Title: A single-channel Kondo impurity in the large s limit

Speakers: Abijith Krishnan

Series: Quantum Matter

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Abstract: The single-channel Kondo impurity problem is a classic example of strongly coupled physics. In the Kondo problem, a single magnetic impurity is placed in a metal -- the resulting system exhibits interesting properties such as a resistance minimum as a function of temperature. The problem was solved by Wilson's numerical renormalization group and later by the Bethe ansatz technique. The Bethe ansatz exactly diagonalizes the Kondo hamiltonian for arbitrary impurity spin s and numerically computes the impurity free energy for all temperatures. In this talk, I'll present an alternate analytic solution for the Kondo problem at large s that builds on recent results in boundary conformal field theory. This solution allows us to access analytically intermediate scales of the Kondo problem at large s; our results in this regime agree with the numeric results of the Bethe ansatz.

Zoom link

A single-channel Kondo impurity in the large spin limit

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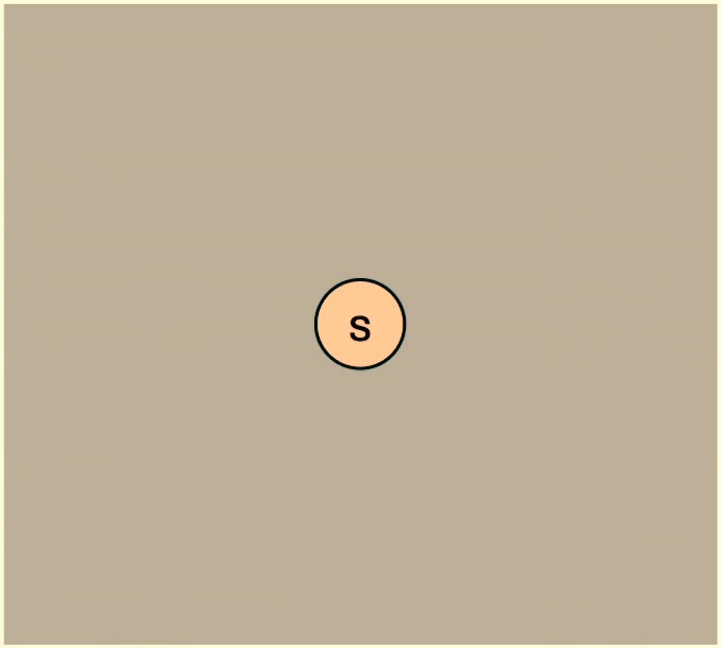
March 13, 2024

Single spin s Kondo impurity in a metal



- One of the first examples of strongly coupled physics
  - Perturbation theory (Kondo, 1964)
  - Numerical RG (Wilson, 1975)
  - Bethe ansatz (Andrei, 1980; Wiegman, 1981; others)
- Experimental signatures include
  - Resistance minimum as function of temperature
  - (Under)screening of impurity

$$H = H_{\text{el}} + J_K\, \vec{S} \cdot \Psi^\dagger \frac{\vec{\sigma}}{2} \Psi(0), \qquad S^2 = s(s+1)$$

Resistance minimum

Two different samples of gold wires with a small concentration of magnetic impurities exhibit resistance minima at ~4 K

(de Haas et al., 1934)

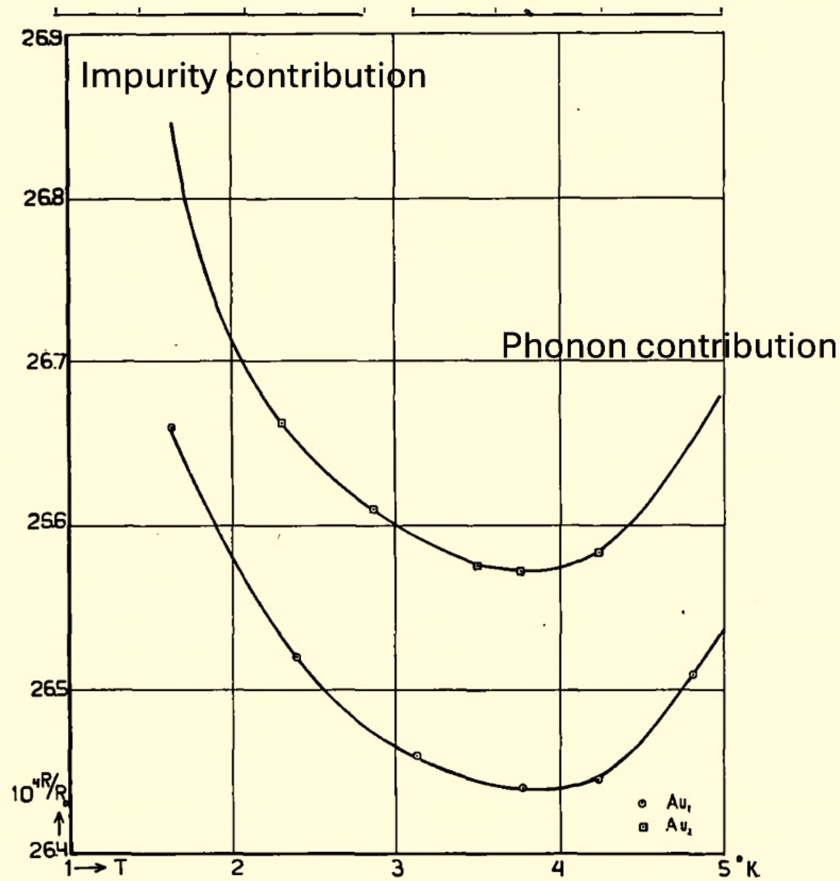


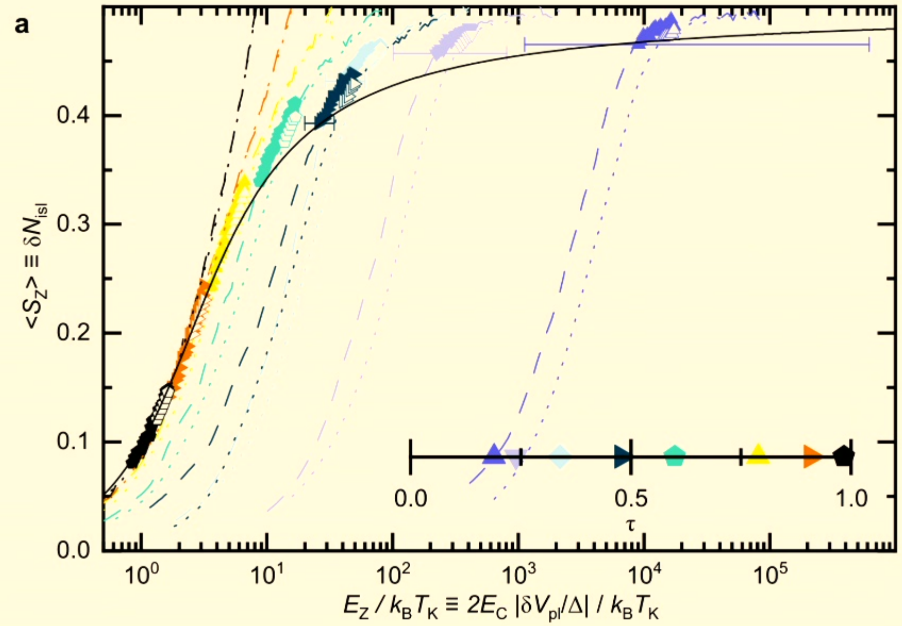
Fig. 1. Resistance of *Au* between 1°K. and 5°K.

Screening of Kondo impurity

A spin impurity of magnitude s=1/2 is completely screened in the IR.

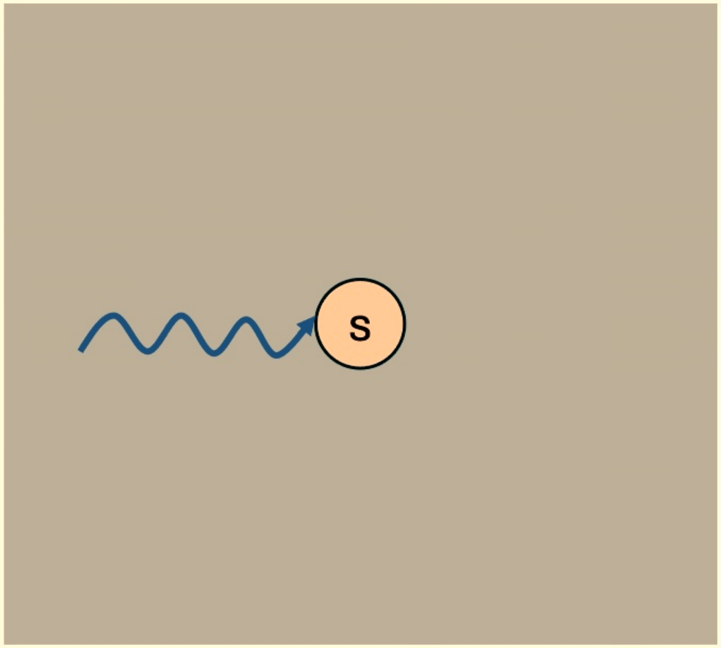
(Piquard et al., 2023)

Note: $\frac{E_Z}{k_B T_K} \propto h$ tunes system between fixed points, as we'll see later



Black curve: Bethe ansatz prediction for zero-temperature magnetization
Dashed lines: experimental results at finite temperature
Solid shapes: experimental results in $E_Z \gg k_B T$ regime

Reduction to 1D problem

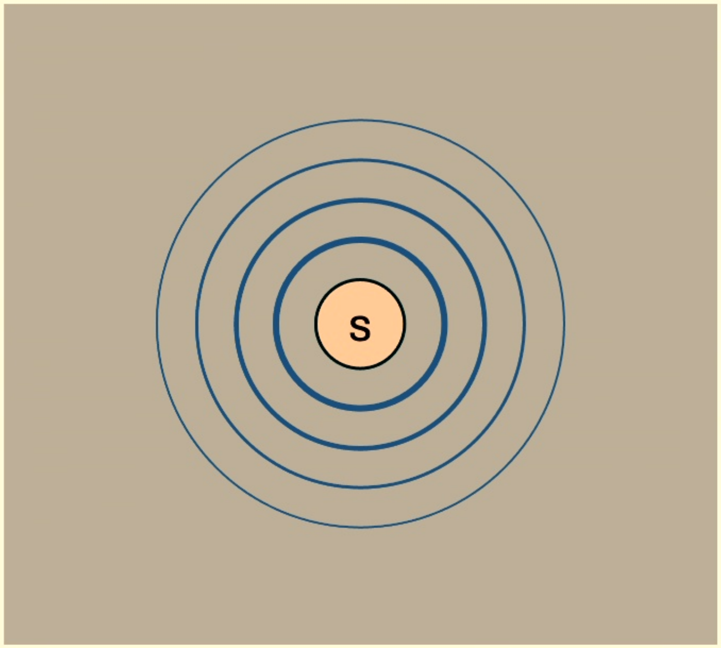


$$H = H_{\mathrm{el}} + J_K \, \vec{S} \cdot \Psi^\dagger \frac{\vec{\sigma}}{2} \Psi(0)$$

- We assume Fermi surface is uniform and spherical

- We also assume s-wave scattering

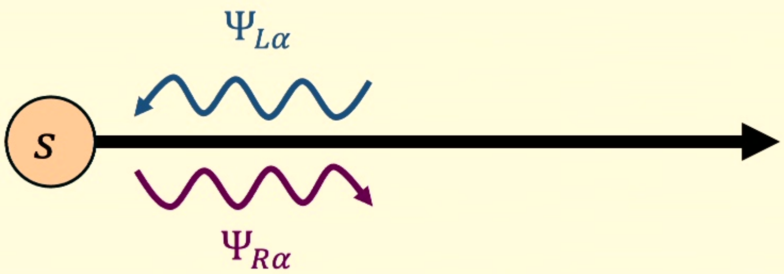
Reduction to 1D problem



$$H = H_{\mathrm{el}} + J_K\, \vec{S} \cdot \Psi^\dagger \frac{\vec{\sigma}}{2}\, \Psi(0)$$

- Each incoming wave contributes equally to each outgoing wave.
- We group incoming waves and outgoing waves near the Fermi surface with the same energy and label them left and right movers respectively.

Reduction to 1D problem



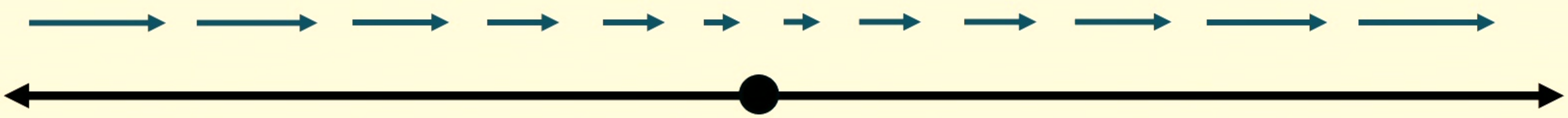
- We get a "folded" action for left and right movers on the half-line with Fermi velocity v_F
- We could also "unfold" the action so that we have just a left or right mover living on the full real line

$$S = S_{\text{spin}} + \int d\tau \int_0^\infty dx \, \left(\Psi^\dagger_{L\alpha} (\partial_\tau + i v_F \partial_x) \Psi_{L\alpha} + \Psi^\dagger_{R\alpha} (\partial_\tau - i v_F \partial_x) \Psi_{R\alpha}\right)$$

$$+ J \int d\tau \, \vec{S} \cdot \Psi^\dagger \frac{\vec{\sigma}}{2} \Psi(0)$$

Qualitative phase diagram

$$S_{\text{int}} = J \int d\tau\, \vec{S} \cdot \Psi^\dagger \frac{\vec{\sigma}}{2} \Psi(0)$$



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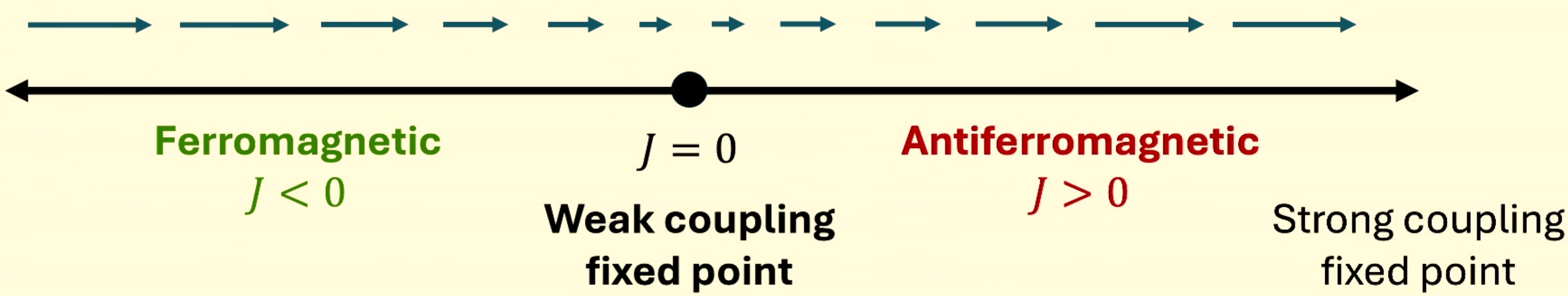
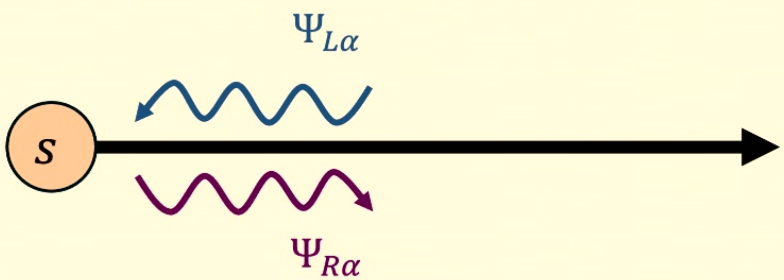


- First accessed by perturbation theory in J by Kondo
- $\frac{dJ}{d\ell} = -\beta(J) = \frac{J^2}{2\pi}$

Strong coupling fixed point ($J_K \gg 1$)

$$H_{\text{discrete}} = t\sum_i (\Psi^\dagger_{i,\alpha}\Psi_{i+1,\alpha} + \Psi^\dagger_{i+1,\alpha}\Psi_{i,\alpha}) + J_K\,\vec{S}\cdot\Psi^\dagger_0\frac{\vec{\sigma}}{2}\Psi_0, \qquad \vec{S}\cdot\Psi^\dagger_0\frac{\vec{\sigma}}{2}\Psi_0 \sim -\left(\vec{S}+\Psi^\dagger_0\frac{\vec{\sigma}}{2}\Psi_0\right)^2$$



Remaining electrons are forbidden from entering impurity site – that would increase total spin back to s, or violate Pauli exclusion

Impurity state, if aligned in +z direction, looks like

$$\frac{1}{2}\sqrt{4-\frac{1}{s}}\,|s,s\rangle\otimes\left|\frac{1}{2},-\frac{1}{2}\right\rangle - \frac{1}{2}\sqrt{\frac{1}{s}}\,|s,s-1\rangle\otimes\left|\frac{1}{2},+\frac{1}{2}\right\rangle = \left|s-\frac{1}{2},s-\frac{1}{2}\right\rangle$$

Qualitative phase diagram

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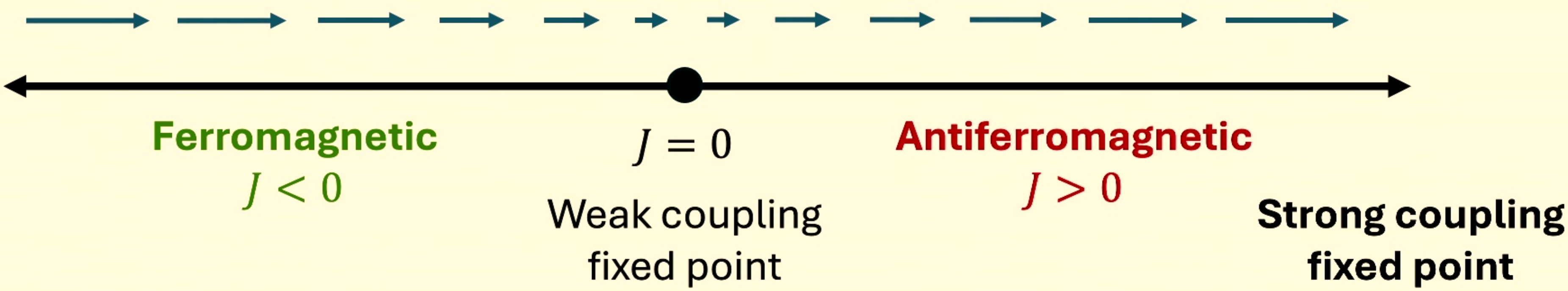
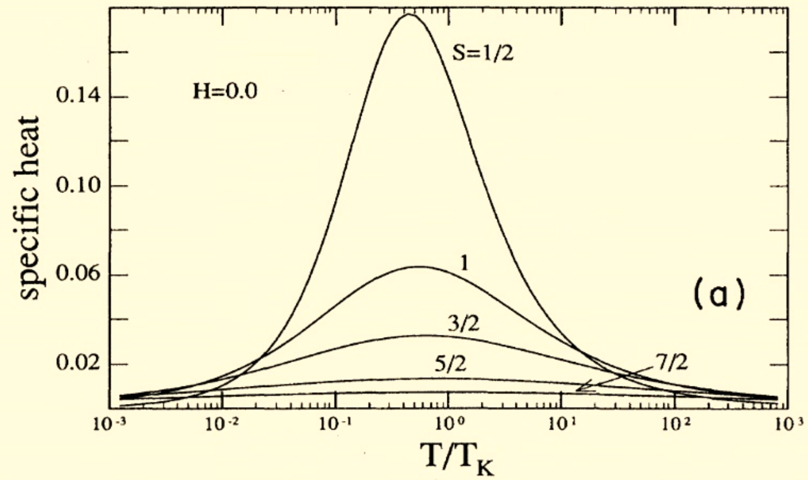


- Impurity spin of magnitude s is screened to $s - 1/2$, remaining electrons see hard wall at impurity
- Can be characterized with boundary conformal field theory (BCFT) (Affleck, 1995)
    - First irrelevant operator at strong coupling fixed point gives low T observables

Successes of the Bethe ansatz solution

- Produces, up to numerical precision, the thermodynamic behavior of the system at all scales (not just near the fixed points) and all values of impurity spin

- Reproduces analytically the behavior of thermodynamic quantities (specific heat, magnetic susceptibility) near fixed points



(Sacramento and Schlottman, 1989)

Qualitative phase diagram

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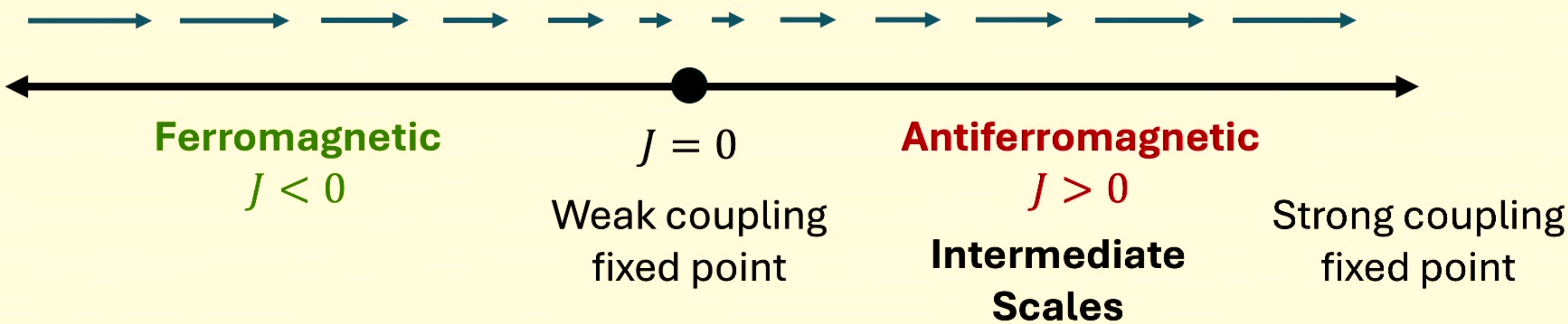
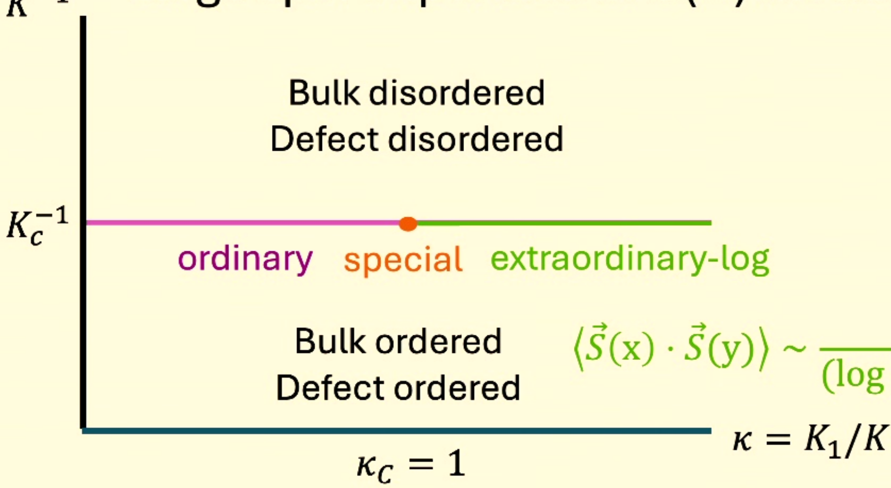


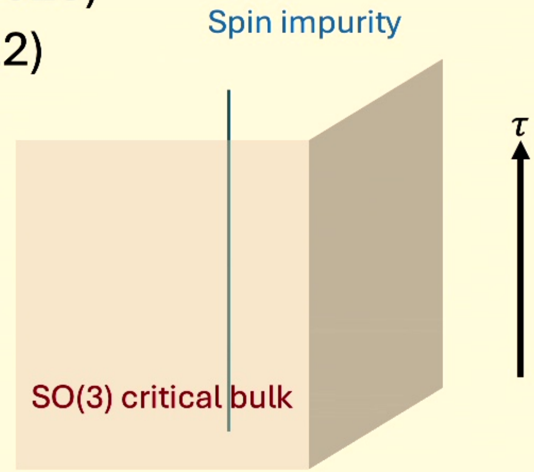
- Observables understood numerically from Bethe ansatz
- Analytic expressions and qualitative understanding at intermediate scales are currently lacking

Another approach: BCFT

- Boundary conformal field theory (BCFT) – study of the boundaries of systems with conformally invariant bulk
  - Extraordinary-log universality class in O(N) models with boundaries/defects (Metlitski, 2020), (* and Metlitski, 2023)
  - Large spin impurities in O(N) models (Cuomo et al, 2022)



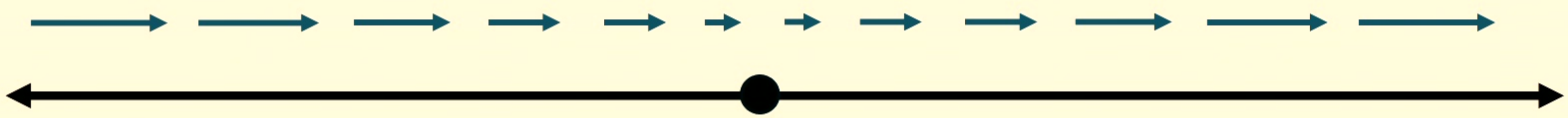
$$\langle \vec{S}(\mathrm{x}) \cdot \vec{S}(\mathrm{y}) \rangle \sim \frac{1}{(\log|\mathrm{x}-\mathrm{y}|)^q}$$



$$\Delta_S = \frac{11}{4\pi^2 s^2} + \mathcal{O}(s^{-3})$$

Qualitative phase diagram

$$S_{\text{int}} = J \int d\tau \, \vec{S} \cdot \Psi^\dagger \frac{\vec{\sigma}}{2} \Psi(0)$$



Ferromagnetic
$J < 0$

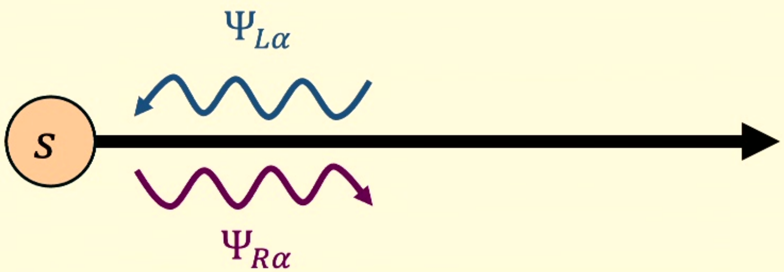
$J = 0$
Weak coupling fixed point

Antiferromagnetic
$J > 0$
Intermediate Scales

Strong coupling fixed point

- Observables understood numerically from Bethe ansatz
- Analytic expressions and qualitative understanding at intermediate scales are currently lacking

Reduction to 1D problem



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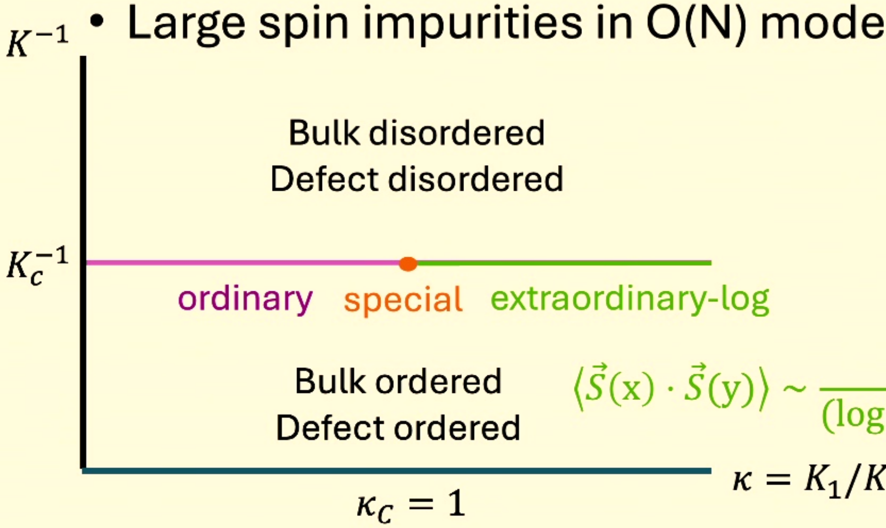

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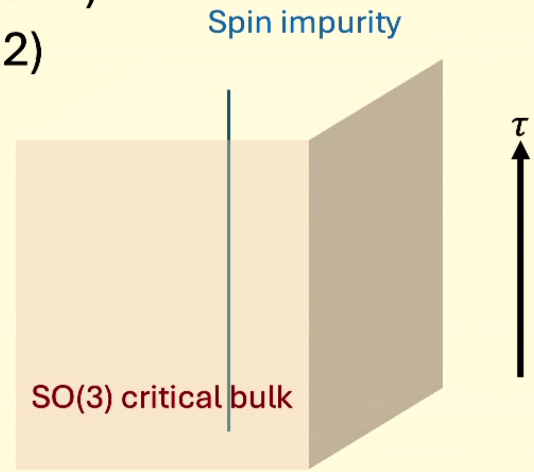


$$\Delta_S = \frac{11}{4\pi^2 s^2} + \mathcal{O}(s^{-3})$$

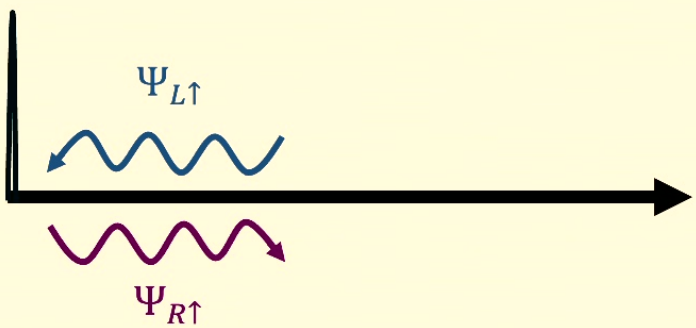
The large s limit

- Approach: expand in $1/s$ instead.
- Aim: capture all scales analytically for large s with BCFT techniques.
- Strategy
  - Consider infinite s limit (impurity spin direction is frozen)
  - Take s large and finite. Restore the $SU(2)$ symmetry order by order in $1/s$
  - Compute the RG flow induced by the spin fluctuations
  - Compute thermodynamic observables from the action and beta function

Infinite s

- Take $s \to \infty$, keep sJ fixed.
- Spin action is $S_B = is\int_0^{1/T} d\tau \int_0^1 du\, \vec{n}\cdot(\partial_\mu \vec{n} \times \partial_\tau \vec{n})$, $\vec{S} = s\vec{n}$
  - For $s \to \infty$, fluctuations are suppressed, spin is "frozen." Take direction of frozen spin to be positive z-direction.

$V(x) = (sJ/2)\delta(x)$



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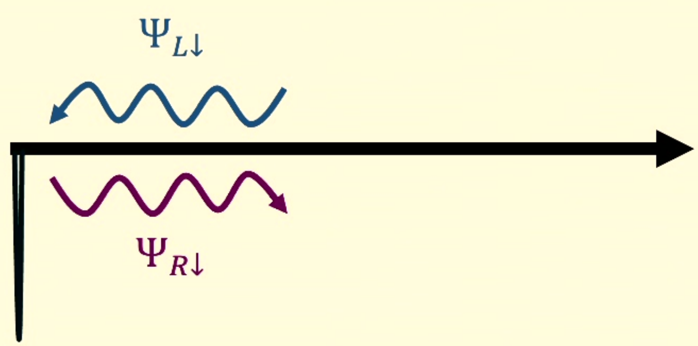
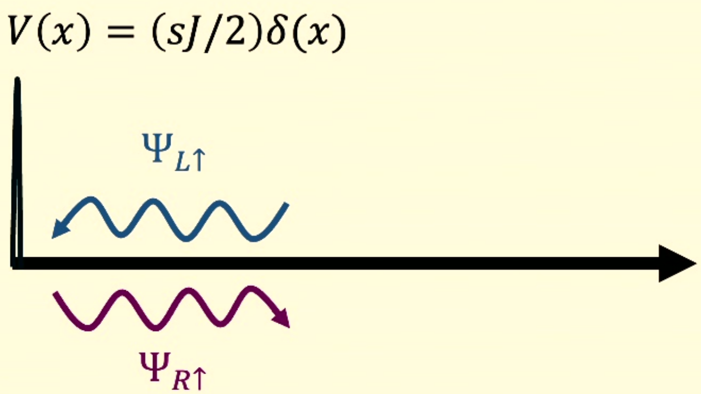
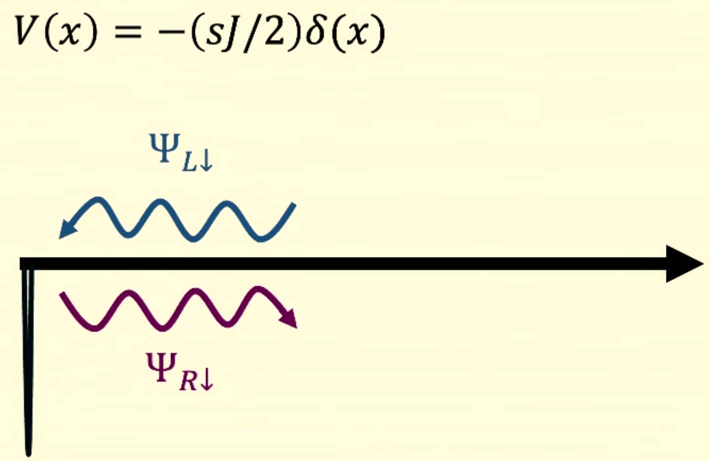


Infinite s phase shift

- $H_{\text{unfolded}} = -i\partial_x + (sJ/2)\delta(x)$.
- Induces a phase shift $\rho = 2\tan^{-1} sJ/4$ between right and left movers.
  - $\rho \to sJ/2$ for small J, $\rho \to \pi$ for large J.
- $\Psi_{R\uparrow}(0^+) = e^{-i\rho}\Psi_{L\uparrow}(0^+), \Psi_{R\downarrow}(0^+) = e^{i\rho}\Psi_{L\downarrow}(0^+)$.





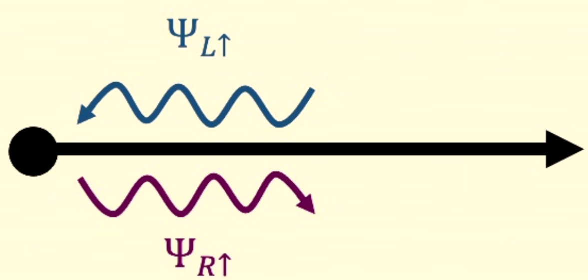
Infinite s action

$$S_{\text{frozen}}(\rho) = \int \mathrm{d}\tau \int_0^\infty \mathrm{d}x [\Psi^\dagger_{L\alpha}(\partial_\tau + i\partial_x)\Psi_{L\alpha} + \Psi^\dagger_{R\alpha}(\partial_\tau - i\partial_x)\Psi_{R\alpha}]$$

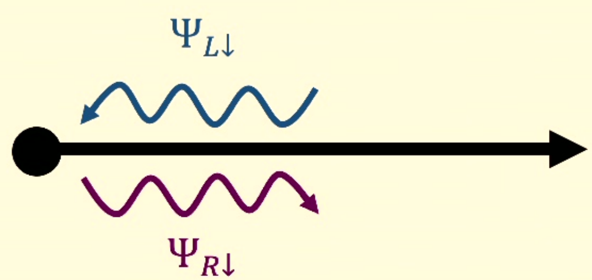
$$\left\langle \Psi_{R\uparrow}(x,\tau)\Psi^\dagger_{L\uparrow}(x',0)\right\rangle = \frac{e^{-i\rho}}{2\pi(\tau - i(x+x'))}, \quad x, x' > 0,$$

$$\left\langle \Psi_{L\uparrow}(x,\tau)\Psi^\dagger_{R\uparrow}(x',0)\right\rangle = \frac{e^{i\rho}}{2\pi(\tau + i(x+x'))}, \quad x, x' > 0,$$

$\Psi_{R\uparrow} = e^{-i\rho}\Psi_{L\uparrow}$



$\Psi_{R\downarrow} = e^{i\rho}\Psi_{L\downarrow}$



Infinite s phase shift

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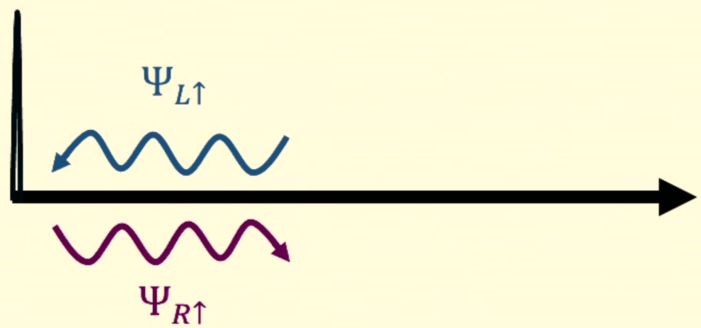
$V(x) = (sJ/2)\delta(x)$



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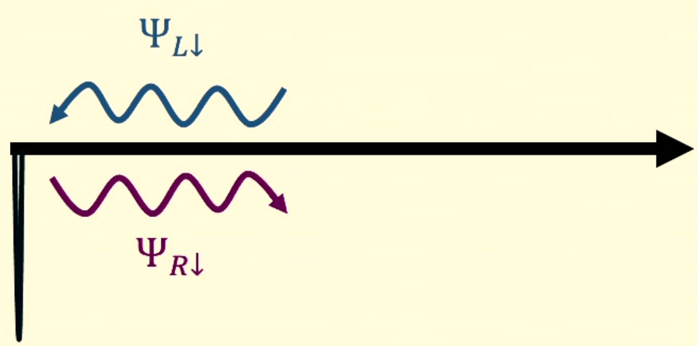

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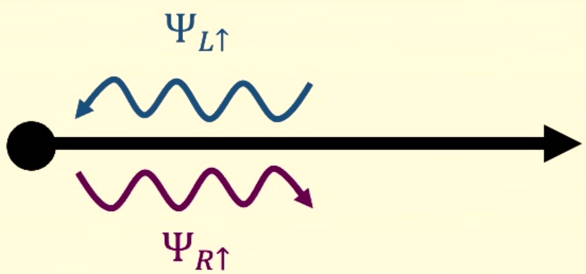

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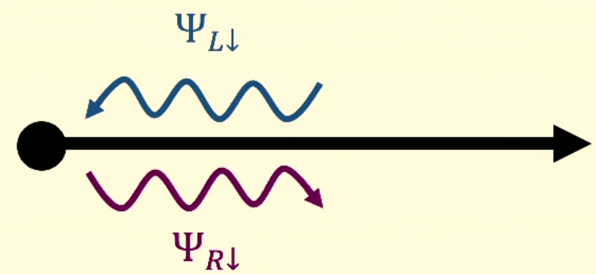
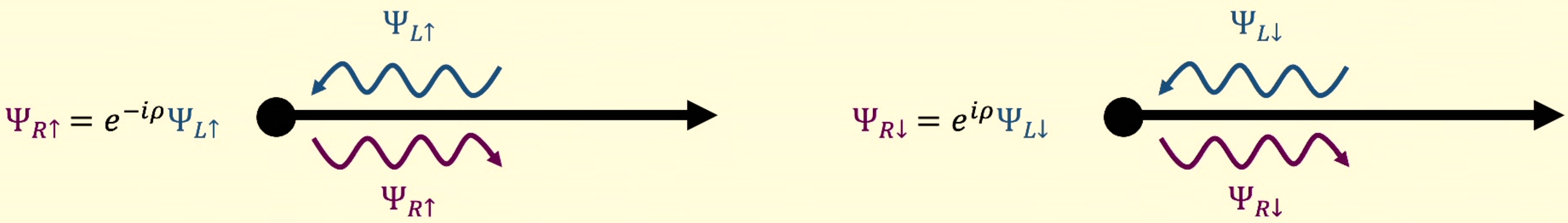


Infinite s, boundary operators

- $\Psi_R^\dagger \frac{\sigma^3}{2} \Psi_R(0^+)$: Tunes the phase shift of the action.
- $\Psi_R^\dagger \frac{\sigma^i}{2} \Psi_R(0^+)$, $\quad i \in \{1,2\}$: **Tilts** the boundary impurity spin. Forms a vector under remaining $U(1)$ symmetry.



The large s limit

- Approach: expand in $1/s$ instead.
- Aim: capture all scales analytically for large s with BCFT techniques.
- Strategy
  - Consider infinite s limit (impurity spin direction is frozen)
  - **Take s large and finite. Restore the $SU(2)$ symmetry order by order in $1/s$**
  - Compute the RG flow induced by the spin fluctuations
  - Compute thermodynamic observables from the action and beta function

Effective action for large, finite s

When s is large but finite, $S_{\text{frozen}}(\rho)$ breaks $SU(2)$ symmetry.

$$S_{\text{eff}} = S_{\text{frozen}}(\rho) + S_B + S_{\text{int}} + S_{\text{cont}}$$

- S_B: impurity free spin action
- S_{int}: the coupling between the spin and the boundary operators
- S_{cont}: boundary contact terms

Last two terms are fixed by $SU(2)$ symmetry.

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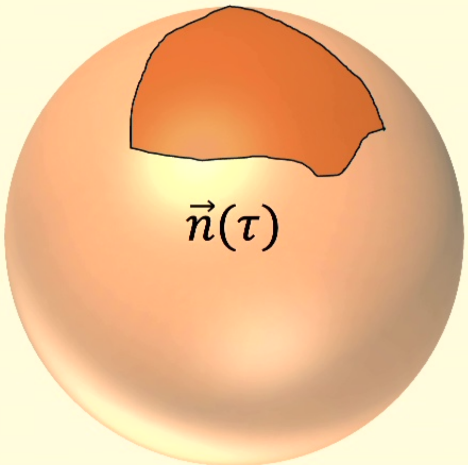
Last two terms are fixed by $SU(2)$ symmetry.

Free spin action

Spin action is the usual Berry phase

$$S_B = is \int_0^{1/T} d\tau \int_0^1 du\, \vec{n} \cdot (\partial_\mu \vec{n} \times \partial_\tau \vec{n}), \qquad \vec{S} = s\vec{n}$$



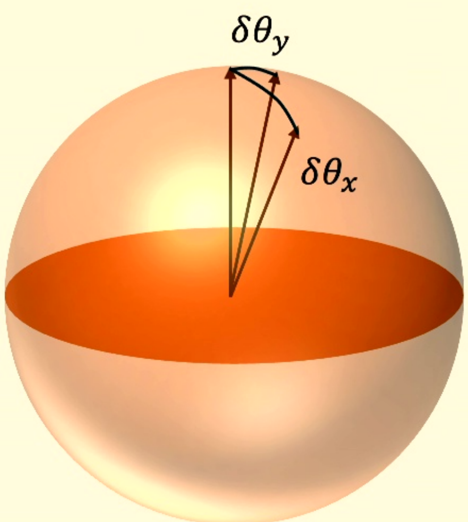
Take $\vec{n} = (\pi_1, \pi_2, \sqrt{1 - \vec{\pi}^2})$. Then,

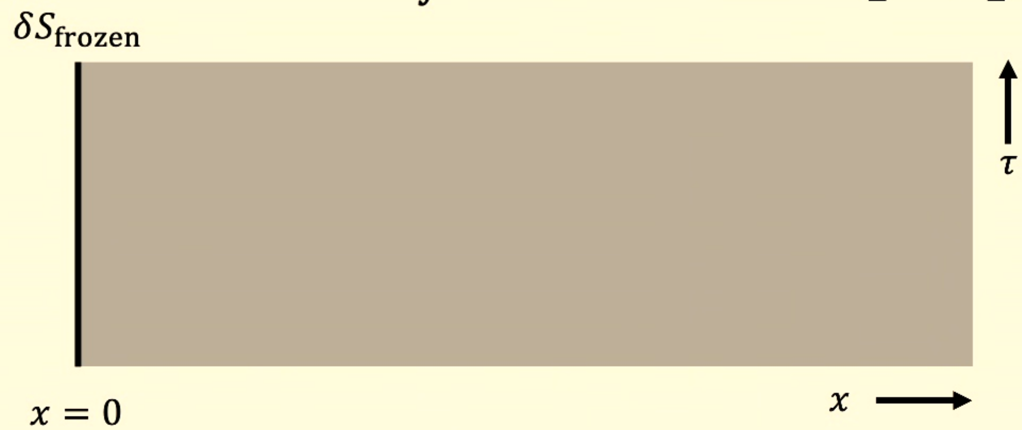
$$S_B = is/2 \int_0^{1/T} d\tau\, (\pi_1 \partial_\tau \pi_2 - \pi_2 \partial_\tau \pi_1) + \mathcal{O}(\pi^4).$$

Spin-fermion interactions

We construct S_{int} to restore the broken $SU(2)$ symmetry.

$$\Psi \to \left(1 - i\,\theta_a \sigma^a/2 + \mathcal{O}(\theta^2)\right)\Psi \qquad \delta S_{\text{frozen}} = -\theta^i \int d\tau\, j_x^i(0^+,\tau)\,, \qquad j_x^i = \frac{1}{2}\left(\Psi_{\rm R}^\dagger \frac{\sigma^i}{2}\Psi_{\rm R} - \Psi_{\rm L}^\dagger \frac{\sigma^i}{2}\Psi_{\rm L}\right)$$



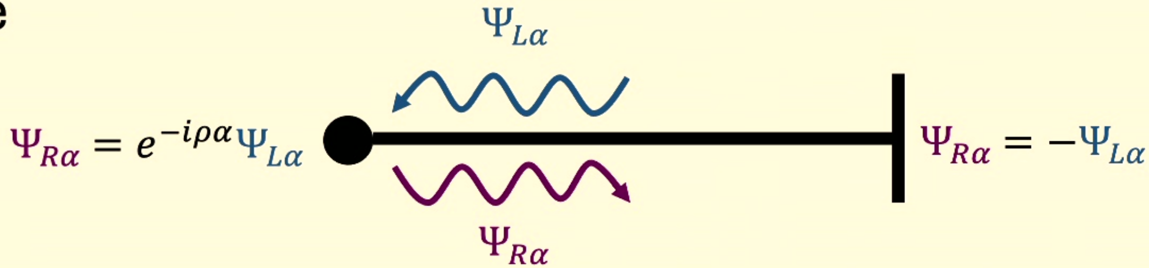


$$S_{\text{int}}(\rho) = \int d\tau\, \epsilon^{ij}\pi^i j_x^j(0^+,\tau) + \kappa\vec{\pi}^2\Psi_{\rm R}^\dagger \frac{\sigma^3}{2}\Psi_{\rm R}, \qquad \kappa = -\frac{\sin(2\rho)}{4}$$

Contact terms

$$S_{\text{cont}} = \int d\tau\, \delta m_\pi \vec{\pi}^2 + i\frac{\delta s_B}{2}\int d\tau(\pi_1\partial_\tau\pi_2 - \pi_2\partial_\tau\pi_1).$$

δm_π fixed by rotational invariance



On length L system, for $\omega \sim 1/L$, $S_{\text{int}} = \left(\frac{\rho}{\pi} - \frac{\sin(2\rho)}{2\pi}\right)\int d\omega\, \omega\tilde{\pi}_1(\omega)\tilde{\pi}_2(-\omega)$.

Set $\delta s_B = -\rho/\pi + \sin(2\rho)/(2\pi)$ to restore quantized Berry phase.

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  - Compute thermodynamic observables from the action and beta function

RG sketch

- Integrate modes with $\Lambda < \omega < \Lambda e^{\delta\ell}$, where ω is conjugate to τ, Λ is a UV cutoff, and $\delta\ell \ll 1$, and then rescale the action.

- $\delta S_{\text{int}} = -\frac{1}{2}\int_{e^{-\delta\ell}\Lambda^{-1}<|\tau_1-\tau_2|<\Lambda^{-1}} d\tau_1\, d\tau_2\;\; \epsilon^{ij}\epsilon^{kl}\pi^i(\tau_1)\pi^k(\tau_2) j_x^j(0^+,\tau_1) j_x^l(0^+,\tau_2)$

- $\delta S_{\text{int}} = \frac{\sin^2\rho}{\pi s}\delta\ell \int d\tau\, \Psi_{\mathrm{R}}^\dagger \frac{\sigma^3}{2}\, \Psi_{\mathrm{R}}(0^+) \Rightarrow \delta\rho = \frac{\sin^2\rho}{\pi s}\delta\ell$

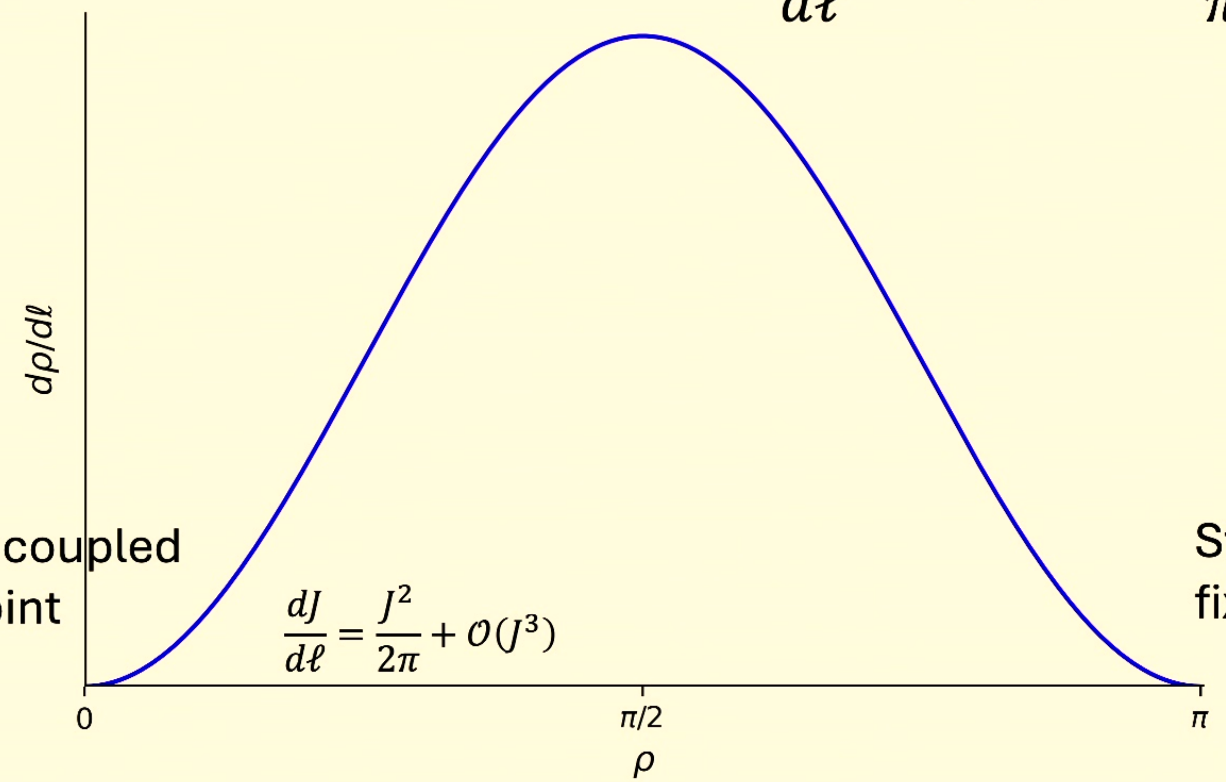
- $\frac{d\rho}{d\ell} = -\beta(\rho) = \frac{\sin^2\rho}{\pi s} + \mathcal{O}(s^{-2}),\;\; \rho(\ell) = \frac{\pi}{2} - \tan^{-1}\left(\cot\rho_0 - \frac{\ell}{\pi s}\right),\; \rho_0 = \rho(0)$

- For IR cutoff T, $\rho(T) = \frac{\pi}{2} - \tan^{-1}\left(\cot\rho_0 - \frac{\log\left(\frac{\Lambda}{T}\right)}{\pi s}\right) = \frac{\pi}{2} - \tan^{-1}\left(\frac{\log\left(\frac{T}{T_0}\right)}{\pi s}\right)$.

- Here, $T_0 = \Lambda e^{-\pi s \cot\rho_0}$, is a reference temperature at which $\rho = \pi/2$.

RG result

$$\frac{d\rho}{d\ell} = -\beta(\rho) = \frac{\sin^2\rho}{\pi s} + \mathcal{O}(s^{-2}),$$



Weakly coupled fixed point

$$\frac{dJ}{d\ell} = \frac{J^2}{2\pi} + \mathcal{O}(J^3)$$

Strongly coupled fixed point

Effective ferromagnetic coupling to $s - 1/2$

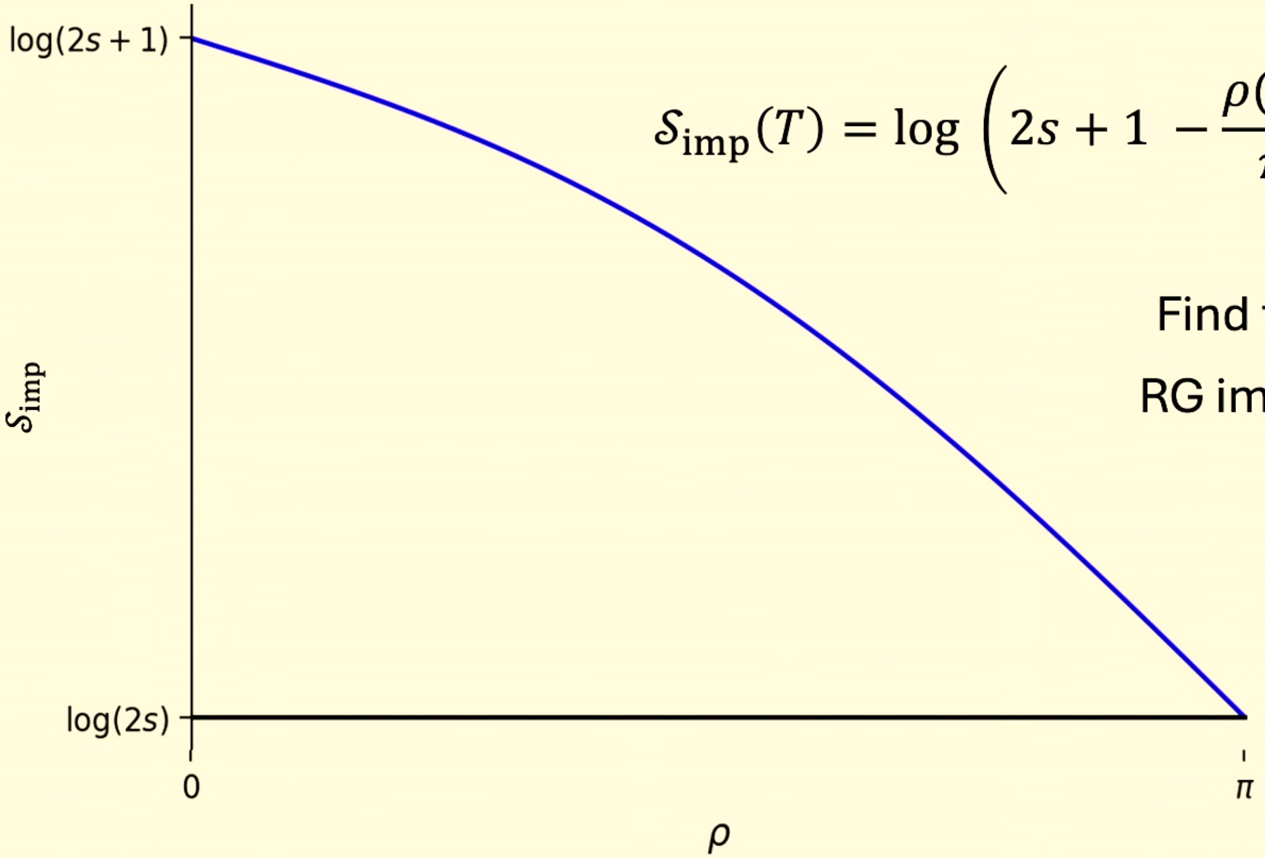
Partition function

$$Z \approx Z_{\text{frozen}} Z_{\text{spin}} \left(1 + \left\langle S_{\text{int}}^2 \right\rangle - \langle S_{\text{cont}} \rangle + \cdots \right)$$

- $Z_{\text{frozen}} = Z_{\text{bulk}} = e^{\frac{\pi c}{6} LT}$, where $c = 2$ is the bulk central charge
- $Z_{\text{spin}} = 2s + 1$
- $\left\langle S_{\text{int}}^2 \right\rangle = 0$
- $\langle S_{\text{cont}} \rangle = \frac{\delta s_B}{2s} = -\frac{\rho}{2\pi s} + \frac{\sin(2\rho)}{4\pi s}$

$$Z_{\text{imp}} = 2s + 1 + \delta s_B = 2s + 1 - \frac{\rho}{\pi} + \frac{\sin(2\rho)}{2\pi}$$

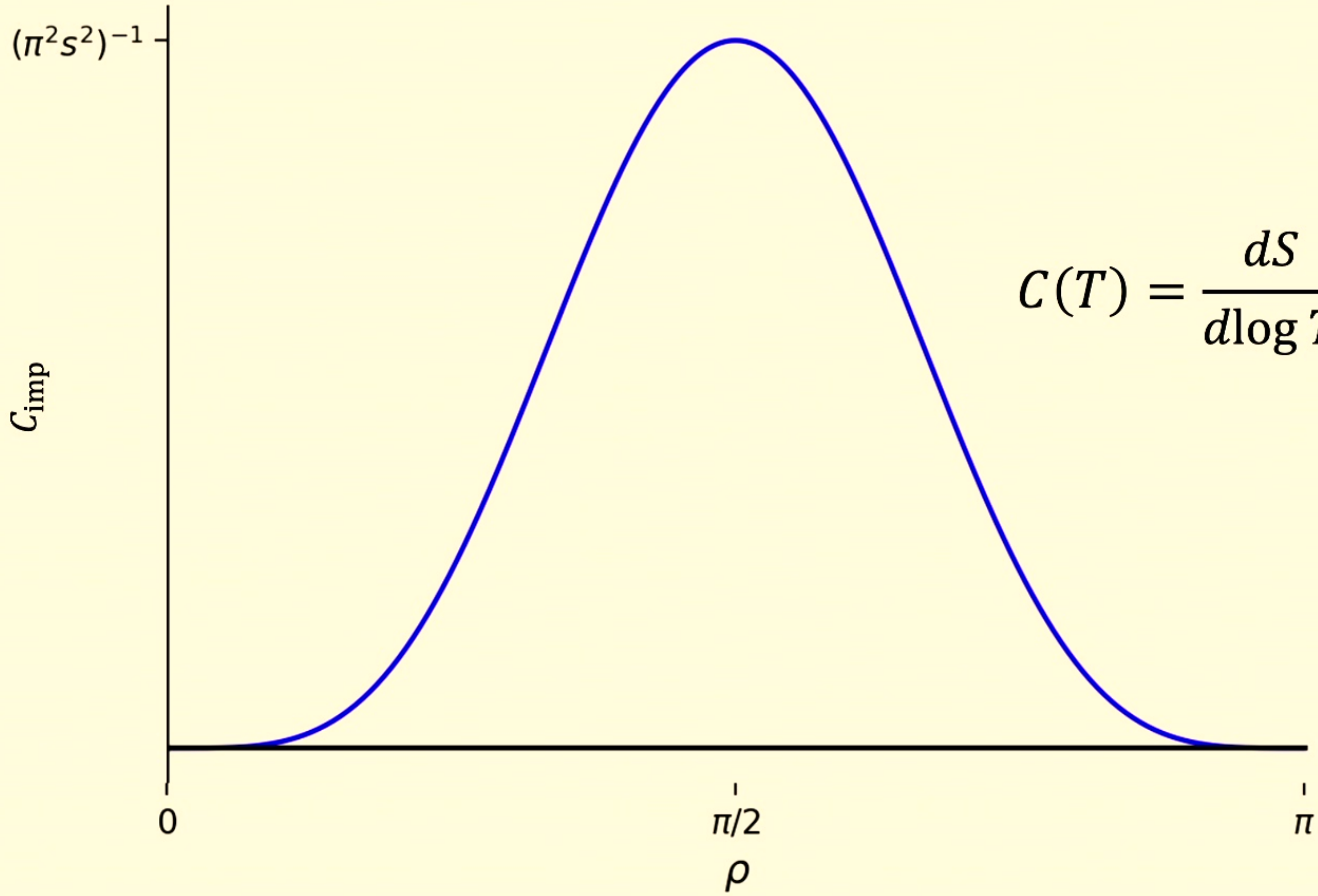
Impurity entropy



$$\mathcal{S}_{\text{imp}}(T) = \log\left(2s + 1 - \frac{\rho(T)}{\pi} + \frac{\sin(2\rho(T))}{2\pi}\right) + \mathcal{O}(s^{-2})$$

Find temperature dependence by RG improving $\rho(\ell) \to \rho\big(\log(\Lambda/T)\big)$

Heat capacity



$$C(T) = \frac{dS}{d\log T} \approx \frac{\sin^4(\rho(T))}{\pi^2 s^2} + \mathcal{O}(s^{-3})$$

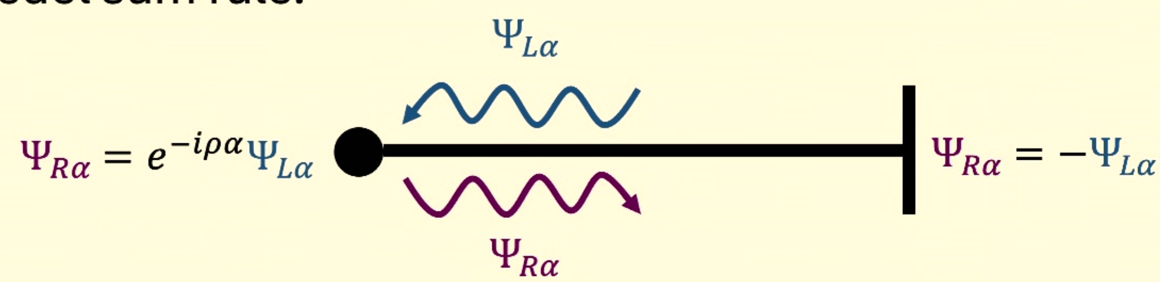
Coupling to a magnetic field

$$S_{\text{eff}}(h^a) = S_{\text{eff}}(0) \; - (s + \delta s_M) \int d\tau \, h^a n^a + \int d\tau \int_{0^+}^{\infty} dx \, h^a j_0^a(x,\tau)$$

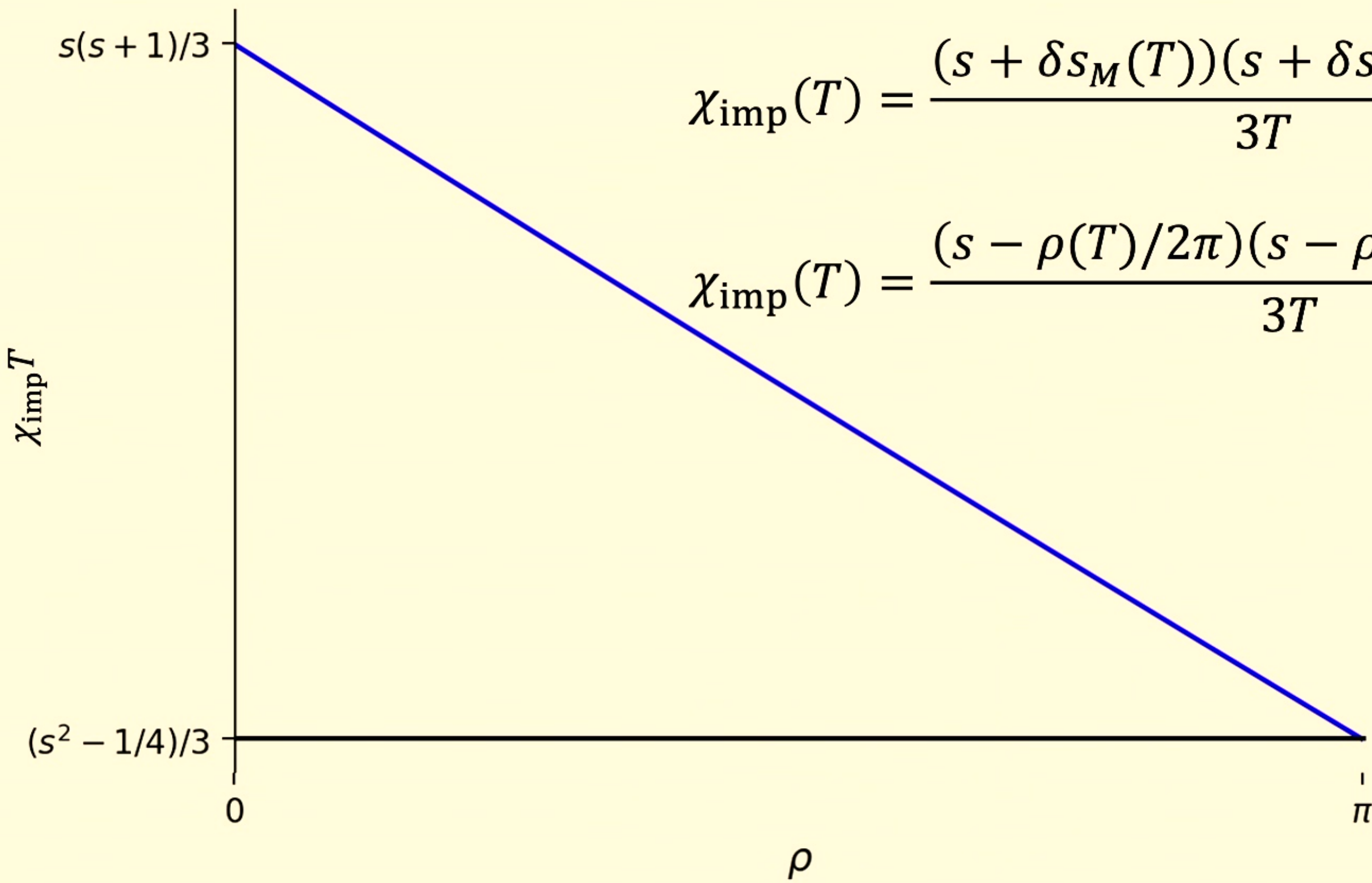
$$j_0^a = \frac{1}{2}(\Psi_{\text{R}}^{\dagger} \frac{\sigma^i}{2} \, \Psi_{\text{R}} + \Psi_{\text{L}}^{\dagger} \frac{\sigma^i}{2} \, \Psi_{\text{L}})$$

δs_M fixed by spin quantization on finite system: $\langle j_0^3 \rangle = \frac{\rho}{2\pi L}$, so $\delta s_M = -\frac{\rho}{2\pi}$.

This is the Friedel sum rule.



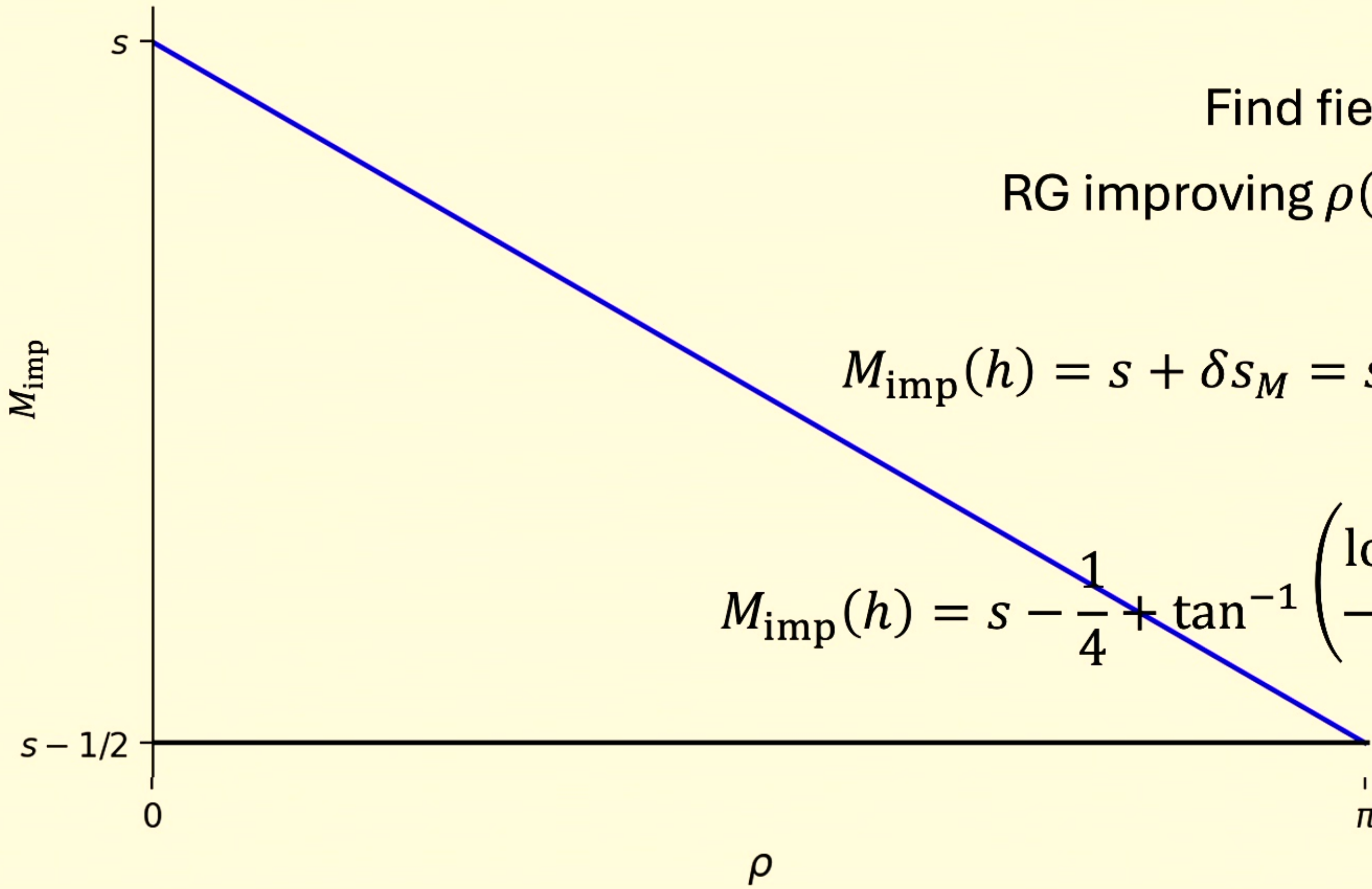
Spin susceptibility, finite T



$$\chi_{\mathrm{imp}}(T) = \frac{(s+\delta s_M(T))(s+\delta s_M(T)+1)}{3T} + \mathcal{O}(s^0)$$

$$\chi_{\mathrm{imp}}(T) = \frac{(s-\rho(T)/2\pi)(s-\rho(T)/2\pi+1)}{3T} + \mathcal{O}(s^0)$$

Zero temperature magnetization



Find field dependence by

RG improving $\rho(\ell) \to \rho\big(\log(\Lambda/h)\big)$

$$M_{\text{imp}}(h) = s + \delta s_M = s - \frac{\rho(h)}{2\pi} + \mathcal{O}(s^{-2})$$

$$M_{\text{imp}}(h) = s - \frac{1}{4} + \tan^{-1}\left(\frac{\log\left(\frac{h}{T_0}\right)}{\pi s}\right) + \mathcal{O}(s^{-2})$$

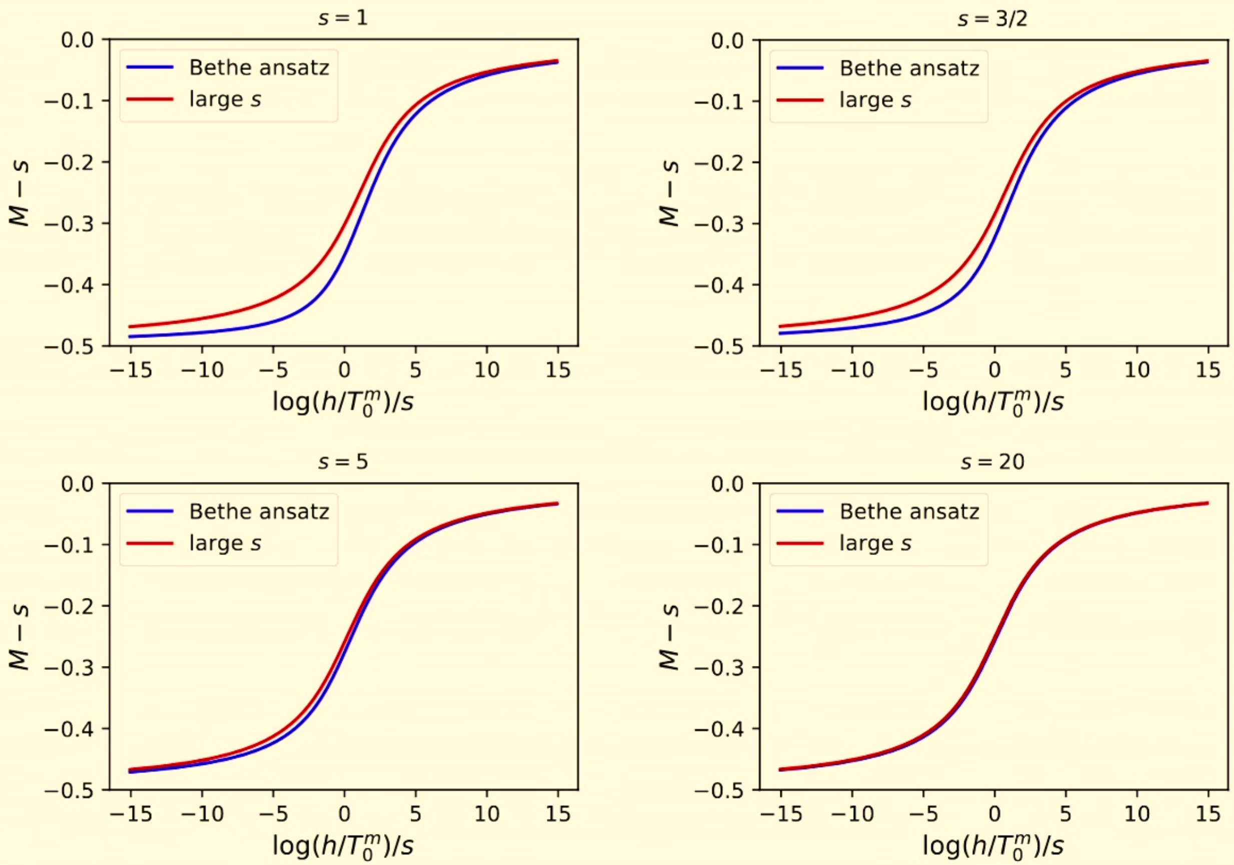
Compare with Bethe ansatz results

- Agreement at low and high T for specific heat and susceptibility
  - $C \sim s^2 (\log T/T_K)^{-4}$ for $T \ll T_K$ and $T \gg T_K$
  - $\chi \sim s(s+1)(1 - (\log T/T_K)^{-1})$ for $T \ll T_K$, $\chi \sim (s^2 - 1/4)(1 - (\log T/T_K)^{-1})$ for $T \gg T_K$
  - At reference temperature T_K, phase shift is $\mathcal{O}(1)$.

- Analytic agreement at large s for the zero-temperature magnetization if reference scale T_0 equals microscopic scale $2T_1$:
  - $M_{\text{Bethe}} \approx s - \frac{1}{4} - \tan^{-1}\left(\frac{\log\left(\frac{h}{2T_1}\right)}{\pi s}\right) = s - \frac{\rho(h)}{2\pi}$.
  - However, $\mathcal{O}(1/s)$ error in M_{Bethe} implies $\mathcal{O}(1)$ error in $\log\left(\frac{T_0}{2\mathrm{T}_1}\right)$

- Numerical calculations from Bethe ansatz use yet another microscopic scale $T_0^m = \sqrt{\frac{e}{2\pi}} T_1$.

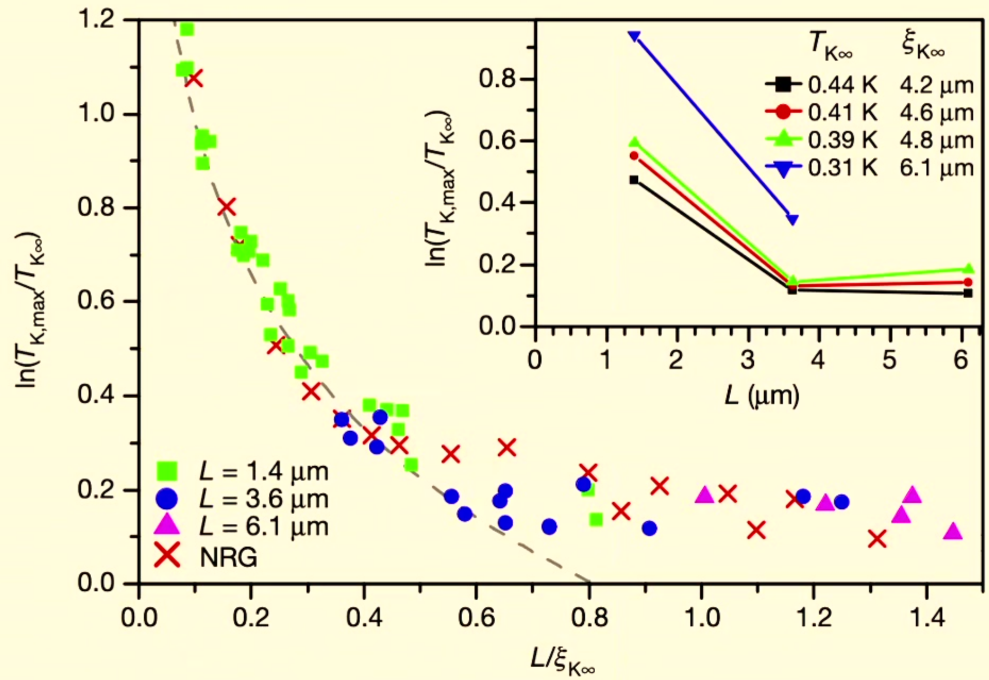
Zero temperature magnetization



Future directions: other Kondo signatures

- Can we obtain the resistance minimum analytically at large s?
  - Hint: magnetoresistance decreases with h
  - $R(h) \propto \cos^2 \rho_{\text{qp}}(h)$, where ρ_{qp} is the quasiparticle phase shift (Andrei, 1981)

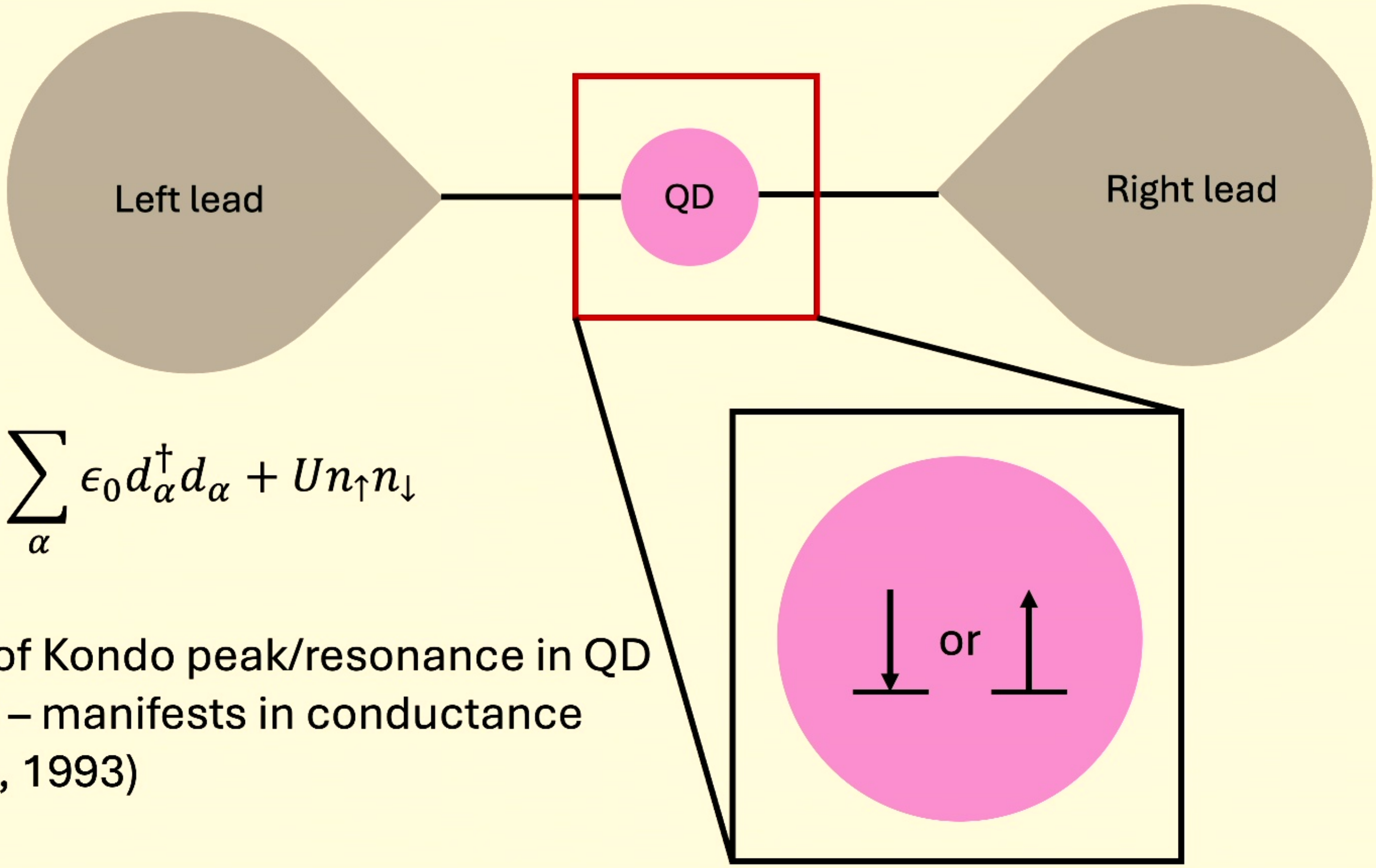
- Can we calculate the Kondo screening cloud?



(Borzenets et al., 2020)

Form Kondo impurity in a quantum dot, measure oscillations of T_K after placing effective barrier L away from impurity

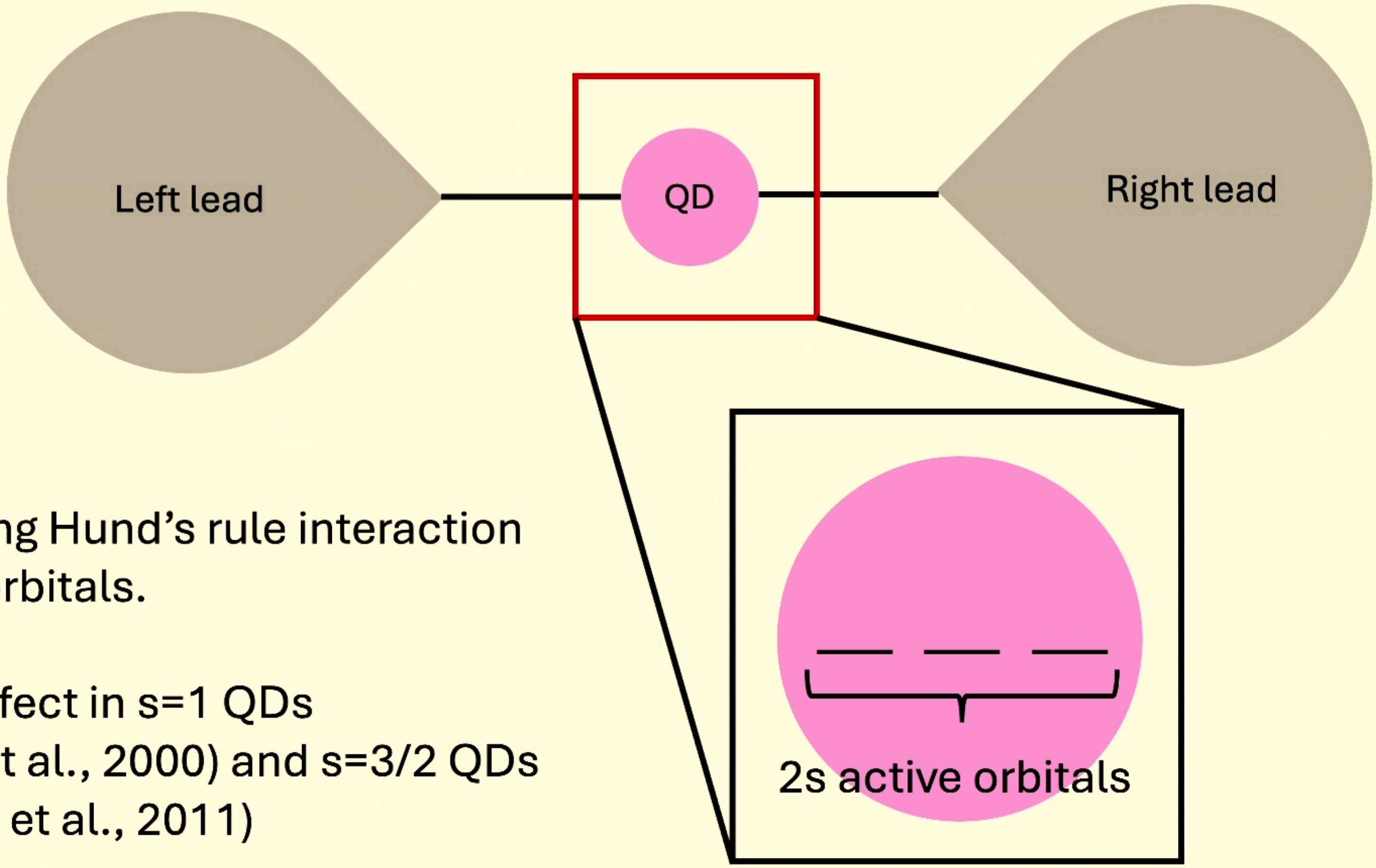
Future directions: transport in quantum dots



$$H_{QD} = \sum_{\alpha} \epsilon_0 d_\alpha^\dagger d_\alpha + U n_\uparrow n_\downarrow$$

Existence of Kondo peak/resonance in QD DOS at FS – manifests in conductance (Meir et al., 1993)

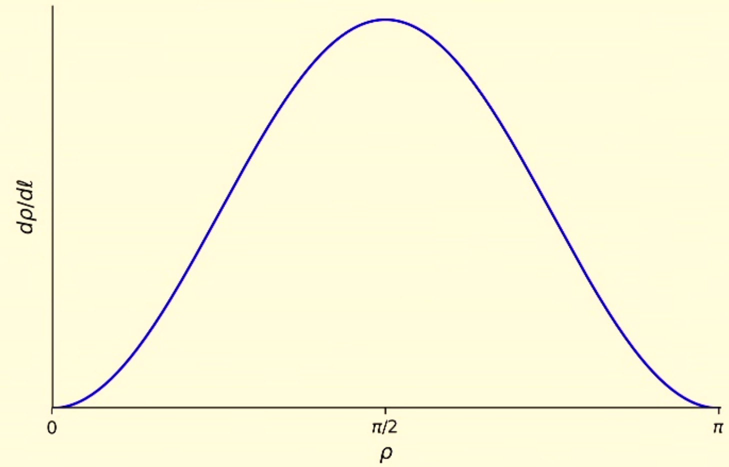
Future directions: transport in quantum dots



Add strong Hund's rule interaction to align orbitals.

Kondo effect in s=1 QDs (Sasaki et al., 2000) and s=3/2 QDs (Klochan et al., 2011)

Conclusion

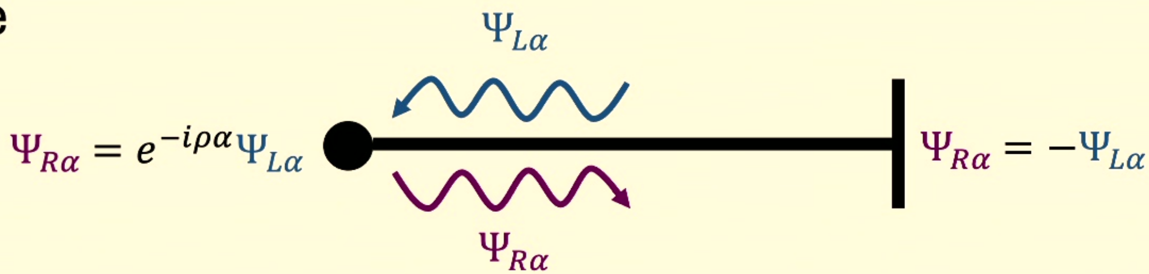


- Effective action for large s Kondo impurity
  - $S_{\text{eff}} = S_{\text{frozen}}(\rho) + S_B + S_{\text{int}} + S_{\text{cont}}$
- RG equation for phase shift at boundary
  - $\frac{d\rho}{d\ell} = -\beta(\rho) = \frac{\sin^2\rho}{\pi s} + \mathcal{O}(s^{-2})$
- Thermodynamic observables (impurity entropy, specific heat, magnetic susceptibility, zero temperature magnetization)

Contact terms

$S_{\text{cont}} = \int d\tau\, \delta m_\pi \vec{\pi}^2 + i\frac{\delta s_B}{2}\int d\tau(\pi_1\partial_\tau\pi_2 - \pi_2\partial_\tau\pi_1).$

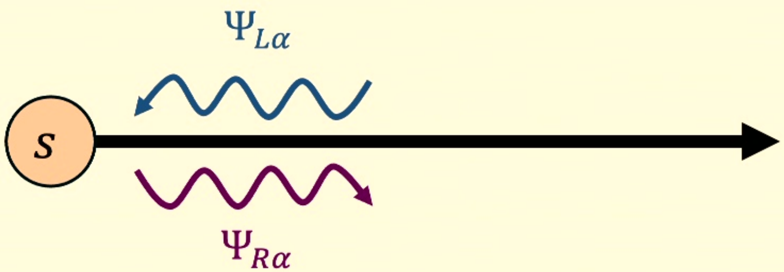
δm_π fixed by rotational invariance



On length L system, for $\omega \sim 1/L$, $S_{\text{int}} = \left(\frac{\rho}{\pi} - \frac{\sin(2\rho)}{2\pi}\right)\int d\omega\, \omega\tilde{\pi}_1(\omega)\tilde{\pi}_2(-\omega).$

Set $\delta s_B = -\rho/\pi + \sin(2\rho)/(2\pi)$ to restore quantized Berry phase.

Reduction to 1D problem



- We get a “folded” action for left and right movers on the half-line with Fermi velocity v_F
- We could also ”unfold” the action so that we have just a left or right mover living on the full real line

$$S = S_{\text{spin}} + \int d\tau \int_0^\infty dx \ \left(\Psi^\dagger_{L\alpha} \left(\partial_\tau + i v_F \partial_x\right)\Psi_{L\alpha} + \Psi^\dagger_{R\alpha} \left(\partial_\tau - i v_F \partial_x\right)\Psi_{R\alpha}\right)$$

$$+J \int d\tau \, \vec{S} \cdot \Psi^\dagger \frac{\vec{\sigma}}{2} \Psi(0)$$

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  - $S_{\text{eff}} = S_{\text{frozen}}(\rho) + S_B + S_{\text{int}} + S_{\text{cont}}$
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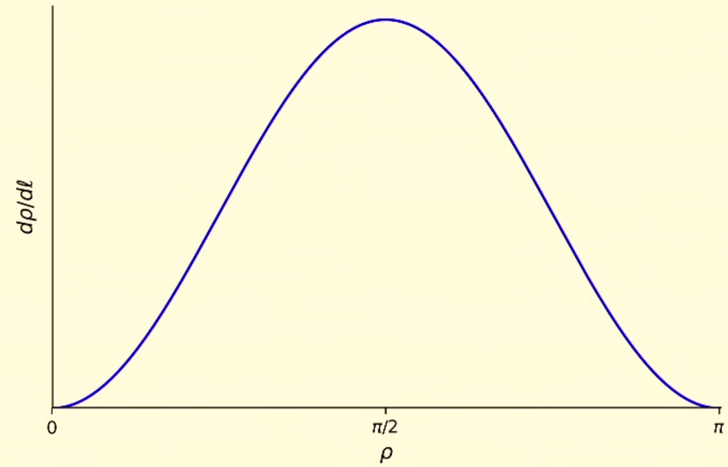

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