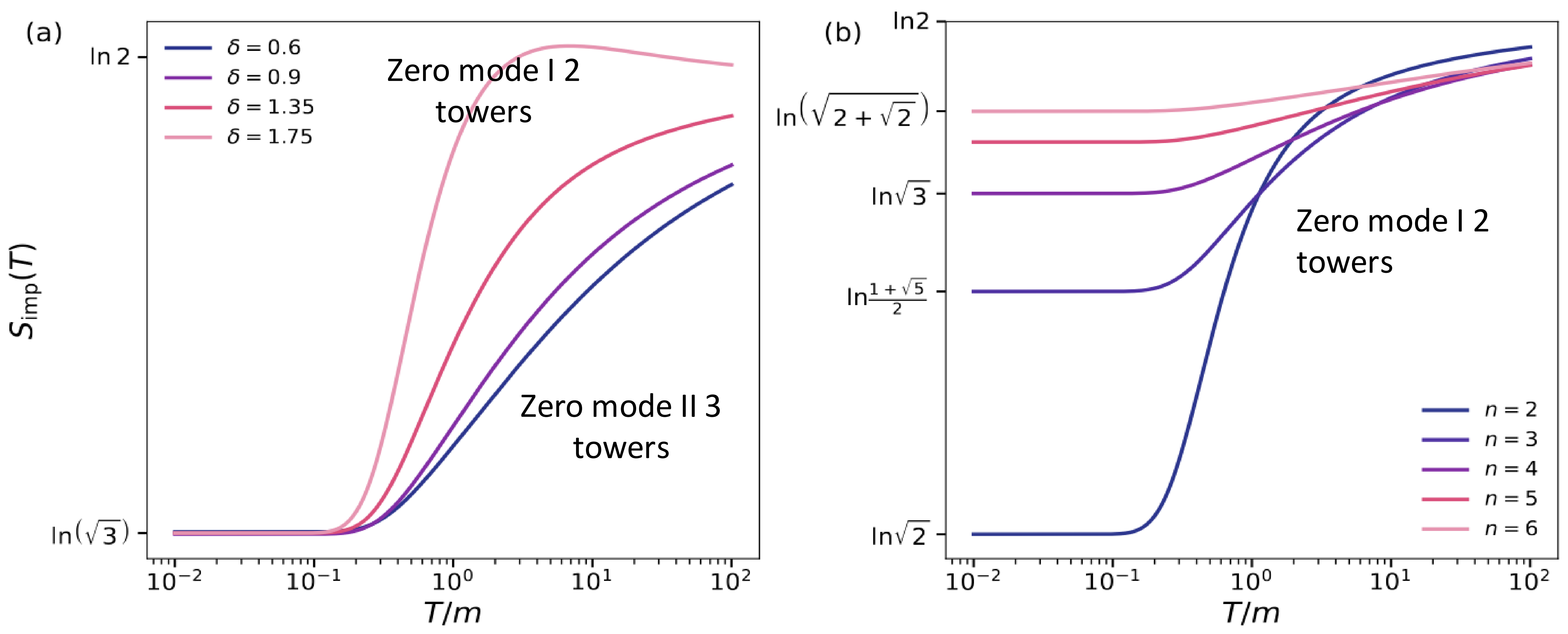
$$F_{\rm imp}^{(\mathcal{T}_2)} = \frac{T}{4} \int \mathrm{d}\lambda \sum_{v=\pm} \frac{\ln\left[1+\eta_1(\lambda)\right]}{\cosh(\pi(\lambda + \mathrm{i}v\delta))}$$

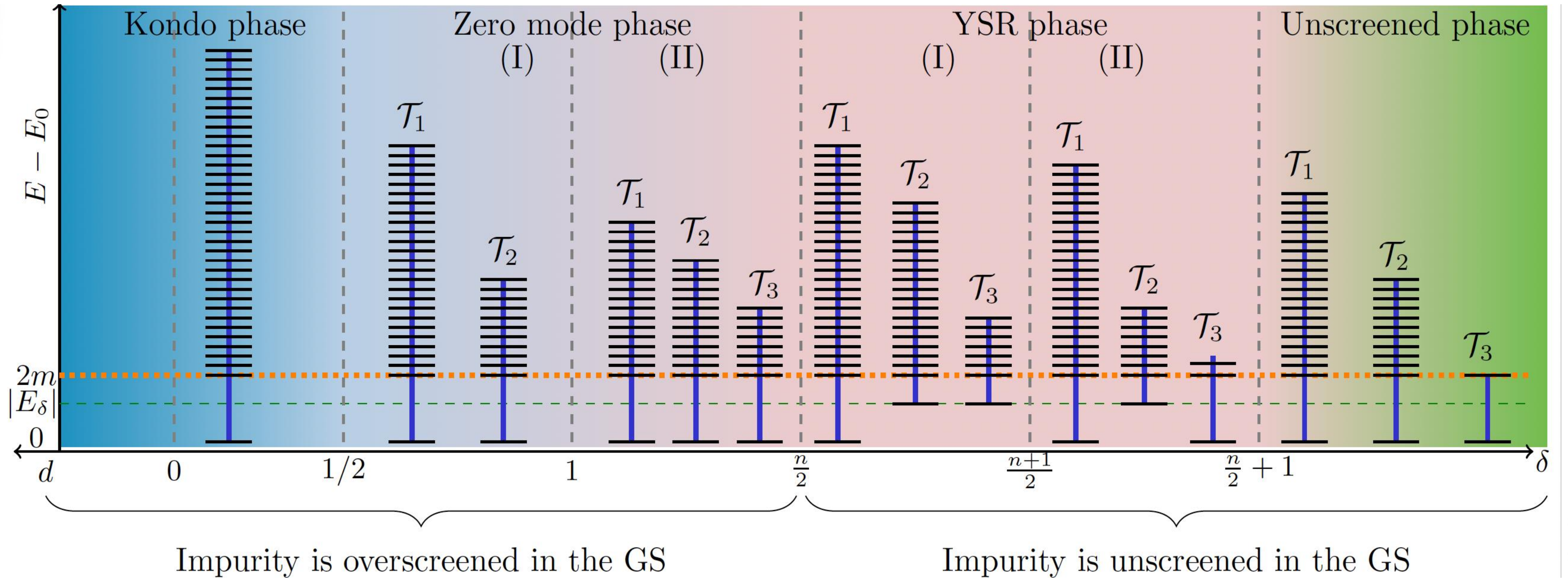
and the zero temperature entropy

$$S_{\rm imp}(T \to 0) = \ln\left(2\cos\left(\frac{\pi}{f+2}\right)\right),$$

Zero mode phase (4 channels, vary *d*)

Zero mode phase (d=0.75, vary *f*)





Impurity Entropy: ***Zero mode* phase (multichannel)**

***Zero mode* phase** $\frac{1}{2} < \delta < \frac{f}{2}$ $(i.e.\ g \lesssim J)$

A boundary string solution $\lambda_\delta = i(\delta - \frac{1}{2})$ appears, it has exactly vanishing energy

$(1 < \delta < \frac{f}{2})$ Zero mode phase II: Three towers - Higher string modes are present

$\mathcal{T}_1$ spanned by the usual bulk string solutions,

$\mathcal{T}_2$ Includes the boundary string solution together with the associated bulk string configuration

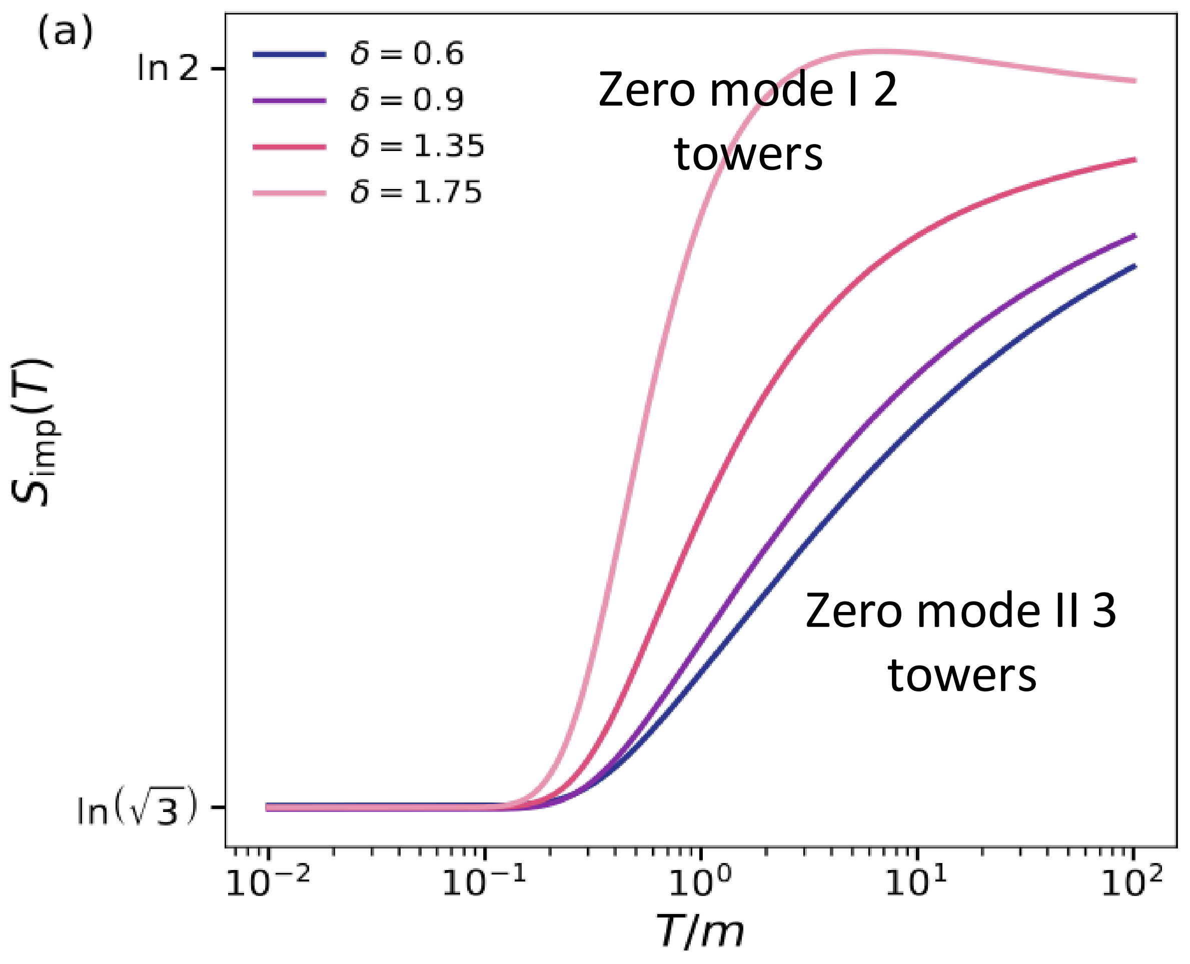
$\mathcal{T}_3$ Contains both the fundamental string solution and λ_δ higher order strings solution $\lambda_\delta + i\ell$

$$F_{\text{imp}}^{(\mathcal{T}_1)} = -\frac{T}{4}\sum_{v=\pm}\int d\lambda \left[\frac{\ln\left(1+\eta_{\lfloor 2\delta\rfloor+1}(\lambda)\right)}{\cosh\left(\pi\left(\lambda + \frac{iv}{2}(2\delta - \lfloor 2\delta\rfloor)\right)\right)} - \frac{\ln\left(1+\eta_{\lfloor 2\delta\rfloor}(\lambda)\right)}{\cosh\left(\pi\left(\lambda + \frac{iv}{2}(\lfloor 2\delta\rfloor + 1 - 2\delta)\right)\right)}\right],$$

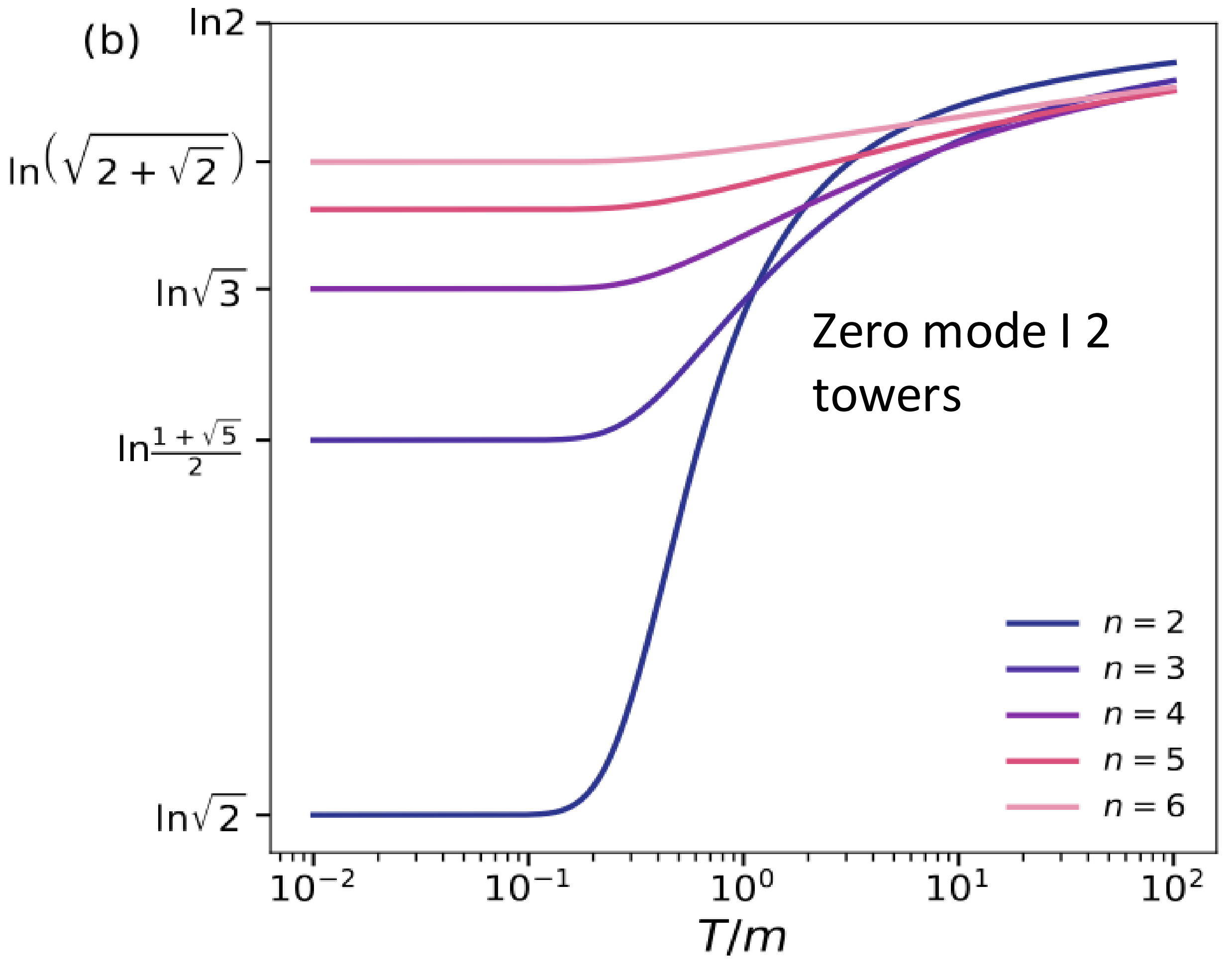
$$F_{\text{imp}}^{(\mathcal{T}_2)} = \frac{T}{4}\sum_{v=\pm}\int d\lambda \left[\frac{\ln\left(1+\eta_{\lfloor 2\delta\rfloor-1}(\lambda)\right)}{\cosh\left(\pi\left(\lambda + \frac{iv}{2}(2\delta - \lfloor 2\delta\rfloor)\right)\right)} - \frac{\ln\left(1+\eta_{\lfloor 2\delta\rfloor-2}(\lambda)\right)}{\cosh\left(\pi\left(\lambda + \frac{iv}{2}(\lfloor 2\delta\rfloor + 1 - 2\delta)\right)\right)}\right],$$

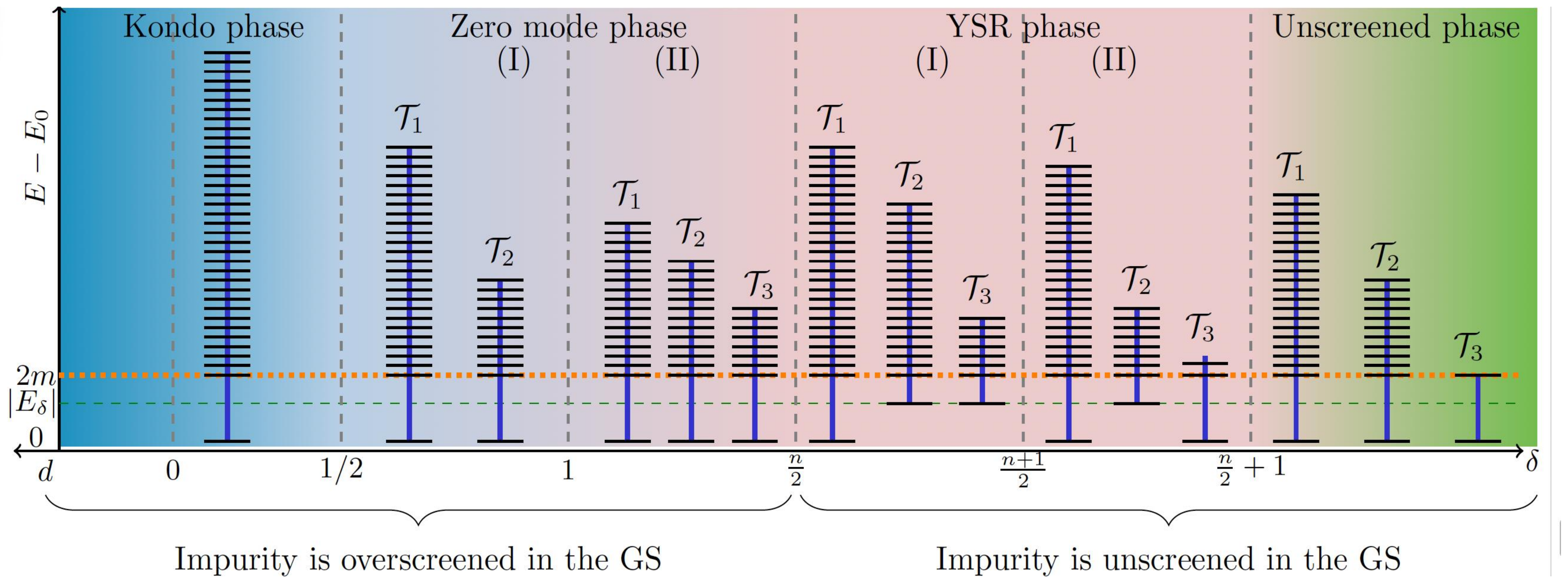
$$F_{\text{imp}}^{(\mathcal{T}_3)} = \frac{T}{4}\sum_{v=\pm}\int d\lambda \left[\frac{\ln\left(1+\eta_{\lfloor 2\delta\rfloor}(\lambda)\right)}{\cosh\left(\pi\left(\lambda + \frac{iv}{2}(\lfloor 2\delta\rfloor + 1 - 2\delta)\right)\right)} + \frac{\ln\left(1+\eta_{\lfloor 2\delta\rfloor-1}(\lambda)\right)}{\cosh\left(\pi\left(\lambda + \frac{iv}{2}(2\delta - \lfloor 2\delta\rfloor)\right)\right)}\right]$$

Zero mode phase (4 channels, vary *d)*



Zero mode phase (d=0.75, vary *f*)



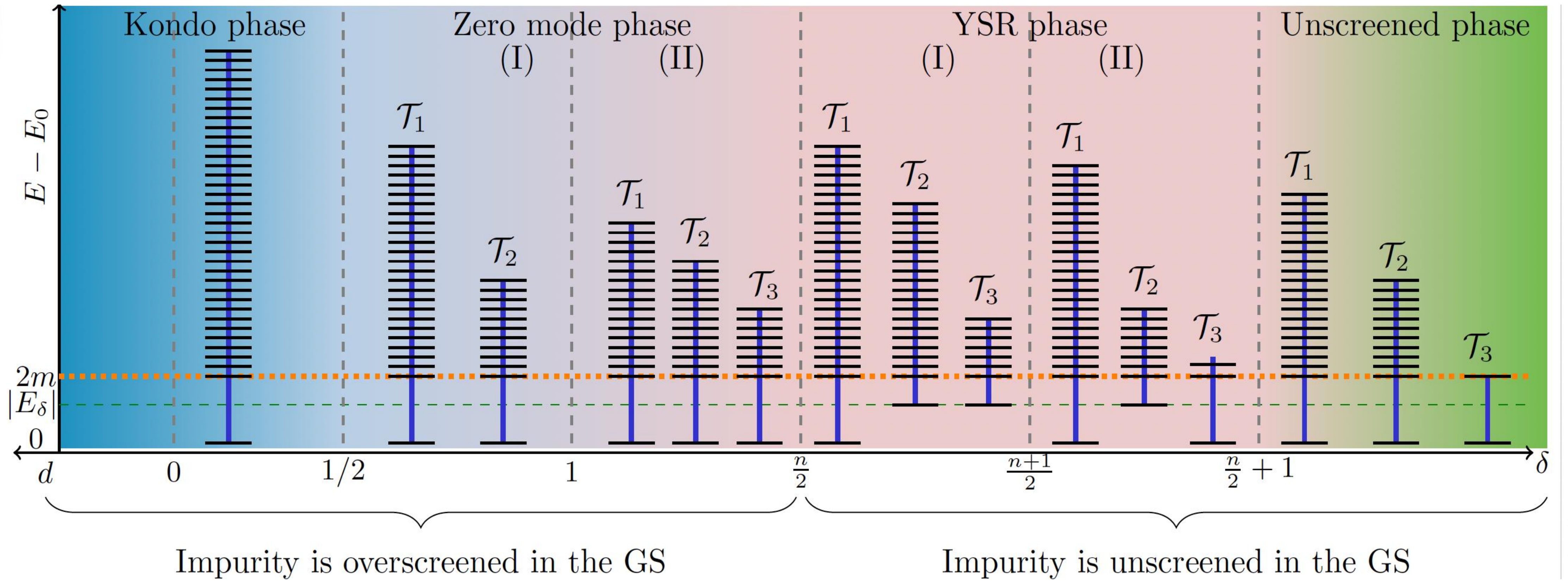


and the zero temperature entropy $S_{\text{imp}}(T \to 0) = \ln\left(2\cos\left(\frac{\pi}{f+2}\right)\right),$

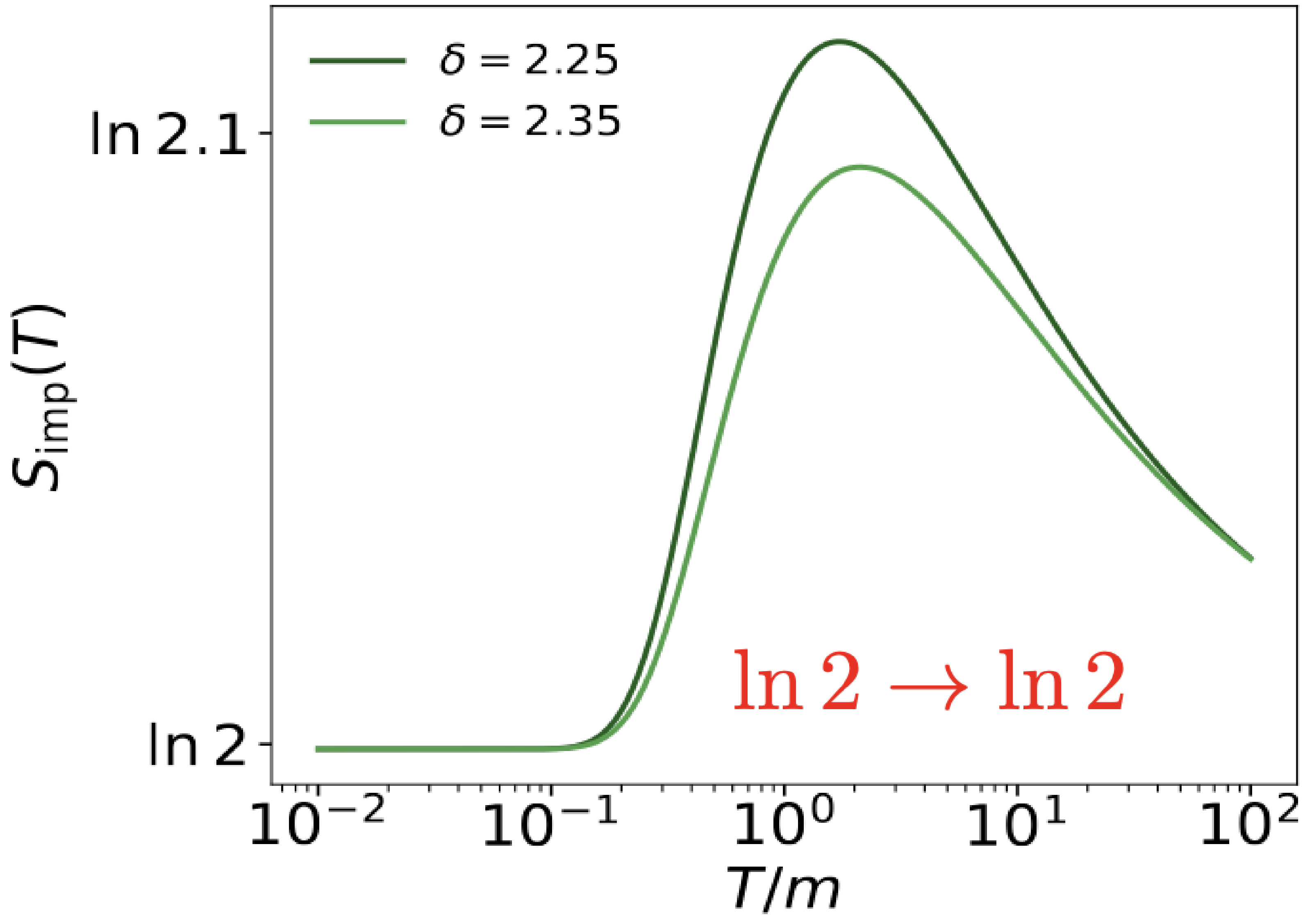
Impurity Entropy: **YSR and Local Moment mode phases (multichannel)**

Now

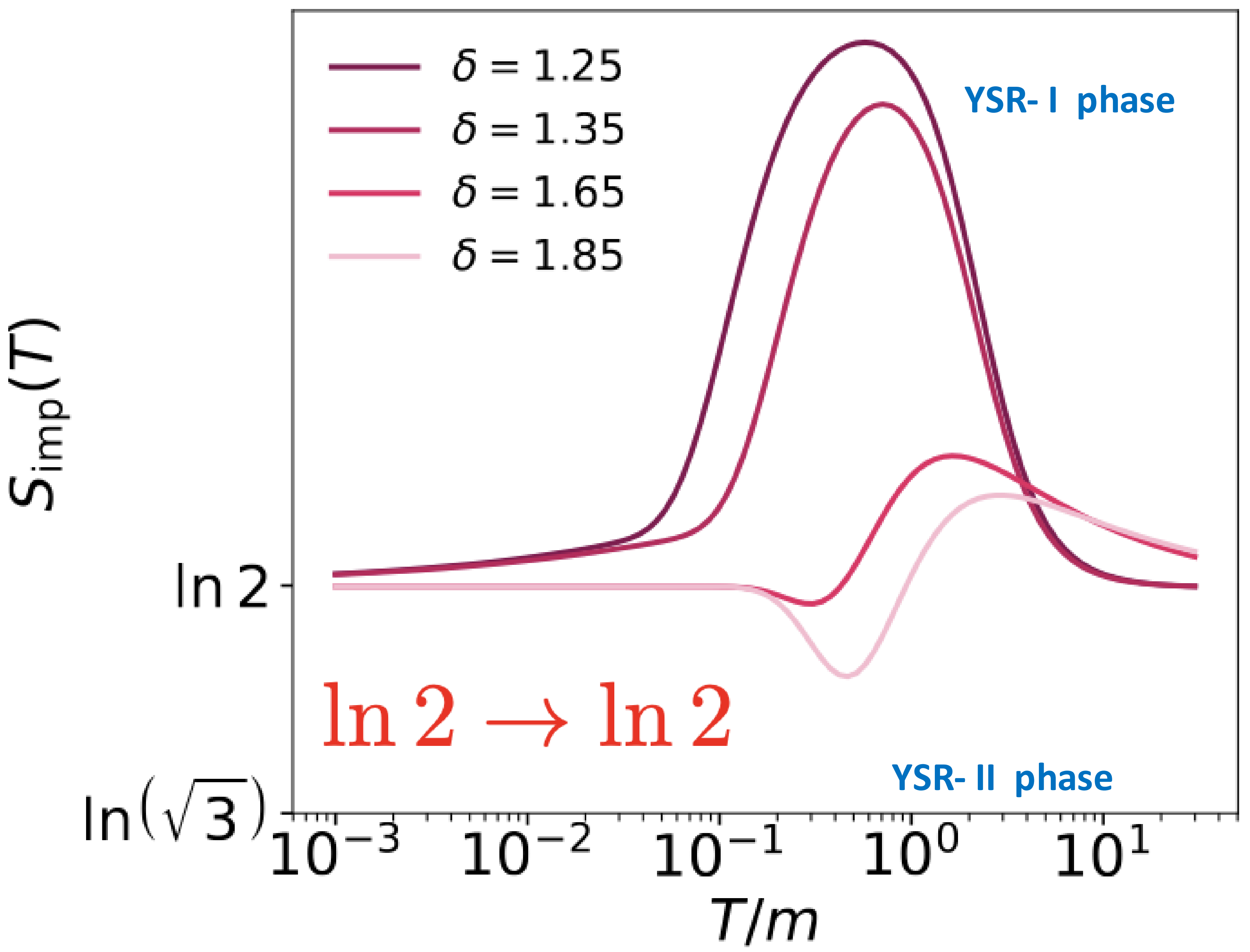
$$\frac{f}{2} < \delta \qquad (i.e.\ J \lesssim g)$$



Local moment phase (2 channels, vary *d)*



YSR phases (2 channels, vary *d)*



overshoots at

intermediate temperatures due to the presence of

boundary states, which become thermally activated

only when

$$T \sim E_\delta$$

Boundary state energy

$$E_\delta = -m\cos\left(\frac{\pi}{2}(f - 2\delta)\right).$$

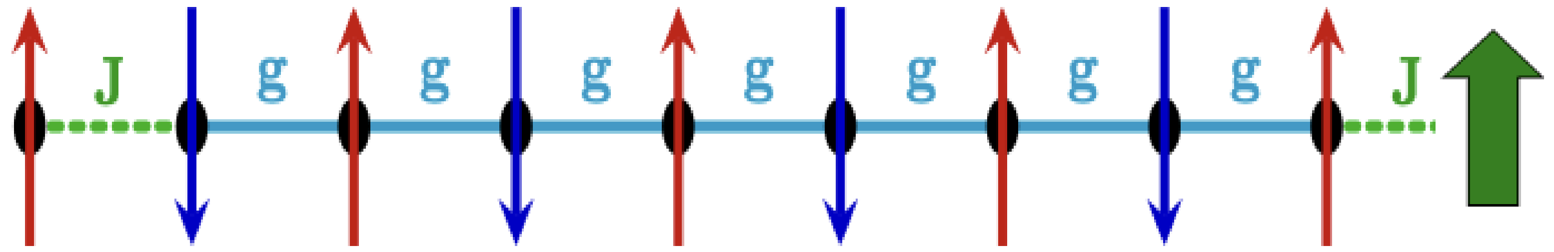
Intermediate summary: The Impurity at the edge of the *f*-SC wires

- In a gapped interacting 1D superconductor, the quantum impurity generates a rich impurity phase diagram, unlike in a Fermi liquid, where only one phase exists, the Kondo phase

- The Kondo phase here shows the same critical low temperature behavior and monotonic impurity entropy flow as in the Fermi Liquid case, <u>although the electrons are gapped</u>

- Additional phases appear with distinct thermodynamic properties. The phase structure is driven by boundary roots which reorganize and split the Hilbert space into excitation towers.

Impurity at the edge of the Spin Chain



- **The Hamiltonian**

$$H = g \sum_{j=1}^{N-1} \vec{\sigma}_j \cdot \vec{\sigma}_{j+1} + J \vec{\sigma}_1 \cdot \vec{\sigma}_0$$

- **The Bethe Ansatz equations** *Wang 1997, Frahm, Zvyagin 1997*

$$\left(\frac{\mu_j - i/2}{\mu_j + i/2}\right)^{2N} \frac{\mu_j - d - i/2}{\mu_j - d + i/2} \frac{\mu_j + d - i/2}{\mu_j + d + i/2} = \prod_{l \neq j}^{M} \frac{(\mu_j - \mu_l - i)(\mu_j + \mu_l - i)}{(\mu_j - \mu_l + i)(\mu_j + \mu_l + i)}$$

- There are M spin momenta $\mu_j, \; j = 1, \cdots M$ yielding:

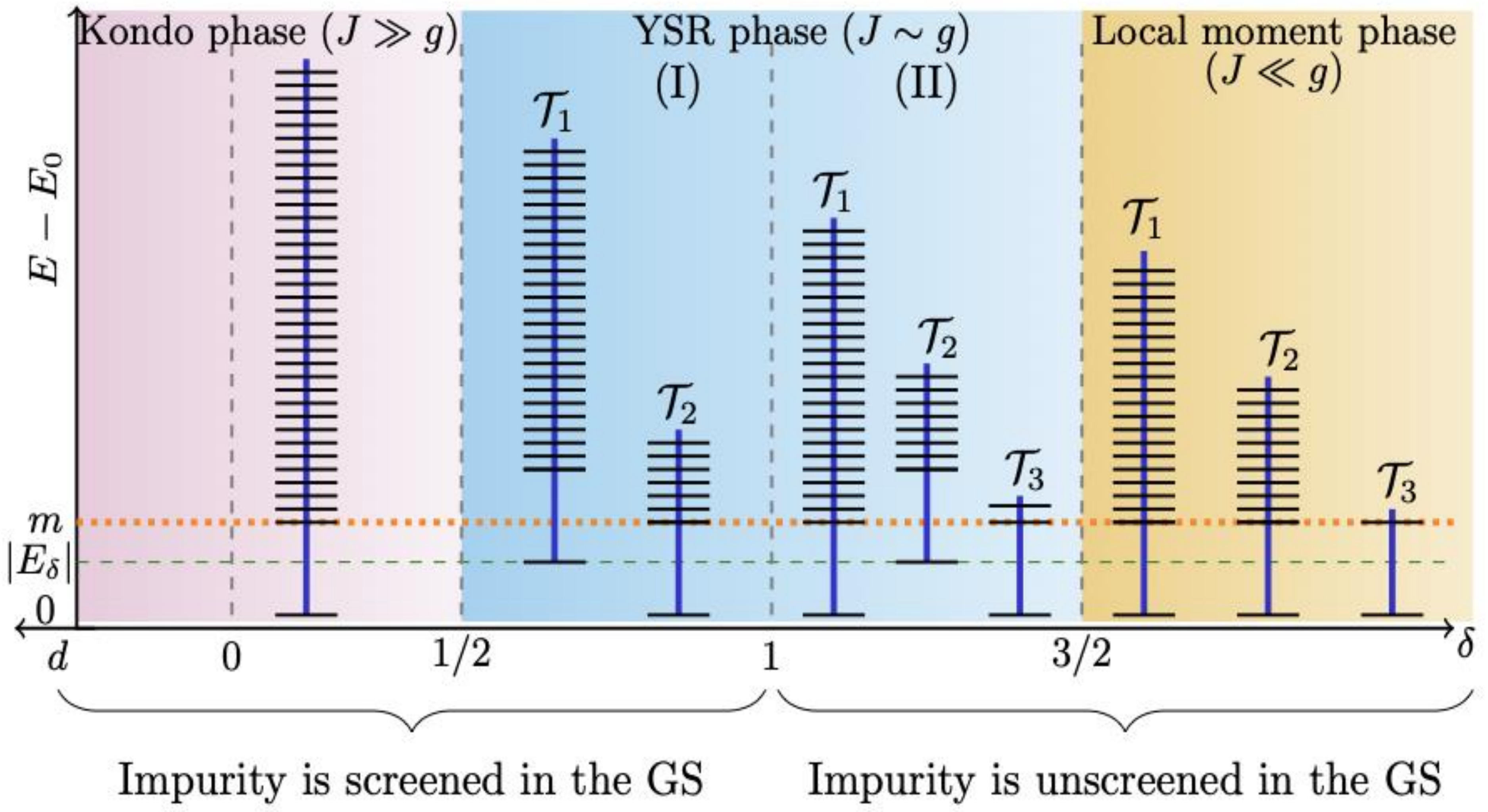
$$E = \sum_j \frac{1}{1 + \mu_j^2} \qquad S^z = \frac{N+1}{2} - M$$

- The impurity parameter $d = d(J) = \sqrt{g/J - 1}$ can be real or imaginary $d = i\gamma$

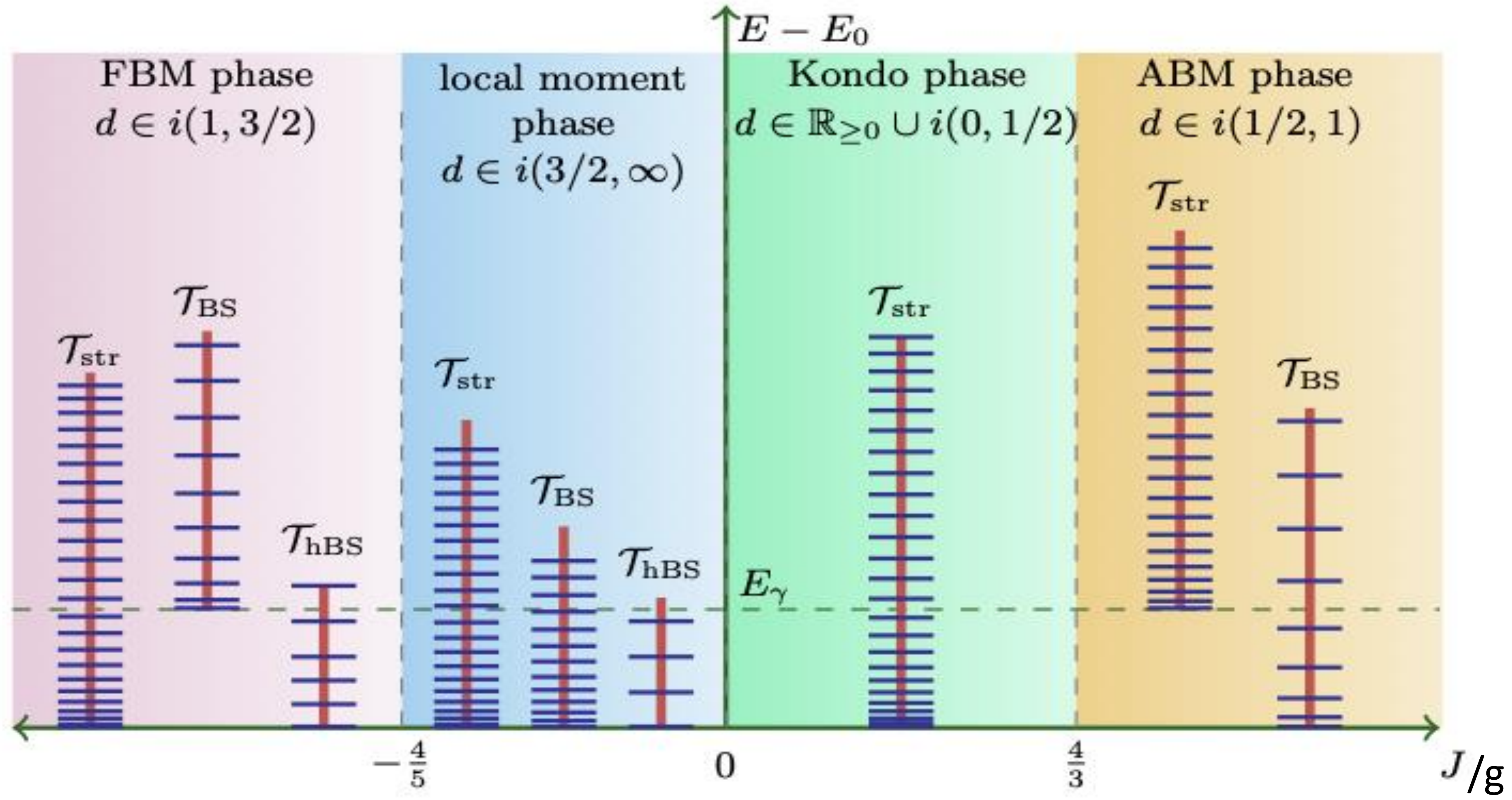
- **It labels the phases**

Outline: Interacting electrons coupled to a local impurity

Phase diagram of the impurity attached to a single channel superconductor

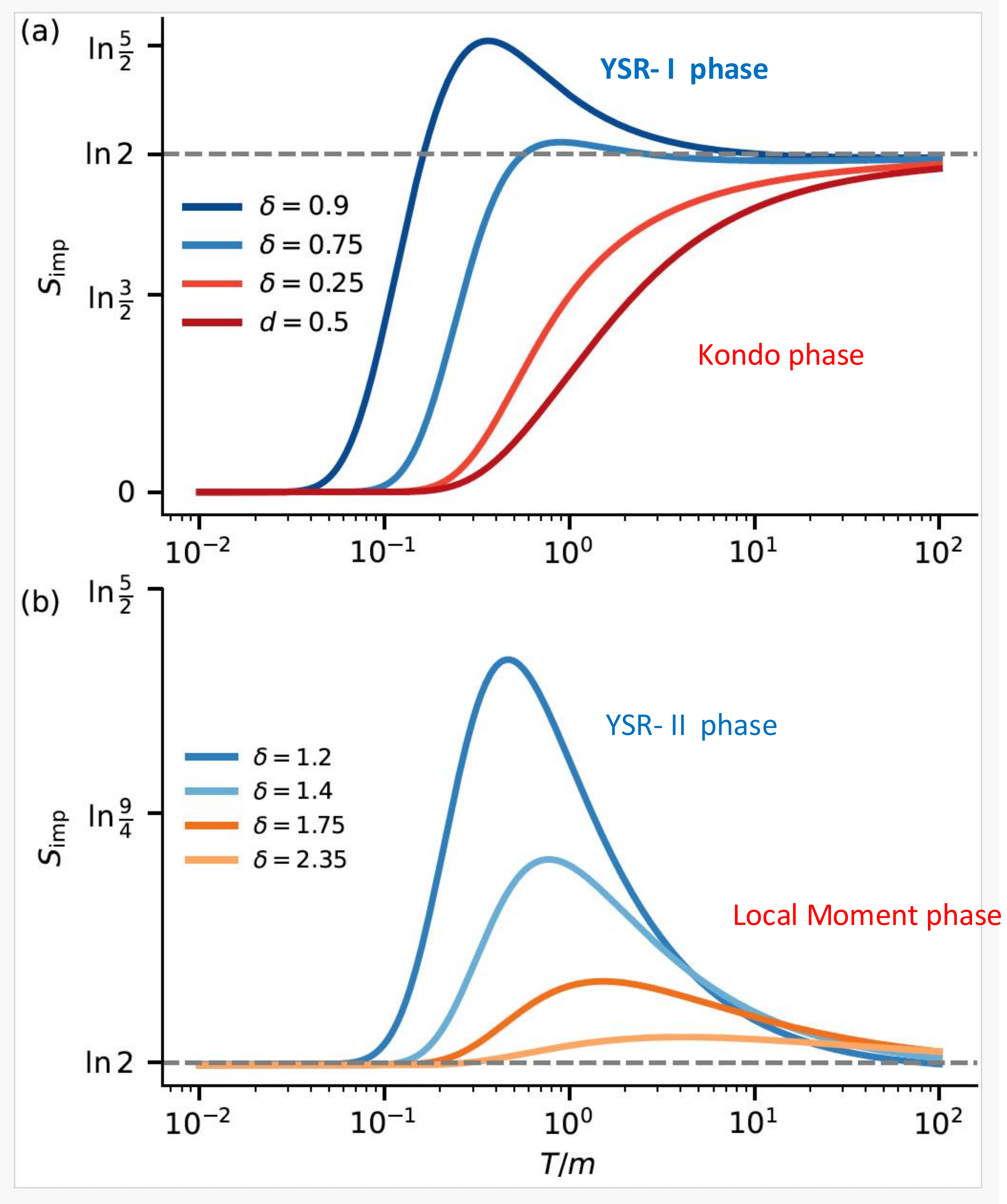


Phase diagram of the impurity attached to a spin chain

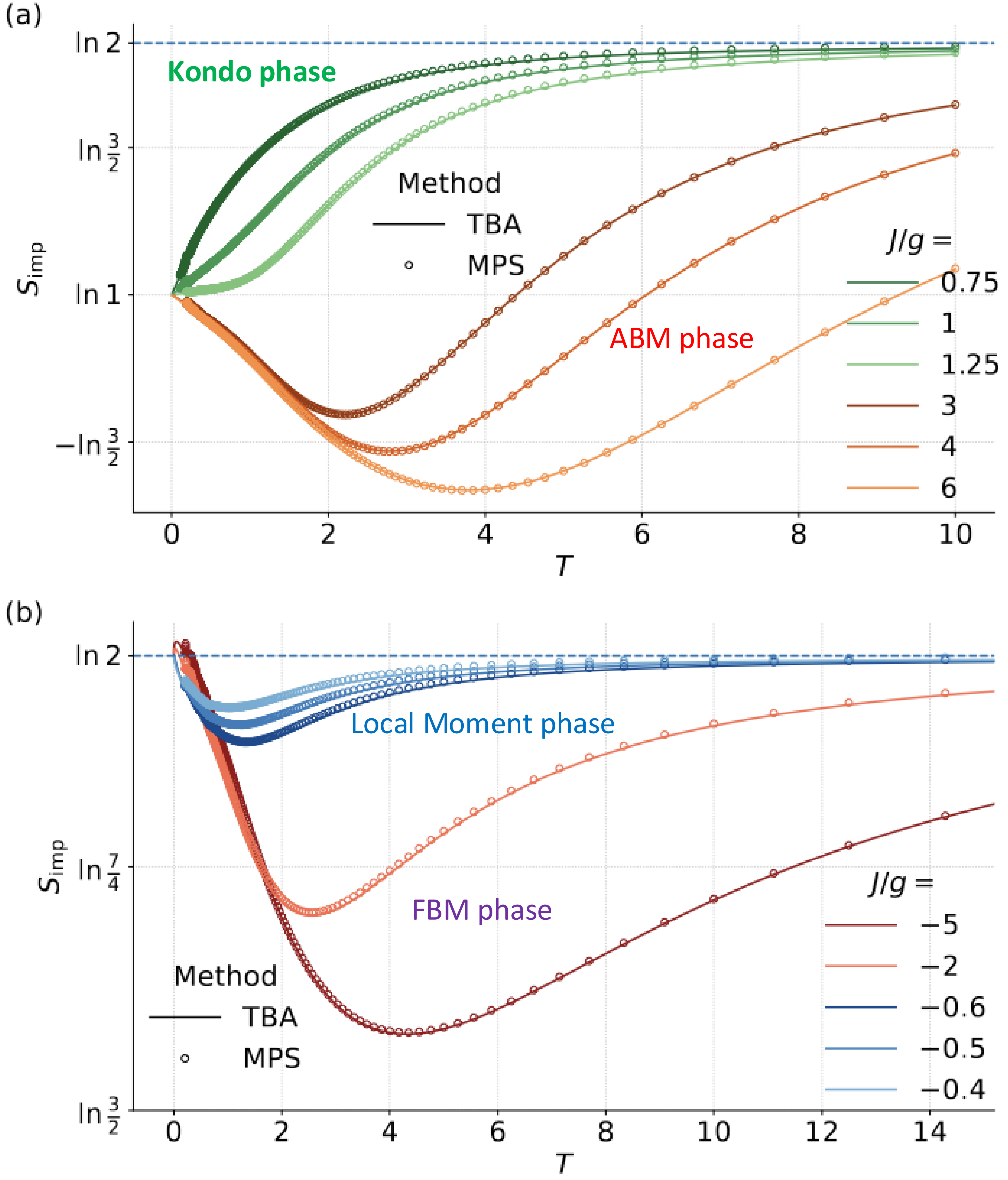


$S_{\mathrm{imp}}(T)$: The impurity entropy as function of the temperature in the various phases (single channel)

Entropy of the impurity attached to a single channel superconductor



Entropy of the impurity attached to a spin chain



The phase diagram: ferromagnetic and antiferromagnetic impurity coupling

- **The antiferromagnetic phases** $J/g > 0$

- The Kondo phase, the impurity is screened via the Kondo effect, only the *string tower* $\mathcal{T}_{str}$ is present.

- The **antiferromagnetic bound-mode (ABM) phase**,

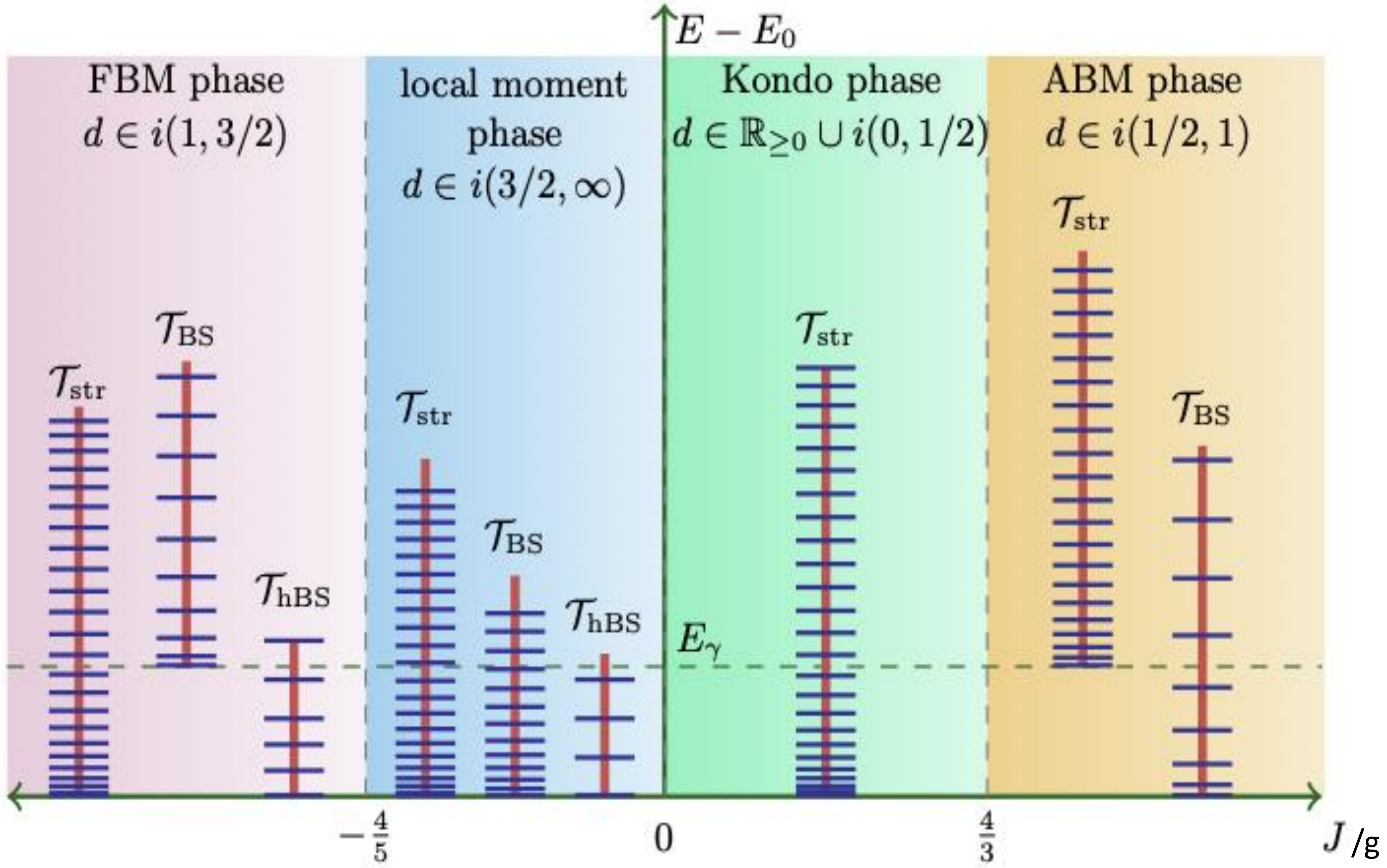
A boundary-string (BS) appears $E_\gamma = 2\pi g/|\sin(\pi\gamma)|$ The tower $\mathcal{T}_{BS}$ over $|BS\rangle$ describes localized screening by the bound mode. The tower $\mathcal{T}_{str}$ is built over the unfilled mode

- **The ferromagnetic phases** $J/g < 0$

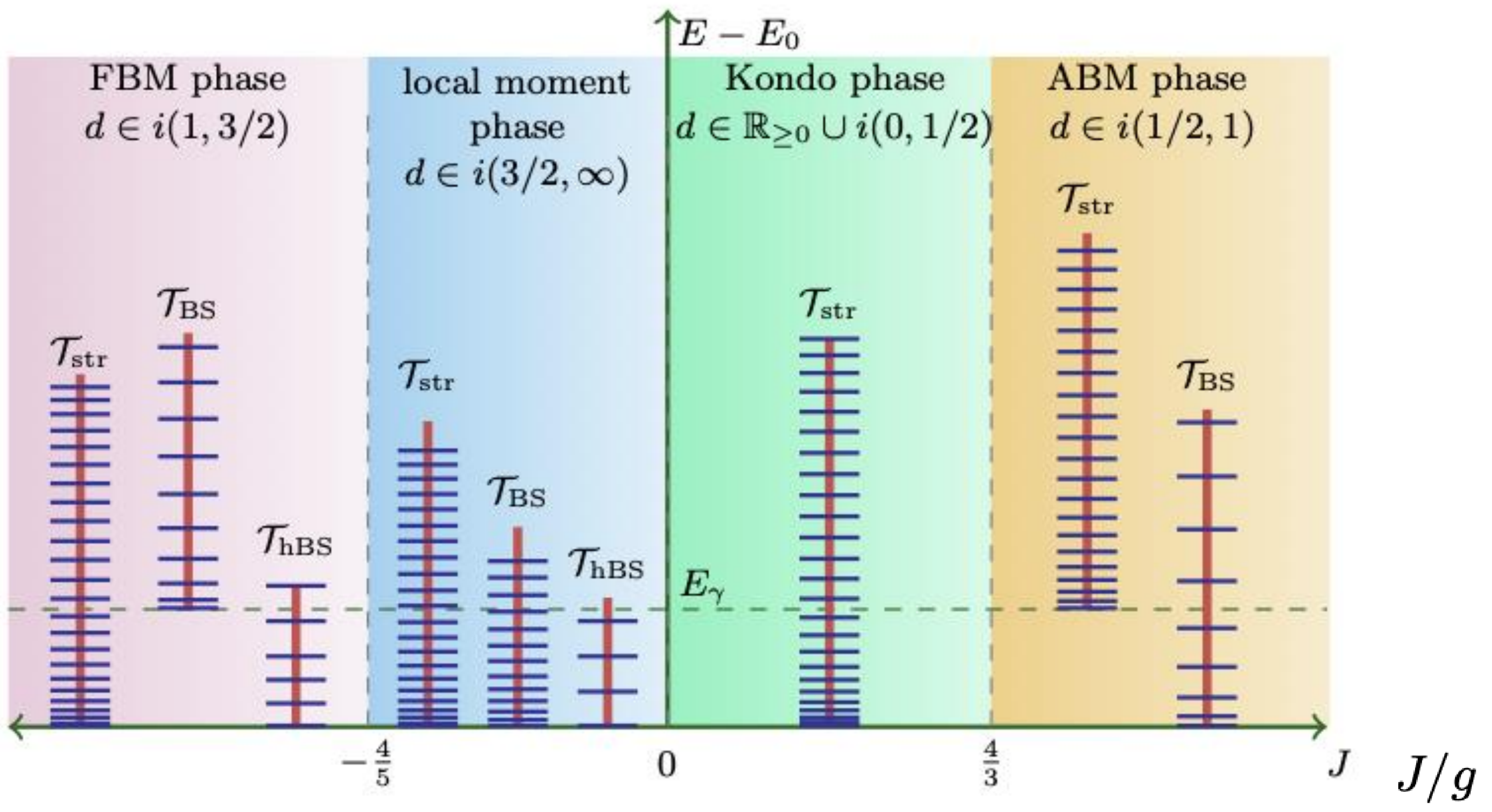
- The ferromagnetic bound state (FBM) phase

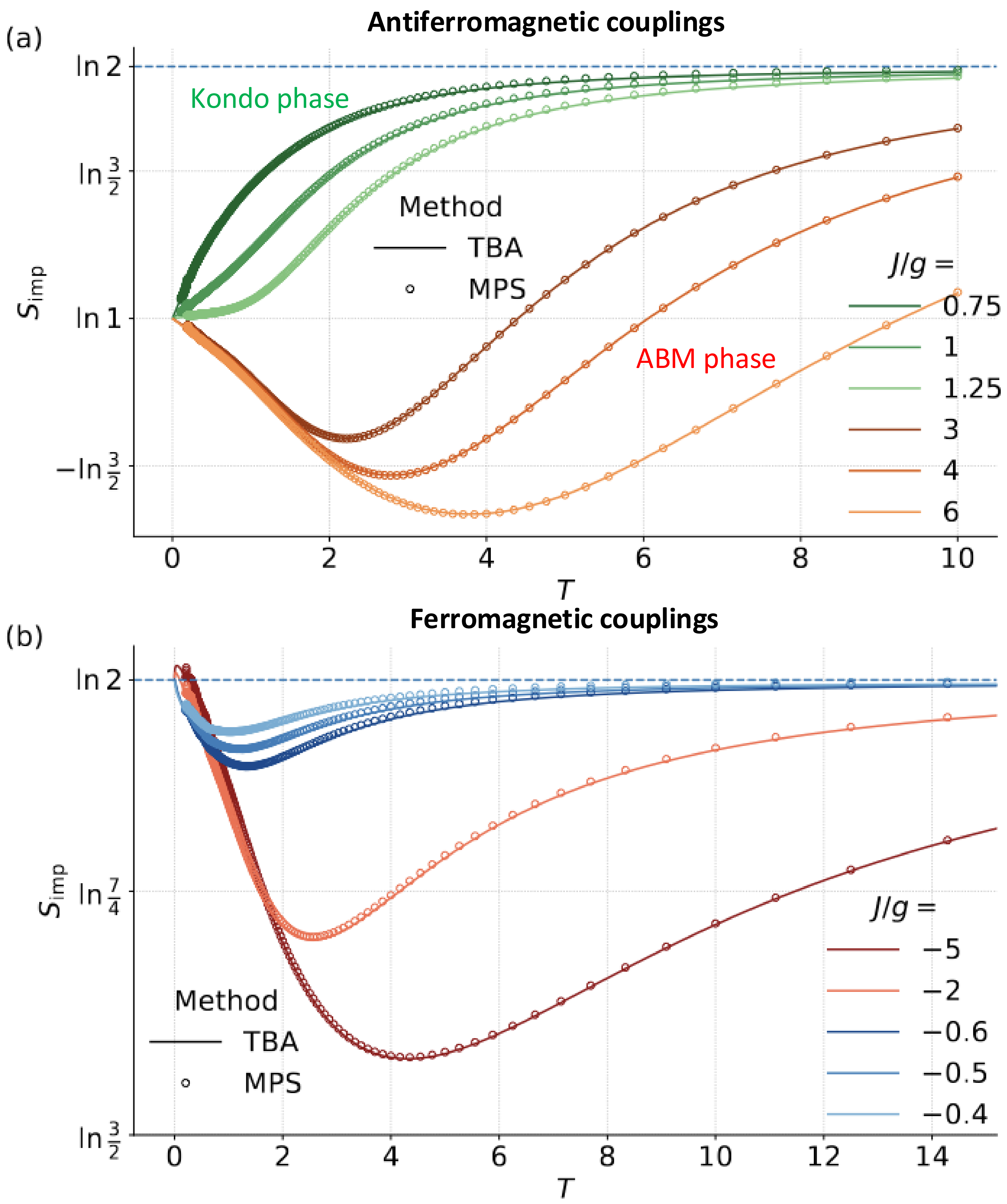
- The Local Moment phase

The spectrum comprises three towers: bulk strings, BS, and higher-order boundary strings (hBS).



The impurity entropy: antiferromagnetic coupling





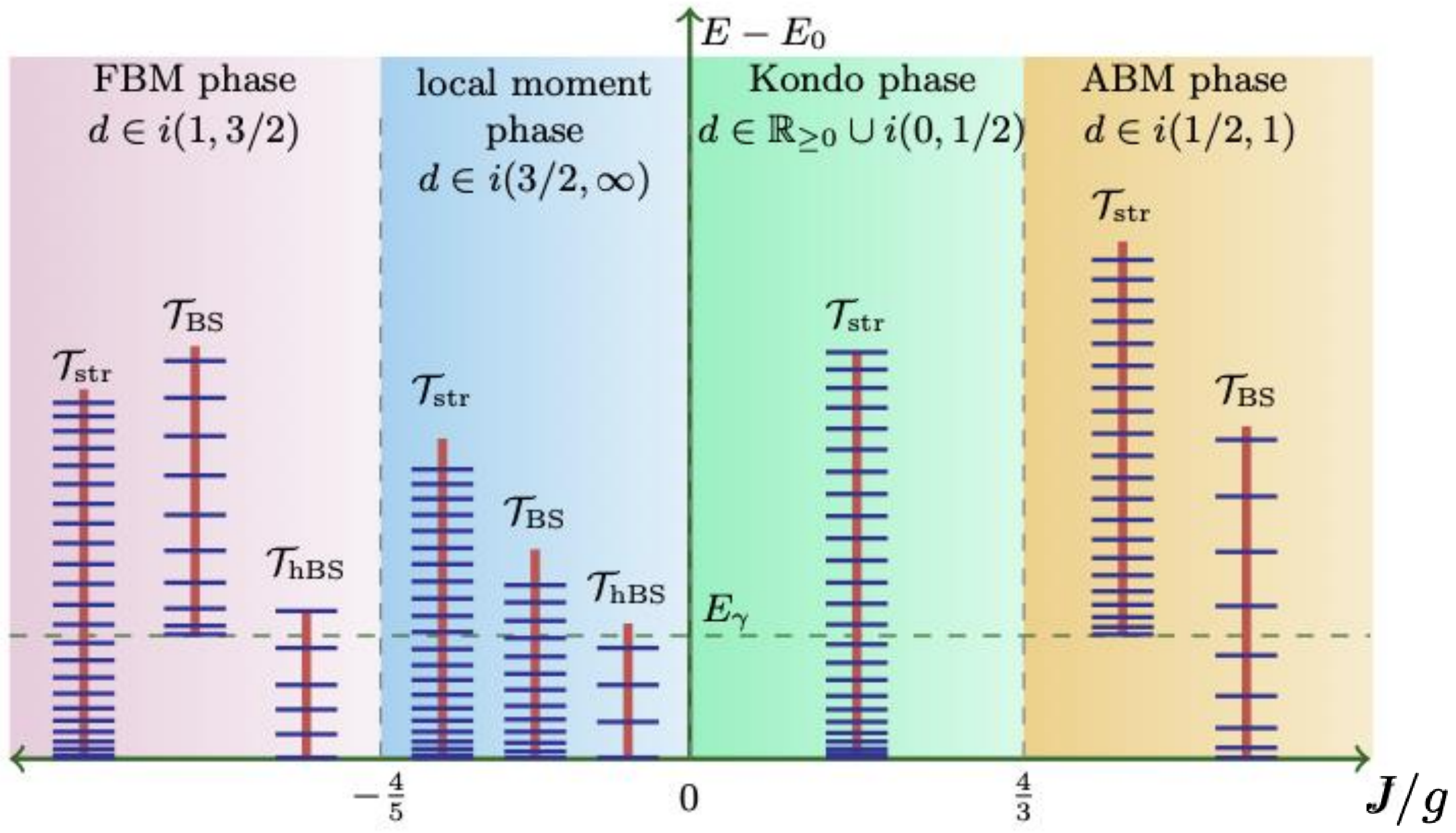
(a) **Antiferromagnetic couplings**:

the impurity goes from complete screening $S_{imp}(T=0)=0$ to asymptotic freedom $S_{imp}(T \to \infty) = \ln 2$.

- **The Kondo phase** $(0 < J/g < 4/3)$: $S_{\rm imp}(T)$ shows monotonic growth

- **The ABM phase** $(J/g > 4/3)$: $S_{\rm imp}(T)$ is non-monotonic, dipping below zero for $g \ll T \ll E_\gamma$ as localized screening removes bulk degrees of freedom from T_{BS} yielding $0 \geq S_{\rm imp} \gtrsim -\ln 2$

The impurity entropy: Ferromagnetic coupling



(b) **Ferromagnetic couplings**: (*FBM and local Moment*, $\gamma > 1$) the impurity is unscreened at both ends, $S_{imp}(T \to \infty) = S_{imp}(0) = \ln 2$; intermediate-$T$ shows non-monotone dips (vanishing as $\gamma \to \infty$ in the local-moment regime)

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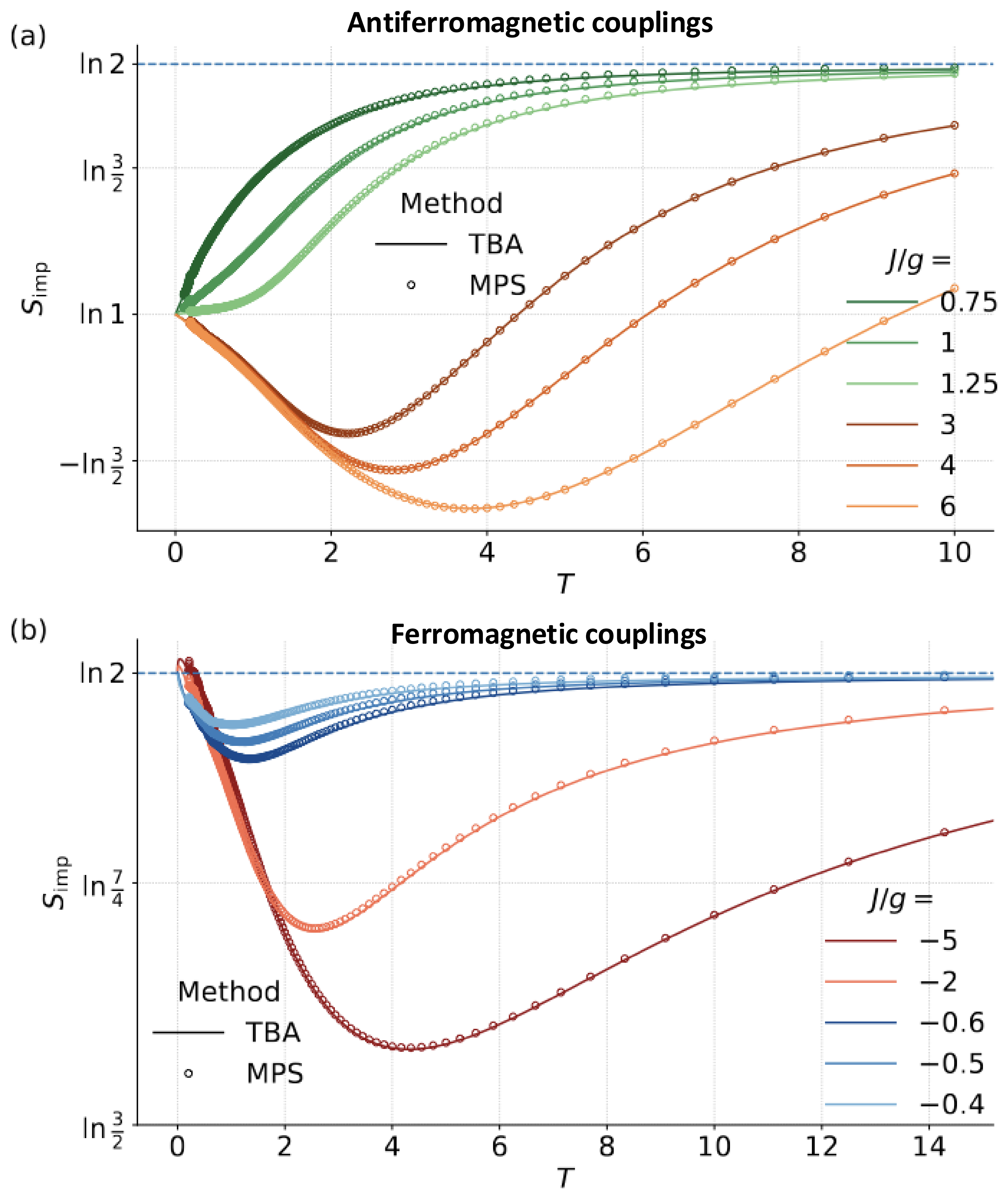


Summary and Outlook

- In a gapped interacting 1D superconductor, a quantum impurity generates a rich impurity phase diagram, unlike in a Fermi liquid, where only the Kondo phase exists; while the Kondo phase here retains the same critical low temperature behavior and monotonic impurity entropy flow as in the Fermi Liquid case, additional phases appear with distinct thermodynamic properties . The phase structure is driven by boundary roots which reorganize the Hilbert space into excitation towers.

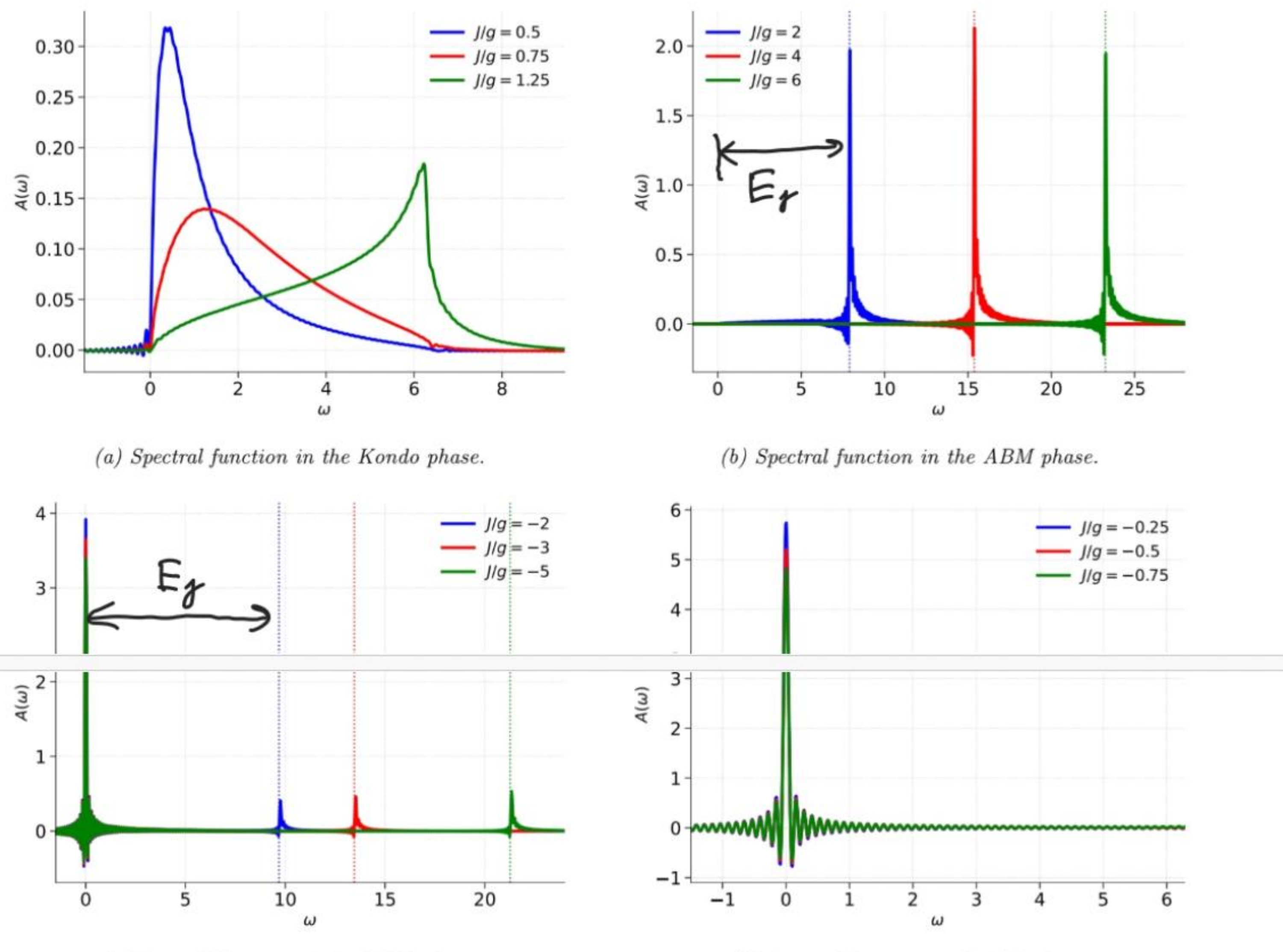
- In a Heisenberg chain an edge impurity generates a rich phase diagram. It is driven by boundary roots which reorganize the Hilbert space into excitation towers, and . $\mathcal{T}_{str}, \mathcal{T}_{BS}$ The activation $\mathcal{T}_{nBS}$ scale $E_\gamma = 2\pi g/|\sin(\pi\gamma)|$ controls the inter-tower mixing.

- A general TBA framework for handling impurities that generate boundary bound-modes, which fragment the Hilbert space into distinct excitation towers. It provides a unified approach to boundary phase transitions and to their thermodynamic signatures as well as their experimental realizations

Summary and Outlook

- Many open questions: does the Hilbert-space fragmentation that drives the impurity thermodynamics also show up quantum dynamics and transport, constraining relaxation and non-equilibrium steady states?

$$A(\omega) = -\frac{1}{\pi} Im\, G^{R}_{\rm imp}(\omega)$$

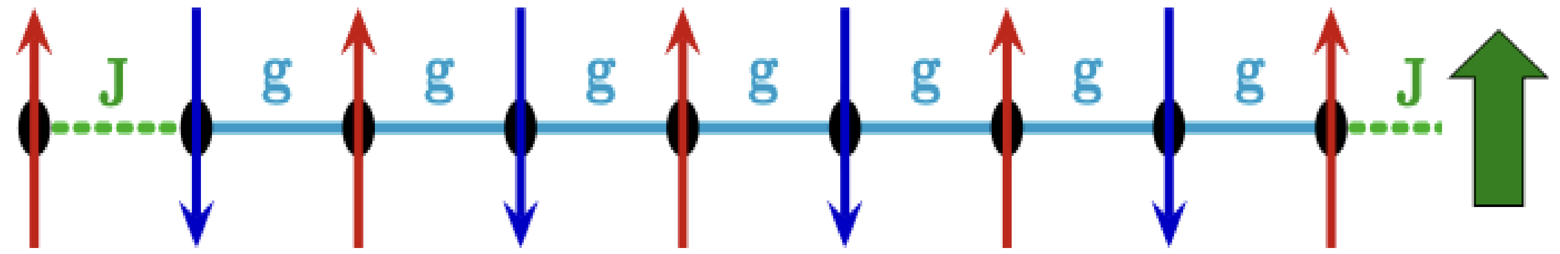


(a) Spectral function in the Kondo phase. (b) Spectral function in the ABM phase. (c) Spectral function in the FBM phase. (d) Spectral function in the US phase.

FIG. 9: Impurity spectral functions $A(\omega)$ for various impurity couplings.

- Does Hilbert space fragmentation arise in higher-dimensional or unconventional superconductors? or in gapped insulators where most studies rely on semiclassical or numerical approaches that may have overlooked such effects?

The Impurity at the edge of the spin chain–
The Bethe Ansatz equations



- The Bethe Ansatz equations for M down spins in a chain with N sites

$$\left(\frac{\mu_j - i/2}{\mu_j + i/2}\right)^{2N} \frac{\mu_j - d - i/2}{\mu_j - d + i/2}\frac{\mu_j + d - i/2}{\mu_j + d + i/2} = \prod_{l \neq j}^{M} \frac{(\mu_j - \mu_l - i)(\mu_j + \mu_l - i)}{(\mu_j - \mu_l + i)(\mu_j + \mu_l + i)}$$

- The energy $E = \sum_j \frac{1}{1+\mu_j^2}$

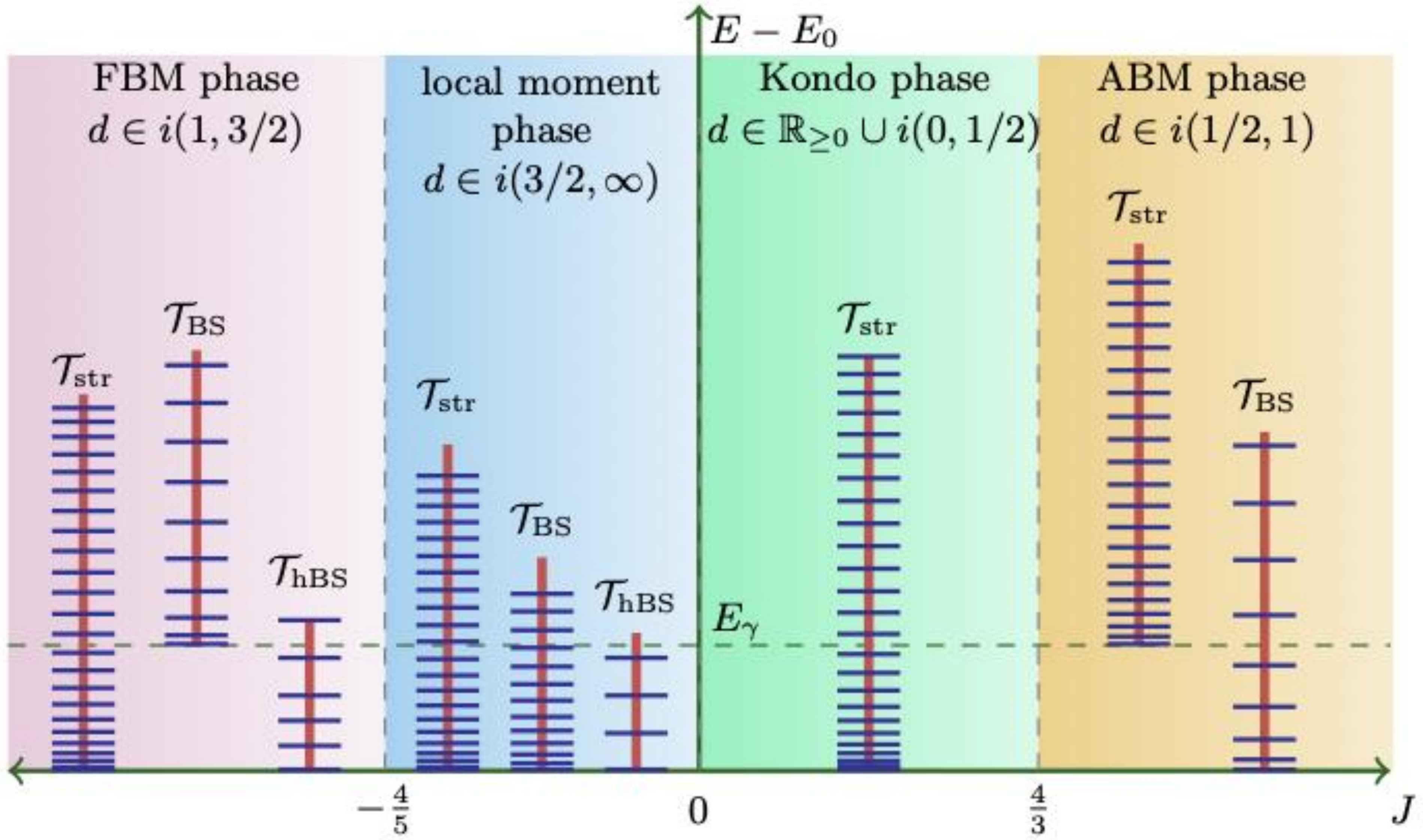
With $d = d(J) = \sqrt{1/J - 1}$ real or $d = i\gamma$

Wang 1997, Frahm, Zvyagin 1997

- The phase diagram: tower structure

The Kondo phase - the impurity is screened via the Kondo effect, and only the string tower is present.

The ABM phase - (antiferromagnetic bound-mode) a boundary-string (BS) tower emerges, describing localized screening by the bound mode, while the string tower is gapped by energy $E_\gamma = 2\pi g/|\sin(\pi\gamma)|$



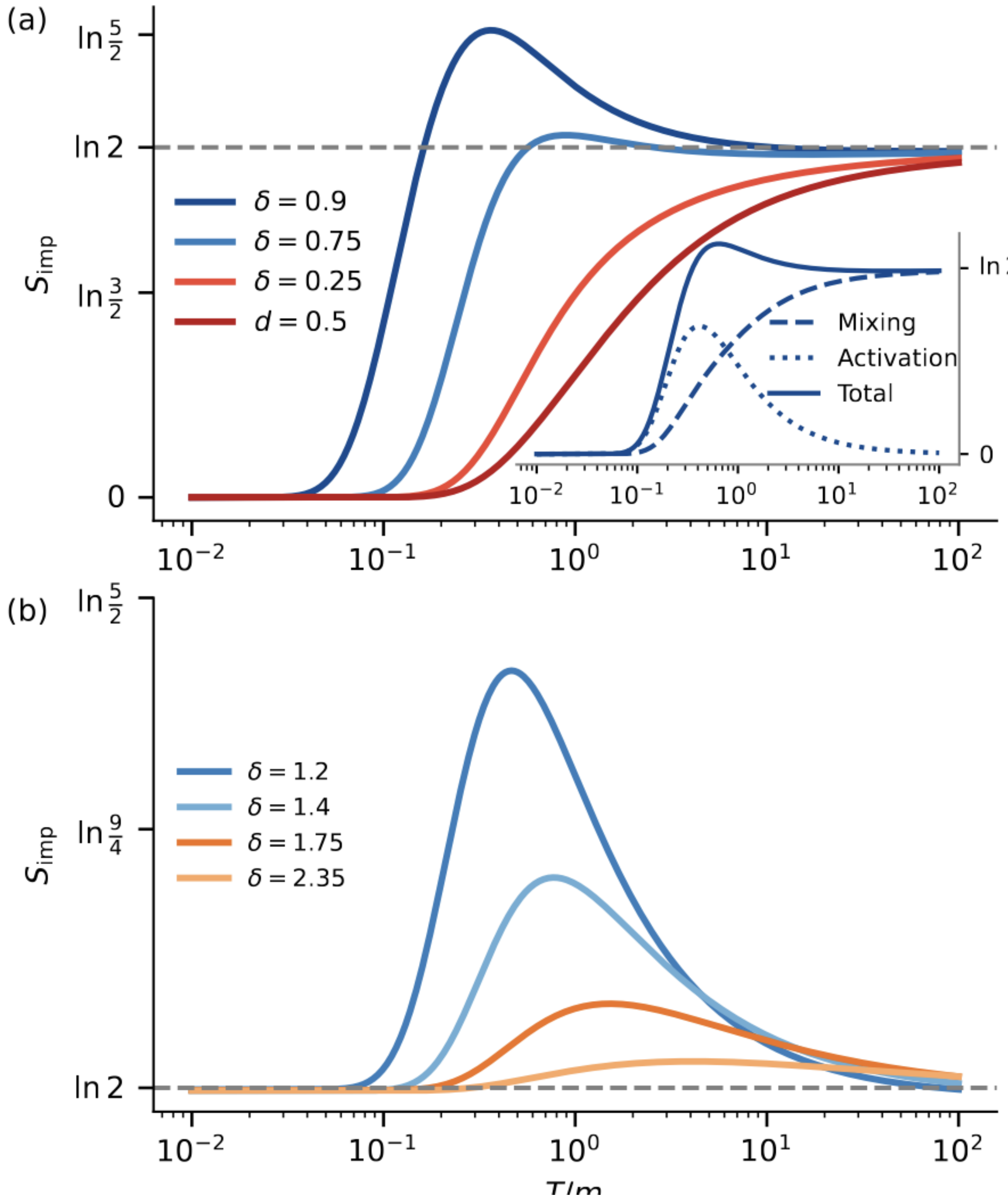
The ferromagnetic regimes- the spectrum comprises three towers: bulk strings, BS, and higher-order boundary strings (hBS).

The FBM - the BS tower is initially gapped, but as ferromagnetic coupling weakens, the gap closes, yielding a fourfold degenerate gs

The Local moment regime – degenerate towers

The Impurity Entropy

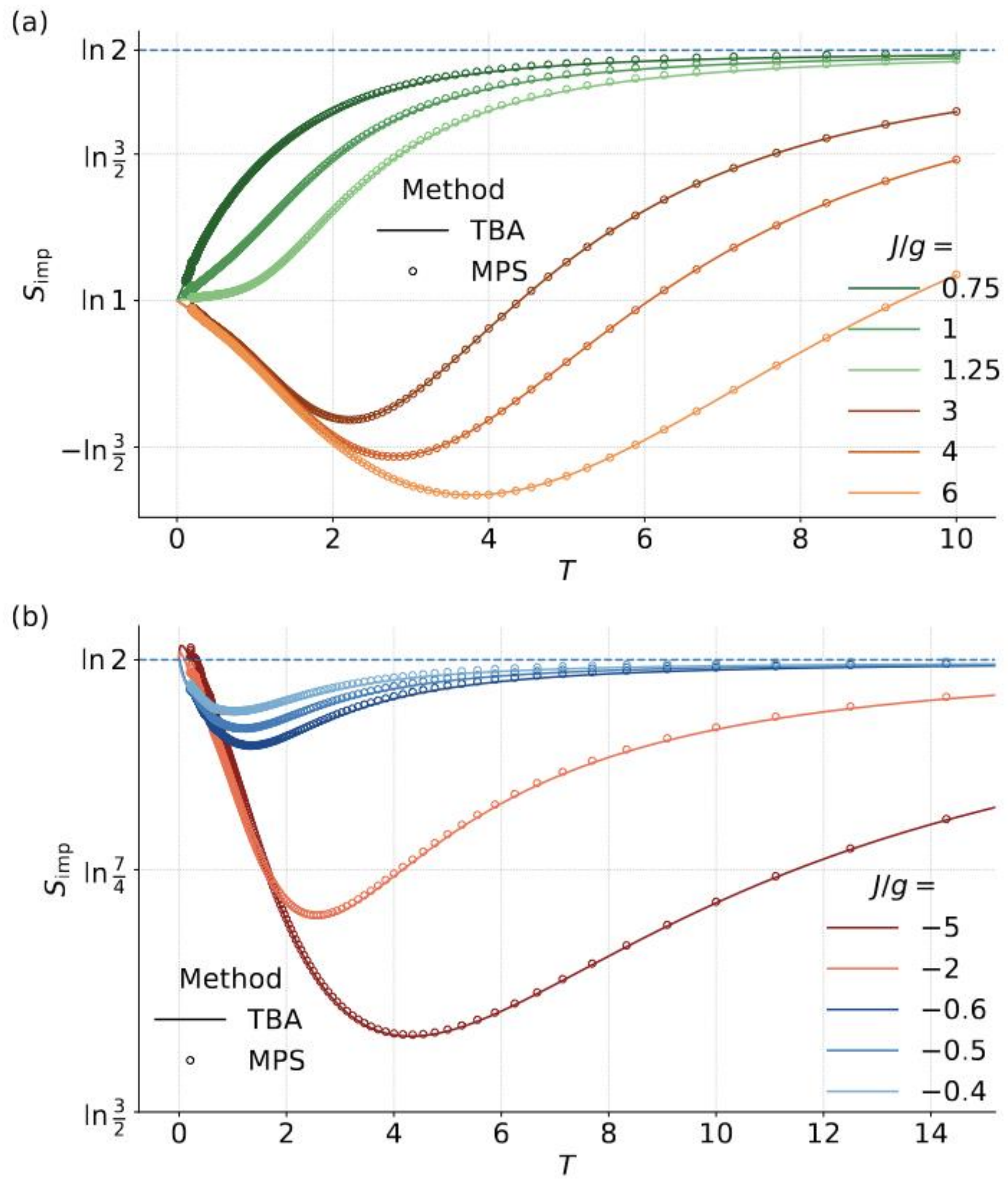
$$Z_0 = e^{-\beta F_{\mathrm{bulk}}(T)}\mathfrak{g}(T)$$



$$\mathfrak{g}(T)$$

universal O(1) boundary factor

$$Z = Z_0\mathfrak{g}_{\mathrm{imp}}(T)$$

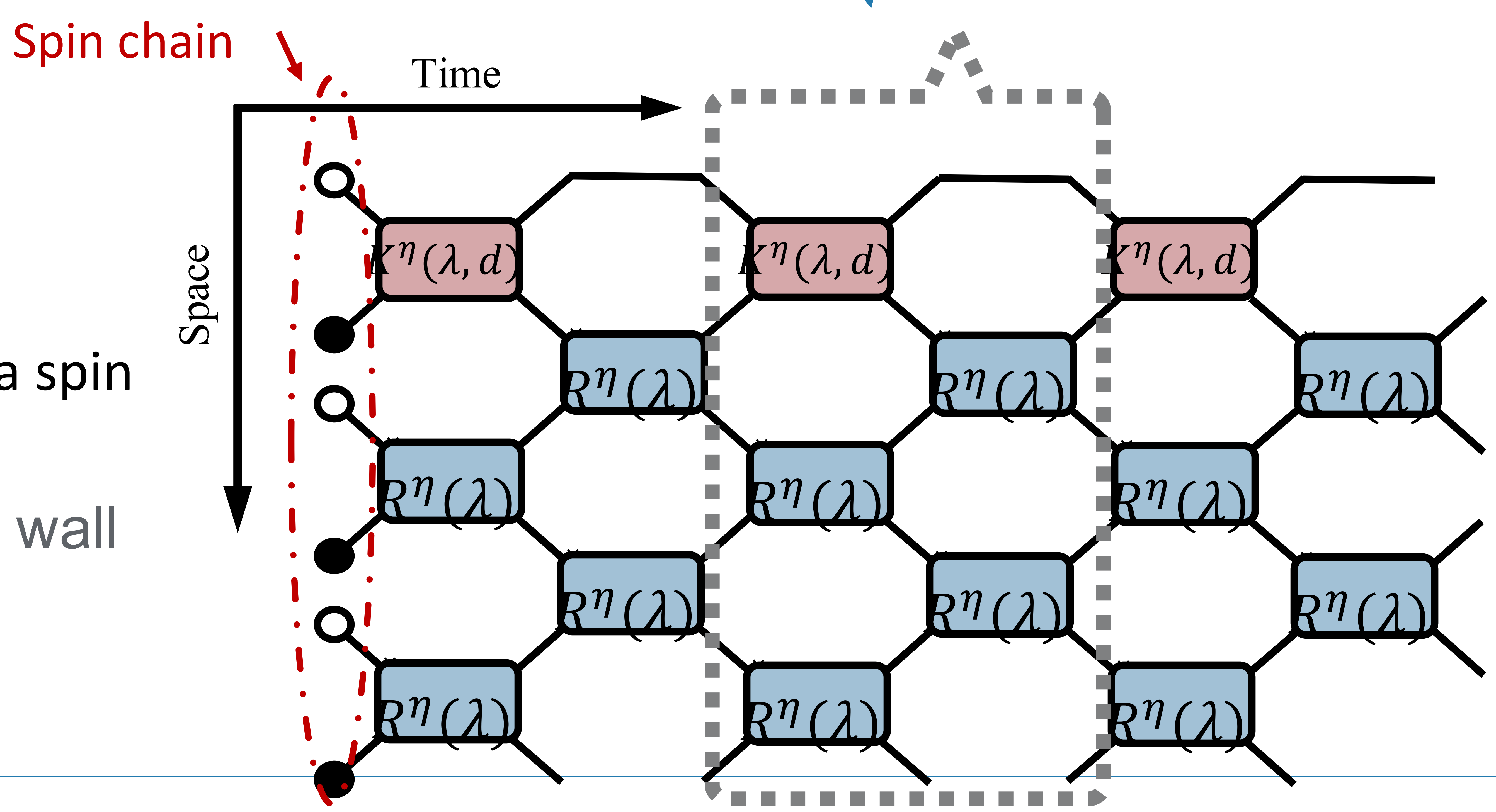


$$F_{\mathrm{imp}}(T) = -\frac{1}{\beta}\ln(Z/Z_0) = -\frac{1}{\beta}\ln\mathfrak{g}_{\mathrm{imp}}(T)$$

Quench Dynamics and Quantum circuits

- Trotterized time evolution: $\exp(-iHt) = \lim_{\delta t \to 0} (\mathbb{U})^{\frac{t}{\delta t}}$ acts on some initial state of a spin chain

- Time slice $\mathbb{U} = K_{0,1} \prod_{j=1}^{L/2-1} R_{2j,2j+1} R_{2j-1,2j}$



- Initial state of a spin chain –

  Néel, domain wall

- Bulk R-matrix

- Boundary K-matrix

The XXX-Kondo model: **Spin chain with an impurity at the edge**

- XXX-Kondo model

$$H = \frac{1}{2}\sum_{j}^{L-1}(\sigma_j^x\sigma_{j+1}^x + \sigma_j^y\sigma_{j+1}^y + \Delta\sigma_j^z\sigma_{j+1}^z) + \frac{J}{2}(\sigma_0^x\sigma_1^x + \sigma_0^y\sigma_1^y + \Delta'\sigma_0^z\sigma_1^z)$$

with

$$\Delta = \cosh(\eta)$$

At the isotropic XXX (Δ=Δ′=1) and the XX (Δ=Δ′=0), model is integrable for any impurity coupling J

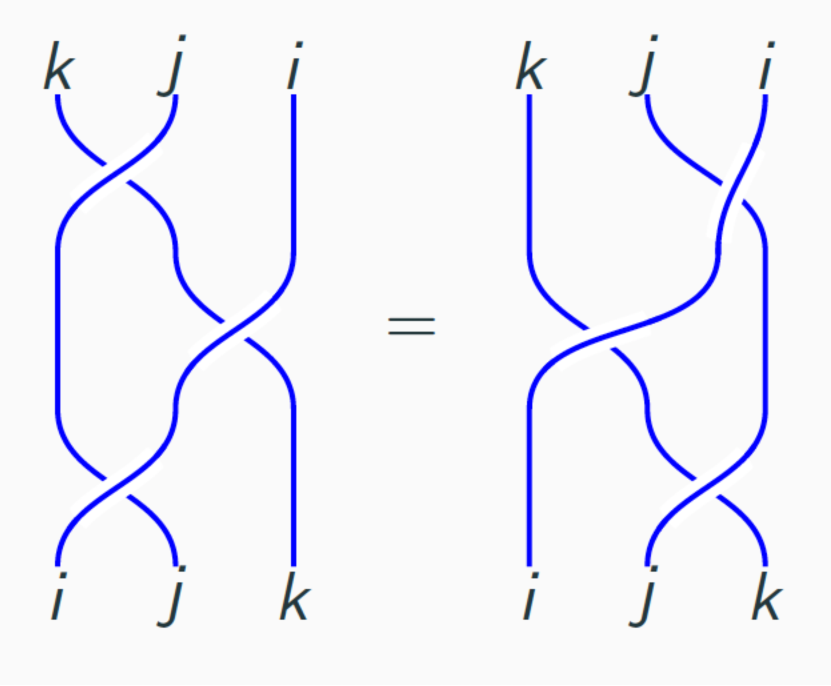
Y P Wang 1997, H Frahm, A Zvyagin 1997

- Integrability based on:

- R-matrix of the six-vertex model

  Satisfies Yang-Baxter equation

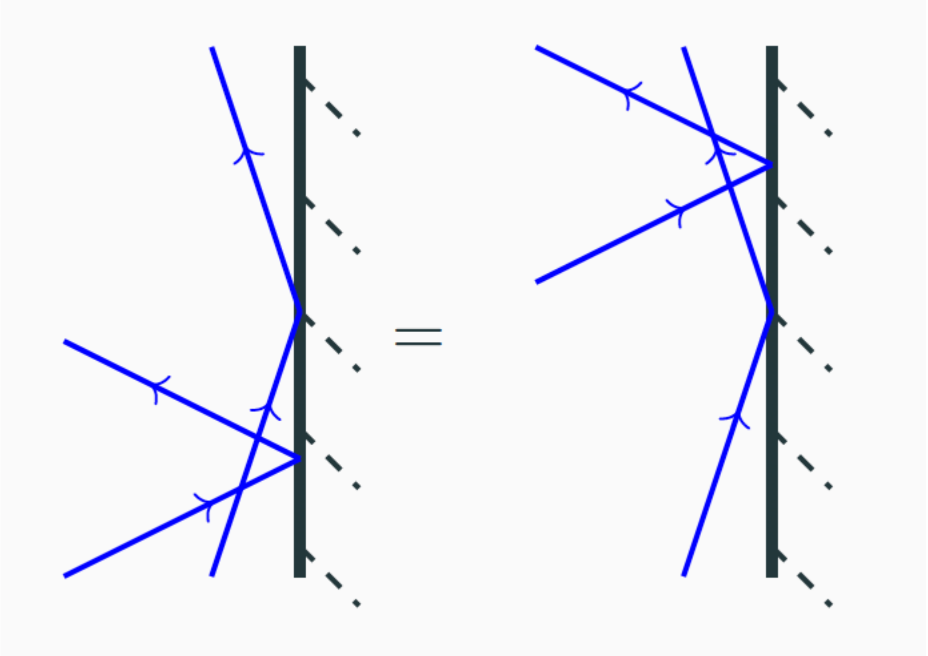
$$\boxed{R^\eta(\lambda)} = \begin{pmatrix} \frac{\sinh(\lambda+\eta)}{\sinh(\eta)} & 0 & 0 & 0 \\ 0 & 1 & \frac{\sinh(\lambda)}{\sinh(\eta)} & 0 \\ 0 & \frac{\sinh(\lambda)}{\sinh(\eta)} & 1 & 0 \\ 0 & 0 & 0 & \frac{\sinh(\lambda+\eta)}{\sinh(\eta)} \end{pmatrix}$$



- Boundary K-matrix

  Satisfies reflection relations

$$\boxed{K^\eta(\lambda, d)} = \check{R}_{01}^\eta(-d)\check{R}_{01}^\eta(\lambda+d)$$



- The Hamiltonian is the logarithmic derivative of the transfer matrix

$$H \propto \frac{d}{d\lambda}\log t(\lambda)\Big|_{\lambda=0}$$

$$t(\lambda) = tr_A\left[R_{AL}(\lambda)\cdots R_{A2}(\lambda)R_{A1}(\lambda)\right]$$

Quench Dynamics and Quantum circuits

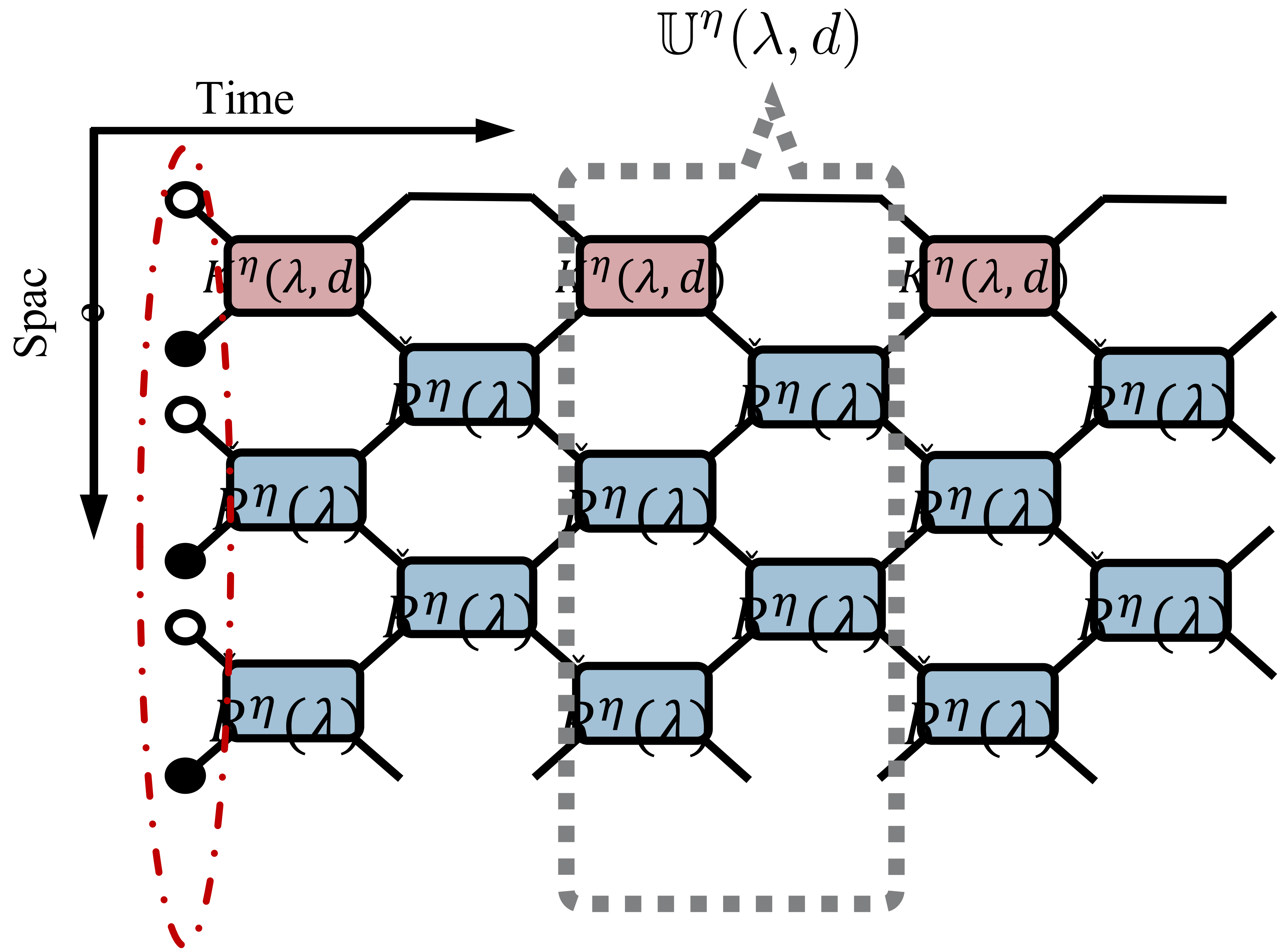
- The Trotterized time evolution of the XXZ – Kondo model:

$$\exp(-iH_{XXZ}t) = \lim_{\delta t\to 0} (\mathbb{U}^{\eta})^{\frac{t}{\delta t}}$$

  - With time slice

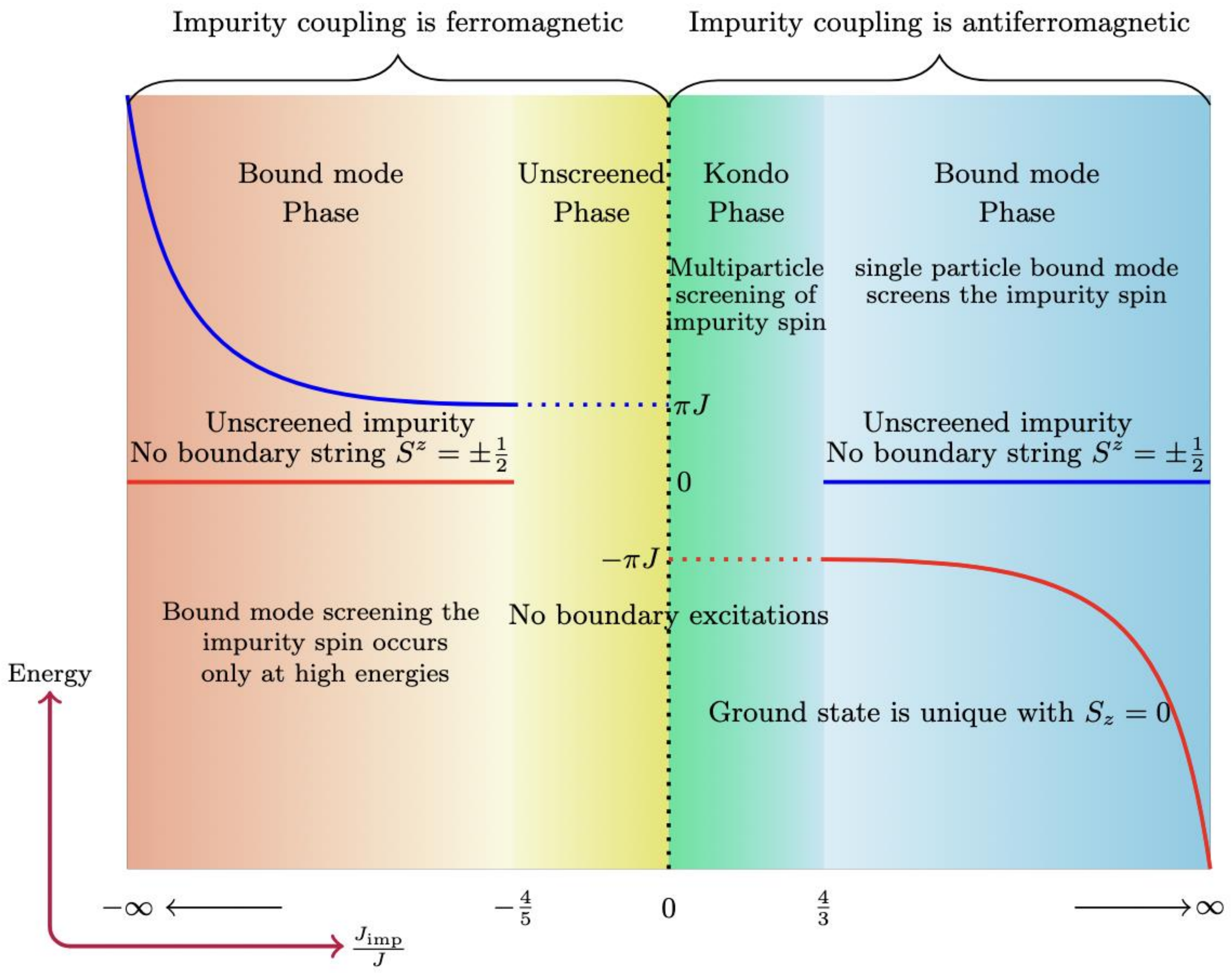
$$\mathbb{U}^{\eta}(\lambda, d) = K^{\eta}_{0,1}(\lambda, d) \prod_{j=1}^{L/2-1} \check{R}^{\eta}_{2j,2j+1}(\lambda)\check{R}^{\eta}_{2j-1,2j}(\lambda)$$

- d, λ and η are free parameters. In the Trotterziation limit choosing $\lambda = -i\delta t \sinh \eta$, the quantum circuit simulates the unitary evolution



XXX Impurity Spin Chain and the Kondo Effect

- Phase diagram of the model

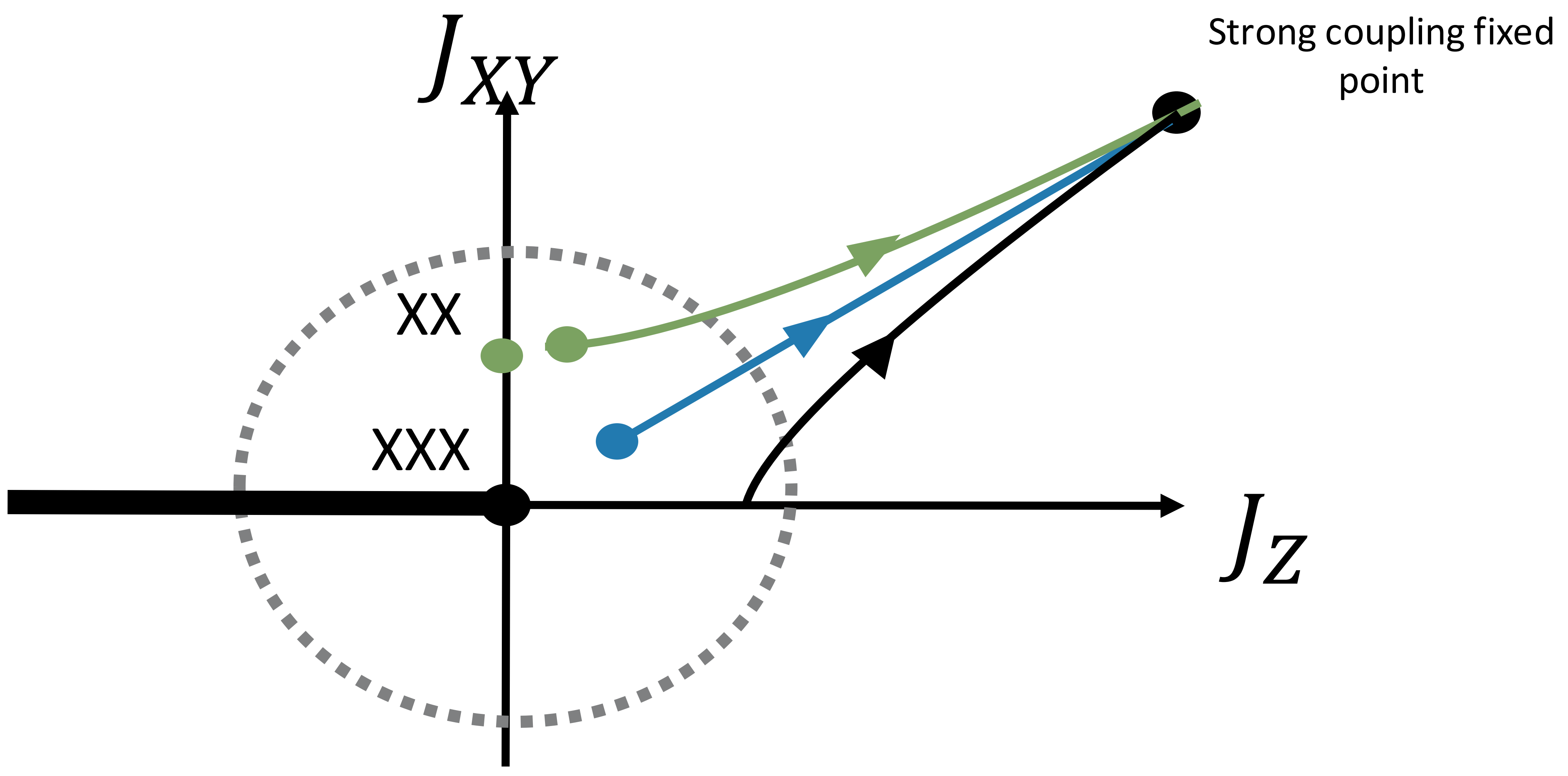


- Kondo phase : Effective low energy description - fermionized spins via Jordan-Wigner, linearize..

$$\mathcal{H} = \frac{1}{6\pi}\left[J(x)^2 + \bar{J}(x)^2\right] - \frac{\lambda}{2\pi}J(x)\cdot\bar{J}(-x) + g(J(0) + \bar{J}(0))\cdot\vec{S}$$

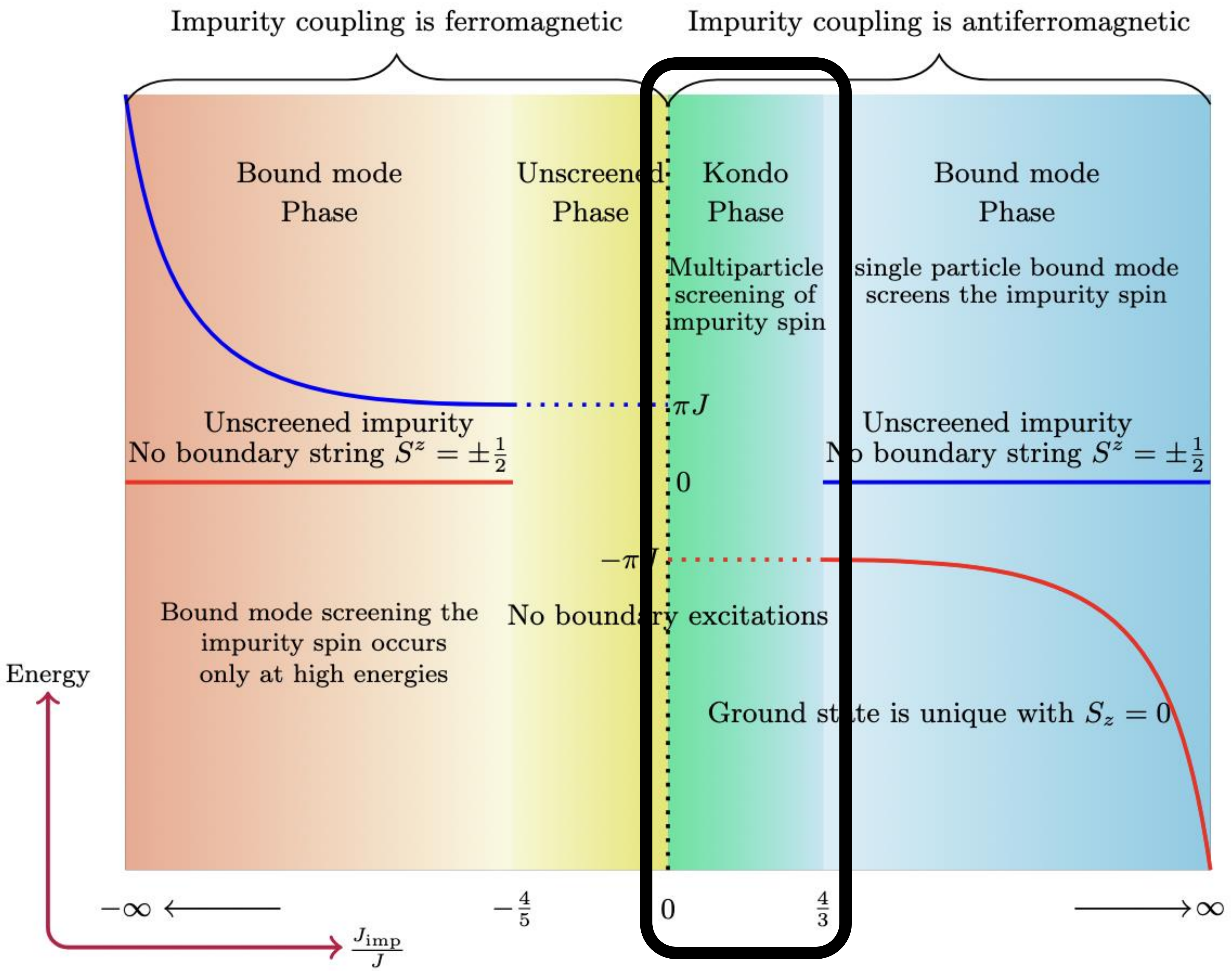
Irrelevant in IR

- RG flows to the strong coupling fixed point

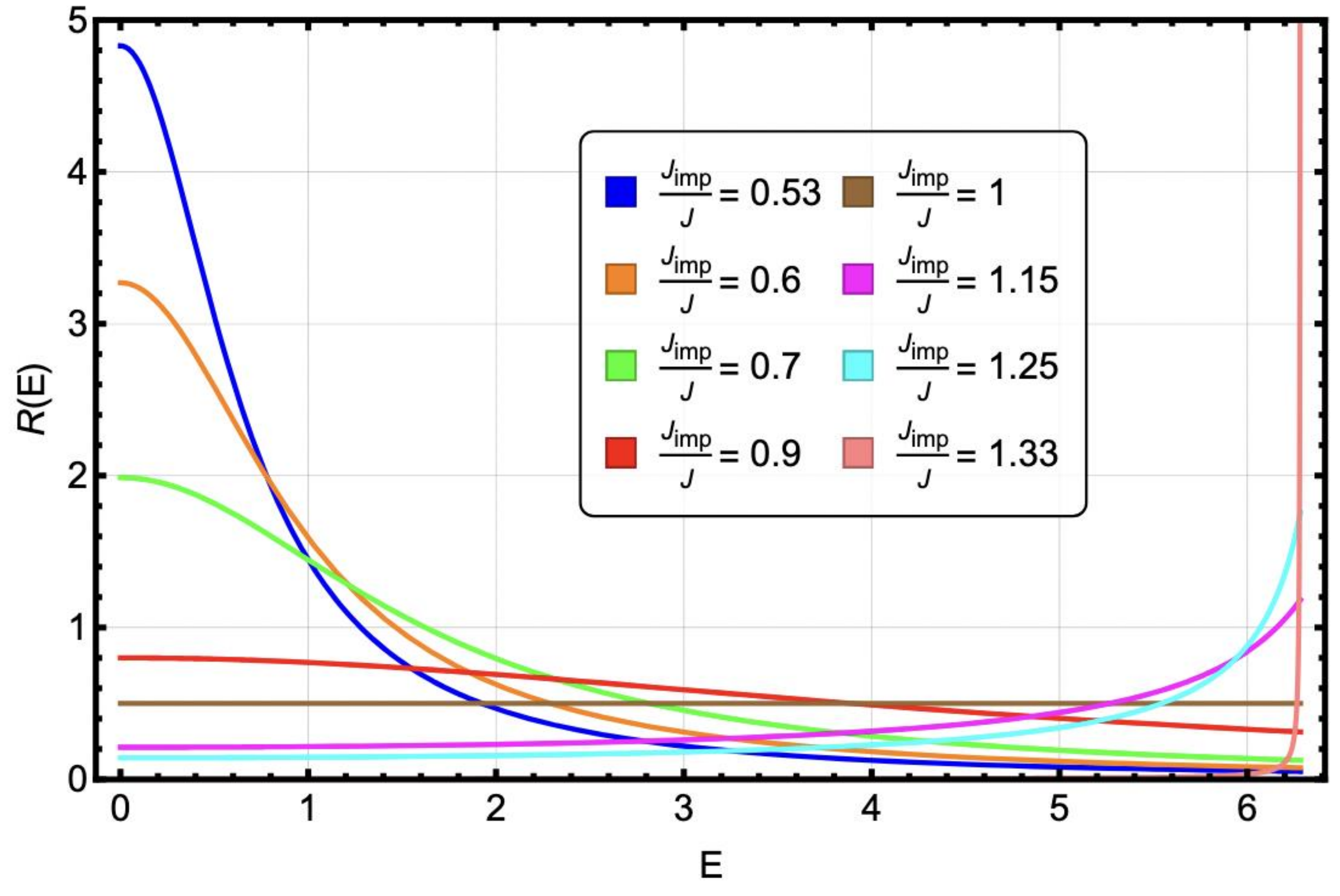


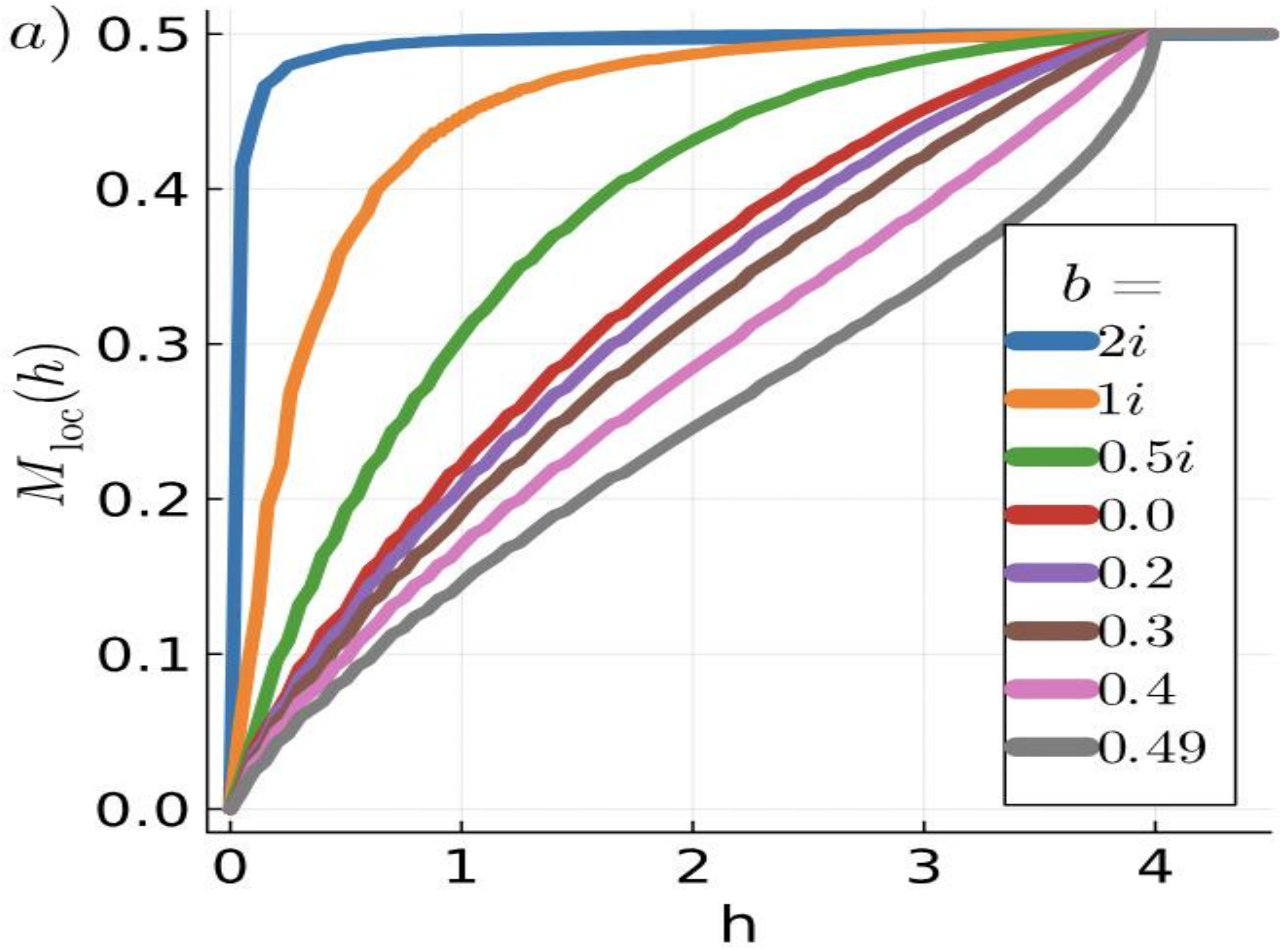
XXX Impurity Spin Chain and the Kondo Effect

Strong correlated Many-body System at $\eta = 0$ (XXX) point



Relative density of state $R(E) = \frac{N}{2}\frac{\rho_{\text{imp}}(E)}{\rho_{\text{bulk}}(E)}$





$$\frac{J_{imp}}{J} = \frac{1}{1 - b^2}$$

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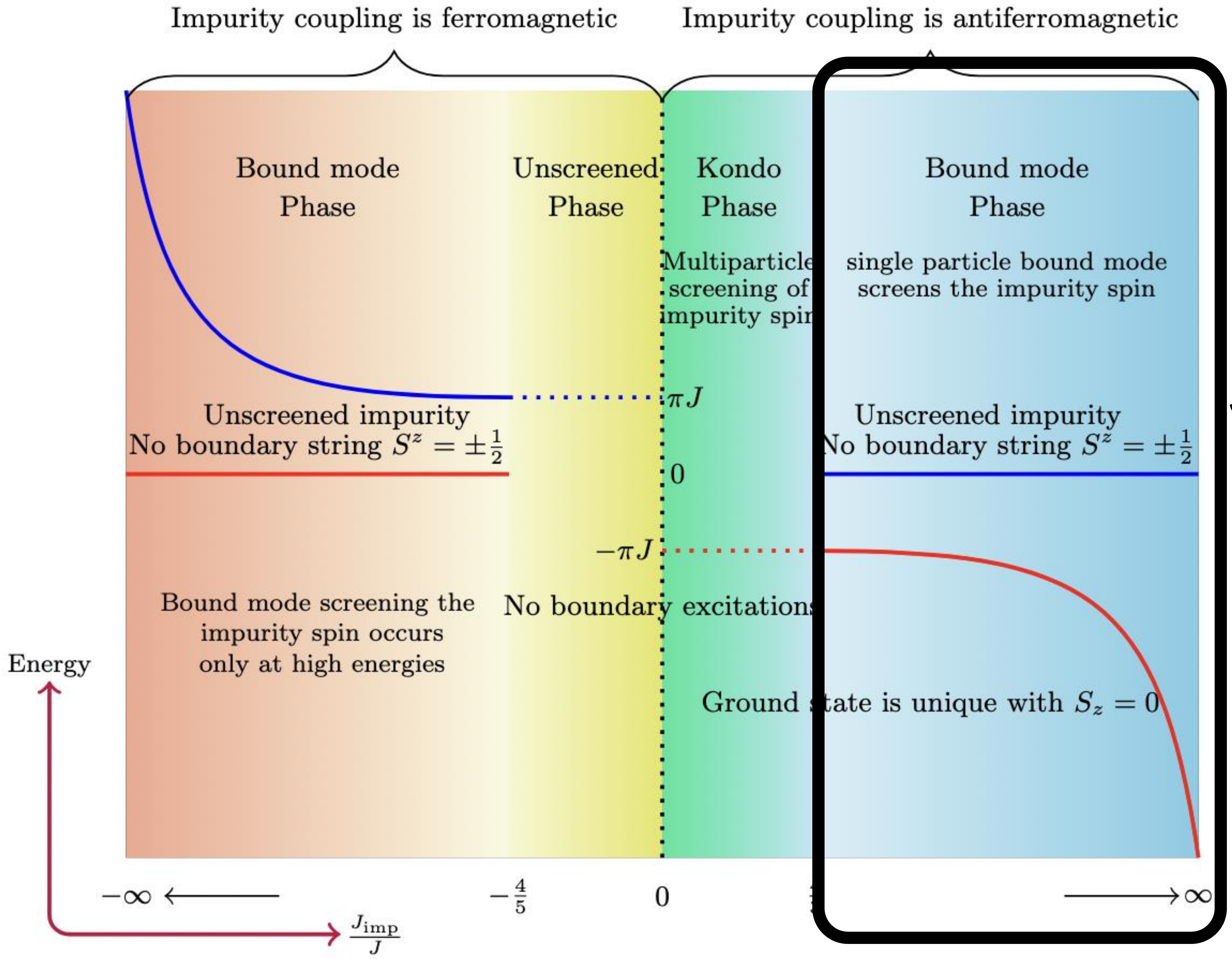
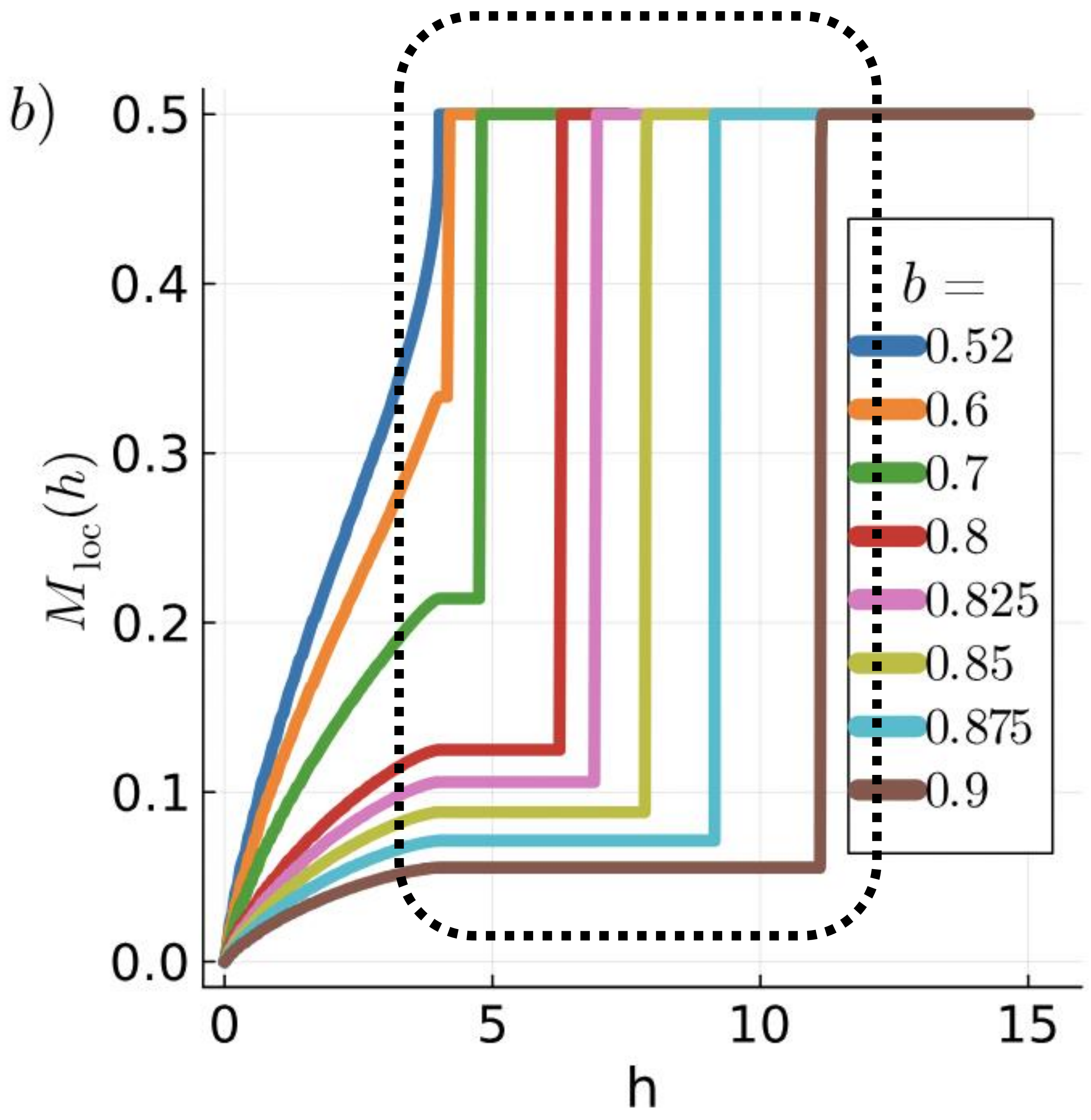
XXX Impurity Spin Chain and the Boundary Mode phase

Strong correlated Many-body System at $\eta = 0$ (XXX) point



Discontinuity indicates Massive bound mode



$$\frac{J_{imp}}{J} = \frac{1}{1-b^2}$$

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XX Impurity Spin Chain and the Kondo Effect

- Spin Hamiltonian when $\eta = i\frac{\pi}{2}$

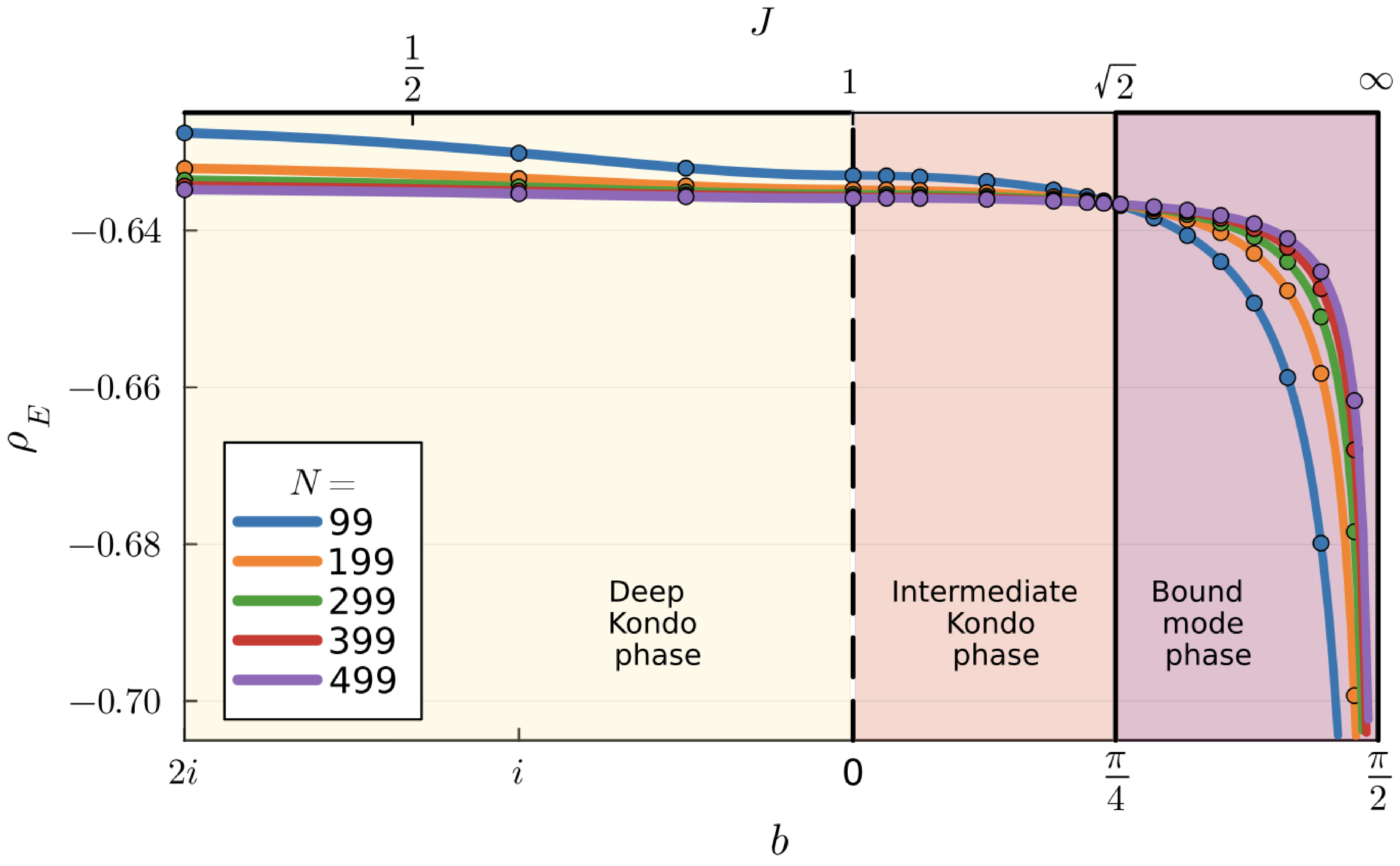
$$H = \sum_{j=1}^{L-1} \frac{1}{2}(\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y) + \frac{J}{2}(\sigma_0^x \sigma_1^x + \sigma_0^y \sigma_1^y)$$

- Same Kondo physics but can be mapped to Free Fermion model.
- Easier to study equilibrium, quenches and noisy effects.

- Spin $\left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i\right) + J\left(c_0^\dagger c_1 + c_1^\dagger c_0\right)$

- **No longer free when we add noise, but still integrable**

Energy density



$$J = \sec b$$

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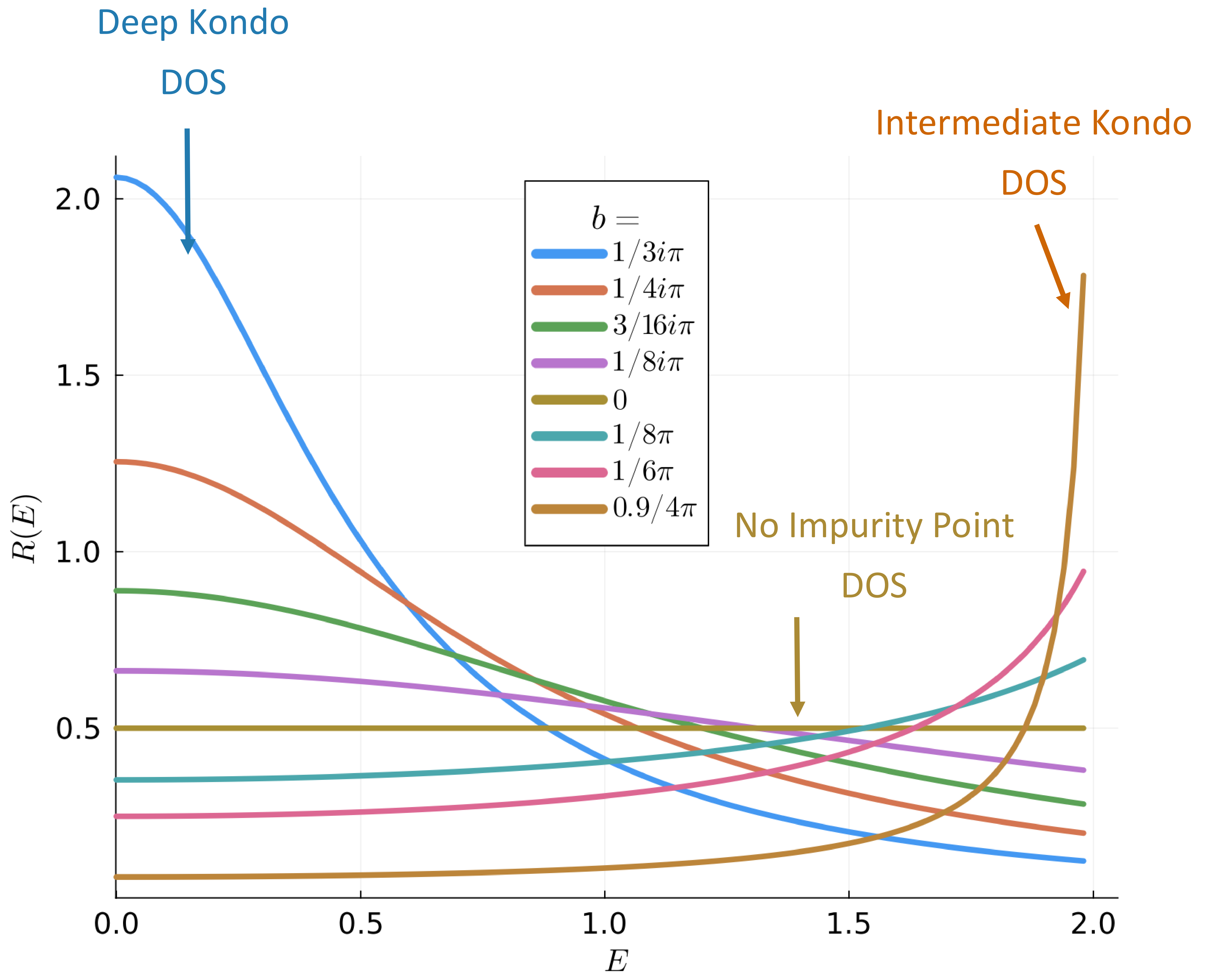
XX Impurity Spin Chain in the Kondo Phase



- DOS in Kondo phase:

$$R(E) = \frac{N}{2} \frac{\rho_{\mathrm{dos}}^{\mathrm{imp}}(E)}{\rho_{\mathrm{dos}}^{\mathrm{bulk}}(E)}$$

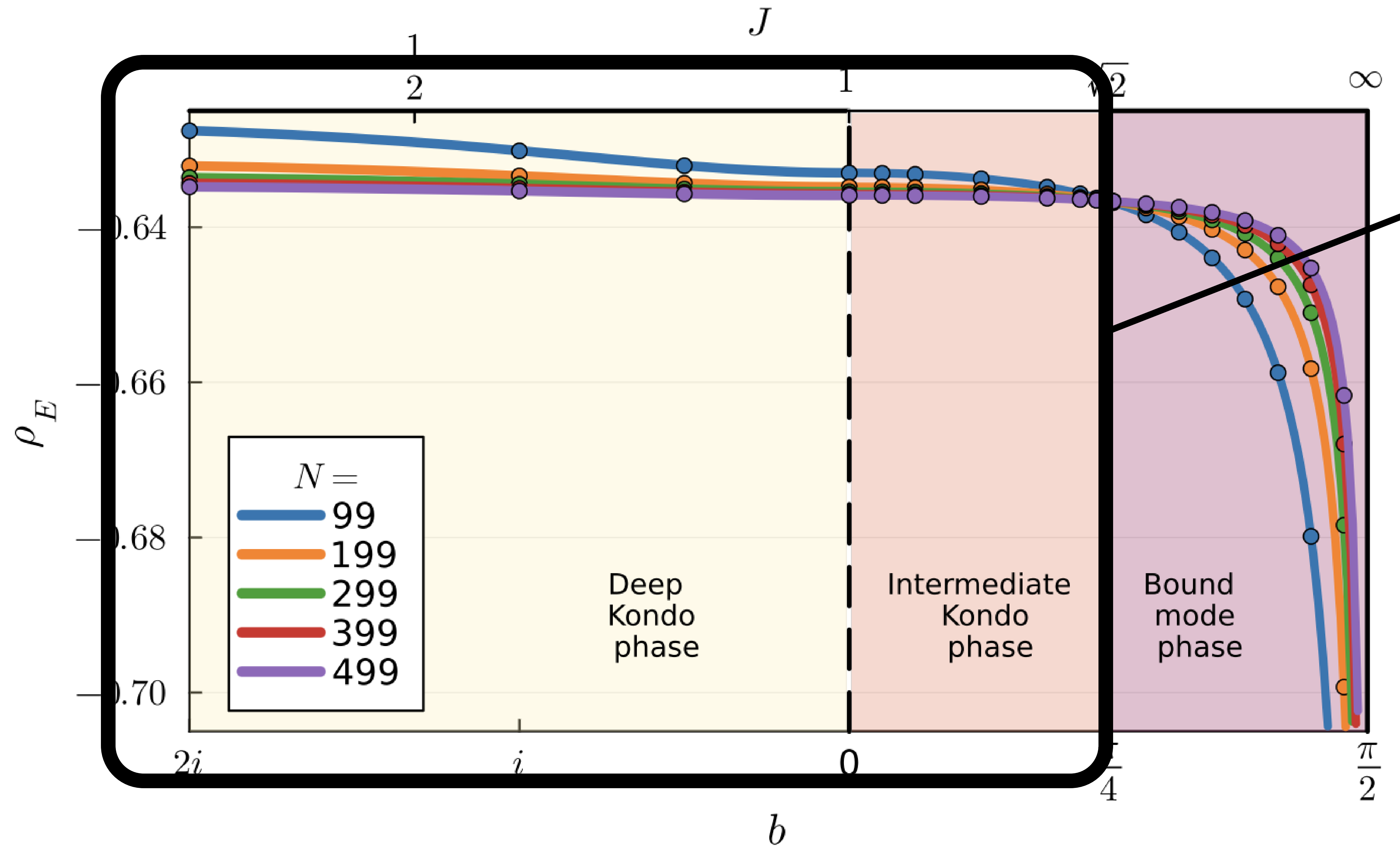
$$= \frac{4\cos(2b)}{E^2\left(\cos(4b) + \cosh\left(2\cosh^{-1}\left(\frac{2}{E}\right)\right)\right)}$$

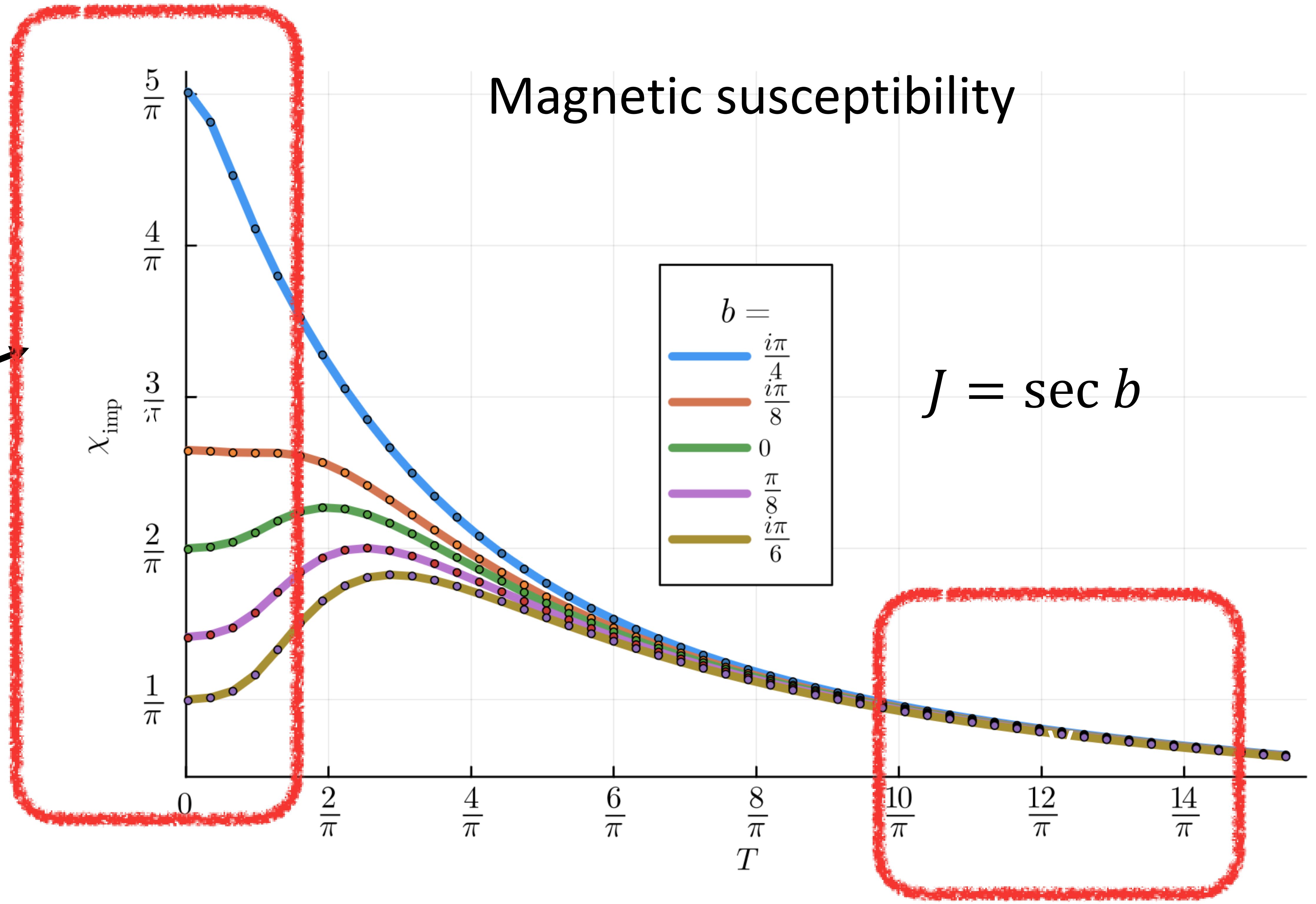
- In the deep Kondo Phase, DOS is a Lorentzian peaked at E=0.

- Moving to the bound mode Phase, DOS starts to peak towards the bound mode regime at E=2.

XX-Impurity Spin Chain and the Kondo Effect

$$H = \sum_{j=1}^{L-1} \frac{1}{2}(\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y) + \frac{J}{2}(\sigma_0^x \sigma_1^x + \sigma_0^y \sigma_1^y)$$





Finite susceptibility at T=0 (Kondo effect)

Susceptibility $\sim T^{-1}$ for High temperature (asymptotic freedom)

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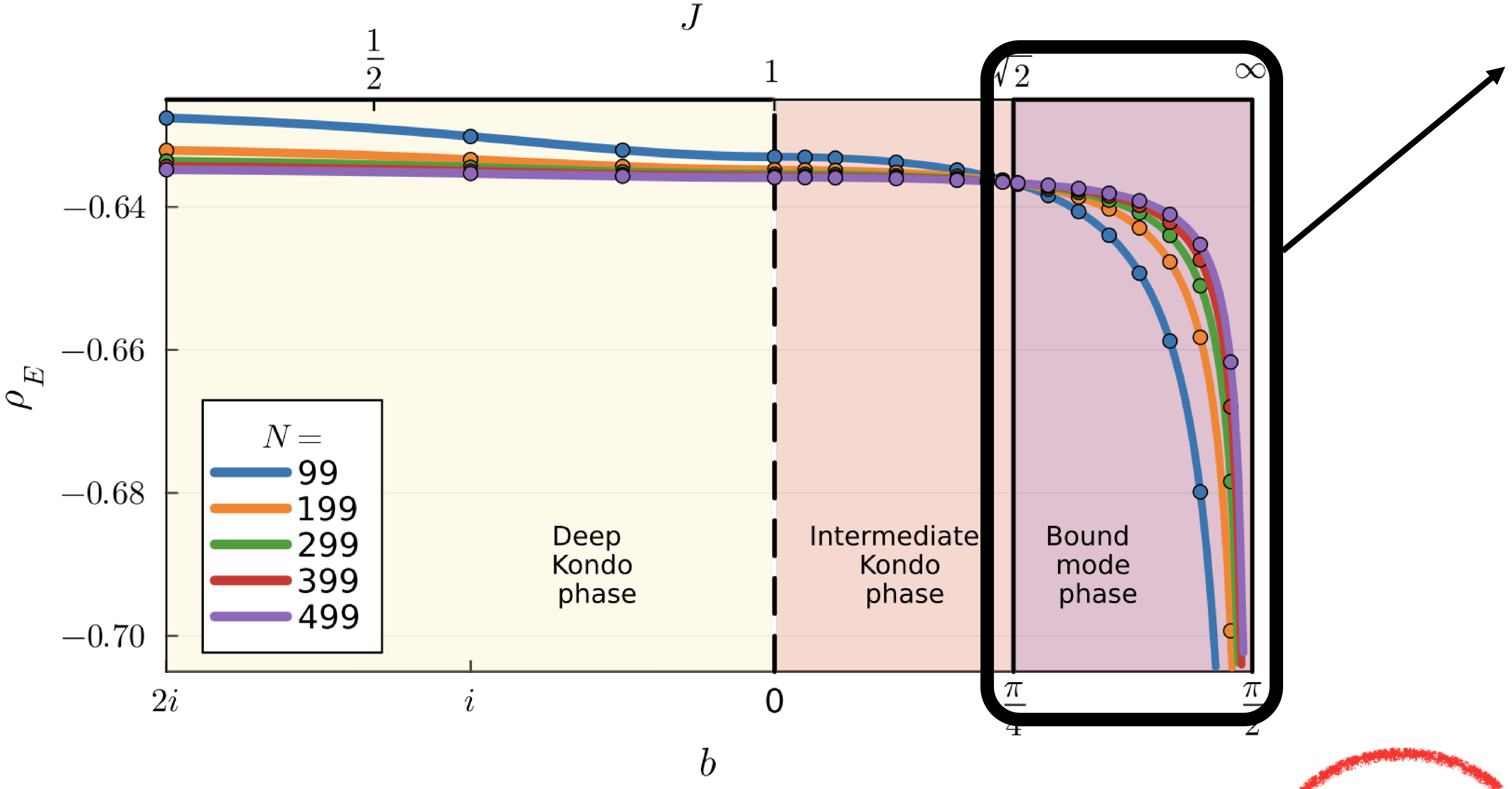
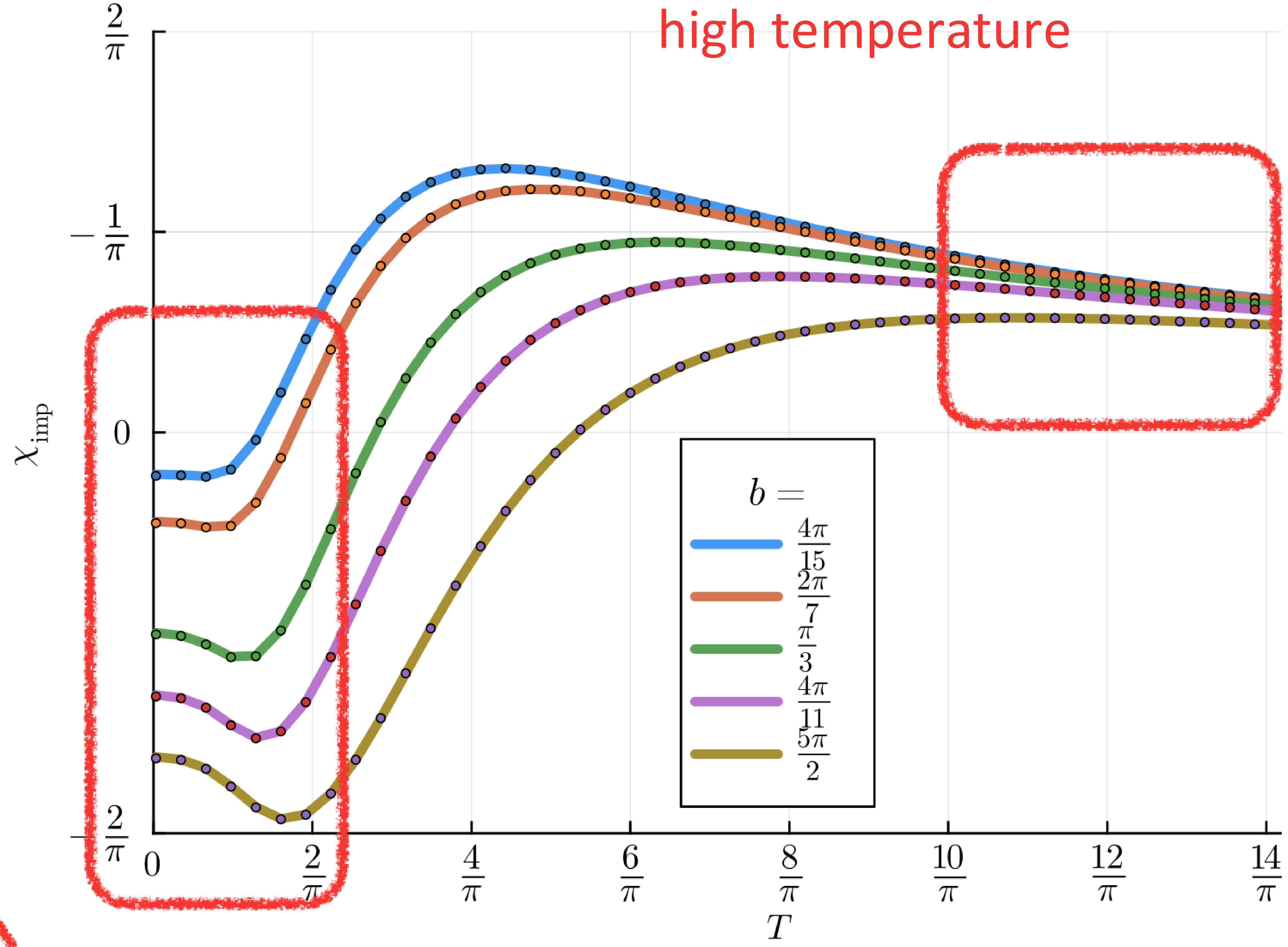
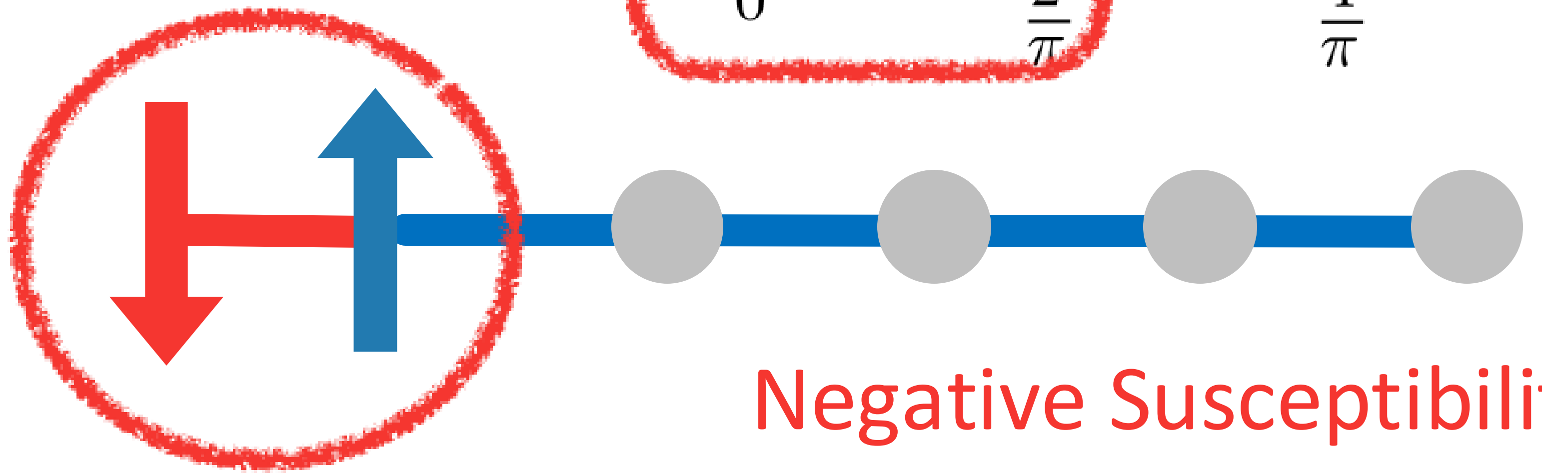
XX- Impurity Spin Chain in the bound mode regime

$$H = \sum_{j=1}^{L-1} \frac{1}{2}(\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y) + \frac{J}{2}(\sigma_0^x \sigma_1^x + \sigma_0^y \sigma_1^y)$$



susceptibility $\sim T^{-1}$ at high temperature





Negative Susceptibility due to bound mode

Singlet

$J = \sec b$

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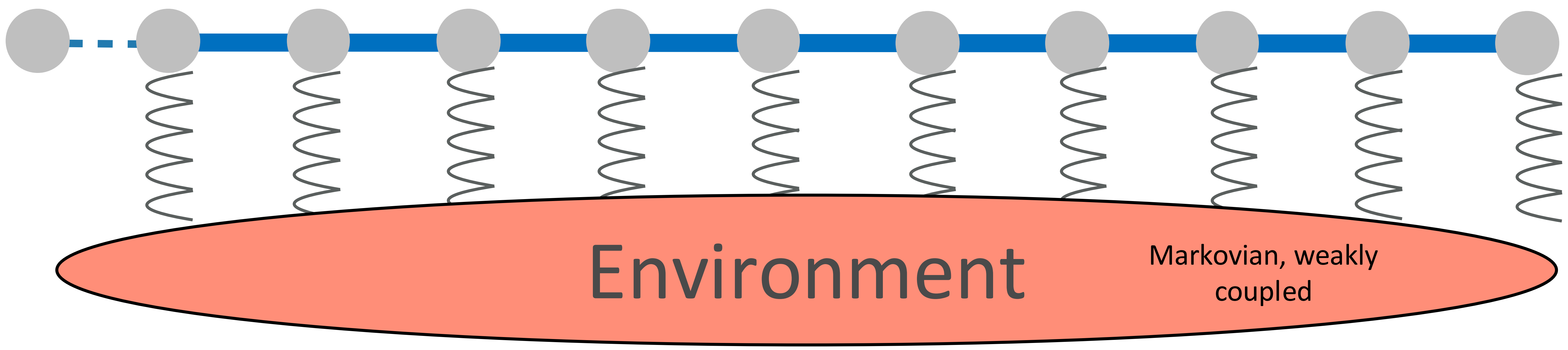
Modeling Noisy Circuit in Trotterized Limit



Liouvillian

$$\frac{d\rho}{dt} = -i[H,\rho] + \sum_i \gamma_i \left(L_i \rho L_i^\dagger - \frac{1}{2}\{L_i^\dagger L_i, \rho\} \right) = \mathcal{L}[\rho(t)]$$

$$H(\eta, d) = \sum_{j=1}^{L-1} \frac{1}{2}(\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \Delta \sigma_j^z \sigma_{j+1}^z) + \frac{J}{2}(\sigma_0^x \sigma_1^x + \sigma_0^y \sigma_1^y + \Delta' \sigma_0^z \sigma_1^z)$$

Lindblad Operator

$L_i = \sigma_i^z$ for dephasing error

- Lindbladian dynamics is Integrable at $\eta = i\frac{\pi}{2}$

Time evolution of the XX-Kondo spin chain in a noisy environment

Reformulate the Lindbladian evolution $i\partial_t \rho(t) = \mathcal{L}[\rho(t)]$

Will show Lindbladian evolution of XX is integrable

- Introduce the 4^N - dim Liouville-Fock space $|m\rangle\langle n| \to |n,m\rangle\rangle$ *Prosen '06*
- The density operator $\rho = \sum_{m,n} \rho_{mn} |m\rangle\langle n| \to \sum_{m,n} \rho_{mn} |n,m\rangle\rangle$
- Define $c_i^\dagger |n,m\rangle\rangle = c_i^\dagger |n\rangle\langle m|, \quad \tilde{c}_i^\dagger |n,m\rangle\rangle = |n\rangle\langle m| c_i$
- The Liouvillian acts as $\mathcal{L}|\rho\rangle\rangle = \frac{d}{dt}|\rho\rangle\rangle$
- The Liouvillian takes the form $\mathcal{L} = -iH + i\tilde{H} + 4\gamma \sum_{i=1}^{L-1} \left(c_i^\dagger c_i \tilde{c}_i^\dagger \tilde{c}_i - \frac{1}{2} c_i^\dagger c_i - \frac{1}{2} \tilde{c}_i^\dagger \tilde{c}_i \right)$ *Medvedyeva, Essler, Prosen '16*
- Denote $c_i^\dagger = c_{i,\uparrow}^\dagger \quad \tilde{c}_i^\dagger = c_{i,\downarrow}^\dagger$ and apply $U = \prod_{i=1}^{N/2} (1 - 2\tilde{c}_i^\dagger \tilde{c}_i)$
- **The Liouvillian --> Kondo-Hubbard model with imaginary coupling**

$$\mathcal{L} = -iJ(c_{0,\sigma}^\dagger c_{1,\sigma} + c_{1,\sigma}^\dagger c_{0,\sigma}) - i \sum_{i=1}^{L-1} (c_{i,\sigma}^\dagger c_{i+1,\sigma} + c_{i+1,\sigma}^\dagger c_{i,\sigma}) + \gamma \sum_{i=1}^{L} (2c_{i,\uparrow}^\dagger c_{i,\uparrow} - 1)(2c_{i,\downarrow}^\dagger c_{i,\downarrow} - 1) - \gamma(L-1)$$

- The model is integrable *Karnaukhov , Egorov '05*

Time evolution of the XX-Kondo spin chain in a noisy environment

- To determine time evolution we need to obtain the spectrum of the Liouvillian.

  The Lindbladian eigenvalue problem $\mathcal{L}|\rho_n\rangle\rangle = E_n|\rho_n\rangle\rangle$

  i. analytically for the noisy XX chain (we shall need also some overlaps)
  ii. numerically for the noisy XXX chain (with similar results as XX)

- The evolution of observable $\hat{O}$ from an initial density matrix ρ_i

$$O(t) = \mathrm{Tr}\{\hat{O}(t)\rho_i\}$$

with

$$\frac{d\hat{O}}{dt} = \mathcal{L}(\hat{O}) = \left[\hat{O}, H\right] + i\sum_{j=1}^{L-1}\gamma\left[L_j\hat{O}L_j^\dagger - \frac{1}{2}\left\{L_j^\dagger L_j, \hat{O}\right\}\right]$$

- Study the time evolution of the **impurity magnetization** $S_0^z(t)$

Time evolution of the XX-Kondo spin chain in a noisy environment

- **Impurity magnetization** can be expressed in terms of the 2-point correlator $G(x;y;t) = \mathrm{Tr}\left\{c_x^\dagger c_y \rho(t)\right\}$

$$S_0^z(t) = 2G(0,0,t) - 1$$

- The time-dependent two-point correlation function $|G(x,y,t)\rangle\rangle = e^{-i\mathcal{L}t}|G(x,y)\rangle\rangle$

Expand : $$|G(x,y,t)\rangle\rangle = \sum_{k,q} \alpha_{k,q}(x,y)|k,q\rangle\rangle e^{-iE(k,q)t}$$

where $|k,q\rangle\rangle$ are the eigenmodes and $E(k,q)$ is the Liouvillian spectrum: $\mathcal{L}|k,q\rangle\rangle = E(k,q)|k,q\rangle\rangle$

$$\boxed{EG(x,y) = \left[J_x\Delta_x + J_y\Delta_y + 4i\gamma\delta_{x,y} + 2i\gamma(\delta_x + \delta_y - 2)\right] G(x,y),}$$

- The time-dependent **impurity magnetization** $S_0^z(t)=\mathrm{Tr}\sigma_0^z\rho(t)$ can be expressed in terms of the eigenmodes of impurity $S_0^z(k,q) = G_{k,q}(0,0)$ as

$$S_0^z(t)=\sum_{k,q} \alpha_{k,q} S_0^z(k,q) \exp[-iE(k,q)t$$

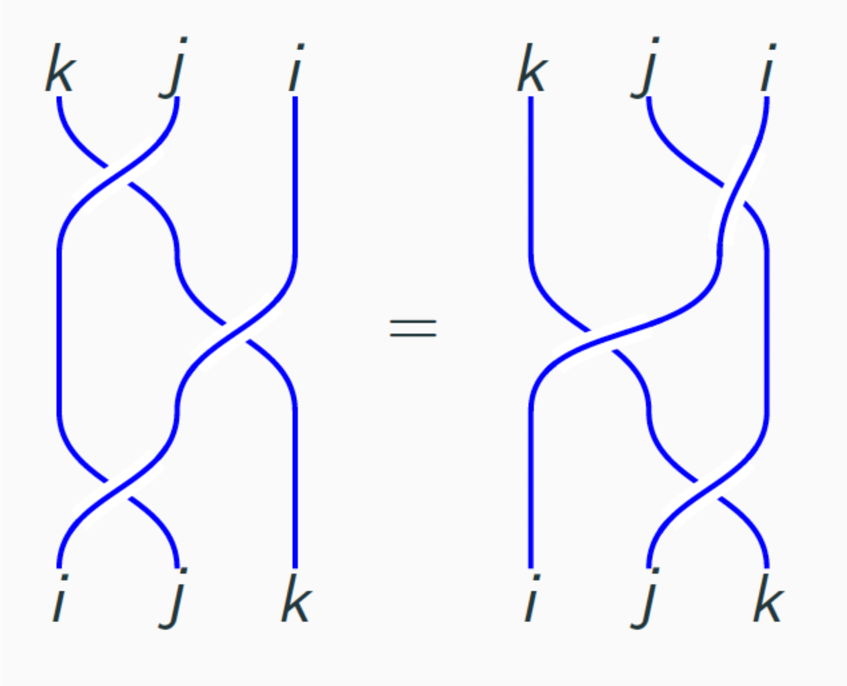
- This requires the knowledge of the Liouvillian spectrum $E(k,q)$, the impurity magnetization of each mode $S_0^z(k,q)$ and the overlap with between the eigenstates and the initial state $\alpha_{k,q}$.

The Liouvillian Spectrum

- The Liouvillian spectrum of the noisy XX-Kondo model

$$EG(x,y) = \left[J_x\Delta_x + J_y\Delta_y + 4i\gamma\delta_{x,y} + 2i\gamma(\delta_x + \delta_y - 2)\right]G(x,y),$$

where $J_x = J$ when x = 0, $J_x = 1$ otherwise, and $\Delta f(x) = f(x+1) + f(x-1)$



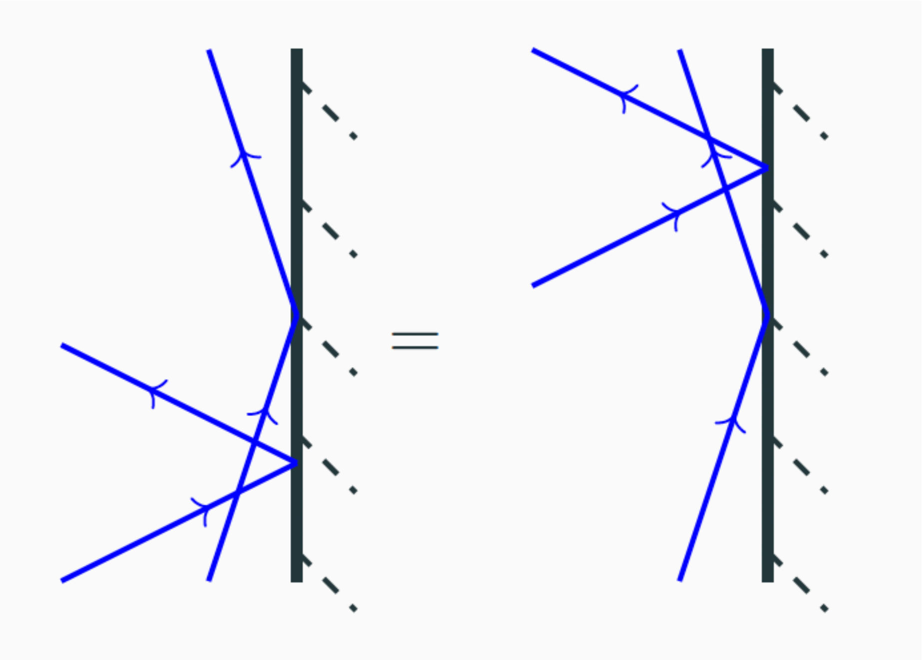
- The solution takes the Bethe Ansatz form

$$G_{k,q}(x,y) = \frac{1}{\mathcal{N}}\mathcal{S}\sum_{\alpha_1,\alpha_2=\pm 1} e^{i\alpha_1 kx + i\alpha_2 qy}\left[A(\alpha_1 k, \alpha_2 q)\theta(x-y) + B(\alpha_2 q, \alpha_1 k)\theta(y-x)\right]$$

with eigenvalues $\boxed{E(k,q) = 2\cos k + 2\cos q - 4i\gamma}$

- Impose boundary conditions: with the boundary and bulk S-matrices

$$\boxed{K(k) = -\frac{e^{ik} + e^{-ik} - 2i\gamma - J^2 e^{ik}}{e^{ik} + e^{-ik} - 2i\gamma - J^2 e^{-ik}} \quad \text{and} \quad S(k,q) = \frac{\sin k - \sin q + 2\gamma}{\sin k - \sin q - 2\gamma}}$$



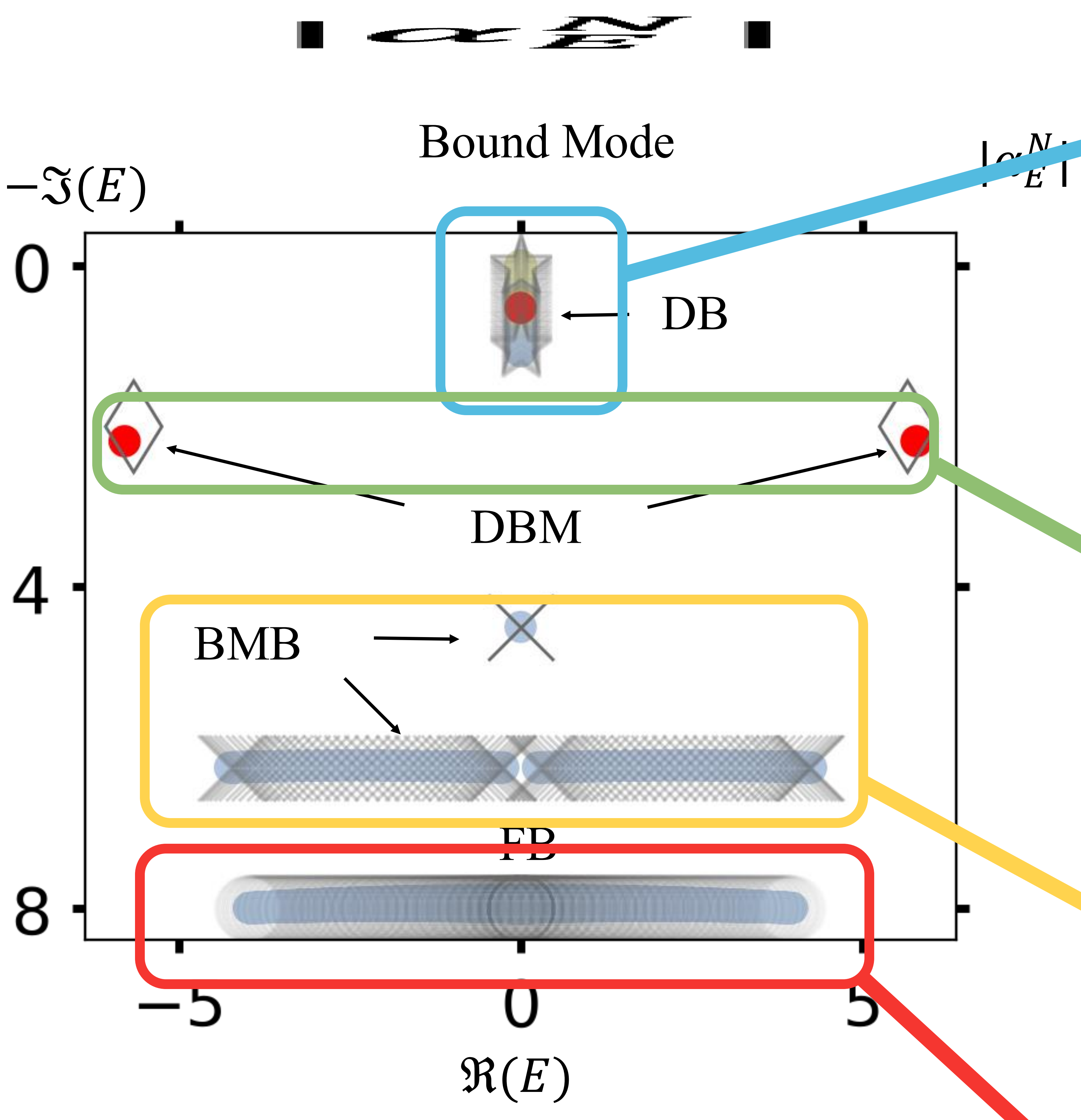
- The momenta *k* and *q* are solutions of the BAE

$$-\frac{2\cos k - 2i\gamma - J^2 e^{ik}}{2\cos k - 2i\gamma - J^2 e^{-ik}}\left(\frac{\sin k - \sin q + 2\gamma}{\sin k - \sin q - 2\gamma}\right)\left(\frac{\sin k + \sin q - 2\gamma}{\sin k + \sin q + 2\gamma}\right) = e^{i2(L+1)k}$$

$$-\frac{2\cos q - 2i\gamma - J^2 e^{iq}}{2\cos q - 2i\gamma - J^2 e^{-iq}}\left(\frac{\sin k - \sin q - 2\gamma}{\sin k - \sin q + 2\gamma}\right)\left(\frac{\sin k + \sin q - 2\gamma}{\sin k + \sin q + 2\gamma}\right) = e^{i2(L+1)q}.$$

- There are 4 classes of solutions, depending on whether the scattering $S(k,q), K(k)$ are regular or not

Eigen-spectrum of the Liouvillian



$\gamma = 2, J = 3$

☆ Diffusive band (DB) When $K \neq 0/\infty, S = 0,$

$$k = \frac{\pi n}{L+1} + \mathcal{O}(L^{-1})$$

$$E_n = 4i\sqrt{\gamma^2 - \sin(k)^2} - 4i\gamma + \mathcal{O}(L^{-3}) \sim -i\frac{k^2}{2\gamma} + \mathcal{O}(L^{-3})$$

◇ Double-bound Mode (DBM)

When $S, K = 0,$ $E_\pm = \pm\sqrt{4J^2 - \gamma^2} - i\gamma$ for $\gamma \gg 1$

$$E_\pm = 4\cos k_\pm + 4i\gamma\left[\sum_{x=1}^{L} \mathcal{N}^2 e^{i4k_\pm x} + \frac{\mathcal{N}}{J^2} - 1\right] + \mathcal{O}(\gamma^2) \text{ for } \gamma \ll 1$$

× Bound Mode band (BMB) When $S \neq 0/\infty, K = 0,$

$$q = \frac{\pi n}{L+1} + \mathcal{O}(L^{-1}) \text{ and } \quad k_\pm = i\log\left(\frac{\pm\sqrt{J^2 - 1 - \gamma^2} - i\gamma}{J^2 - 1}\right)$$

○ Free band (FB) When $S, K \neq 0/\infty$

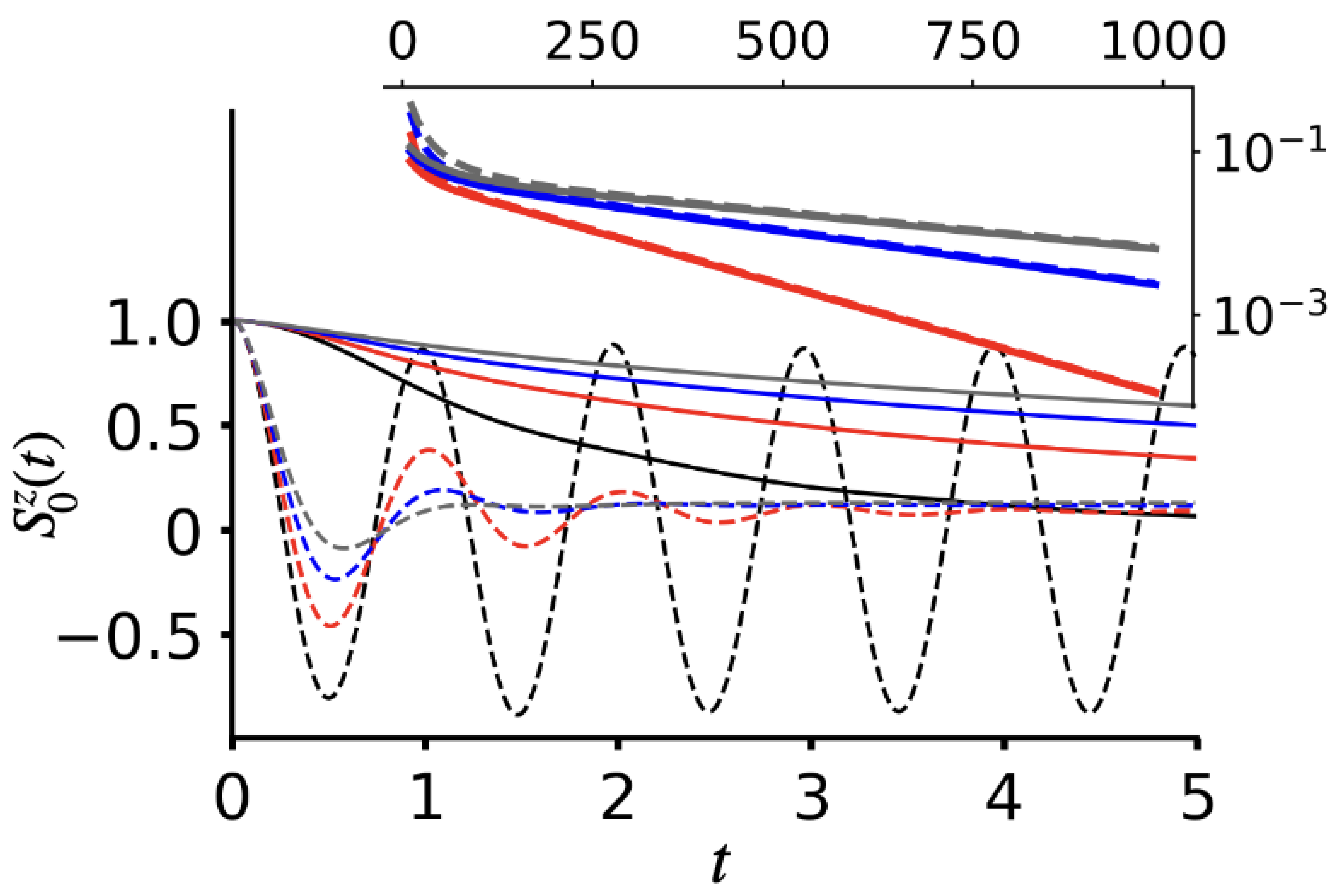
$$k = \frac{\pi n_1}{L+1} + \mathcal{O}(L^{-1}) \text{ and } q = \frac{\pi n_2}{L+1} + \mathcal{O}(L^{-1})$$

Eigen-spectrum of the Liouvillian

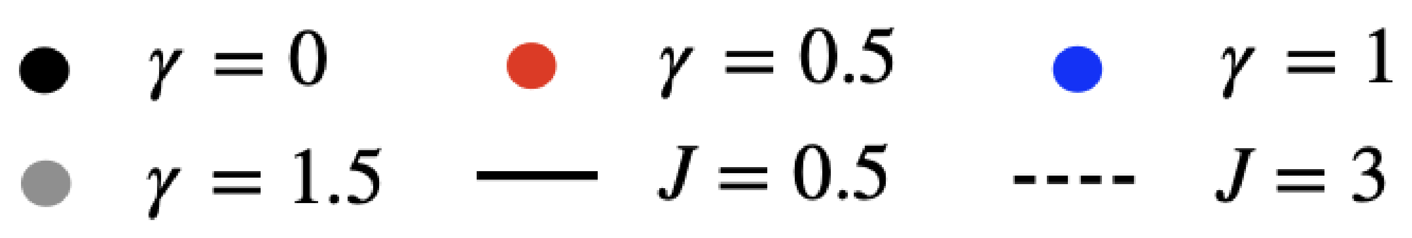
The (J, γ) parameter space. The bound-mode and Kondo regimes separate with the boundary approx. $J = \gamma/2$ for large γ

- **Short time Behavior:** Eigenmodes with Larger $|\alpha_E^N|$ dominates the dynamics, differ from Kondo Regime (Diffusive band) to Bound Mode Regime (Double bound mode)
- **Long time Behavior:** Eigenmodes with smaller $-\Im(E) \sim \gamma^{-1}L^{-2}$ dominates the long time dynamics (decays slower) and result into a Quantum Zeno Effect.

Time evolution of the noisy XX-Kondo spin chain from Néel state



Impurity dynamics of the XX impurity model evolving from a Néel initial state under Lindbladian evolution with and without dephasing noise (for L=40).



- **In the Short time limit,** different behavior in the Kondo and Bound mode regime as function of noise strength γ

  In bound mode regime faster decay as γ increases, *in the Kondo regime* slower decay as γ increases

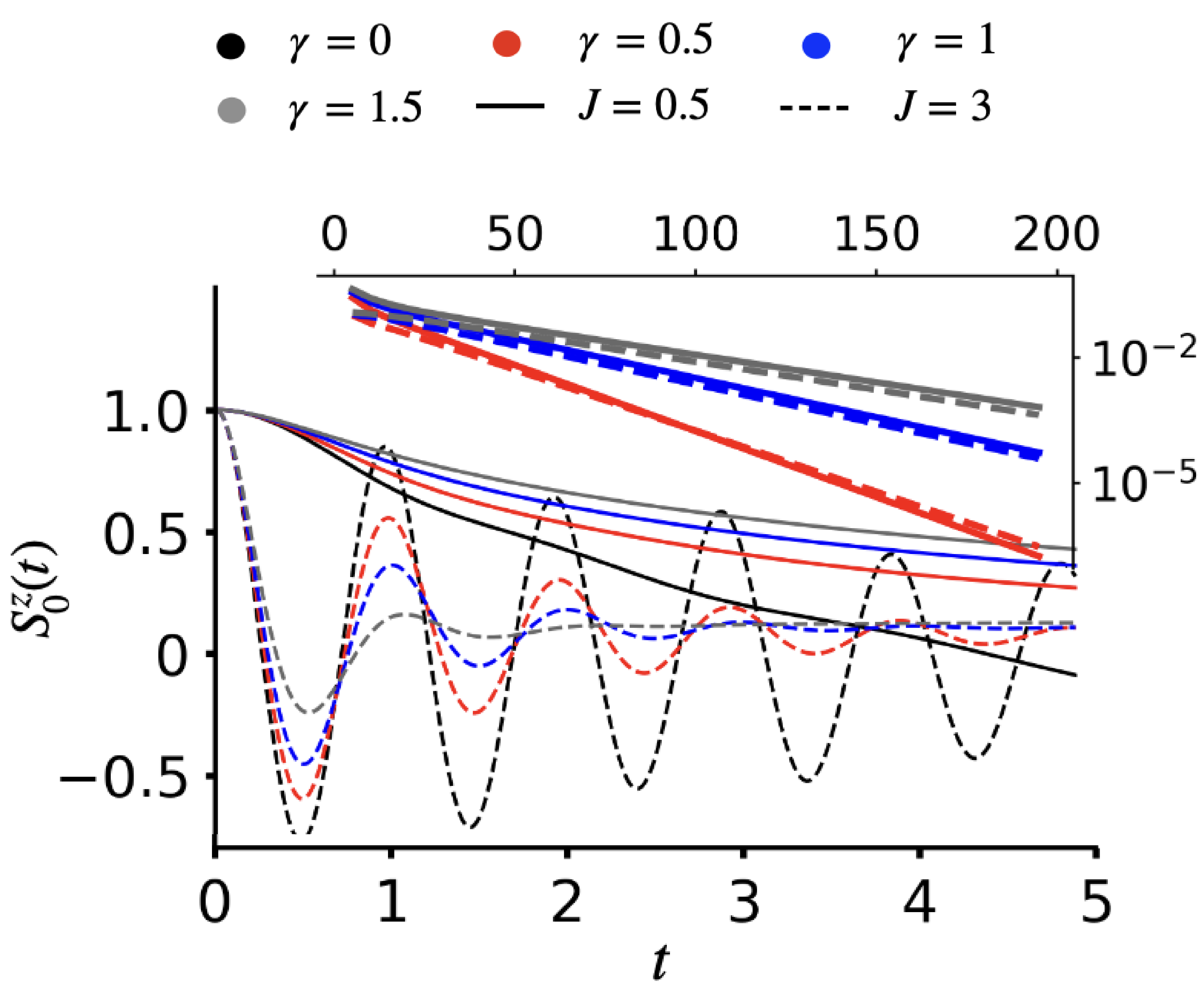
- **In the long time limit**, independent of the boundary coupling, impurity magnetization falls off as $S_0^z(t) \sim e^{-Et}$ with $E = \frac{\pi^2}{2\gamma L^2} + \mathcal{O}(L^{-3})$ in both regimes, slower decay as the noise increases.

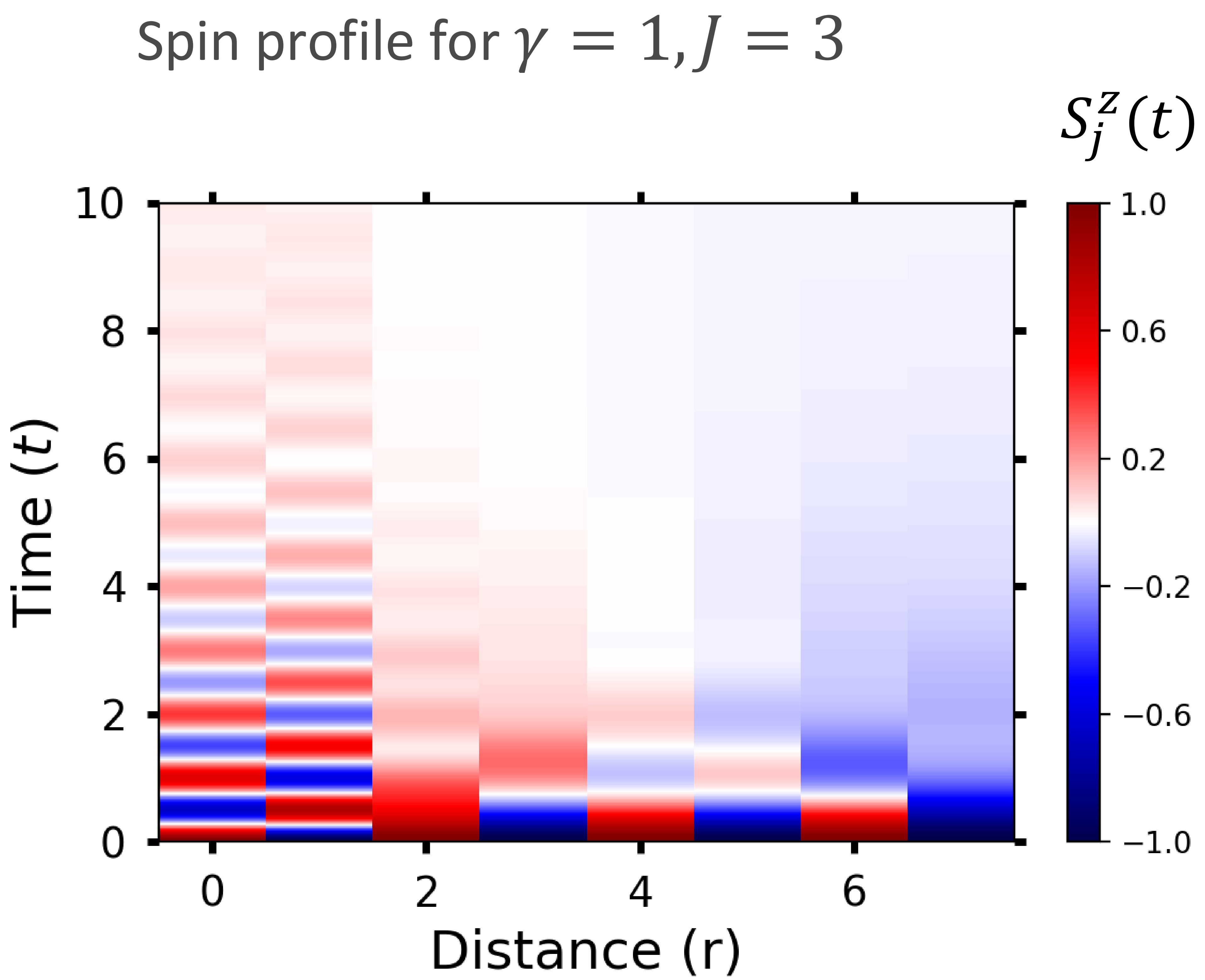
- Consistent with the heating of the bulk induced by Hermitian Lindblad operators.

  Medvedeva, Prosen, Znidaric '16
  Fischer, Maksymenko, Altman '16

- Increasing the bulk noise γ, the bulk temperature increases, leading in the extreme limit to $S_0^z(t) = 1$, due to the asymptotic free nature of Kondo system

Time evolution of the noisy XXX-Kondo spin chain from Néel state

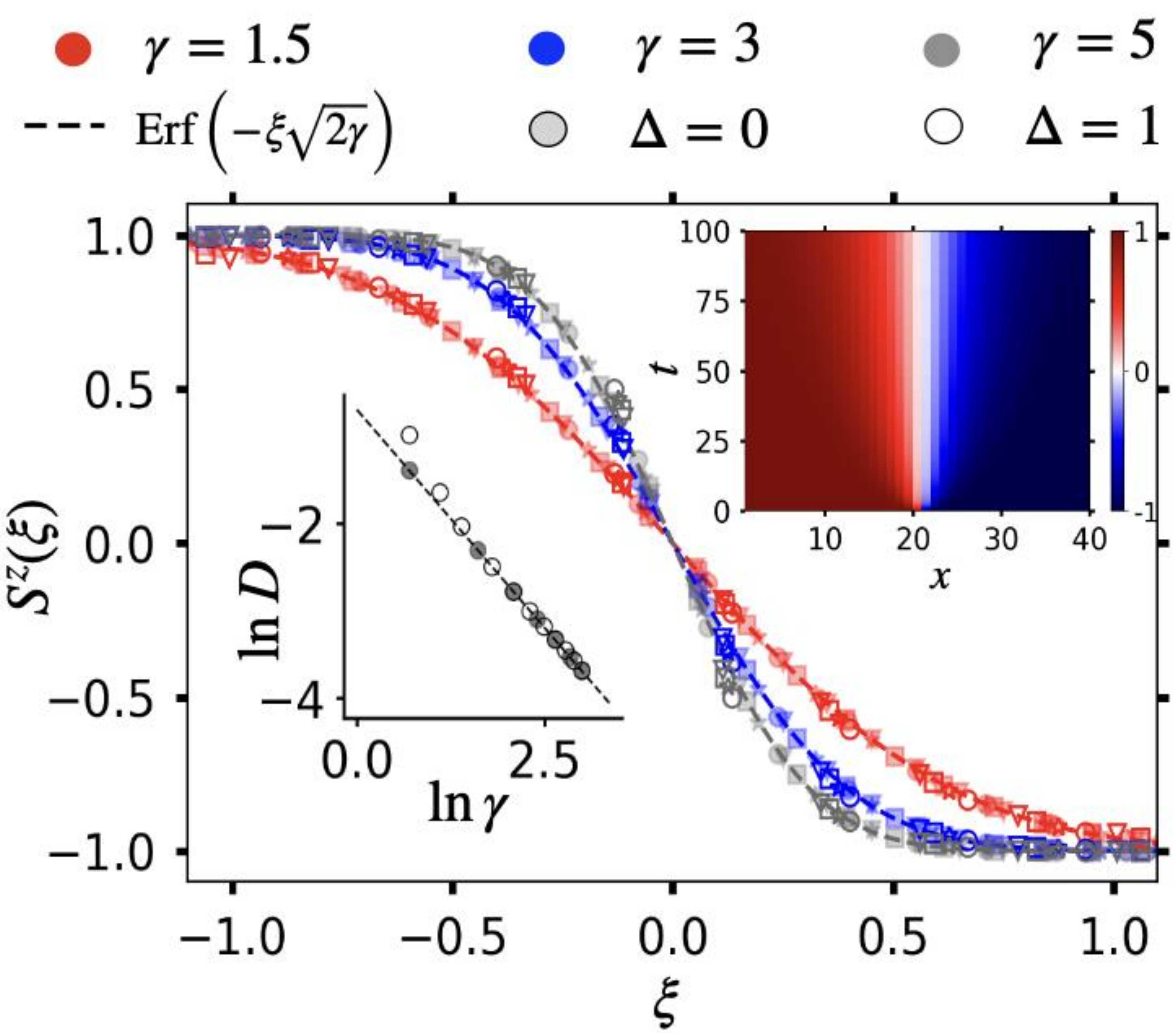




Impurity dynamics of the XXX impurity model evolving from a Néel initial state under Lindbladian evolution with and without dephasing noise.

- Similar behavior as XX chain

Bulk dynamics for a noisy spin chain



- For arbitrary γ, the system is diffusive.

In the continuum limit, as lattice spacing $a \to 0$ the bulk magnetization $S_j^z(t) \to S(x,t)$, and satisfies the diffusion equation $(\partial_t - D\partial_x^2)S(x,t) = 0$.

- For a domain wall initial state $S(x, t=0) = \frac{1}{2} - \Theta(x)$, the diffusion equation solution is

$$S(\xi) = S(x/\sqrt{t}) = -\,\mathrm{erf}(x/\sqrt{Dt})$$

- The data collapses on the curve $S(\xi)$ for both XX and XXX point

Interpretation: the diffusive bulk make the impurity to decay slower and results in a Quantum Zeno Effect

cf Gotta , Giamarchi ’24 and discussion

Conclusions

- Dephasing noise affects impurity behavior differently in the Kondo and bound mode regimes.
  - In the Kondo regime, increasing γ slows the impurity magnetization decay, leading to a quantum Zeno effect.
  - In the bound mode regime, bound mode initially decays faster, but eventually also exhibits the Zeno effect

- The existence of the quantum Zeno effect is due to the bulk transport becoming diffusive when the dephasing noise is introduced

- Increasing the noise does not allow the impurity to communicate with the bulk

Time evolution of the XX-Kondo spin chain in a noisy environment

Reformulate the Lindbladian evolution $i\partial_t \rho(t) = \mathcal{L}[\rho(t)]$

- Introduce the 4^N -dim Liouville-Fock space $|m\rangle\langle n| \to |n,m\rangle\rangle$ *Prosen '06*
- The density operator $\rho = \sum_{m,n} \rho_{mn} |m\rangle\langle n| \to \sum_{m,n} \rho_{mn} |n,m\rangle\rangle$
- The Liouvillian acts as $\mathcal{L}|\rho\rangle\rangle = \frac{d}{dt}|\rho\rangle\rangle$
- Define $c_i^\dagger |n,m\rangle\rangle = c_i^\dagger |n\rangle\langle m|, \quad \tilde{c}_i^\dagger |n,m\rangle\rangle = |n\rangle\langle m| c_i$
- The Liouvillian takes the form $\mathcal{L} = -iH + i\tilde{H} + 4\gamma \sum_{i=1}^{L-1} \left(c_i^\dagger c_i \tilde{c}_i^\dagger \tilde{c}_i - \frac{1}{2} c_i^\dagger c_i - \frac{1}{2} \tilde{c}_i^\dagger \tilde{c}_i \right)$
- Denote $c_i^\dagger = c_{i,\uparrow}^\dagger$ $\tilde{c}_i^\dagger = c_{i,\downarrow}^\dagger$ and apply $U = \prod_{i=1}^{N/2} (1 - 2\tilde{c}_i^\dagger \tilde{c}_i)$
    - The Liouvillian --> Kondo-Hubbard model with imaginary coupling *Medvedyeva, Essler, Prosen '16*

$$\mathcal{L} = -iJ(c_{0,\sigma}^\dagger c_{1,\sigma} + c_{1,\sigma}^\dagger c_{0,\sigma}) - i \sum_{i=1}^{L-1} (c_{i,\sigma}^\dagger c_{i+1,\sigma} + c_{i+1,\sigma}^\dagger c_{i,\sigma}) + \gamma \sum_{i=1}^{L} (2c_{i,\uparrow}^\dagger c_{i,\uparrow} - 1)(2c_{i,\downarrow}^\dagger c_{i,\downarrow} - 1) - \gamma(L-1)$$

The model is integrable *Karnaukhov, Egorov '05*