Spin-spin and charge correlations around a magnetic impurity

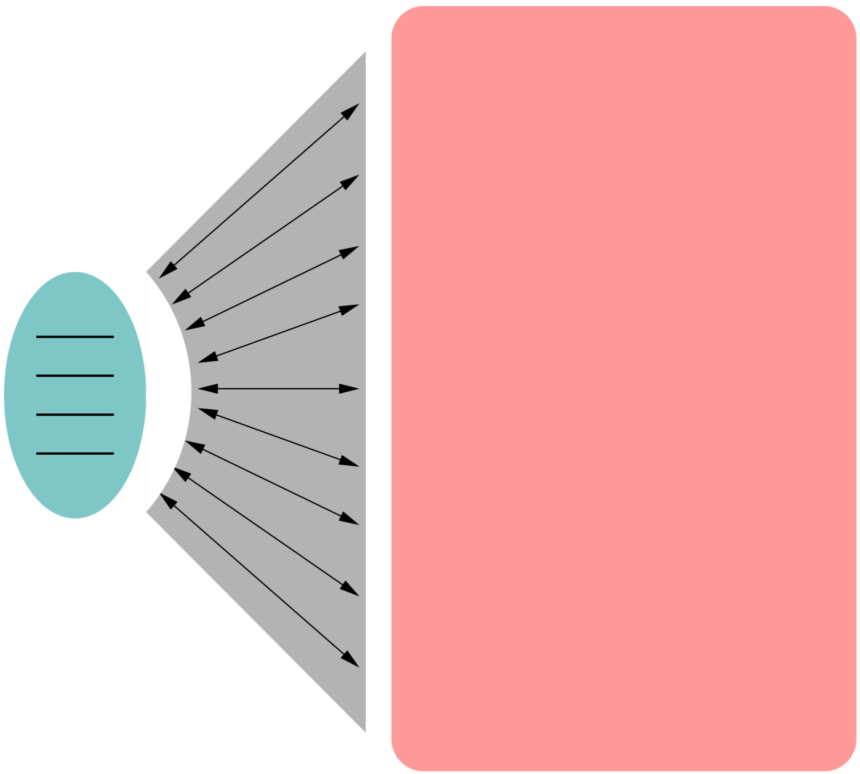
László Borda

Physikalisches Institut, Universität Bonn

Collaborators: I. Affleck, H. Saleur, J. Kroha, M. Garst

L. Borda, PRB **75**, 041307(R) (2007)
I. Affleck, L. Borda, H. Saleur, PRB **77**, 180404(R) (2008)
L. Borda, M. Garst, J. Kroha, submitted to PRB

Quantum impurity systems



Large system: the “environment”
• continuum degrees of freedom
• noninteracting

Small system: the “impurity”
• few degrees of freedom
• can be interacting

Examples:

- spin + fermionic bath:
  Kondo model
- spin + bosonic bath:
  spin-boson model
- spin + fermionic bath
  + bosonic bath:
  Bose Fermi Kondo model

S=1/2 single channel Kondo model

Kondo model:

$$H_K = J\vec{S}\Psi^{\dagger}(0)\vec{s}\Psi(0) + \sum_{k\sigma}\epsilon_k c_{k\sigma}^{\dagger}c_{k\sigma}$$

The system forms a singlet (the impurity gets “screened”) below the Kondo temperature

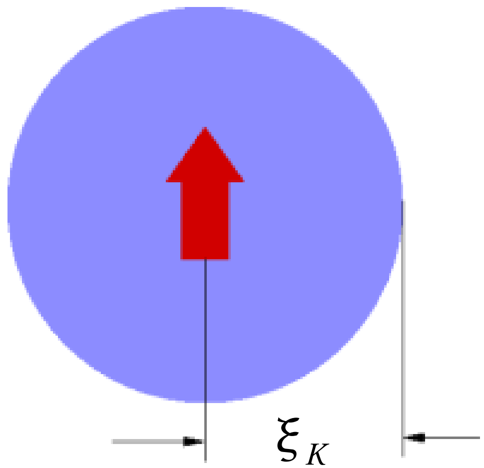
$$T_K = D e^{-\frac{1}{2J\rho_0}}$$ as seen in

$$c_{loc} \sim \frac{T}{T_K}, \qquad \chi_{loc} \sim \frac{1}{T_K}, \qquad \delta\rho_K(T) - \delta\rho_K(0) \sim -\left(\frac{T}{T_K}\right)^2, \qquad T \ll T_K$$

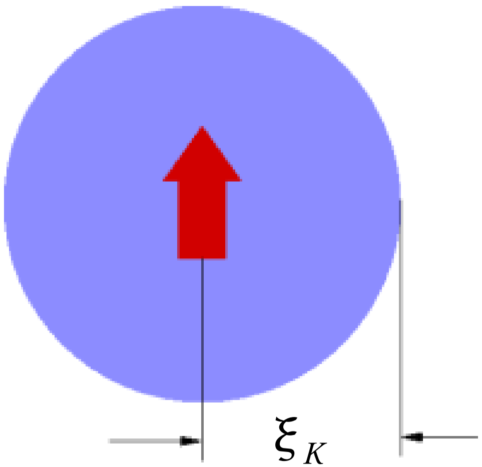
Where is the other part of the singlet? What is its extent?

Comparing the competing kinetic and “binding” energies

$$\frac{\xi_K}{k_F^{-1}} = \frac{\epsilon_F}{T_K} \rightarrow \xi_K = \frac{v_F}{T_K}$$

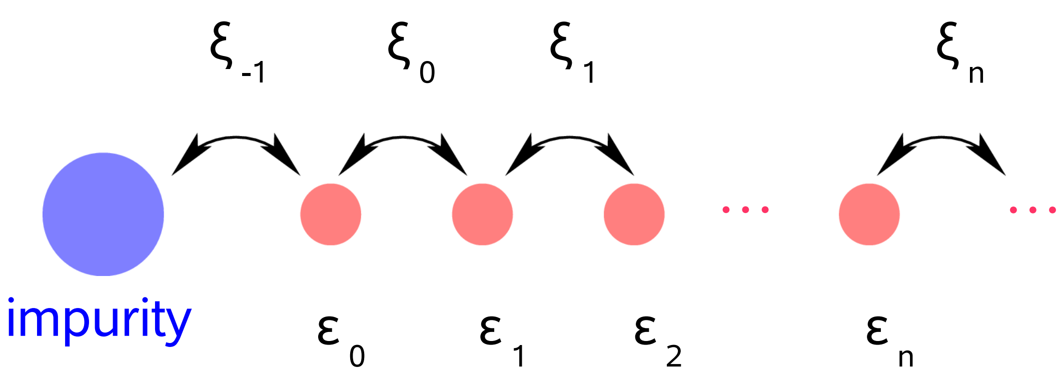


S=1/2 single channel Kondo model



How to compute spatial correlations with NRG?

K.G. Wilson, RMP **47**, 773 (1975)
Review: R. Bulla, T. A. Costi, Th. Pruschke, RMP **80**, 395 (2008)



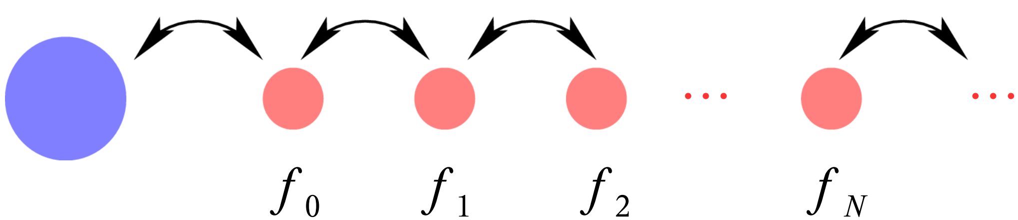
- NRG discretization parameter $\Lambda > 1$
- Logarithmic discretization
- Mapping onto a semi-infinite chain $\xi_n \sim \Lambda^{-n/2}$
- Iterative diagonalization

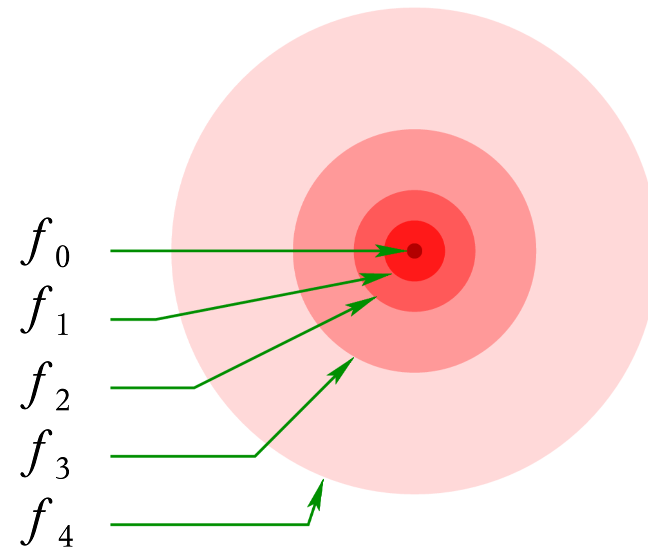
Numerical renormalization group (NRG)

K.G. Wilson, RMP **47**, 773 (1975)
Review: R. Bulla, T. A. Costi, Th. Pruschke, RMP **80**, 395 (2008)

Consequences of logarithmic discretization:

✔ simple truncation scheme
✗ bad resolution at finite energies
✗ bad spatial resolution away from the impurity





The spatial extent of *f* states grows as $\sim k_F^{-1} \Lambda^{N/2}$

How to compute spatial correlations?

Intermezzo: NRG for the two impurity problem

B.A. Jones, C.M. Varma, and J.W. Wilkins, PRL **61**, 125 (1988)

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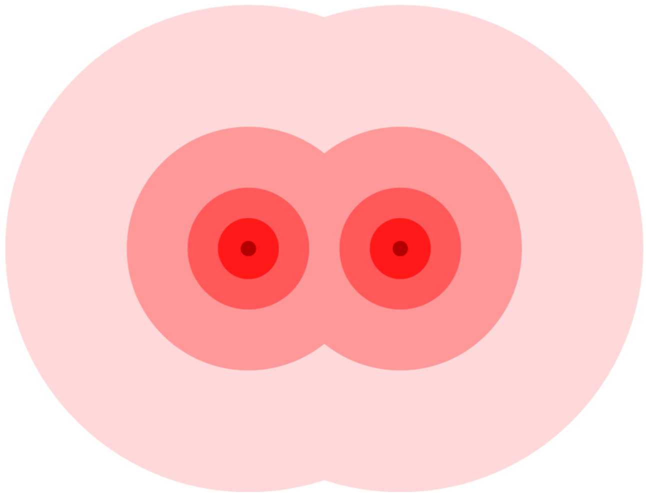
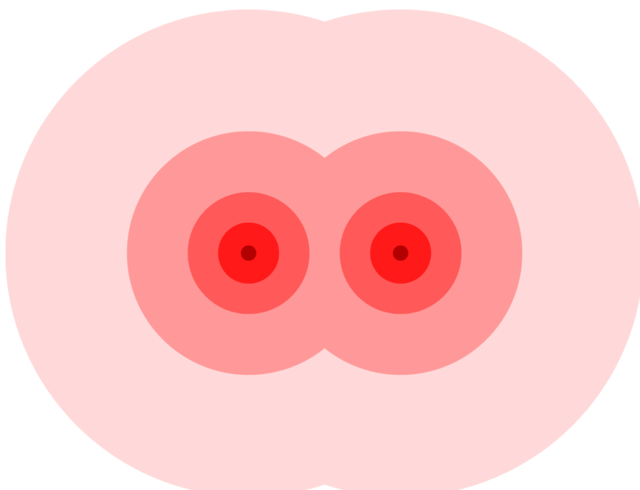


Intermezzo: NRG for the two impurity problem

B.A. Jones, C.M. Varma, and J.W. Wilkins, PRL **61**, 125 (1988)
J.B. Silva *et al.*, PRL **76**, 275 (1996)



$$H = H_0 + J[\vec{S}_1 \cdot \vec{s}_c(1) + \vec{S}_2 \cdot \vec{s}_c(2)], \qquad (1)$$

where H_0 is a structureless half-filled band with the linear dispersion relation $\epsilon_k = v_F(k - k_F)$, the energy measured from the Fermi level.

The overlap between the states $\psi(1)$ and $\psi(2)$ drives us to the more convenient even (+)/odd (−) combinations

$$f_{0\mu\pm} = N_\pm \int_{-D}^{D} c_{\epsilon_k\mu\pm} \sqrt{1 \pm \frac{\sin(kR)}{kR}}\, d\epsilon_k, \qquad (2)$$

[J.B. Silva *et al.*, PRL **76**, 275 (1996)]

The coupling of the two conduction channels to impurity spins rewritten as spatially symmetric $(\vec{S}_1 + \vec{S}_2)$ and asymmetric $(\vec{S}_1 - \vec{S}_2)$ operators yields

$$H = H_0 + \frac{J}{4}(\vec{S}_1 \pm \vec{S}_2) \cdot \sum_{\mu\nu,p=\pm} N_p N_{\pm p} f^\dagger_{0\mu p} \vec{\sigma}_{\mu\nu} f_{0\nu\pm p}\,. \qquad (3)$$

[J.B. Silva *et al.*, PRL **76**, 275 (1996)]

- 3D expression
- $\rho^{1/2}_{e/o}(\varepsilon)$

(In case of 2 impurity problem $\rho_{e/o}(\varepsilon)$ was evaluated at the Fermi energy)

Now: forget about the second impurity!

impurity   another point
where we need good resolution

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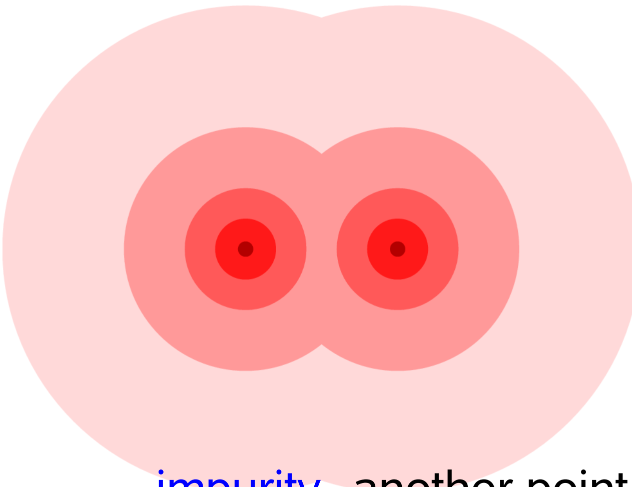

impurity another point
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$\Psi(0)$ $\Psi(x)$

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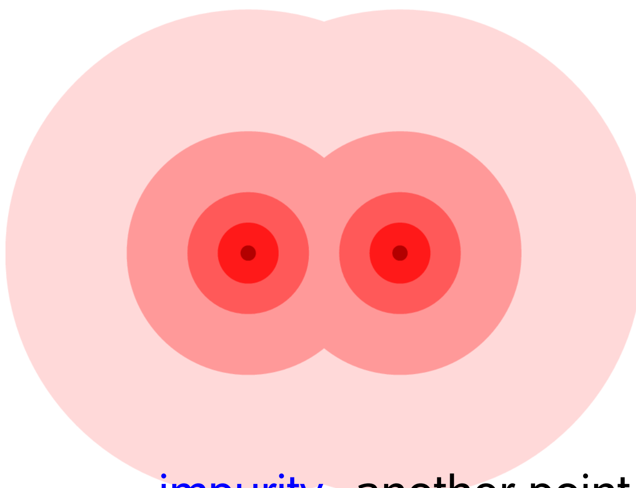

impurity another point
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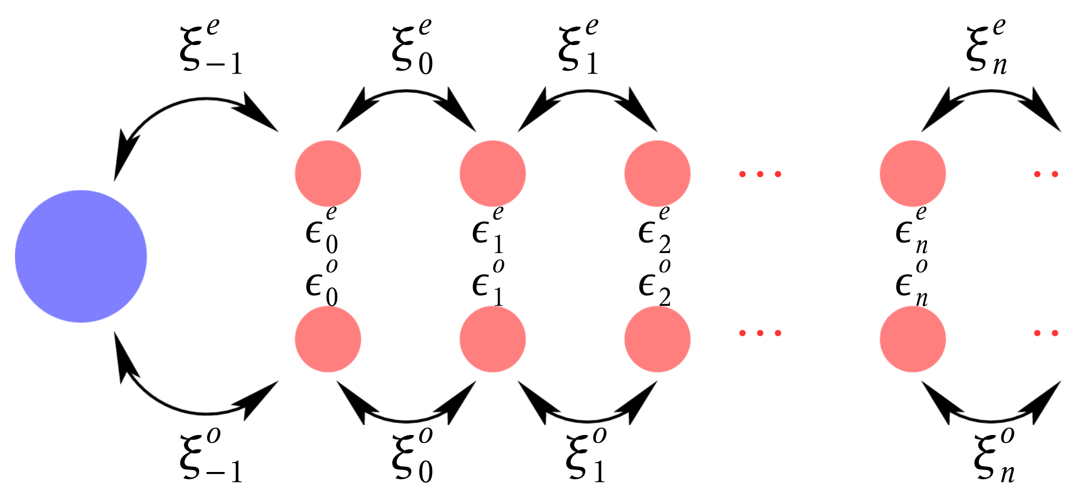
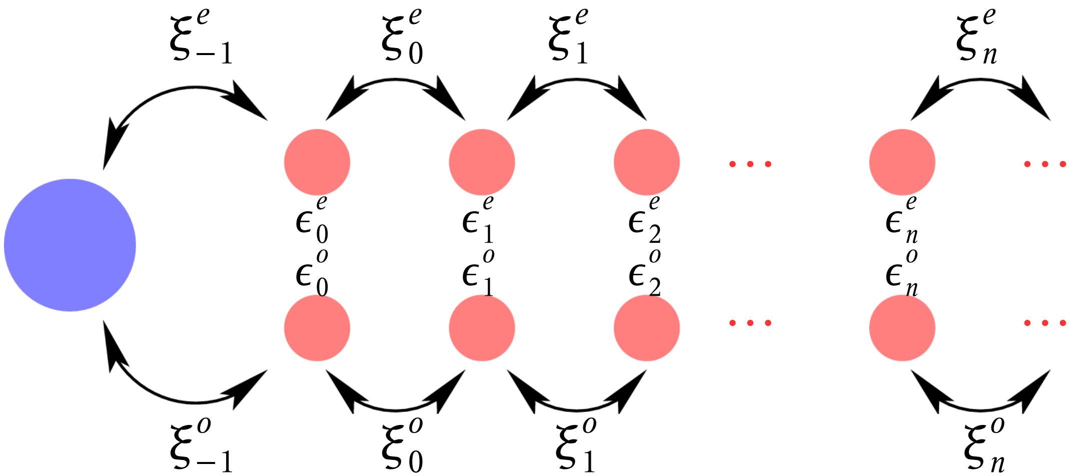
$\Psi(0)$ $\Psi(x)$

$$\Psi_{e/o} = \frac{1}{\sqrt{2}} \left(\Psi(0) \pm \Psi(x) \right)$$

both for even and odd channel:
- logarithmic discretization
- mapping onto Wilson chains





The chain parameters
$\xi_i^{e/o}$ and $\epsilon_i^{e/o}$
depend on the density of states
$\rho^{e/o}(\epsilon, x)$

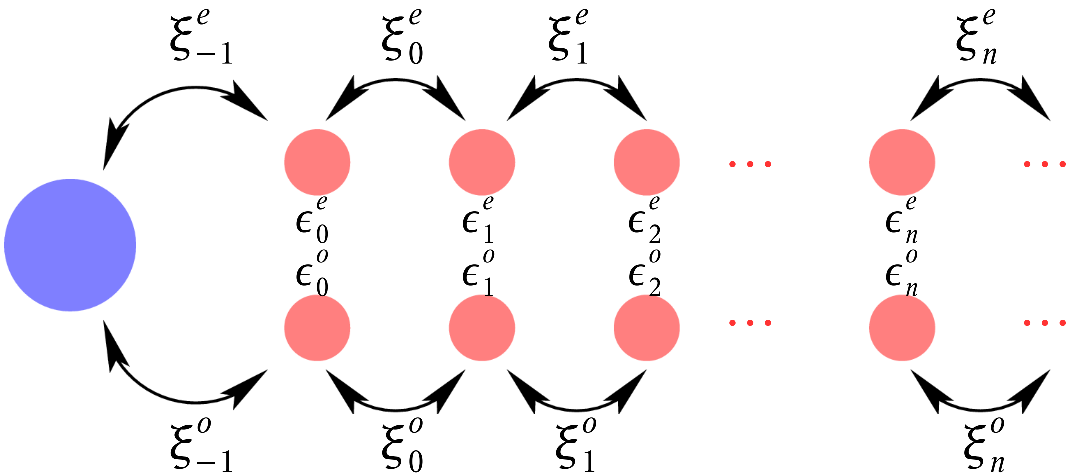
(of course, $\rho^e(\epsilon, x) + \rho^o(\epsilon, x) \equiv \rho_0$)

$$\rho_{1D}^{e/o}(\epsilon, x) = \rho_0 \left[\frac{1}{2} \pm \frac{1}{2} \cos\left(\frac{\epsilon}{v_F} x \right) \right]$$

$$\rho_{2D}^{e/o}(\epsilon, r) = \rho_0 \left[\frac{1}{2} \pm \frac{1}{2} J_0\left(\frac{\epsilon}{v_F} r \right) \right]$$

$$\rho^{e/o}(\epsilon, r) \sim r^{-\frac{D-1}{2}}$$

$$\rho_{3D}^{e/o}(\epsilon, r) = \rho_0 \left[\frac{1}{2} \pm \frac{1}{2} \frac{\sin(\epsilon r / v_F)}{\epsilon r / v_F} \right]$$



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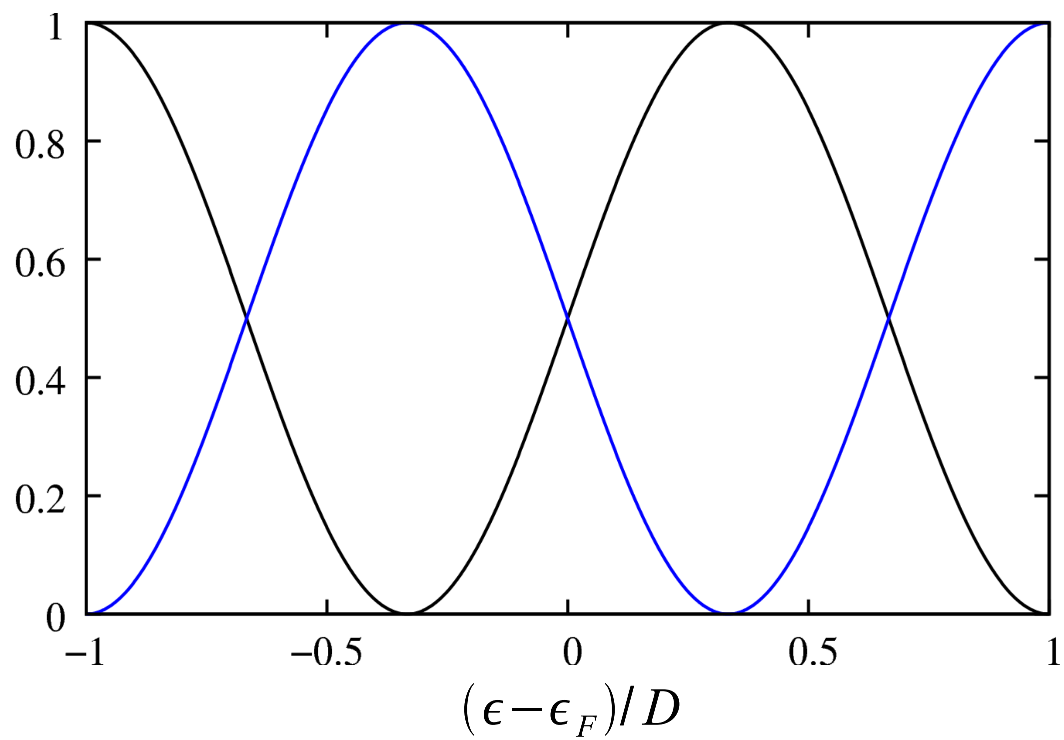
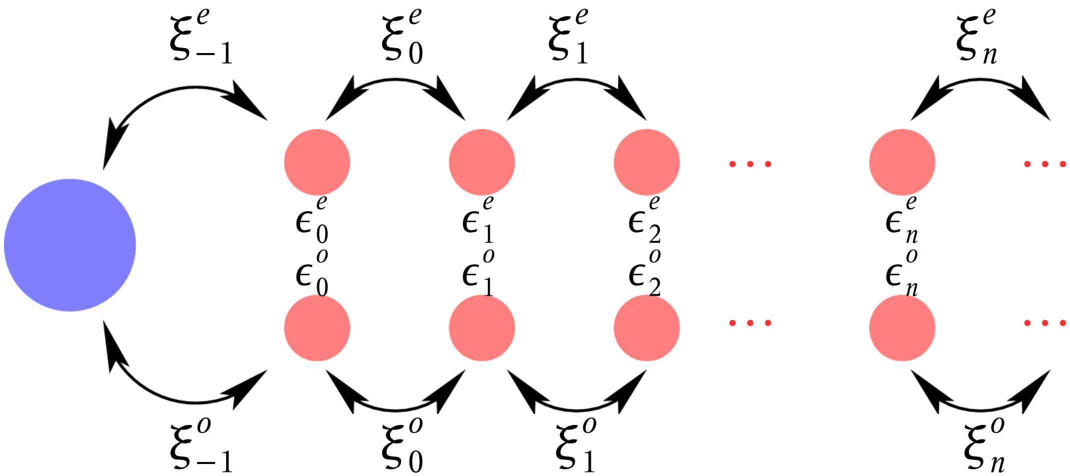
$$\rho^{e/o}_{1D}(\epsilon, x) = \rho_0 \left[\frac{1}{2} \pm \frac{1}{2} \cos\left(\frac{\epsilon}{v_F} x \right) \right]$$

$$x = 1.5 \frac{\pi}{k_F}$$

$\rho^e(\epsilon)$

$\rho^o(\epsilon)$





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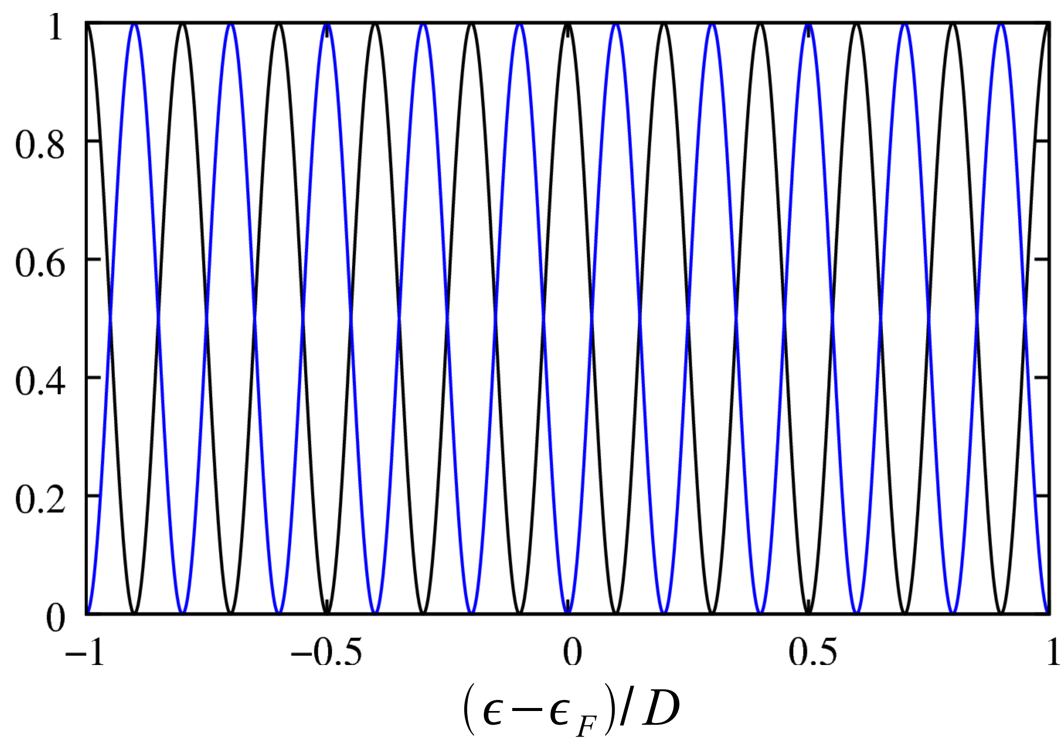
$$x = 10 \frac{\pi}{k_F}$$

$\rho^e(\epsilon)$

$\rho^o(\epsilon)$



S=1/2 single channel Kondo model

A measure of the Kondo correlations:

$$\chi_{t=0}(x) = \langle \vec{S}\,\Psi^\dagger(x)\,\vec{s}\,\Psi(x)\rangle_{t=0}$$

Sum rule (consequence of the singlet ground state):

$$\int_0^\infty \chi_{t=0}(x)\,dx = -\frac{3}{4}$$

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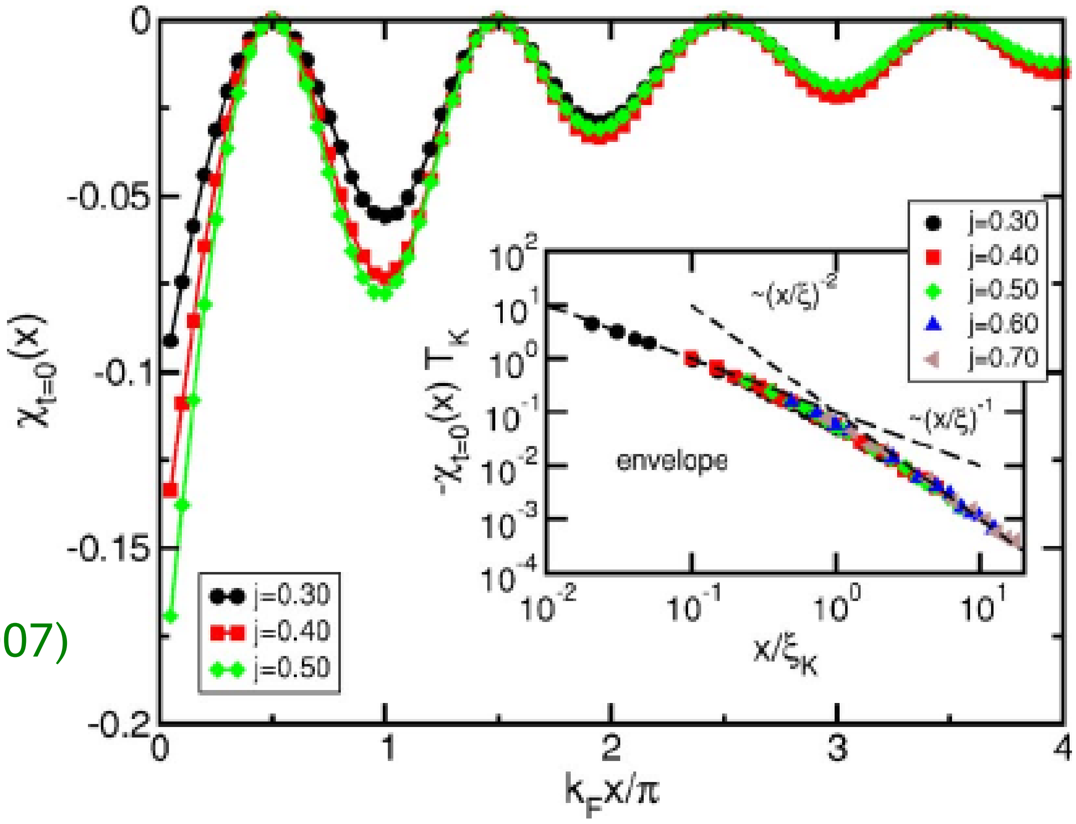

L. Borda, PRB **75**, 041307(R) (2007)

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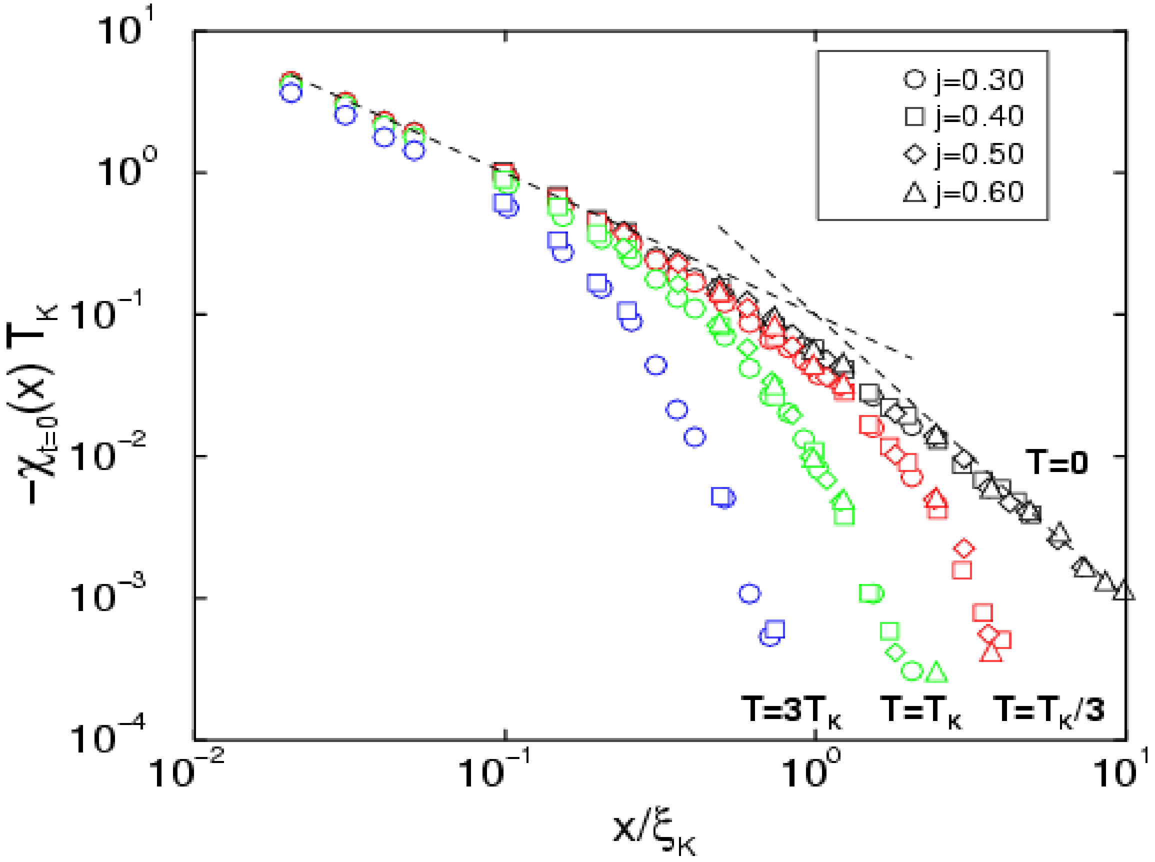

S=1/2 single channel Kondo model

Does the length scale ξ_K show up in the charge oscillations?

One can be skeptical:

- Spin-charge separation? How can a purely spin-dependent interaction affect the charge density?

- What about electron-hole symmetry?

G. Grüner and C. Hargitai, Phys. Rev. Lett. **26**, 772 (1972).
D. Šokčević, V. Zlatić, and B. Horvatić, Phys. Rev. B **39**, 603 (1989).

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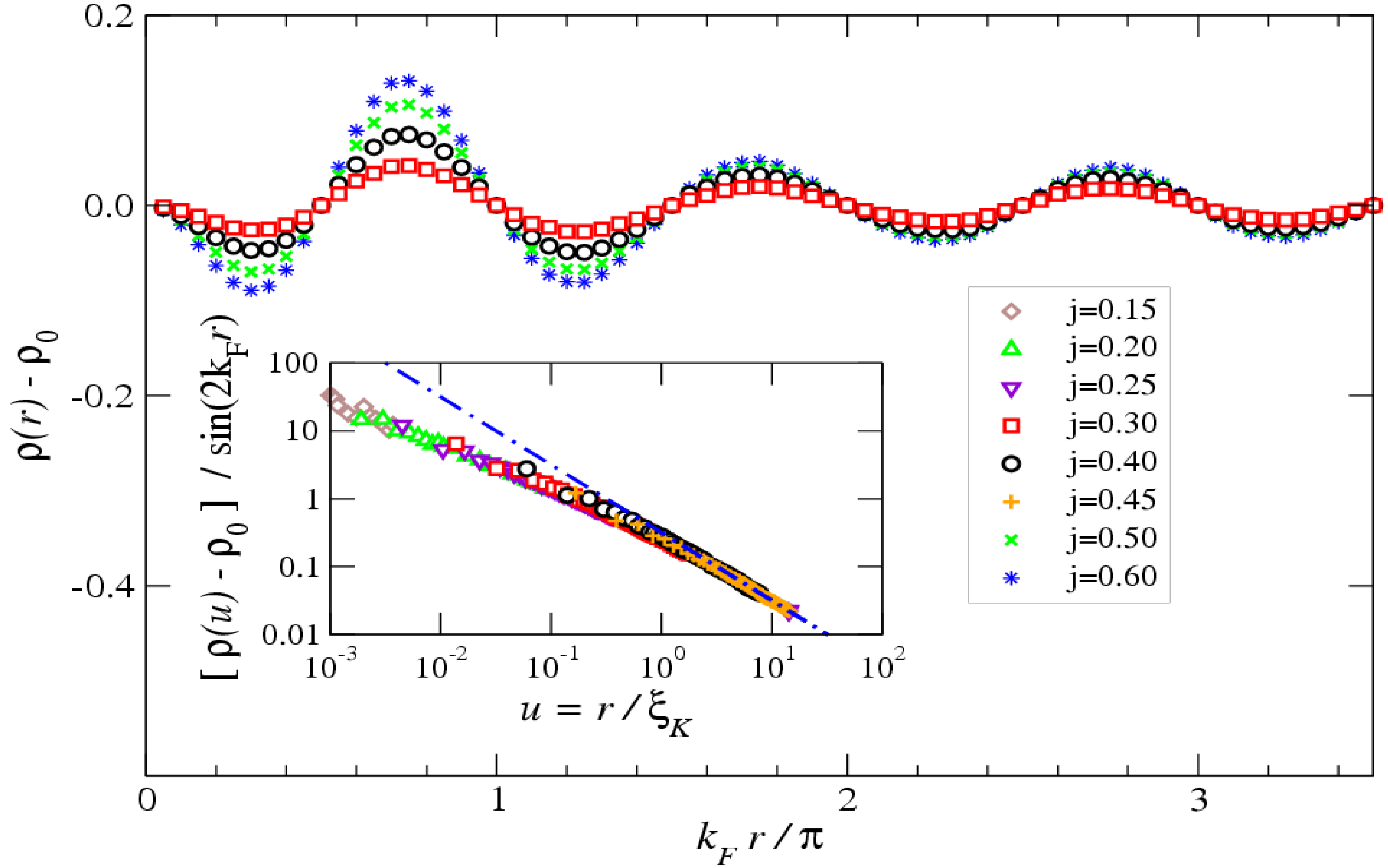

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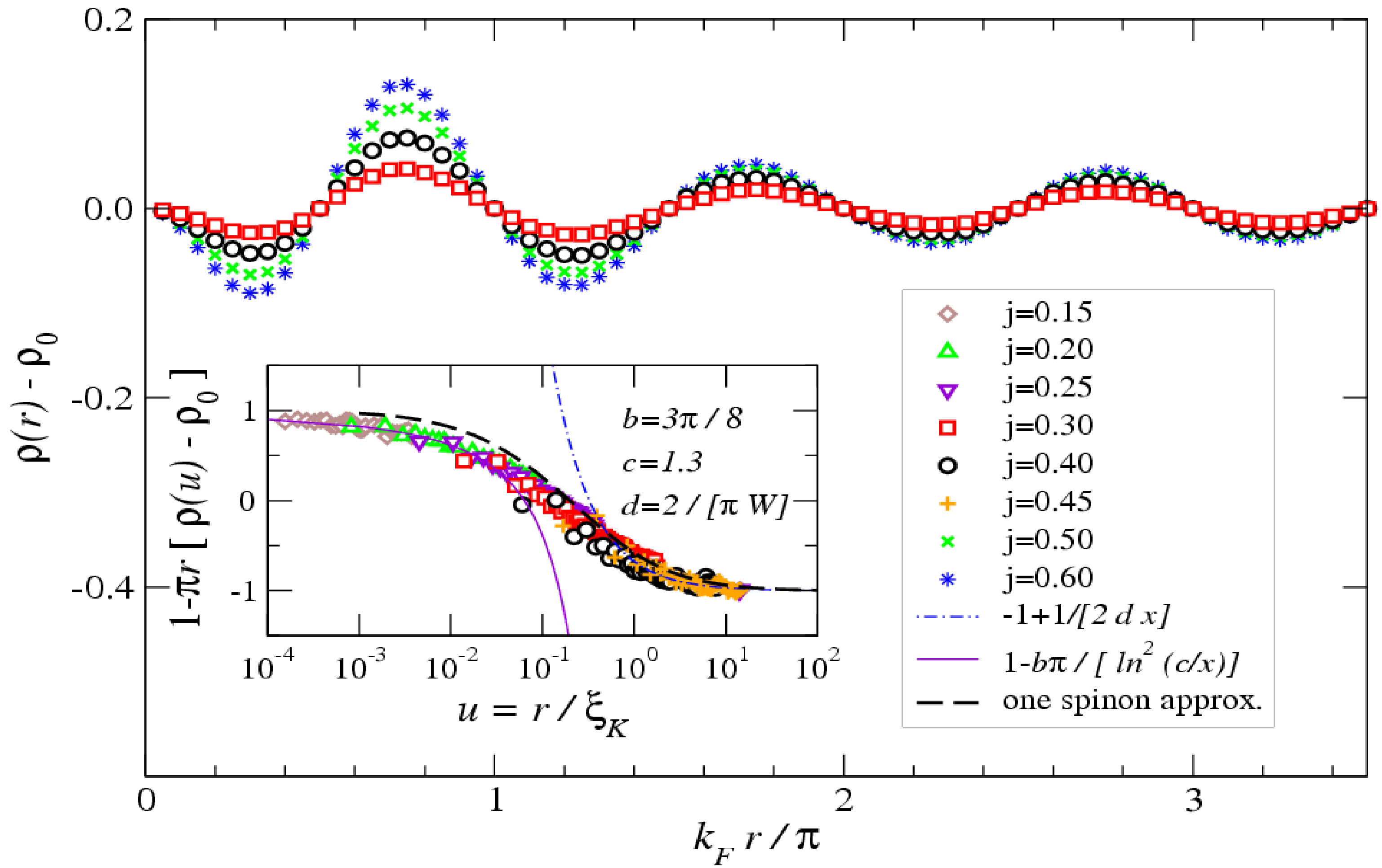

S=1 single channel Kondo model: the “Kondo underscreening cloud”

S=1 single channel Kondo model:

$$H_K = J\vec{S}\Psi^\dagger(0)\vec{s}\Psi(0) + \sum_{k\sigma}\epsilon_k c^\dagger_{k\sigma}c_{k\sigma} \quad (S=1)$$

The low energy physics described by “singular” Fermi liquid

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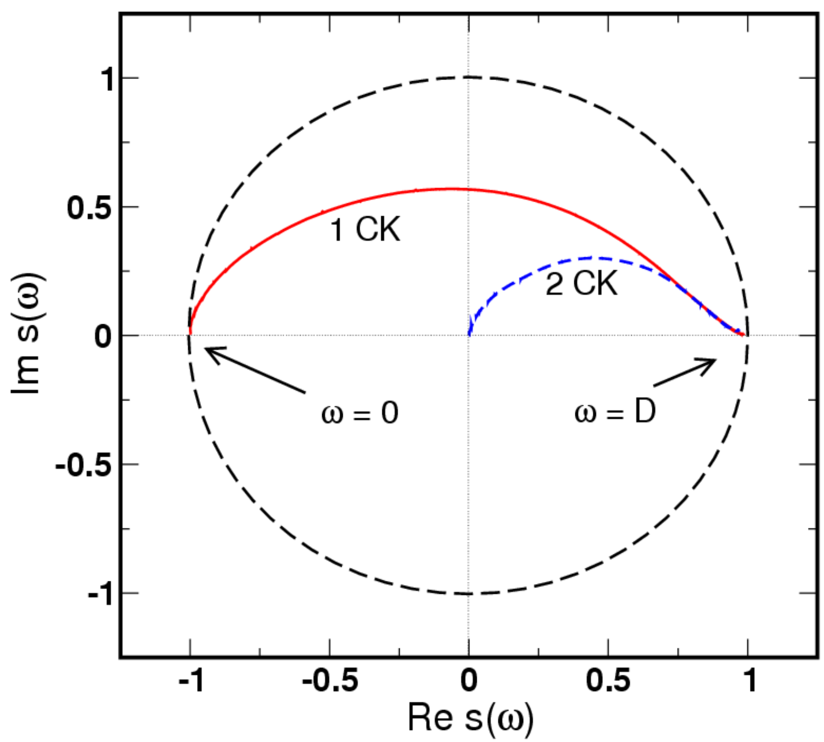

Regular Fermi liquid:

$$|S(\omega=0)|=1$$

$S(\omega)$ analytic around $\omega=0$

Non Fermi liquid:

$$|S(\omega=0)|<1$$

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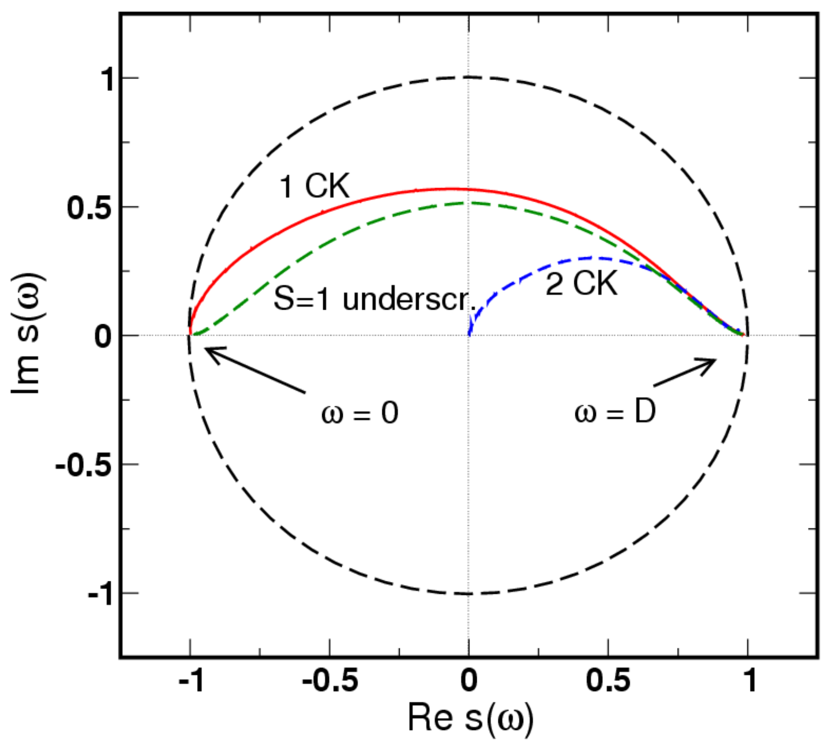

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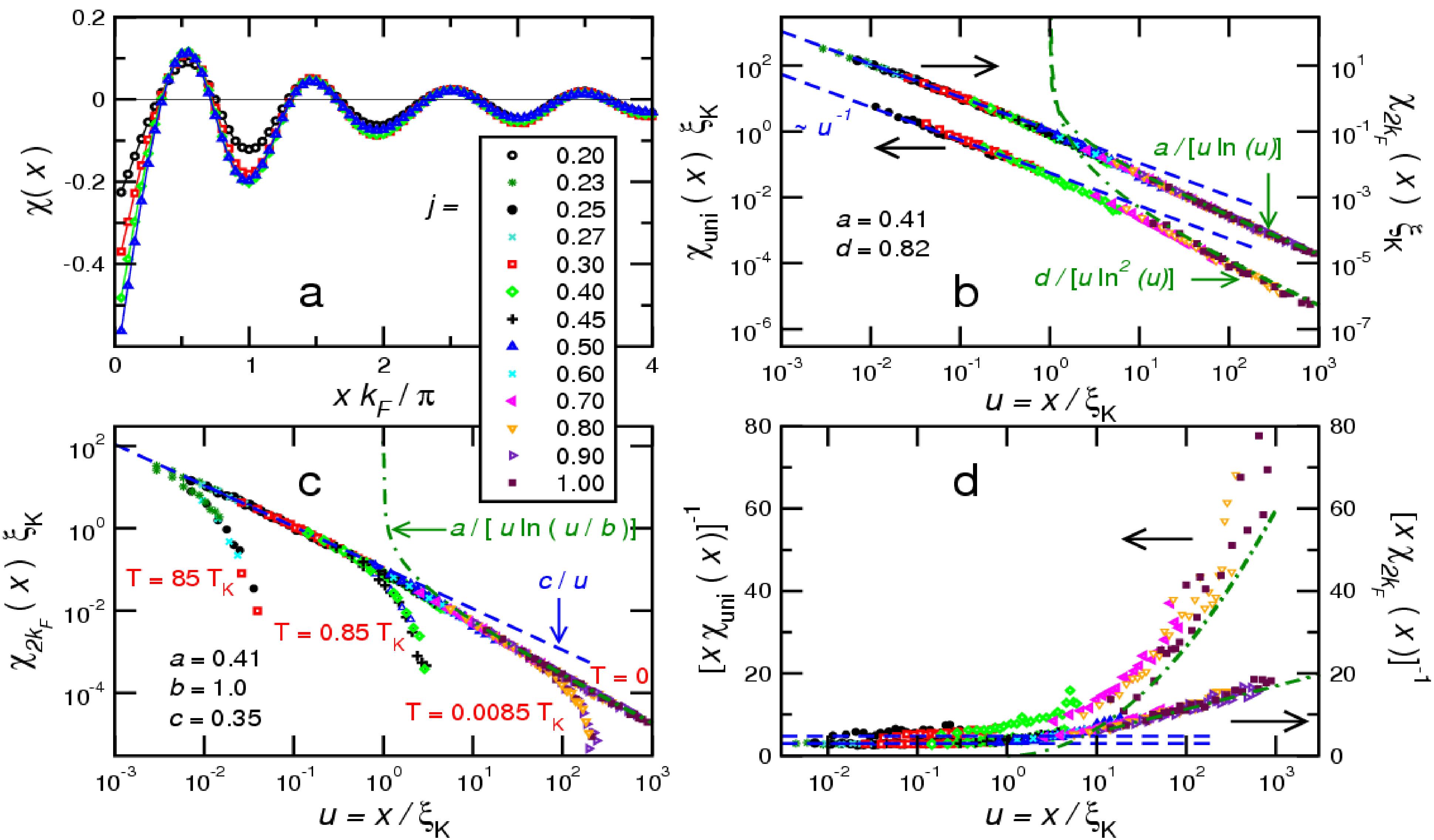
The low energy physics described by "singular" Fermi liquid

as seen in

$$\delta(\omega) = \frac{\pi}{2} - \frac{1}{4\ln(T_K/\omega)}$$

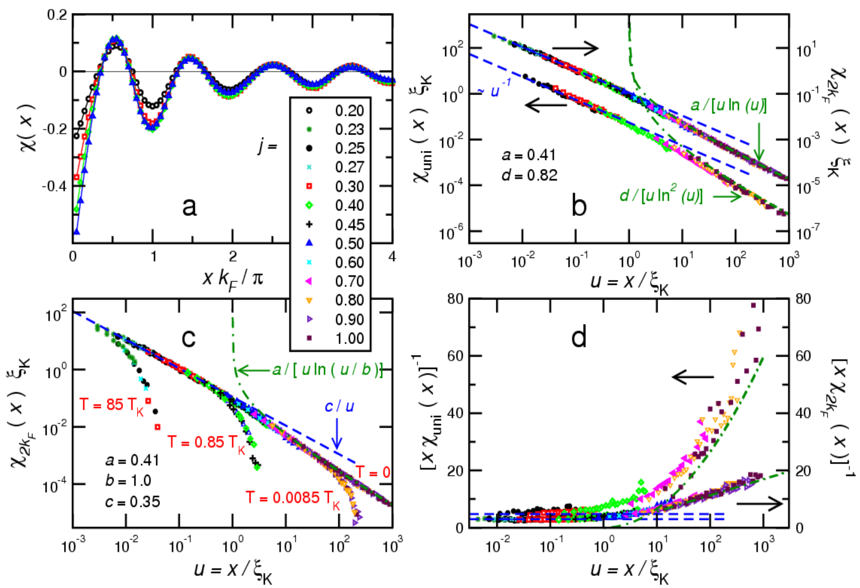
$$\sigma_{inel}(\omega) \sim \frac{1}{\ln^2(T_K/\omega)}$$

S=1 single channel Kondo model: the “Kondo underscreening cloud”



Summary

- NRG for spatial correlations
- Kondo screening cloud
  (and charge oscillations)
- Kondo "underscreening cloud"



Future

- Kondo "overscreening cloud"