Spatial and temporal propagation of Kondo correlations

Frithjof B. Anders
Lehrstuhl für Theoretische Physik II - Technische Universität Dortmund

Deutsche Forschungsgemeinschaft DFG

JÜLICH FORSCHUNGSZENTRUM
John von Neumann Institut für Computing

GIF German-Israeli Foundation for Scientific Research and Development

technische universität dortmund

Collaborators

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Benedikt Lechtenberg

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Time-dependent NRG
FBA, A. Schiller
PRL 95, 196801 (2005),
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Avi Schiller

† (22.6.2013)

Outline

1. Kondo model
   - spatial correlation: $\chi(R,t) = \langle \vec{S}_{\mathrm{imp}} \vec{s}_c(\vec{r}) \rangle (t)$
   - length scale ξ_K
2. Real-time dynamics of quantum impurity systems
   - TD numerical renormalization group
3. Mapping on a two-impurity problem for each distance R
4. Results
   - equilibrium: Kondo cloud
   - propagation of spin correlations
5. Conclusion

1. Spatial Kondo correlations

Kondo model: drosophila of solid state theory

$$H = \sum_{\sigma} \int_{-D}^{D} d\varepsilon \, \varepsilon \, c^{\dagger}_{\varepsilon\sigma} c_{\varepsilon\sigma}$$

J. Kondo, Prog. Theor. Phys 32, 37 (1964)

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J. Kondo, Prog. Theor. Phys 32, 37 (1964)

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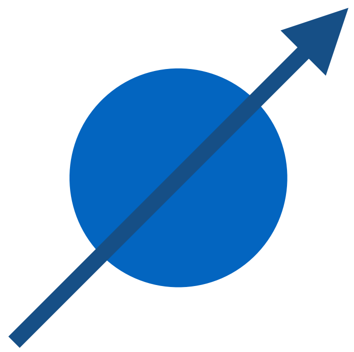
impurity spin



host

$\vec{s}_c(\vec{r})$

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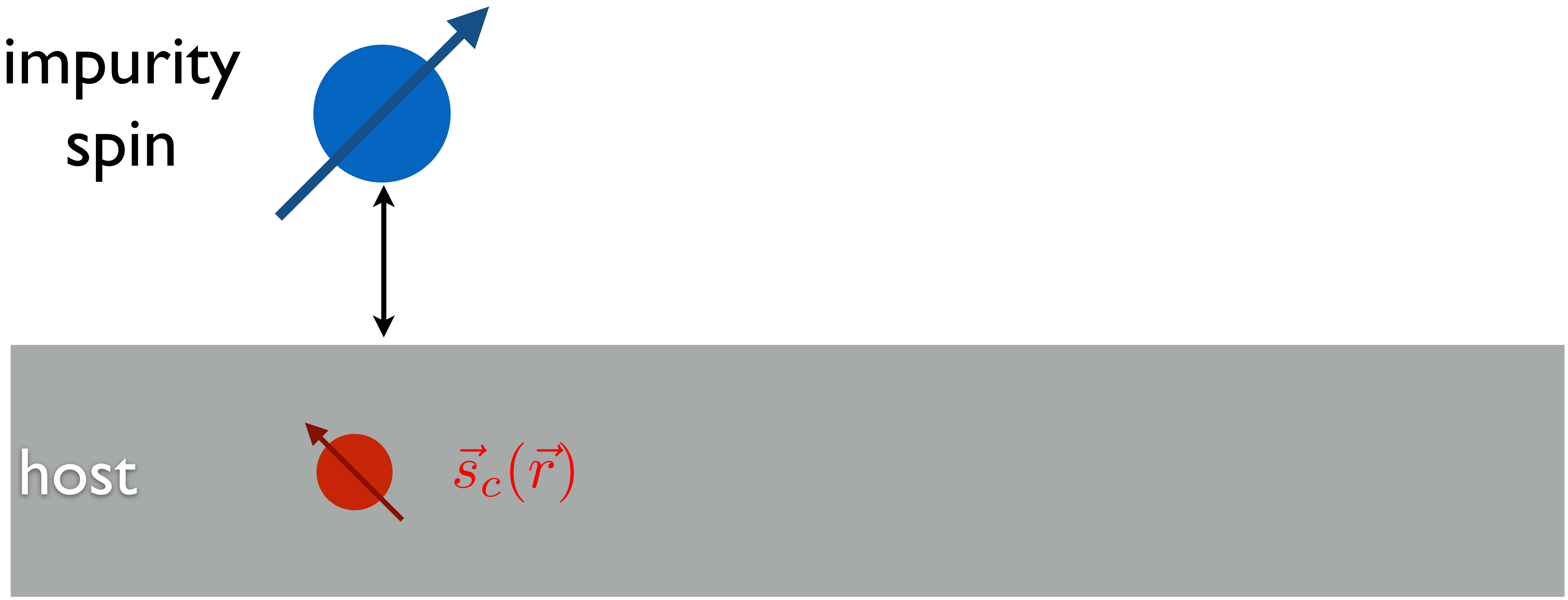

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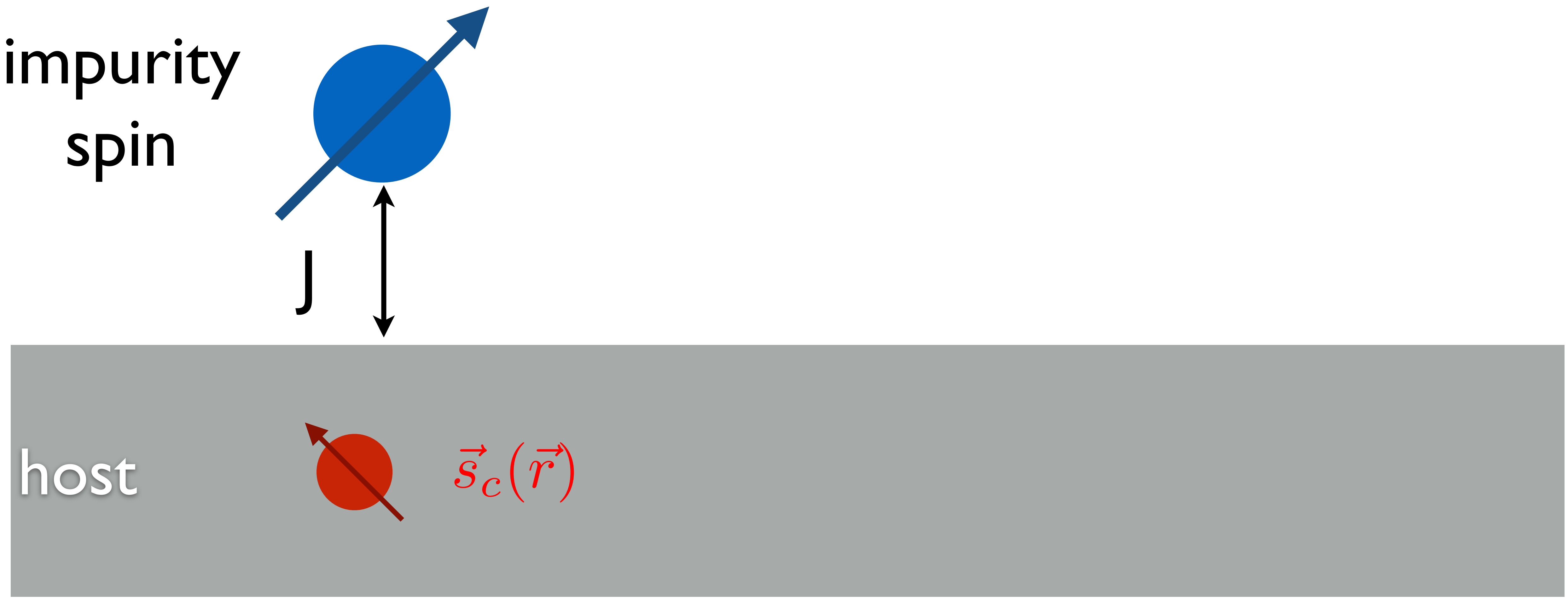

$$H = \sum_\sigma \int_{-D}^{D} d\varepsilon\, \varepsilon\, c^\dagger_{\varepsilon\sigma} c_{\varepsilon\sigma} + J \vec{S}_{\rm imp} \vec{s}_c(0)$$

J. Kondo, Prog. Theor. Phys 32, 37 (1964)

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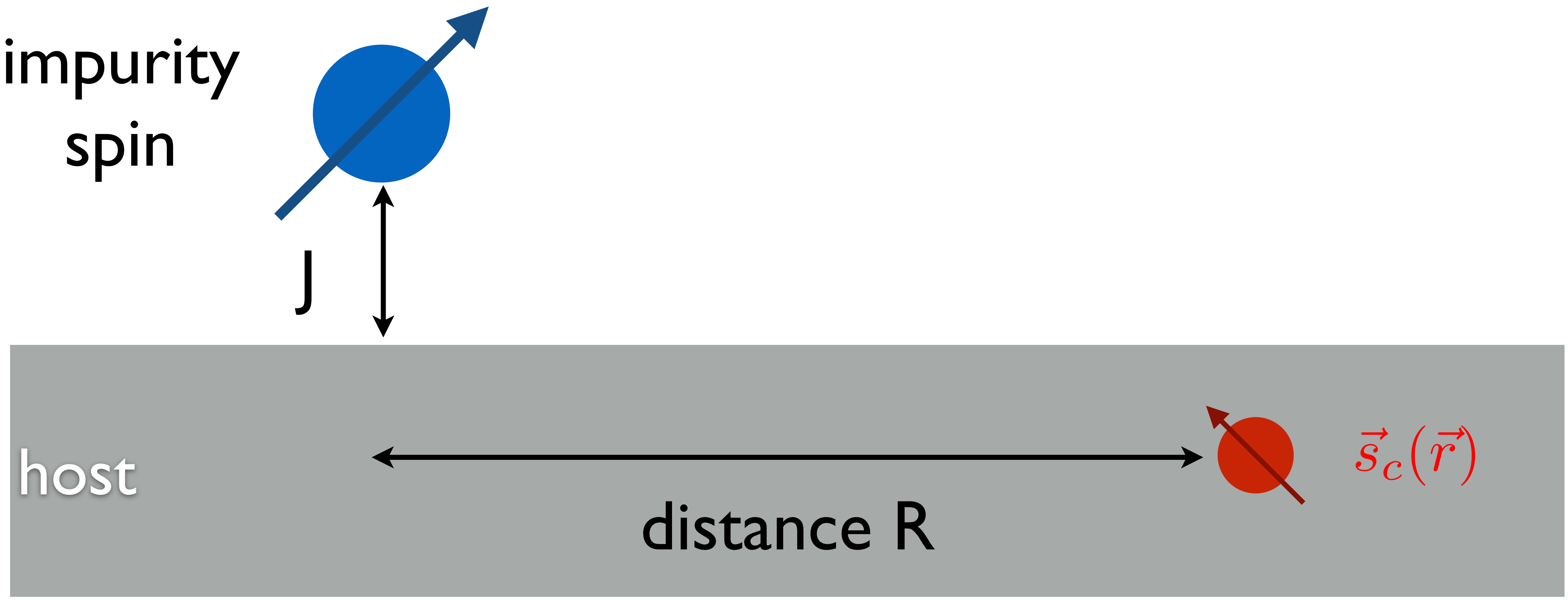

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correlation function:

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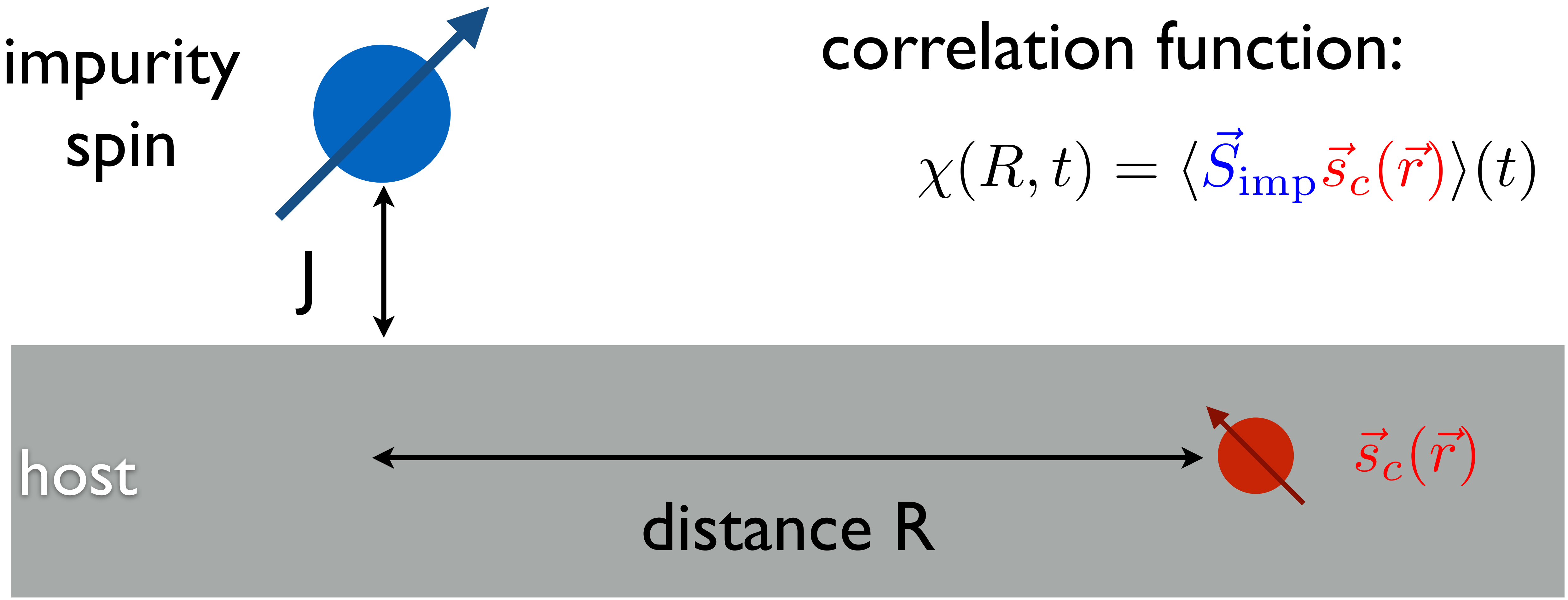

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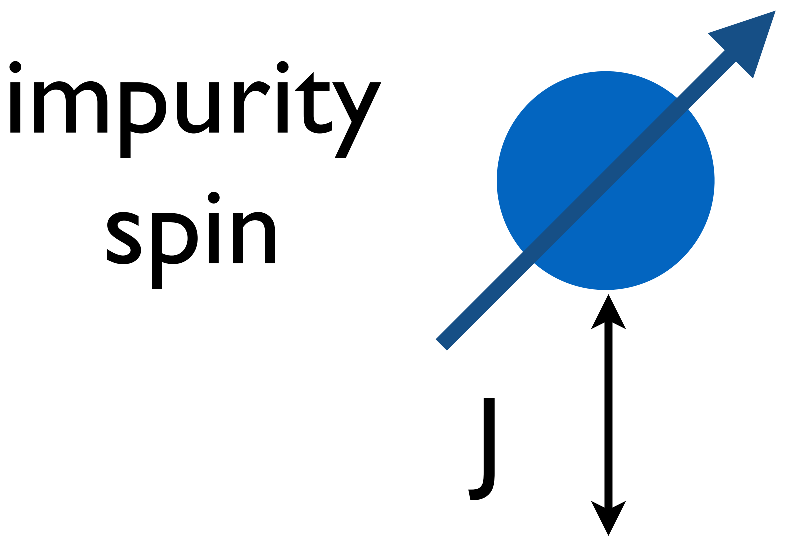

correlation function:

$$\chi(R,t) = \langle \vec{S}_{\rm imp} \vec{s}_c(\vec{r}) \rangle (t)$$

equilibrium: $\chi_\infty(R) = \lim_{t\to\infty} \chi(R,t)$

$$H = \sum_\sigma \int_{-D}^{D} d\varepsilon \, \varepsilon \, c^\dagger_{\varepsilon\sigma} c_{\varepsilon\sigma} + J \vec{S}_{\rm imp} \vec{s}_c(0)$$

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Kondo model: drosophila of solid state theory

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experimental evidence

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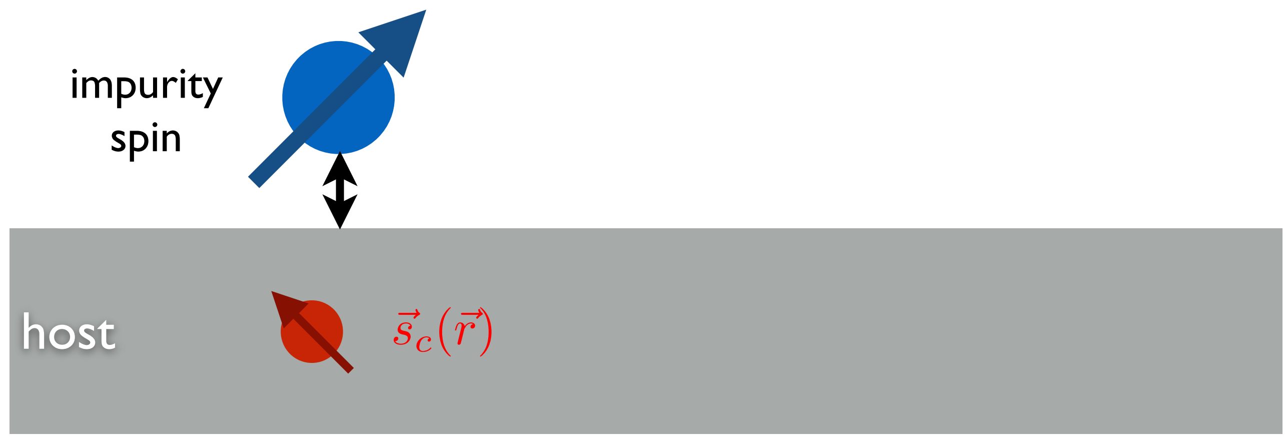

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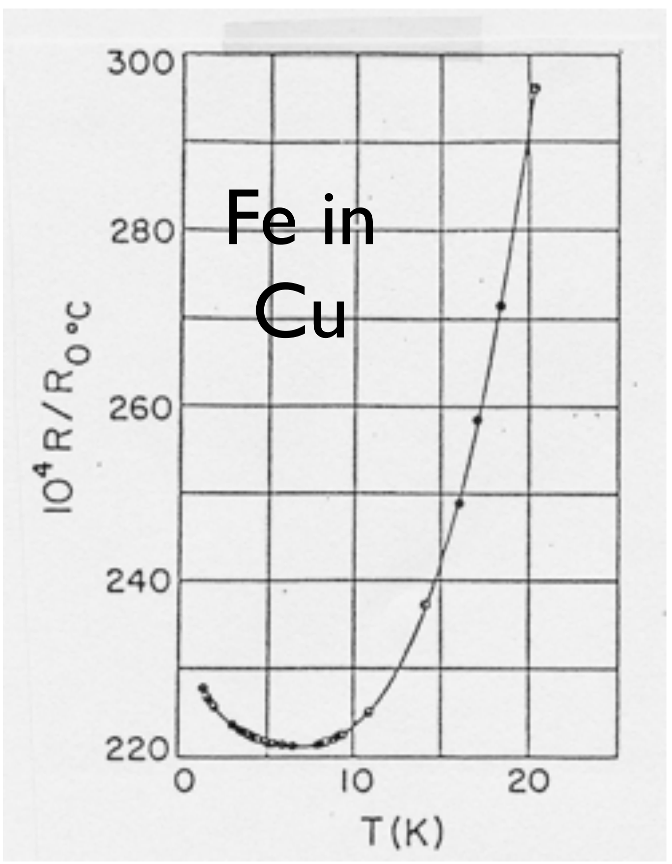

de Haas, de Boer, van den Berg
Physica 1,1115 (1934)

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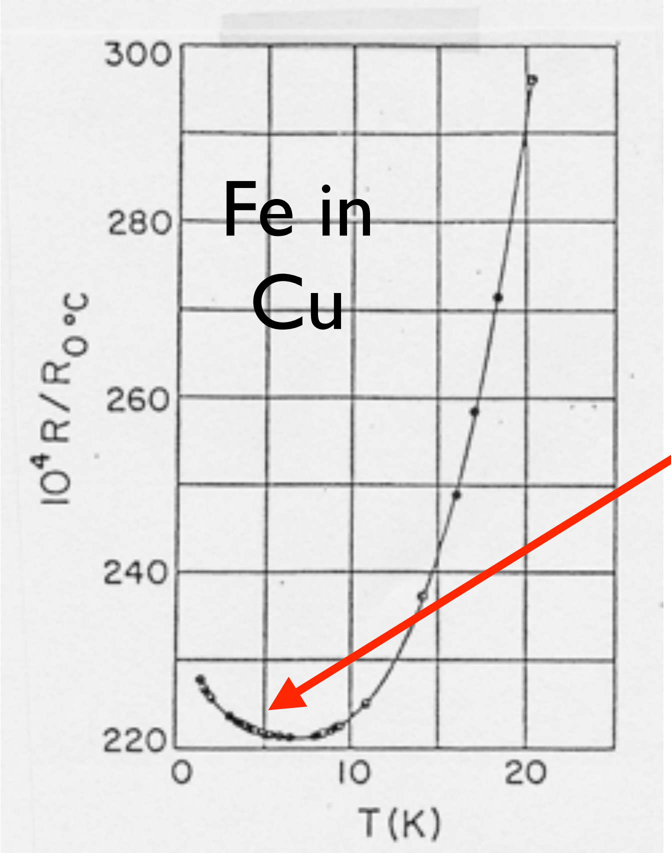


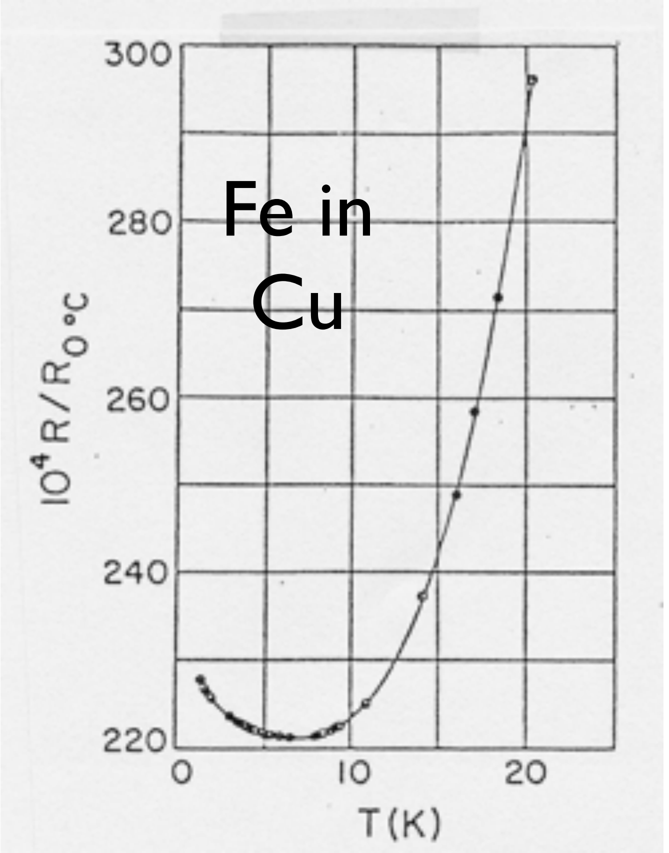
Kondo scale T_K

$$T_K = De^{-\frac{1}{\rho J}}$$

de Haas, de Boer, van den Berg
Physica 1,1115 (1934)

Kondo model: drosophila of solid state theory

experimental evidence



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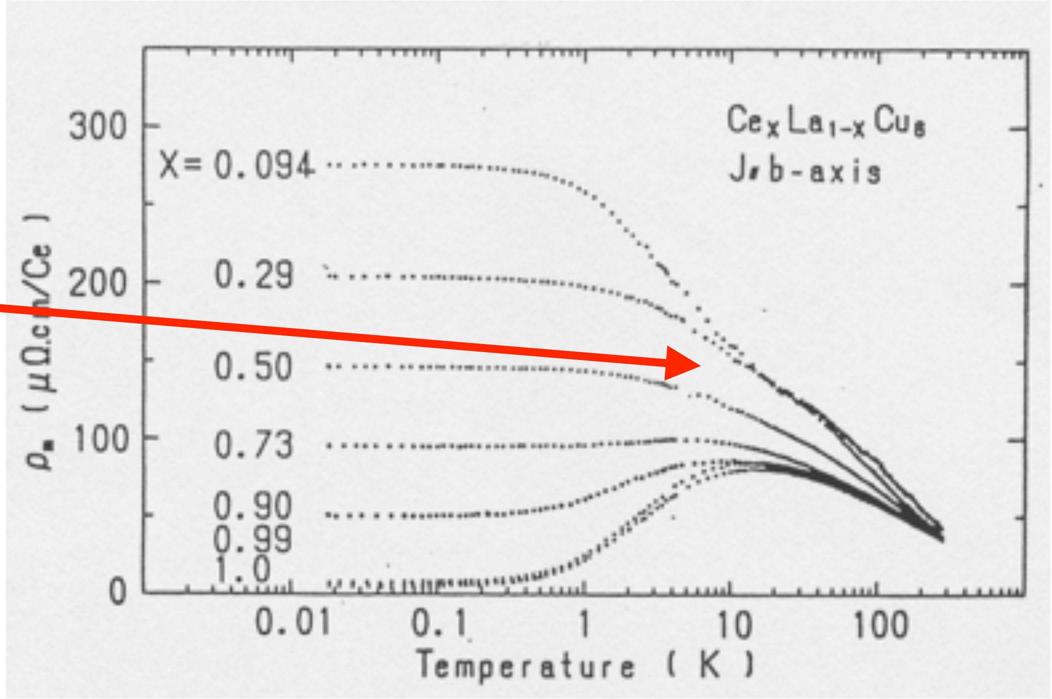
Heavy Fermions



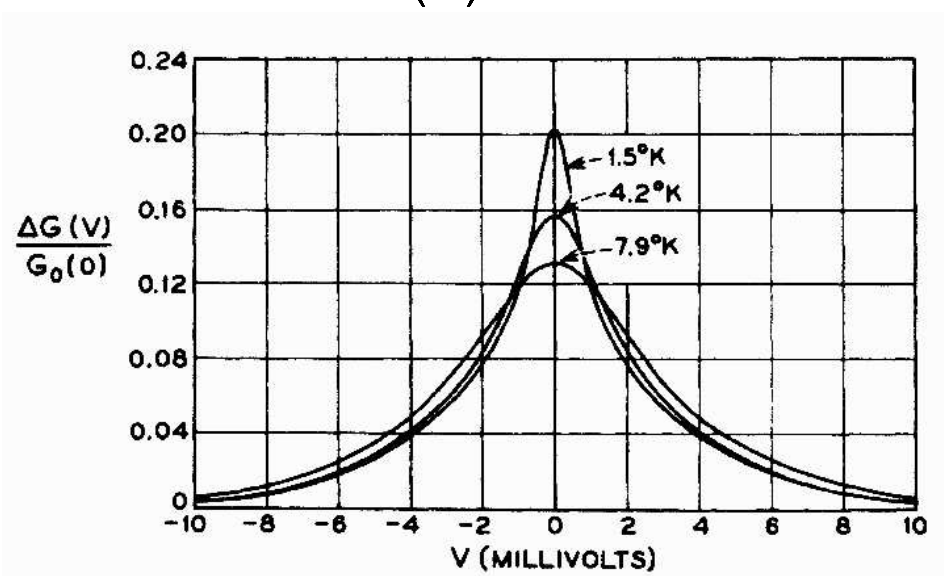
Onuki et al (1987)

Kondo model: drosophila of solid state theory

experimental evidence

Heavy Fermions

G(V) in Ta-I-Al



Wyatt, PRL 13,401 (1964)

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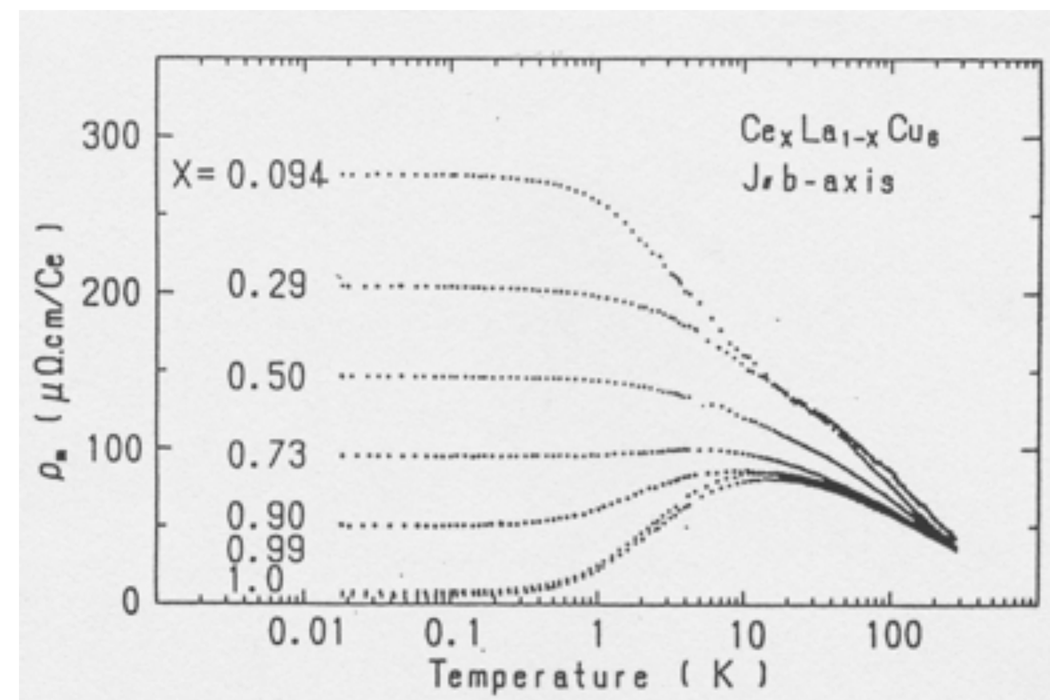
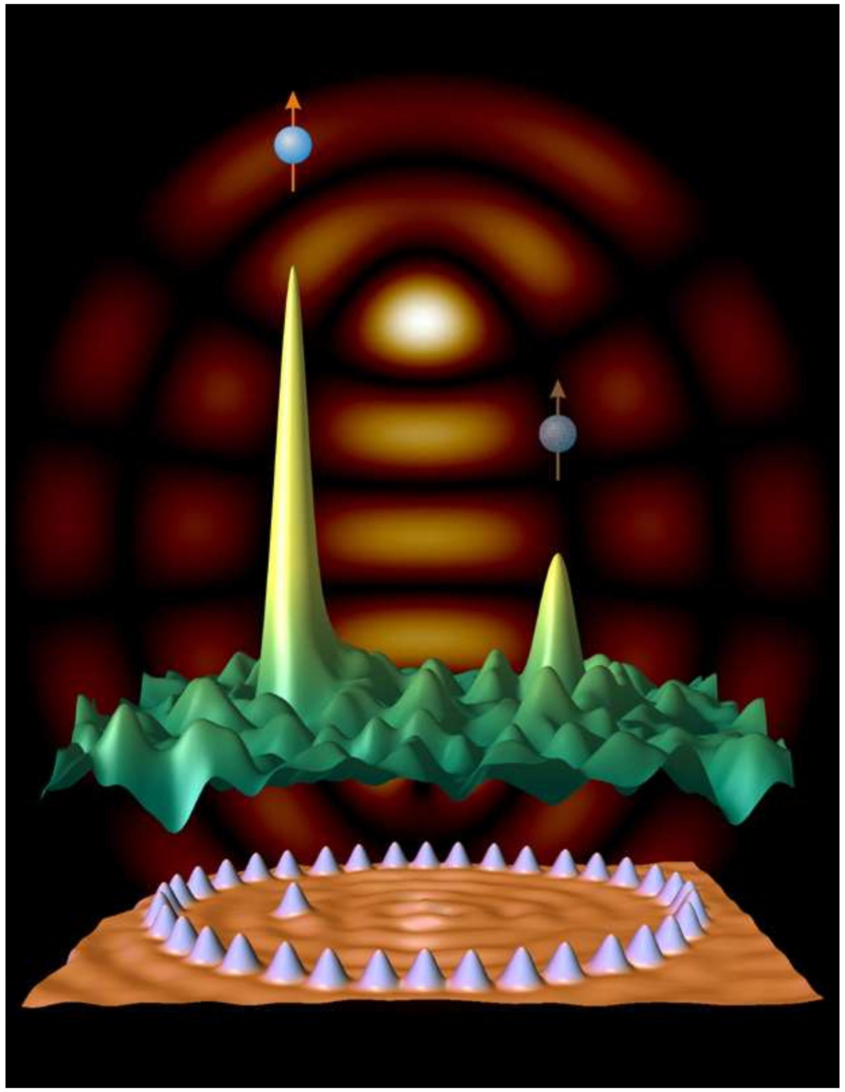


Onuki et al (1987)

Kondo model: drosophila of solid state theory

Quantum-Mirage:
Co on Cu



Manoharan et al,
Nature 403, 512 (2000)

experimental evidence

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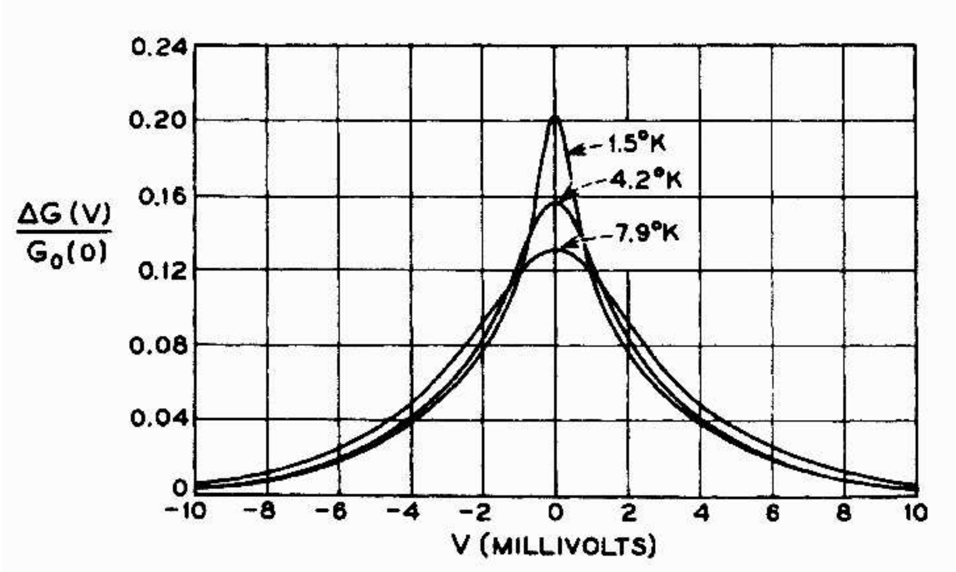

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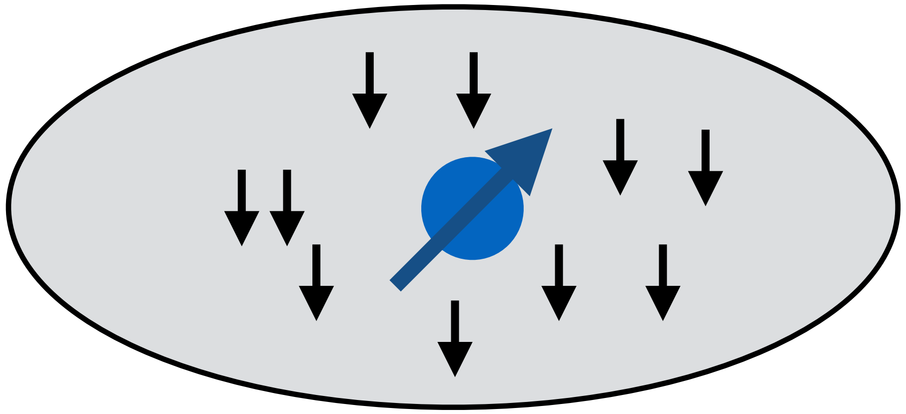
Kondo model: drosophila of solid state theory

T=∞: free spin

K. Wilson, RMP 1975

Kondo model: drosophila of solid state theory

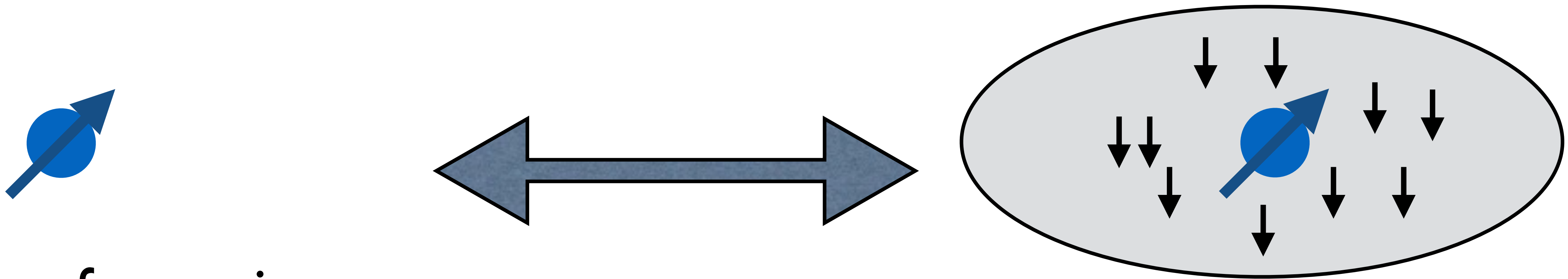
T=∞: free spin



T=0: Kondo singlet

K. Wilson, RMP 1975

Kondo model: drosophila of solid state theory



$T=\infty$: free spin

crossover scale T_K

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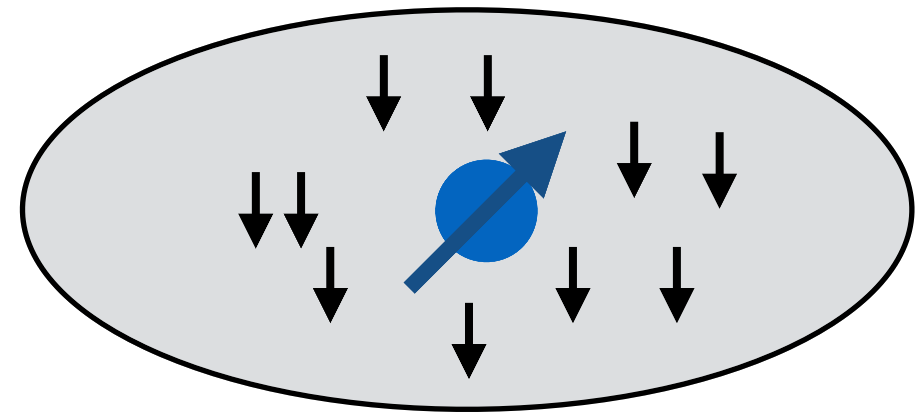

$T=0$: Kondo singlet

two length scales:

K. Wilson, RMP 1975

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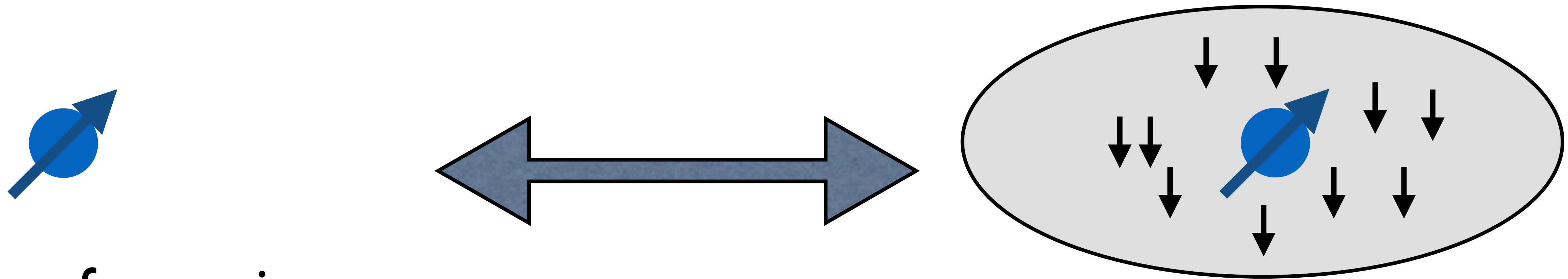


T=∞: free spin

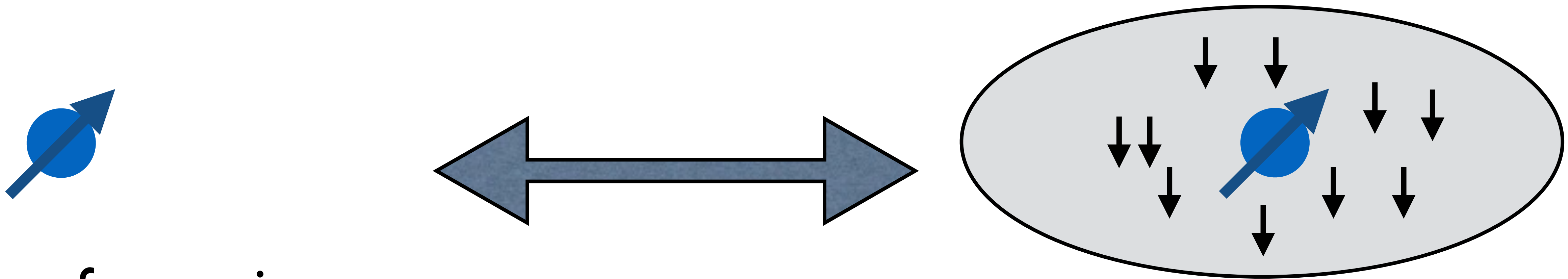
crossover scale T_K

T=0: Kondo singlet

two length scales:

- Fermi wave length : $1/k_F$

Kondo model: drosophila of solid state theory



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ξ_K

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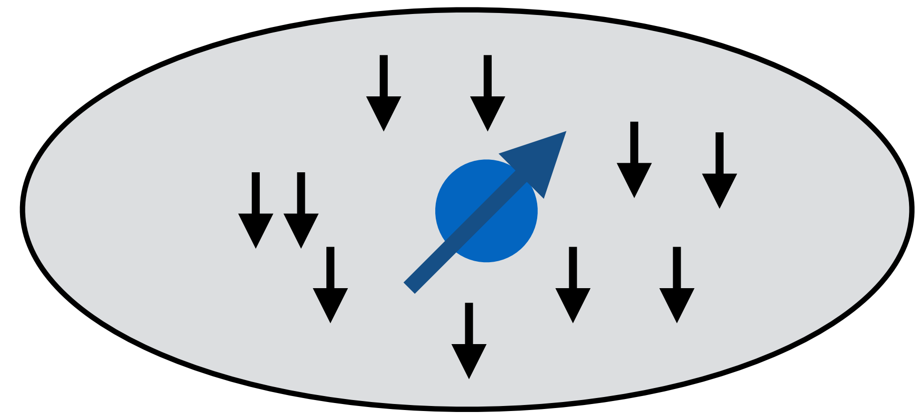

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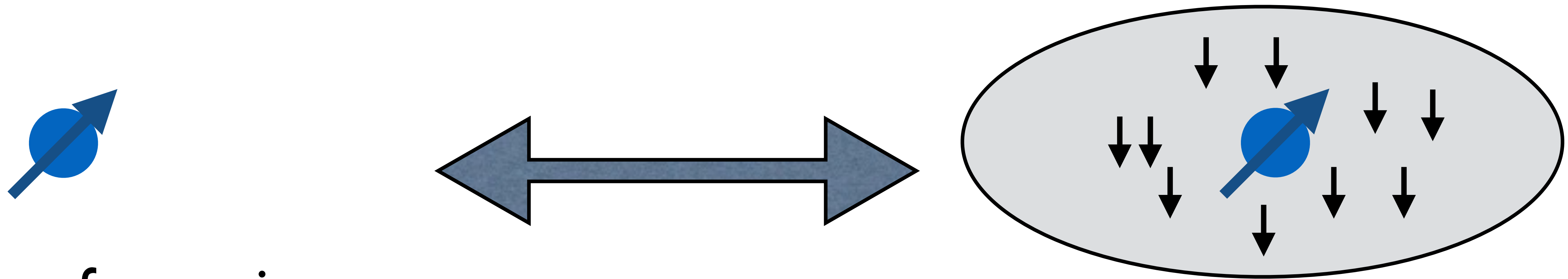

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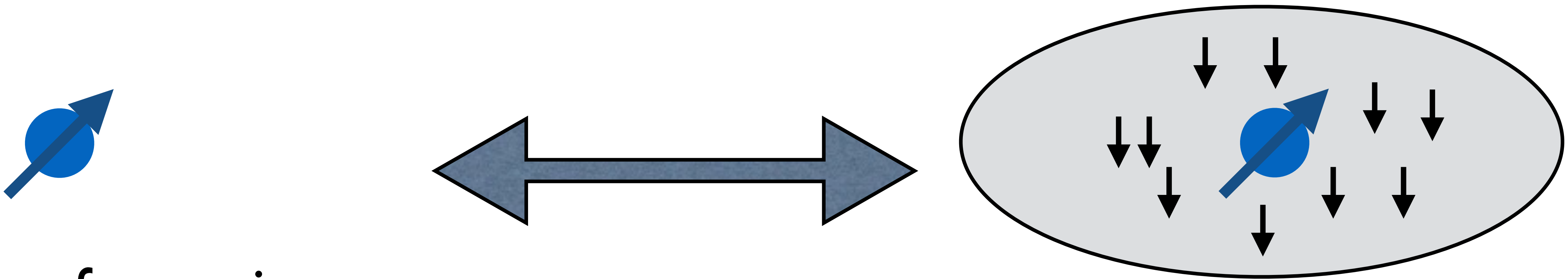

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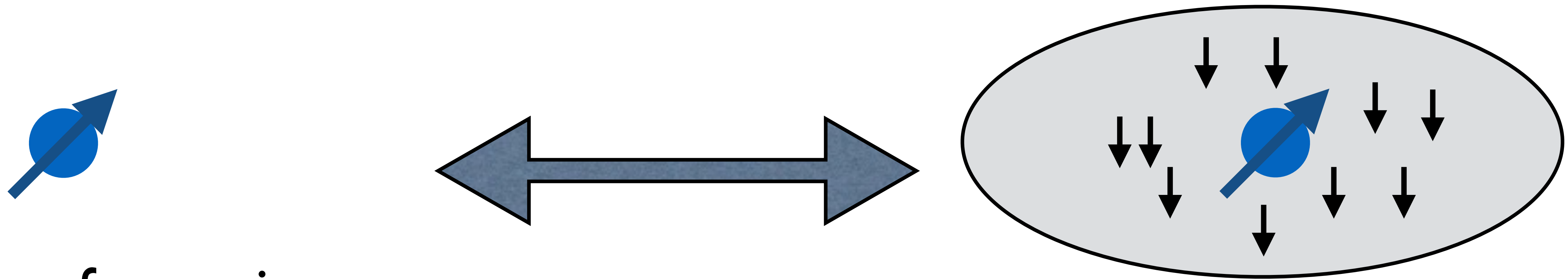

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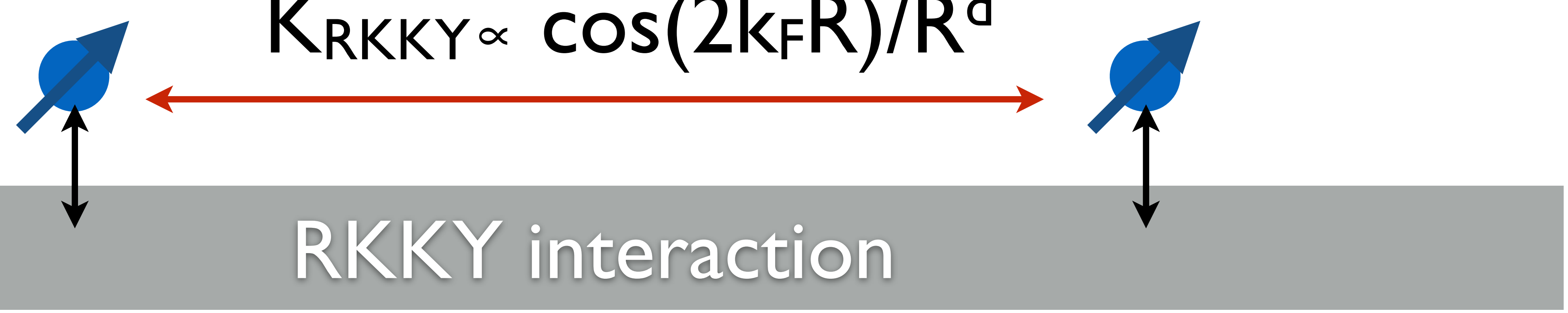
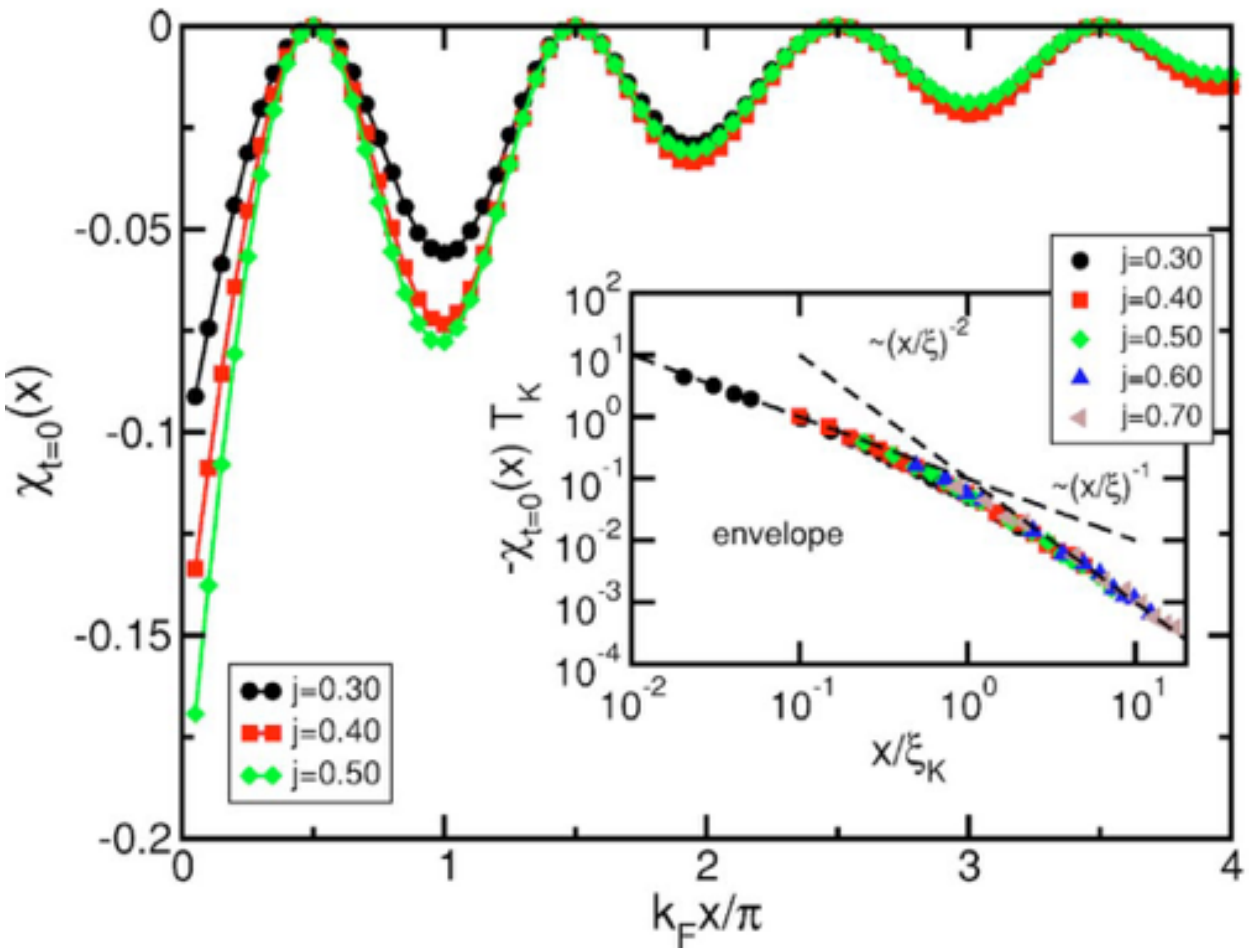
$K_{RKKY} \propto \cos(2k_F R)/R^d$



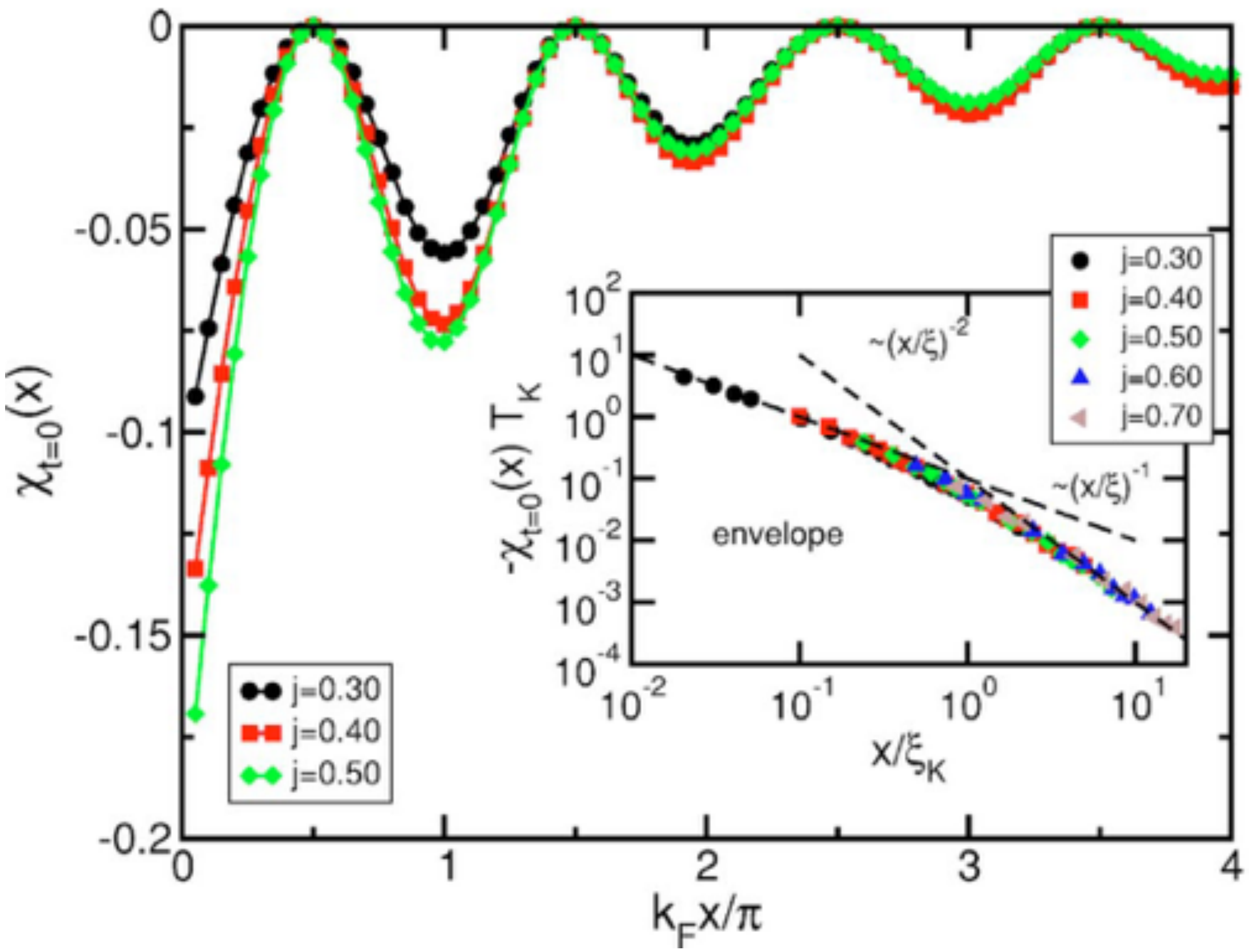
K. Wilson, RMP 1975

spatial correlations in 1D



Borda PRB 2007

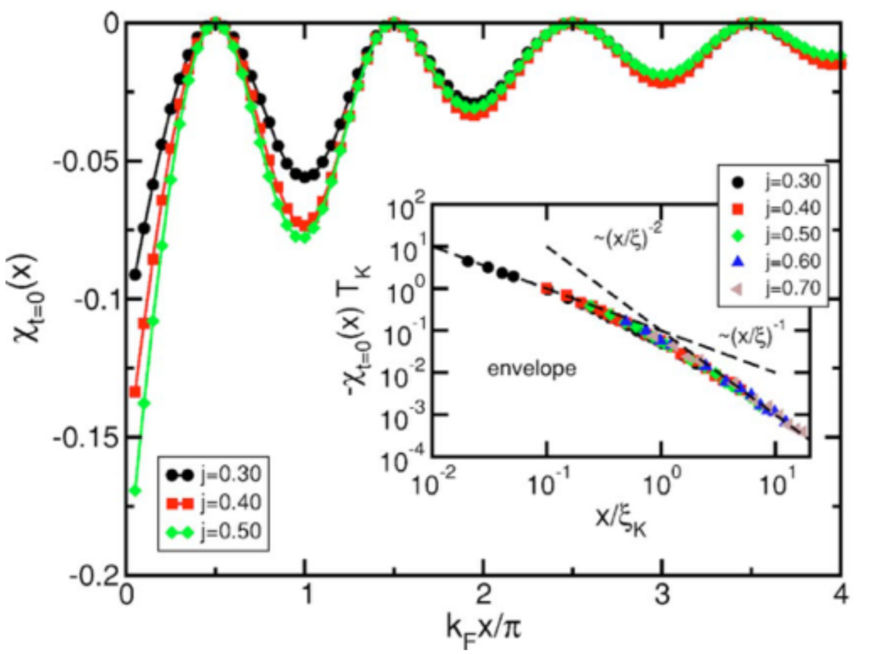
spatial correlations in 1D



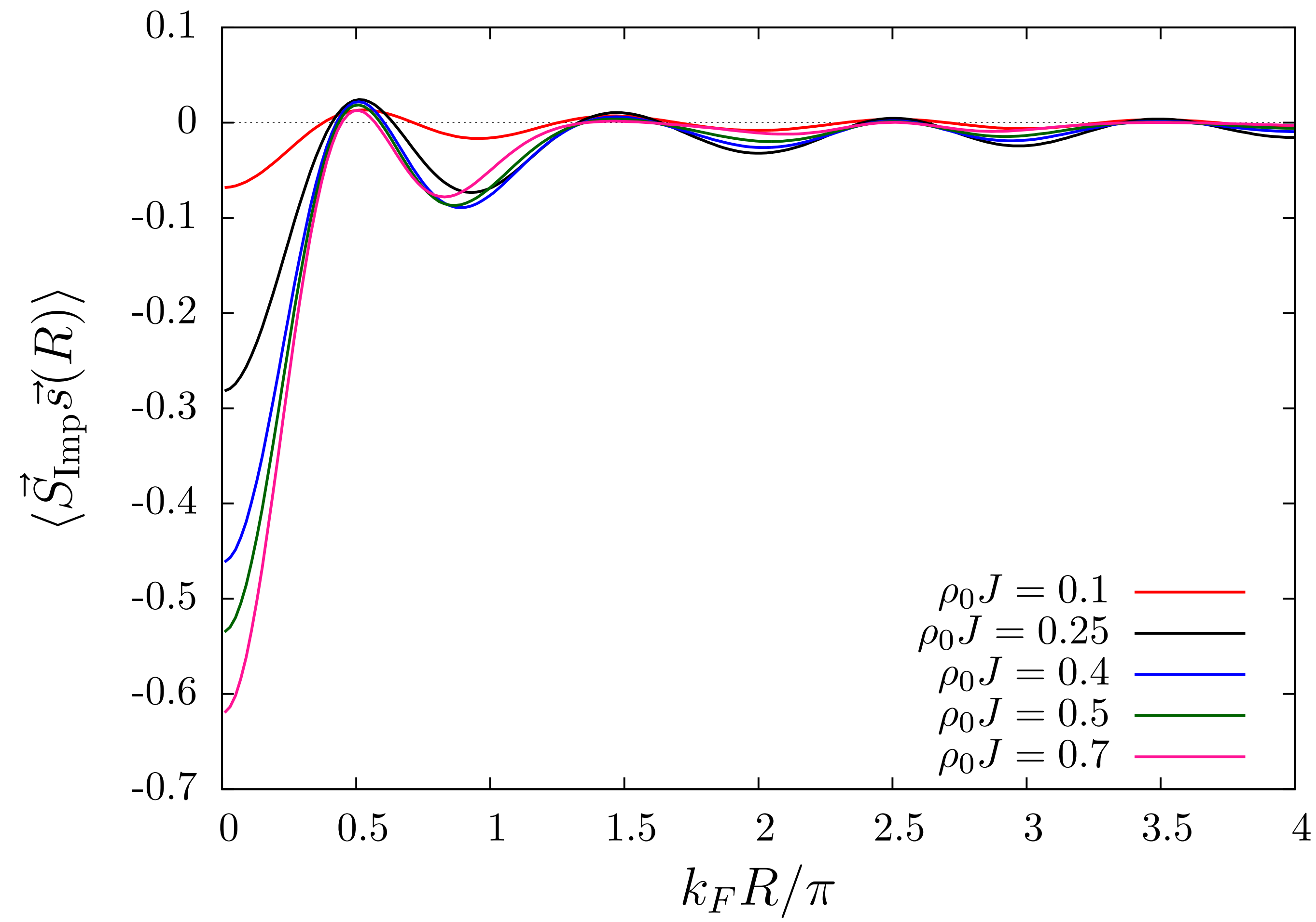
Borda PRB 2007

numerical renormalization group (NRG) calculations

spatial correlations in 1D



Borda PRB 2007



Lechtenberg, FBA, arXiv:1402.1028

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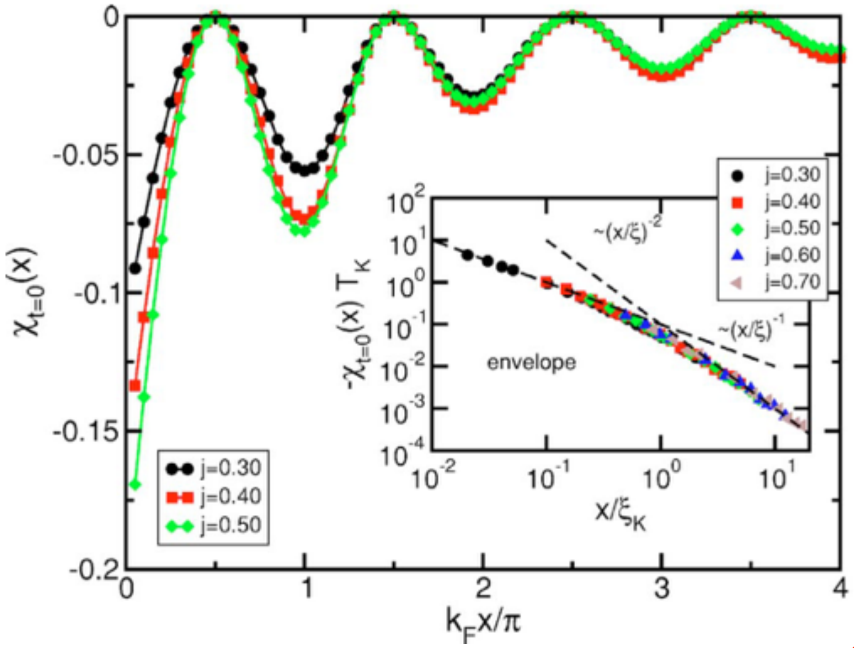
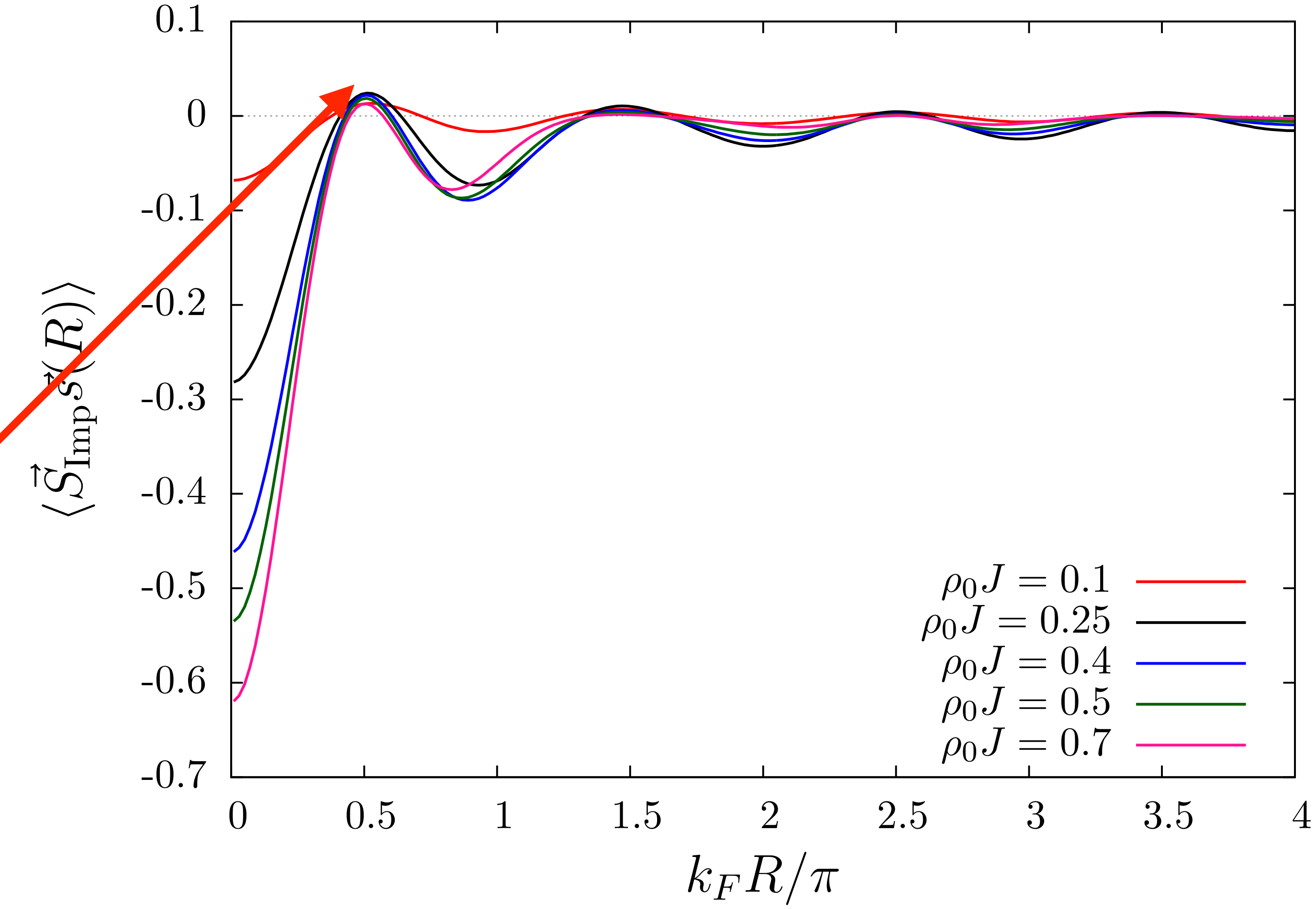


Borda PRB 2007

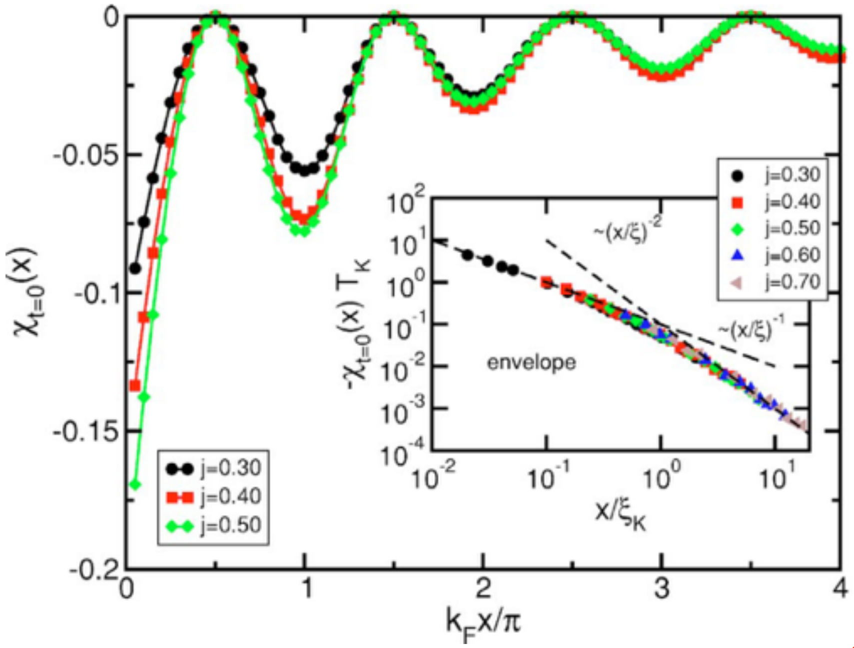


Lechtenberg, FBA, arXiv:1402.1028

- ferro and antiferromagnetic correlations

numerical renormalization group (NRG) calculations

spatial correlations in 1D



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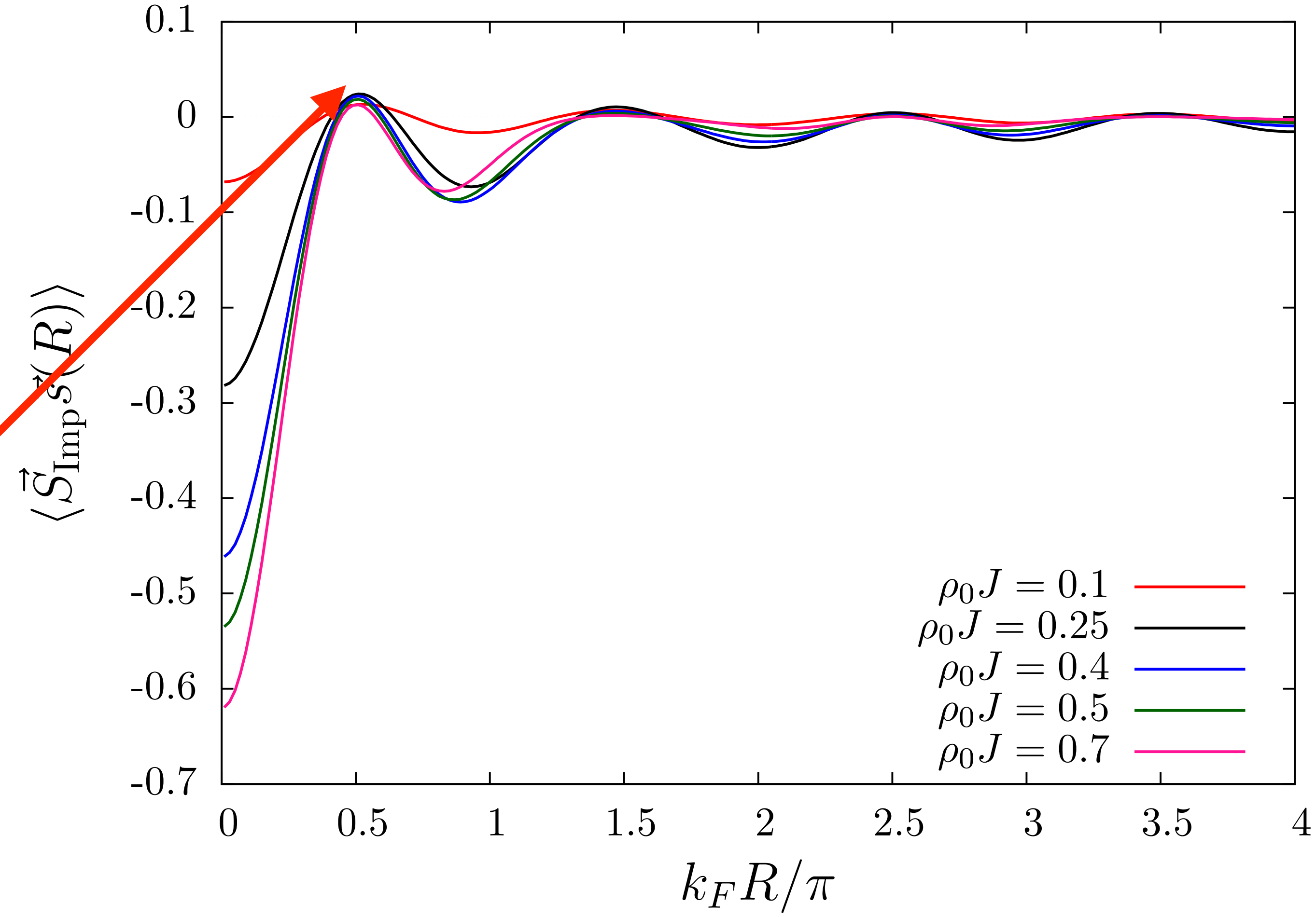
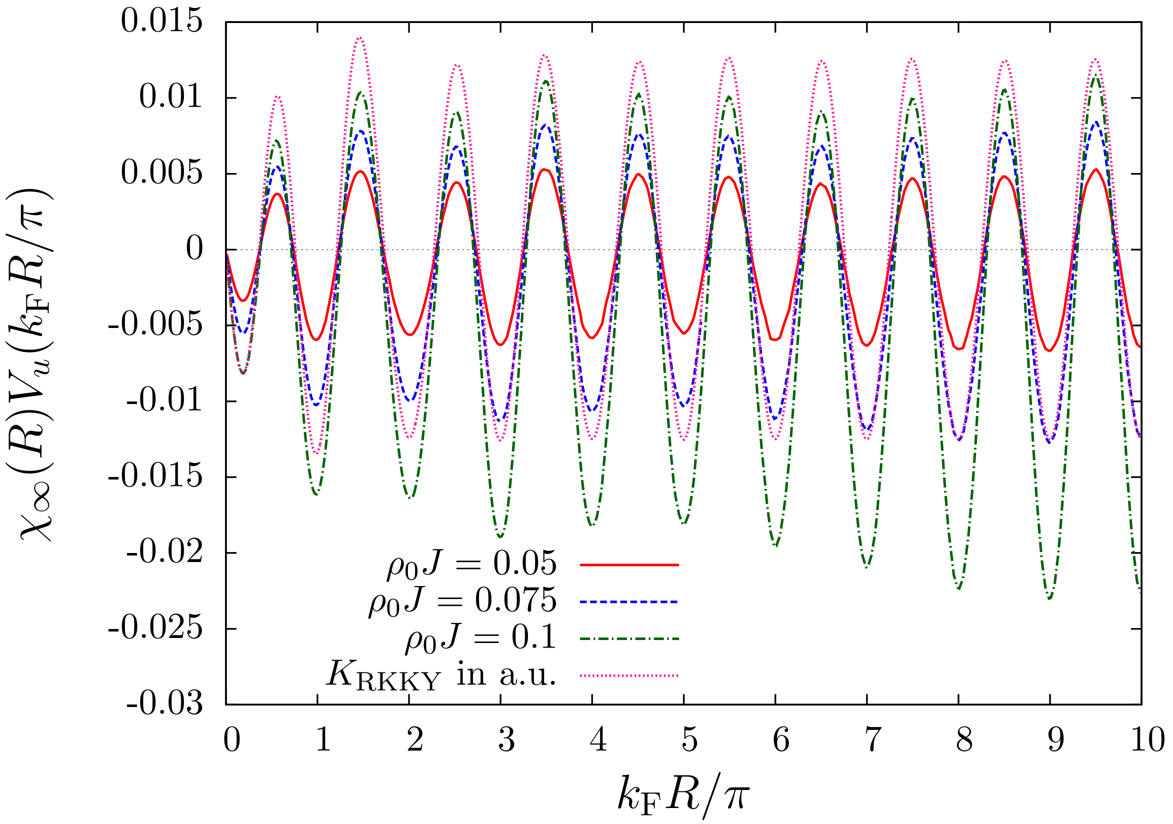


Lechtenberg, FBA, arXiv:1402.1028

- ferro and antiferromagnetic correlations
- exact sum rule: $\int_0^\infty dr r^{d-1} \chi_\infty(R) = -\frac{3}{4}$

numerical renormalization group (NRG) calculations

spatial correlations in 1D

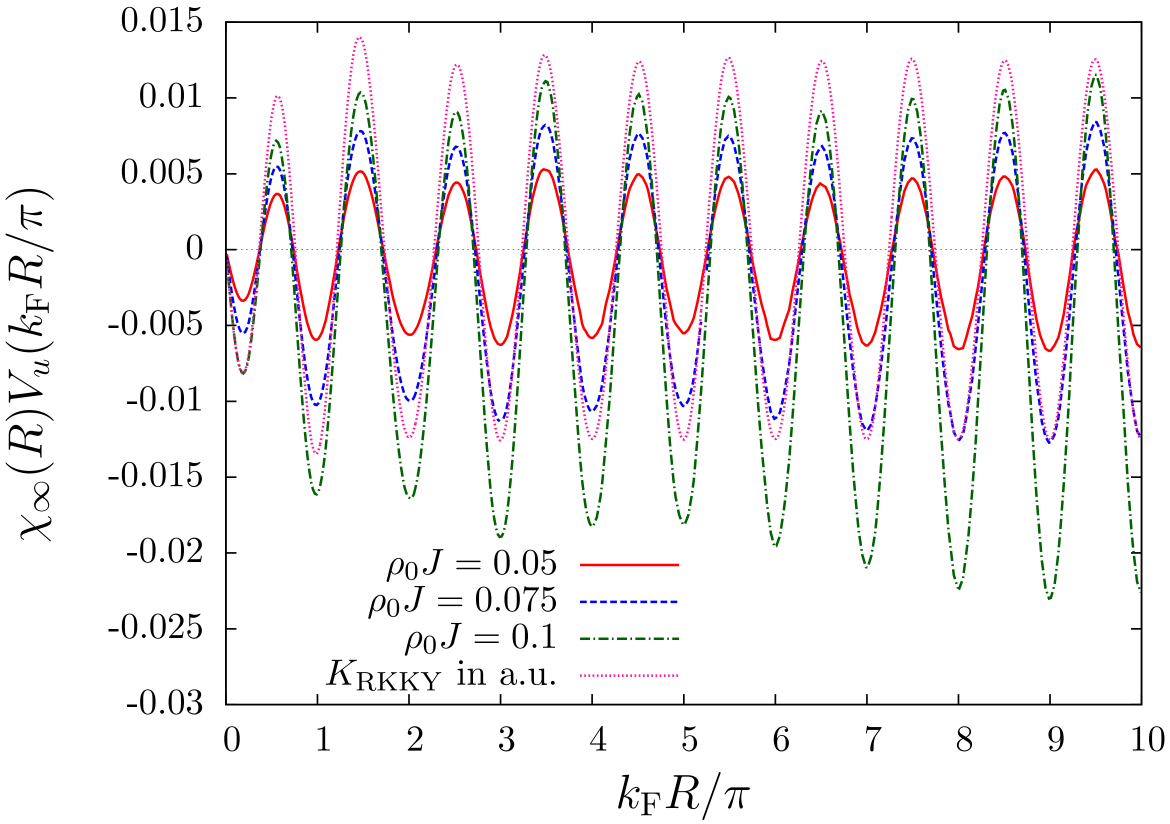


$R < \xi_K$

Affleck et al
Borda 2007

Lechtenberg, FBA, arXiv:1402.1028

spatial correlations in 1D



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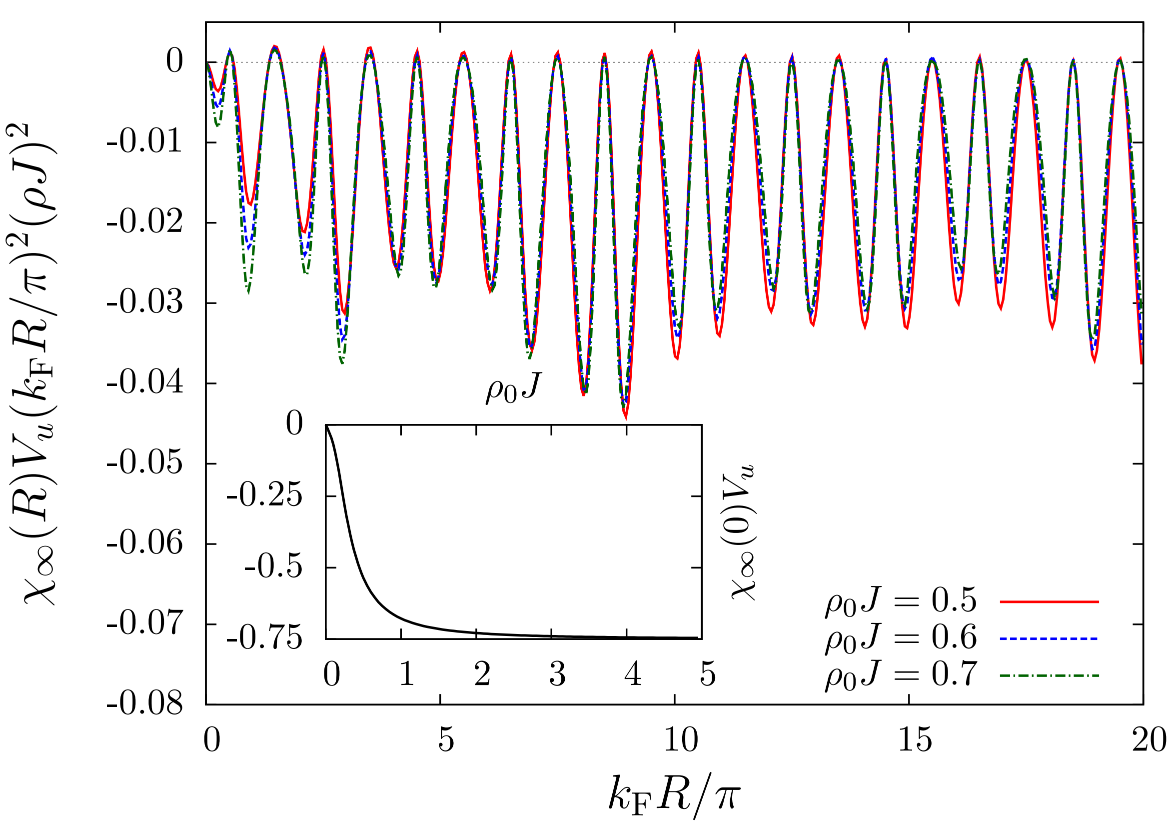

ξ_K<R

Affleck et al
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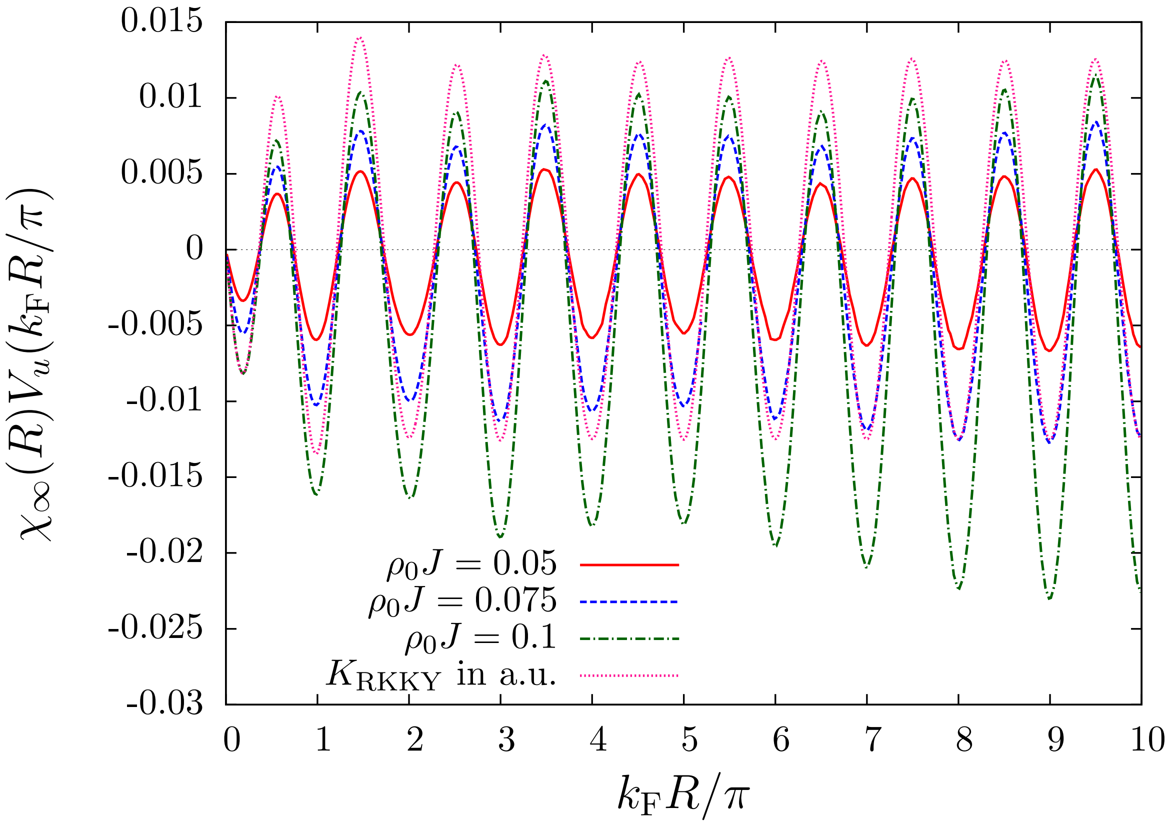
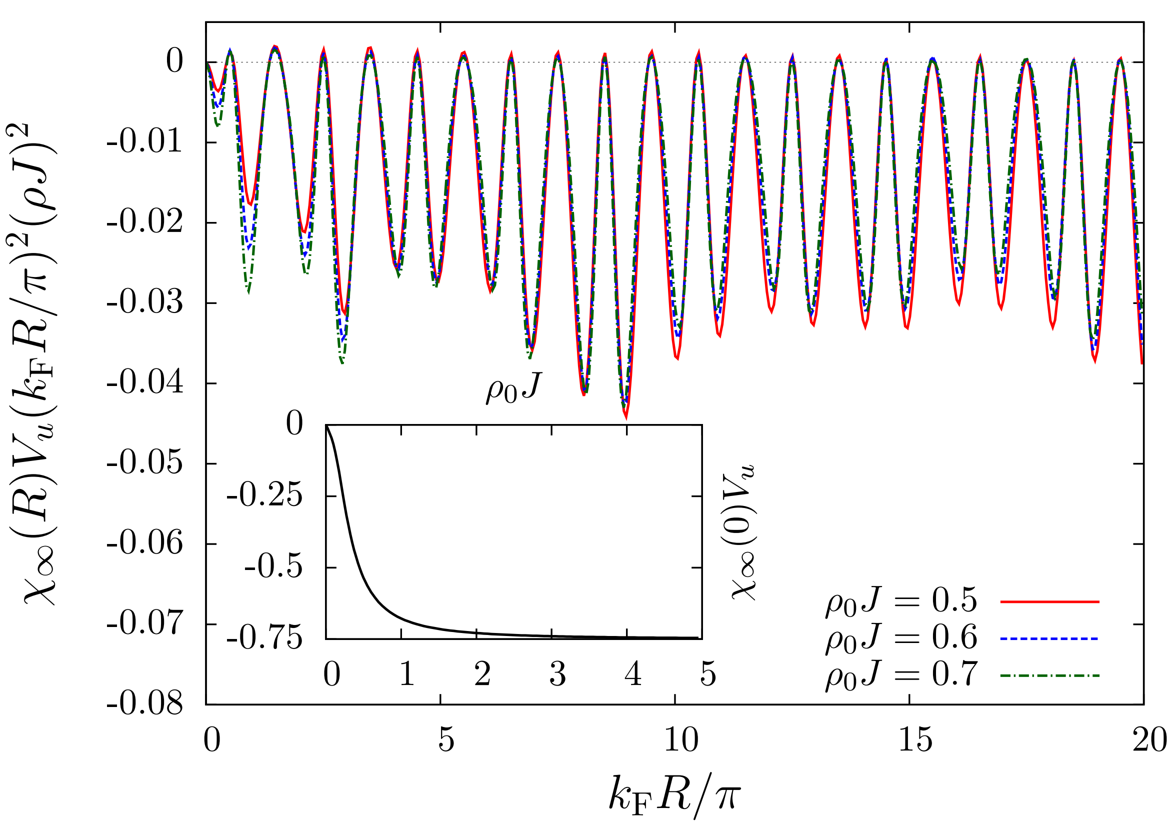
spatial correlations in 1D





$R < \xi_K$

$\xi_K < R$

- crossover from $1/R^d$ to $1/R^{d+1}$ around ξ_K

Affleck et al
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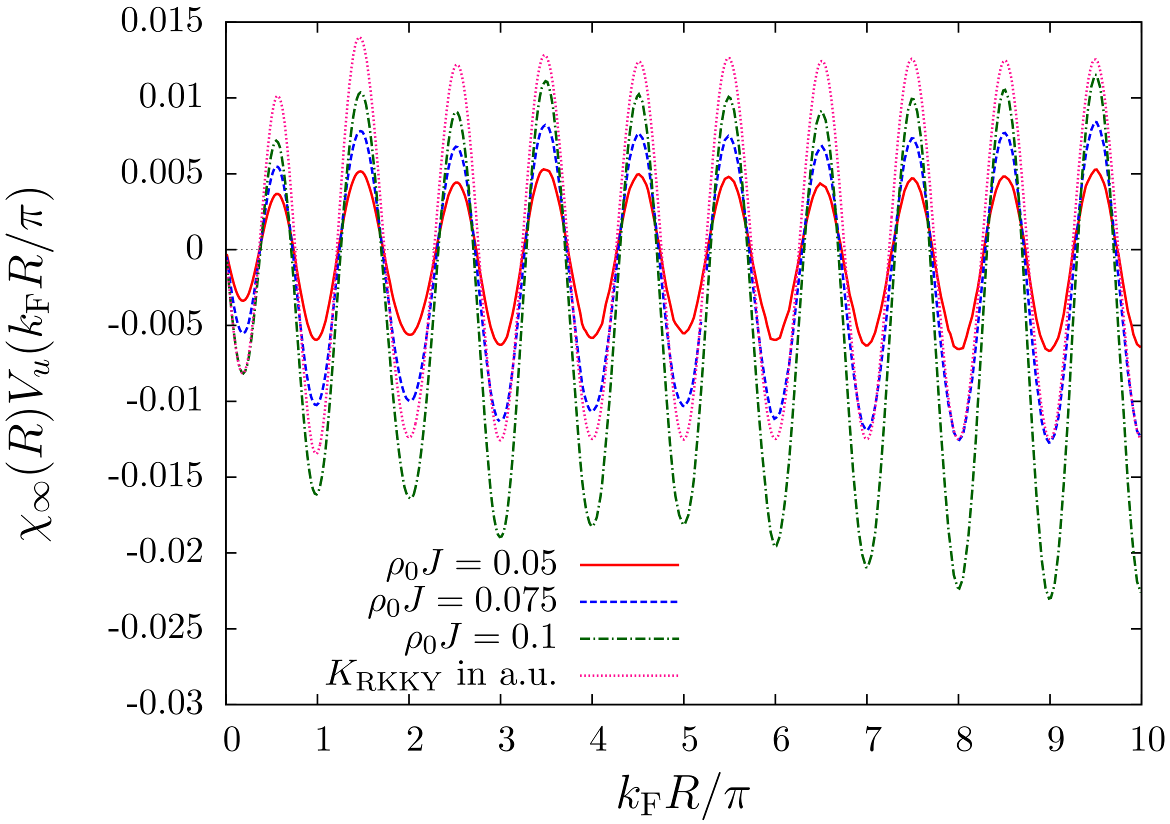
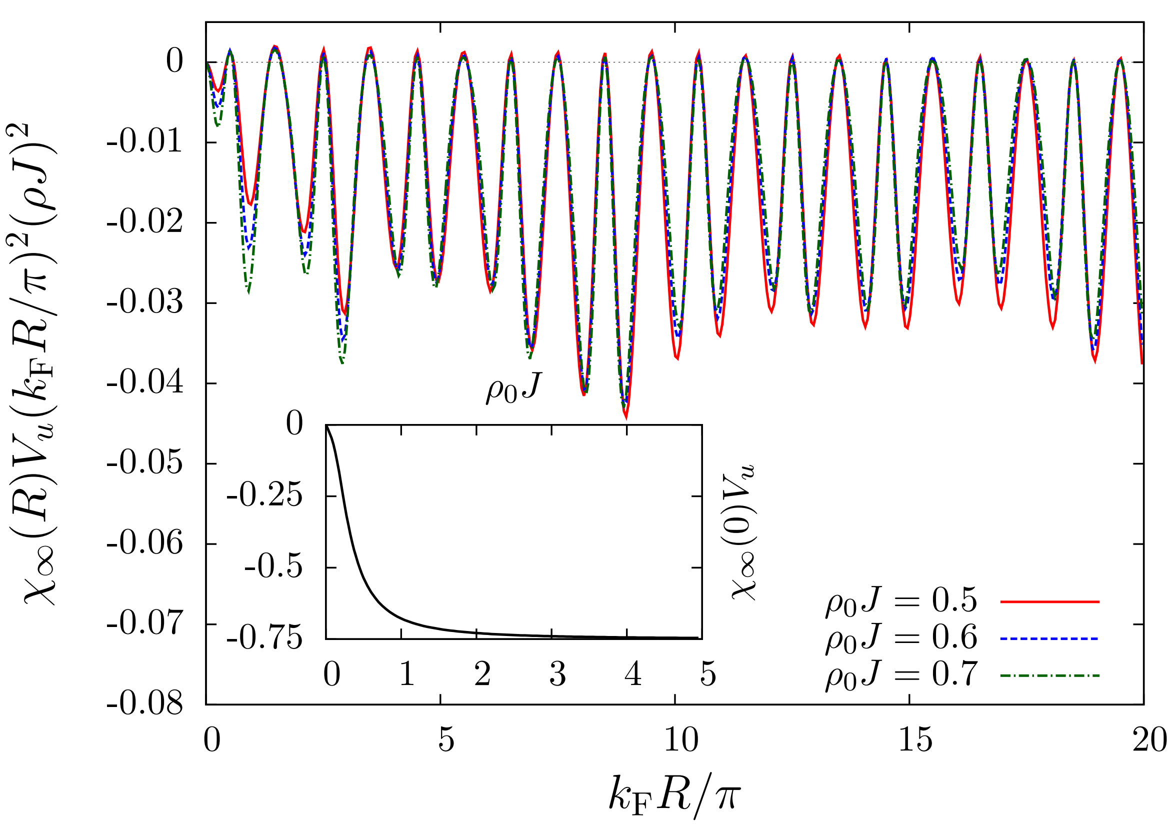
Lechtenberg, FBA, arXiv:1402.1028

spatial correlations in 1D





$R < \xi_K$ $\xi_K < R$

- crossover from $1/R^d$ to $1/R^{d+1}$ around ξ_K
- correlation follow the RKKY interaction

Affleck et al
Borda 2007

Lechtenberg, FBA, arXiv:1402.1028

2. Real-time dynamics in quantum impurity systems

FBA, A. Schiller, PRL **95**, 196801 (2005)
FBA, A. Schiller, PRB **74**, 245113 (2006)

Time-evolution of states

$$i\partial_t|\psi(t)\rangle = H|\psi(t)\rangle$$

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H=const.

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eigenstates of H: $$H|n\rangle = E_n|n\rangle$$

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Can we calculate such a complete basis set?

quantum impurity systems

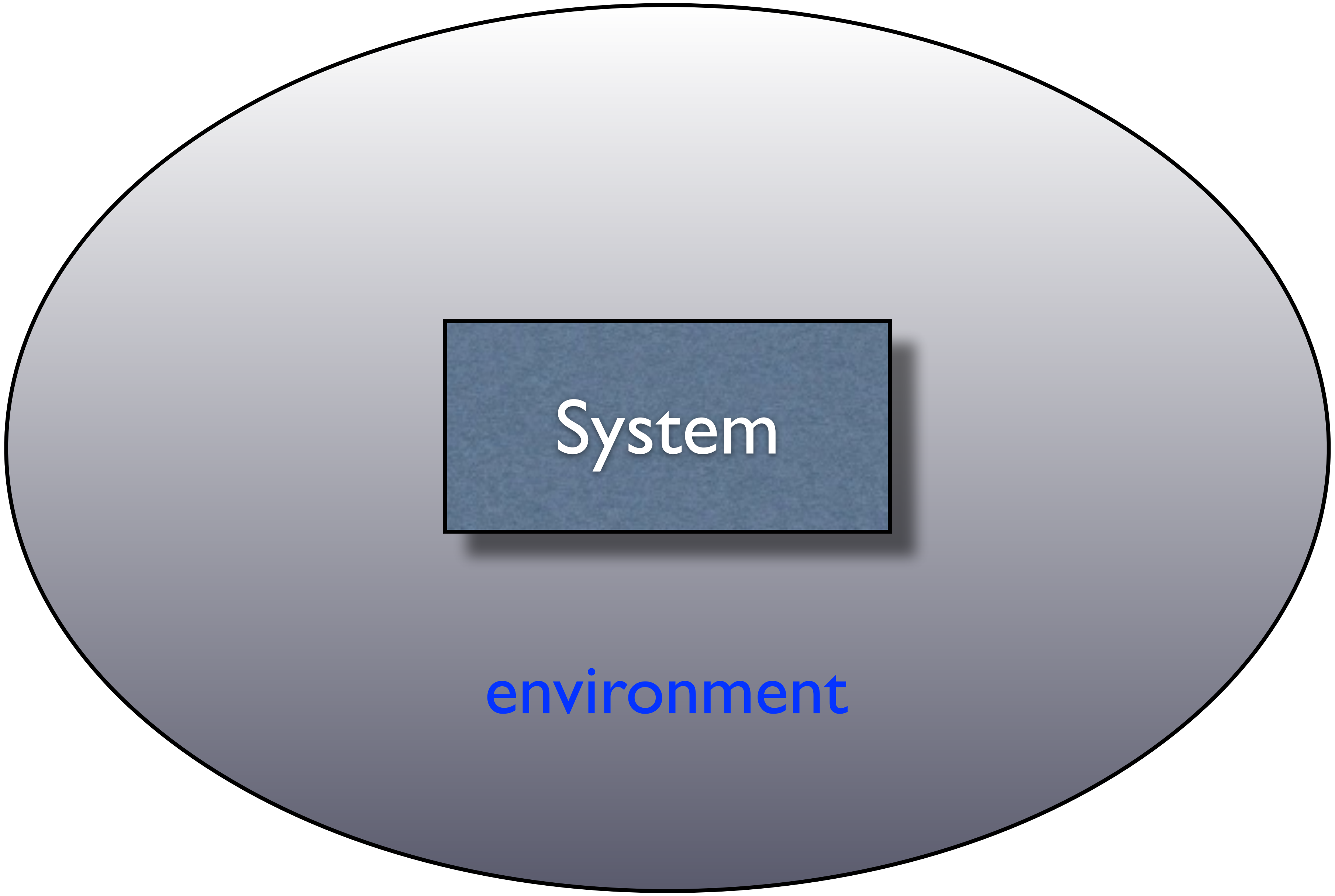
quantum impurity systems

system:

- small
- finite number of DOF

Non-equilibrium dynamics

quantum impurity systems



system:

- small
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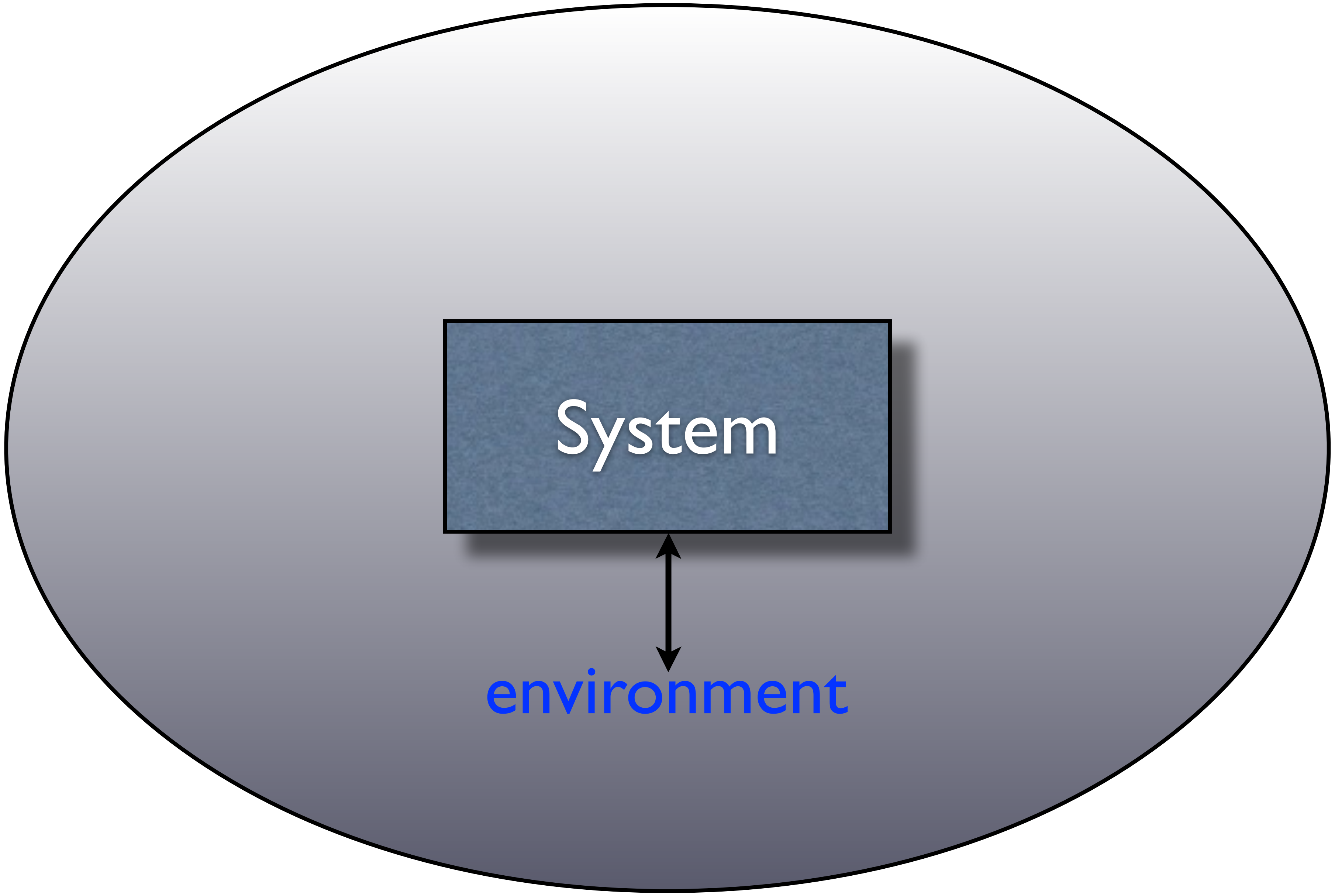
environment:

- infinitely large
- Bosonic or Fermionic baths

quantum impurity systems



system:

- small
- finite number of DOF

environment:

- infinitely large
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coupling between system and bath:

- entanglement
- Kondo effect
- decoherence

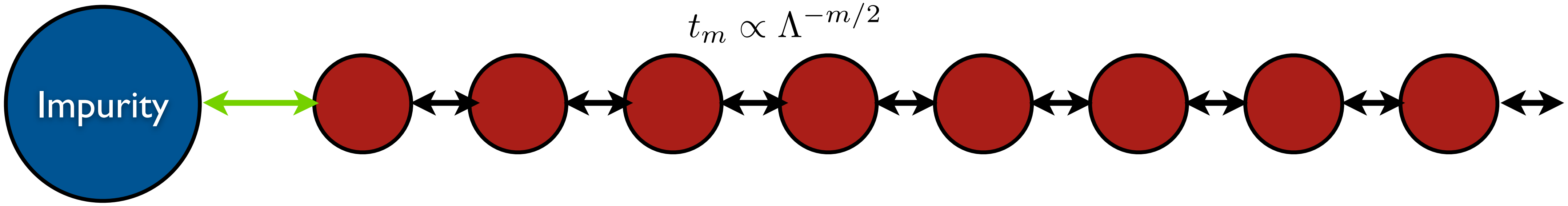
Wilson's numerical renormalisation group

Wilson's numerical renormalisation group

quantum impurity model

- impurity coupled to a energy-continuum

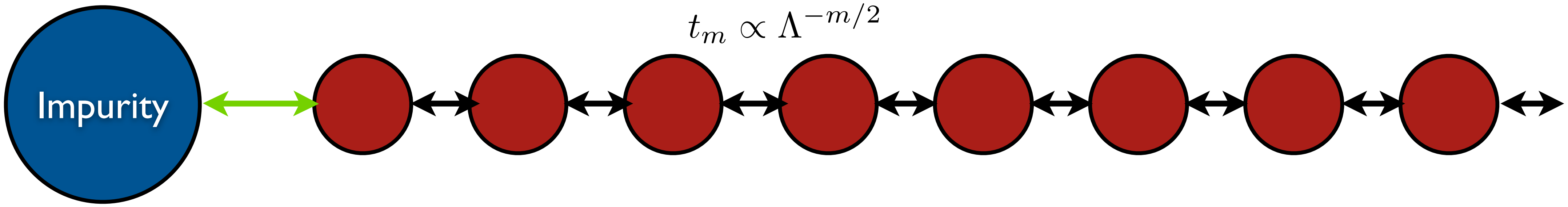
Wilson's numerical renormalisation group



reason: Kondo logarithm contribute equal at each interval

$$I_n = \int_{\Lambda^{-(n+1)}}^{\Lambda^{-n}} \frac{d\varepsilon}{\varepsilon} = \log(\Lambda)$$

Wilson's numerical renormalisation group



- discretization of the energy-continuum

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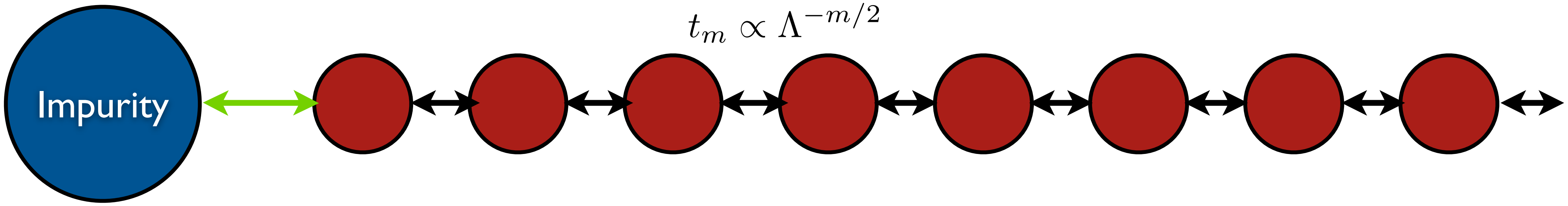
Wilson's numerical renormalisation group

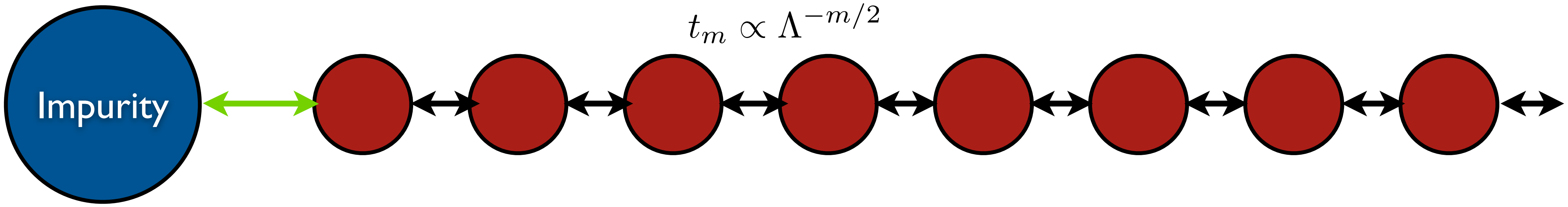


- discretization of the energy-continuum
- separation of energy scales: $t_m \propto \Lambda^{-m/2}$

reason: Kondo logarithm contribute equal at each interval

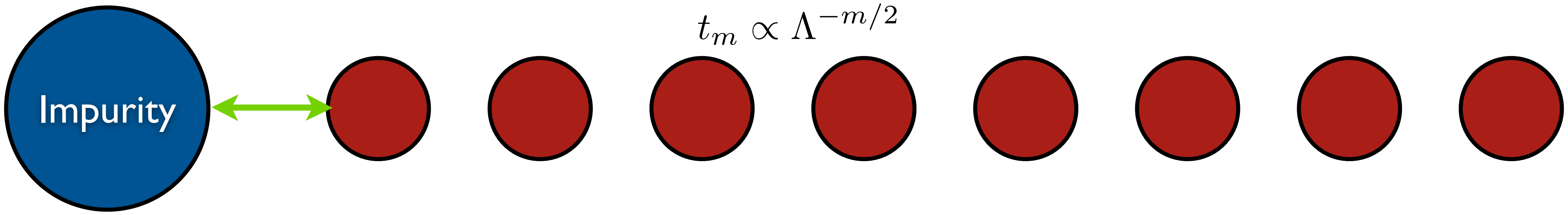
$$I_n = \int_{\Lambda^{-(n+1)}}^{\Lambda^{-n}} \frac{d\varepsilon}{\varepsilon} = \log(\Lambda)$$

Wilson's numerical renormalisation group

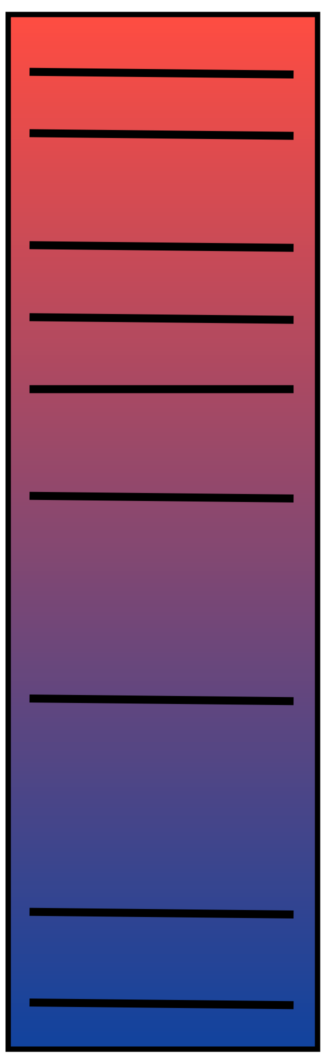


iterative diagonalization

Wilson's numerical renormalisation group



iterative diagonalization: approx. eigenbasis



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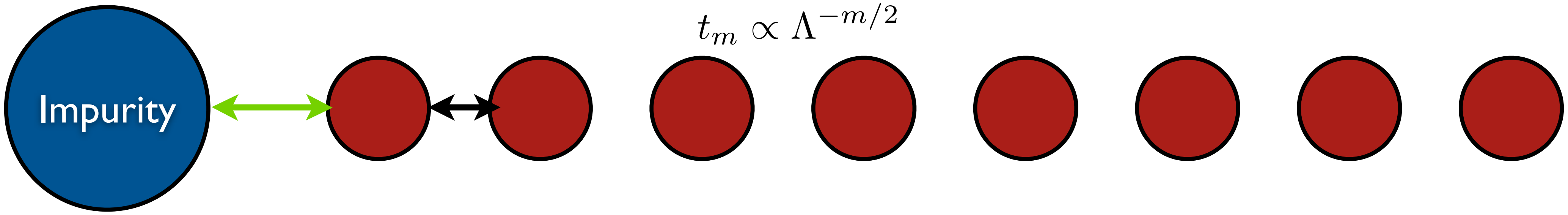

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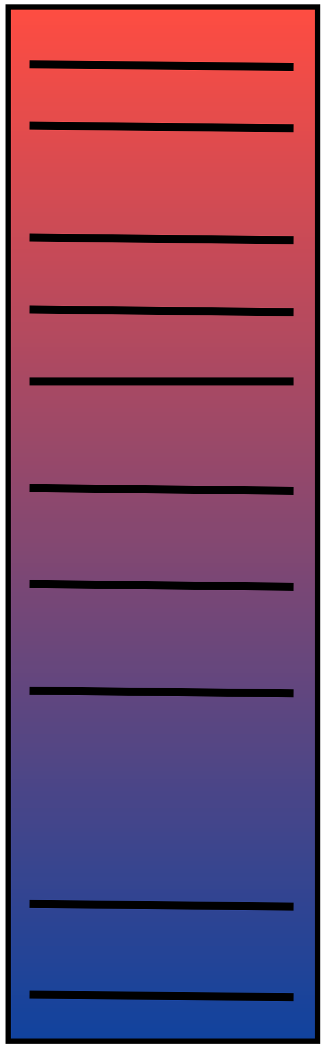

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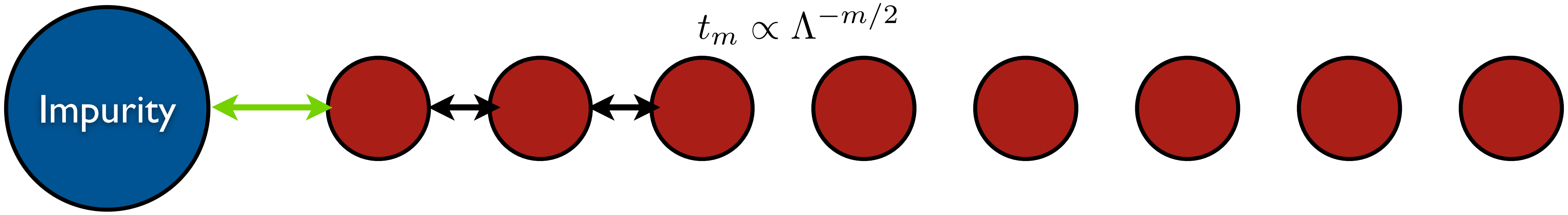

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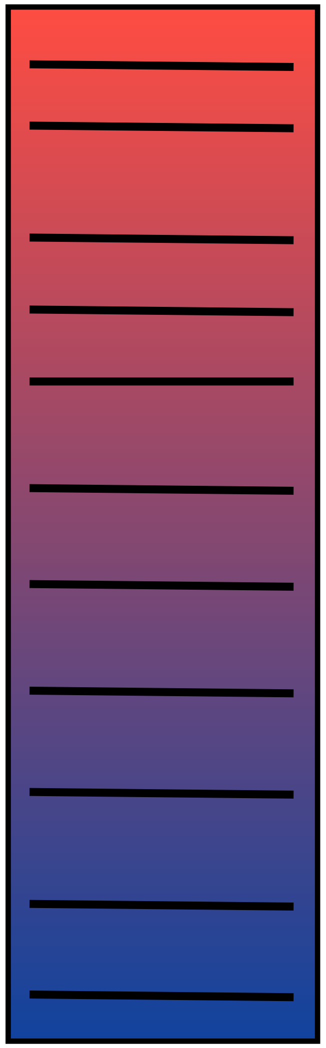

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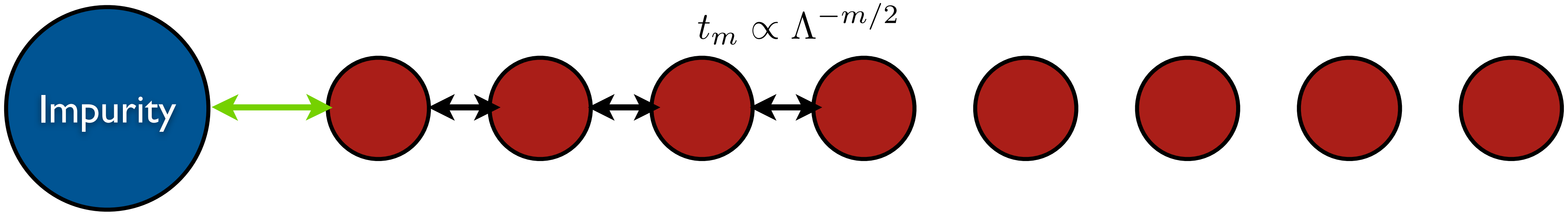

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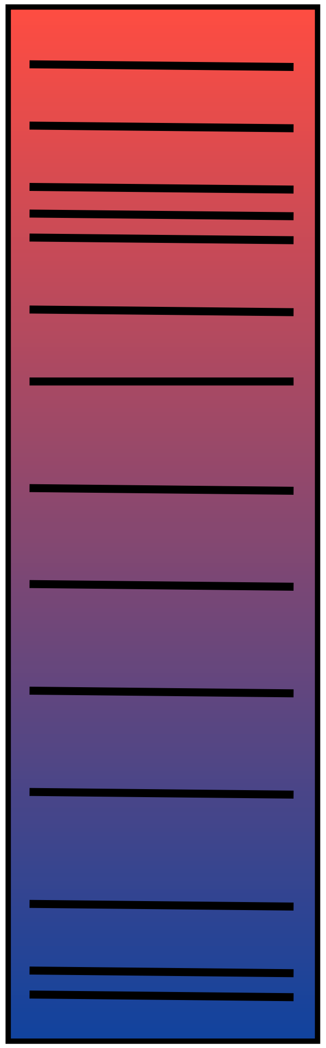

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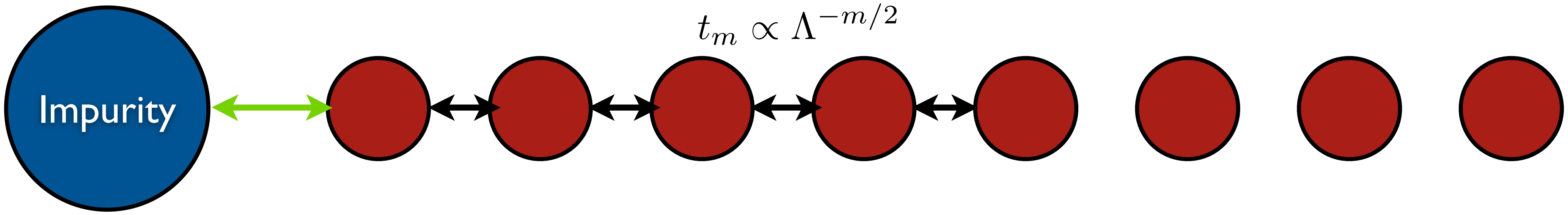

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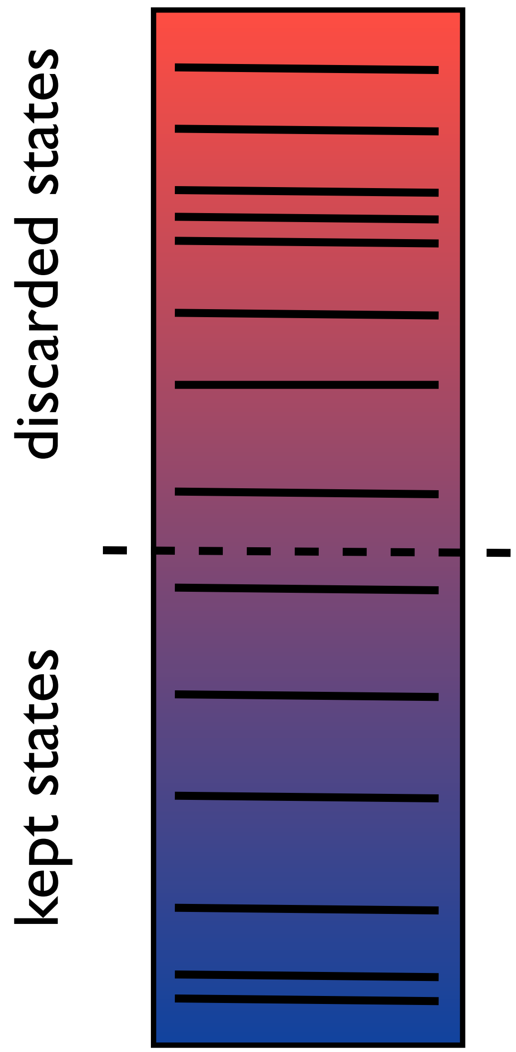

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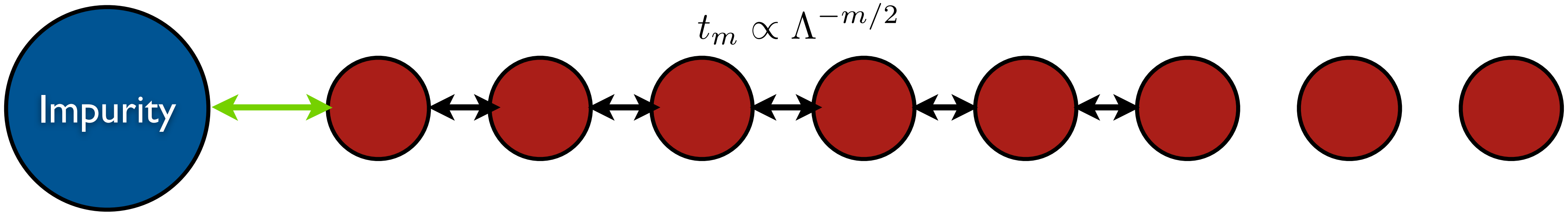

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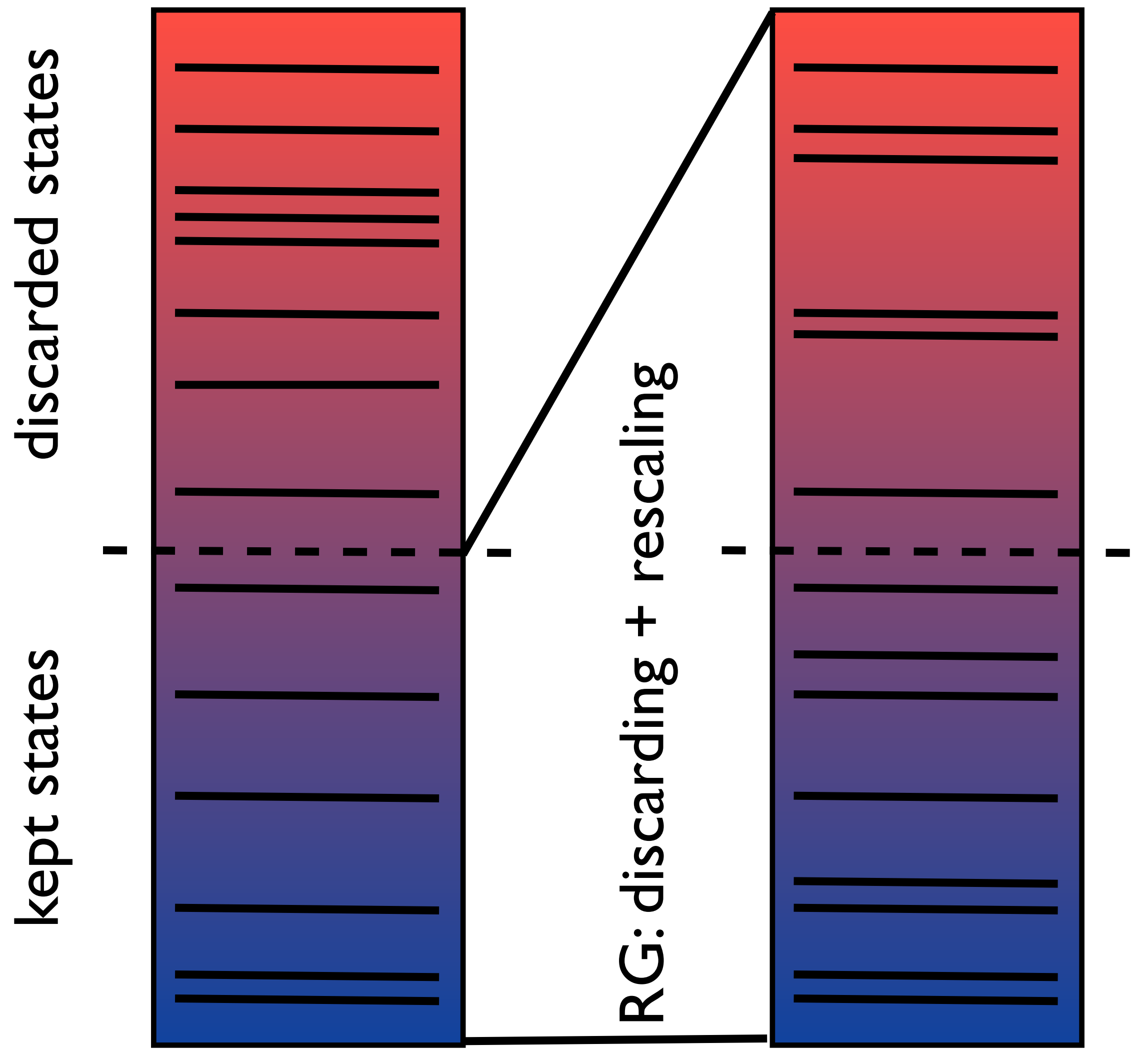

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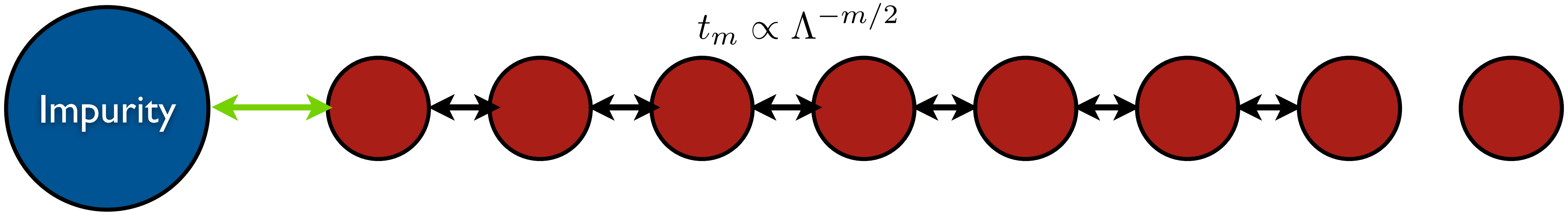

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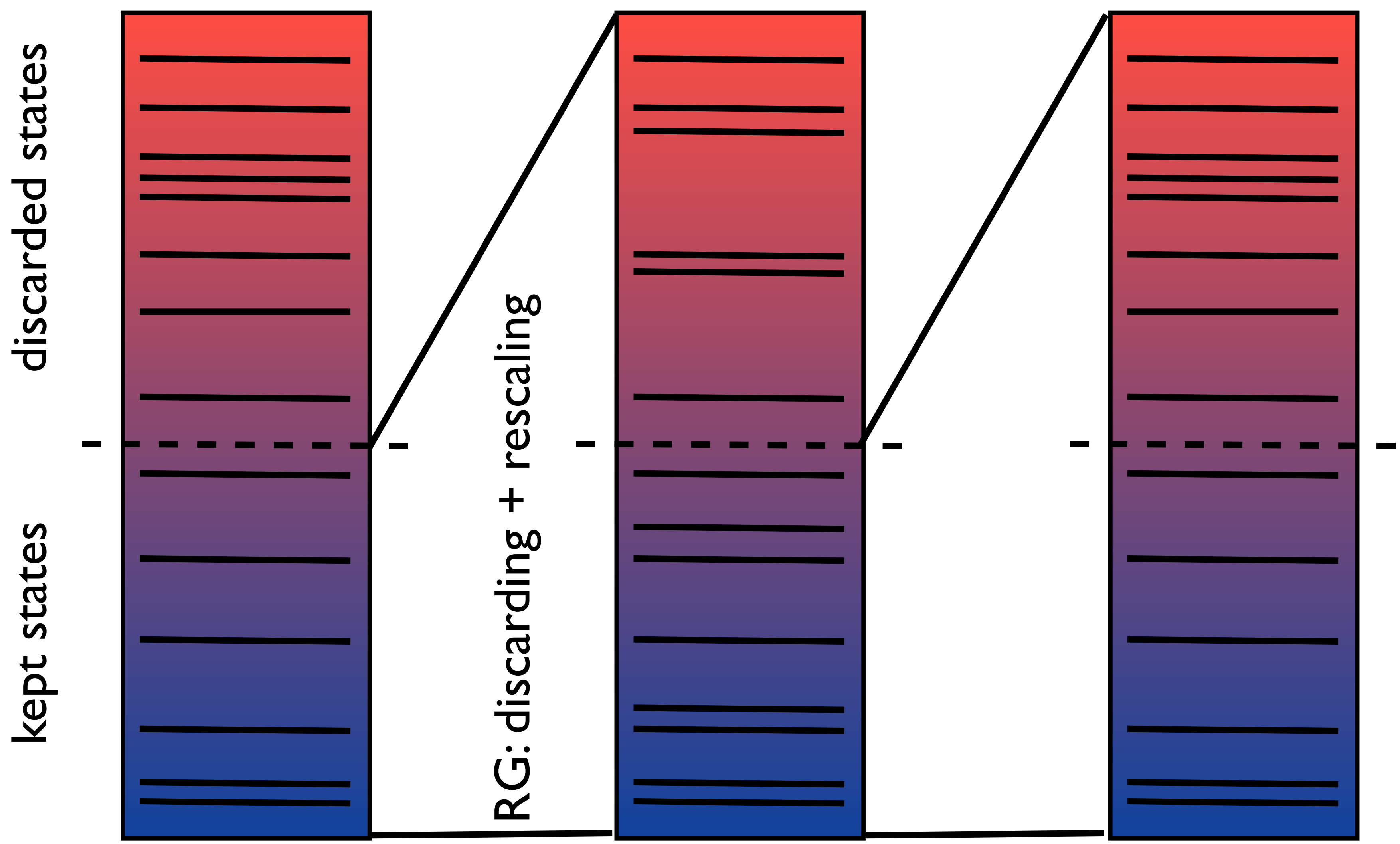

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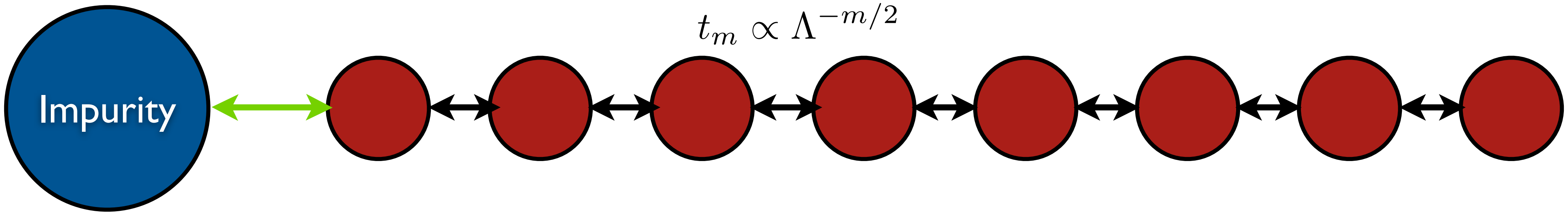

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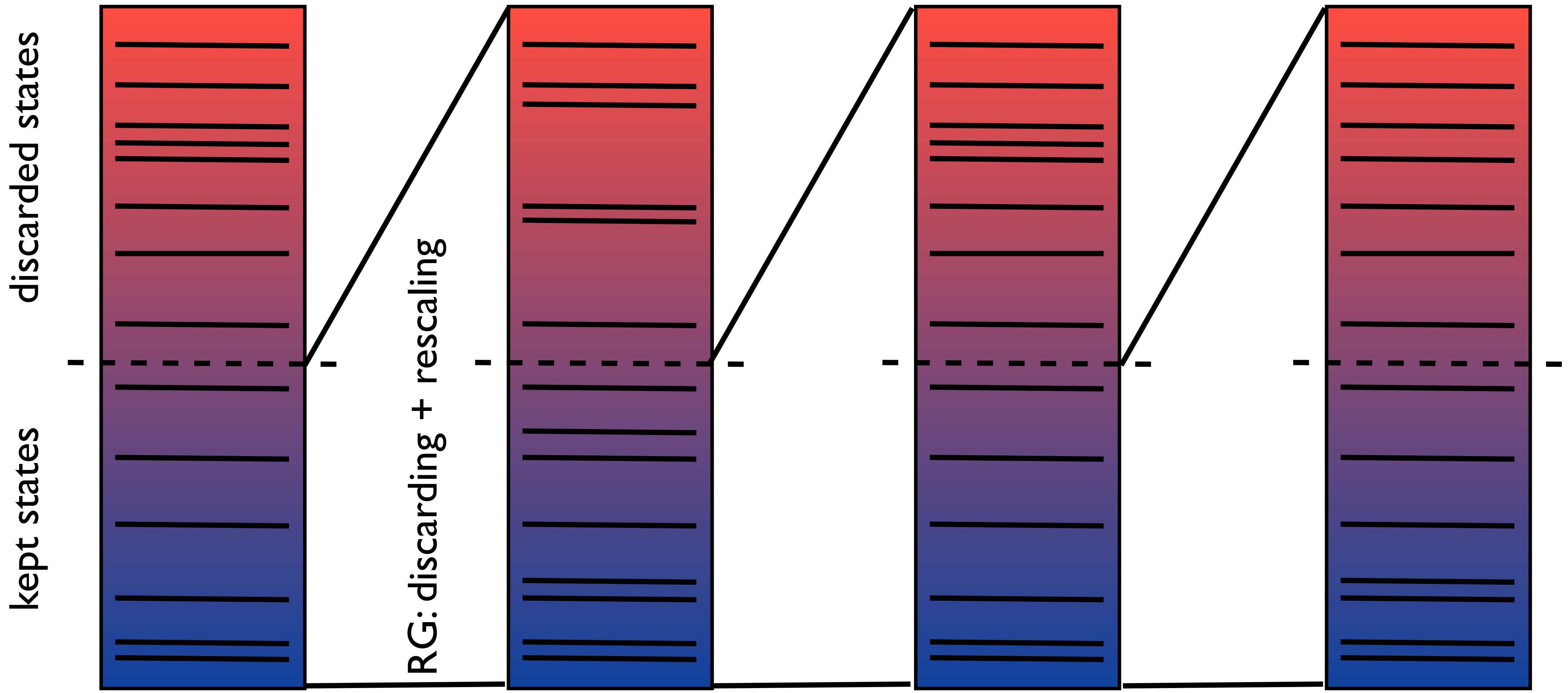

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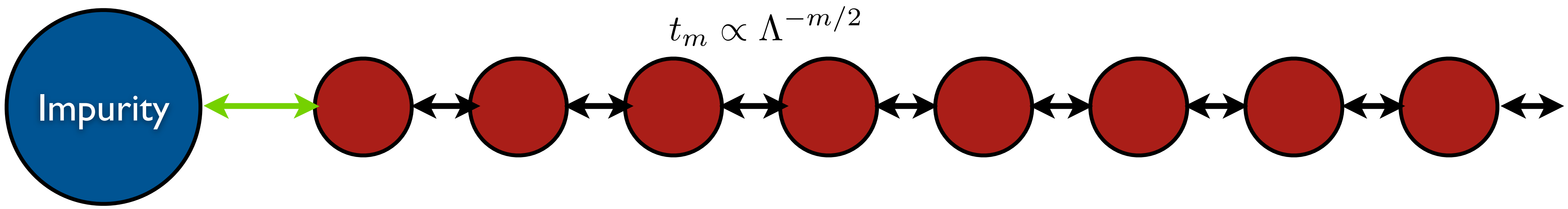

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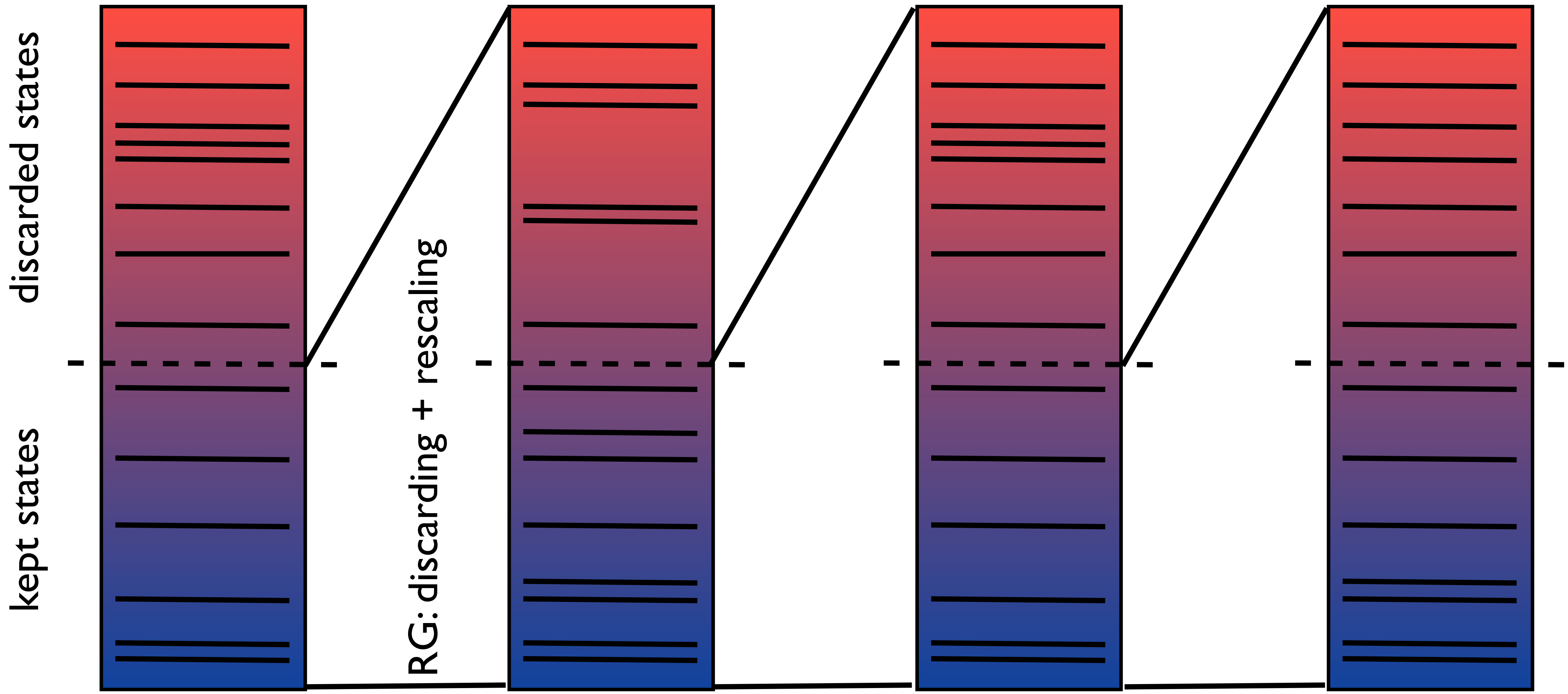

complete basis set

FBA, A. Schiller, PRL **95**, 196801 (2005)
FBA, A. Schiller, PRB **74**, 245113 (2006)

the sum of all discarded high-energy states in the NRG iteration form

- a complete basis set {|l,e;m>}

$$\hat{1} = \sum_m^N \sum_l \sum_e |l, e; m\rangle\langle l, e; m|$$

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- an approximate eigenbasis

$$H|l, e; m\rangle \approx E_l |l, e; m\rangle$$

FBA, A. Schiller, PRL **95**, 196801 (2005)
FBA, A. Schiller, PRB **74**, 245113 (2006)

Real-time evolution of observables

$$\langle \hat{O} \rangle(t) = \sum_m \sum_{l,l}^{l \text{ or } l' \text{ discarded}} \langle l|\hat{O}|l'\rangle e^{i(E_l - E_{l'})t} \rho^{red}_{l'l}(m)$$

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reduced density matrix:

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contains information on

- dissipation
- entanglement with the environment

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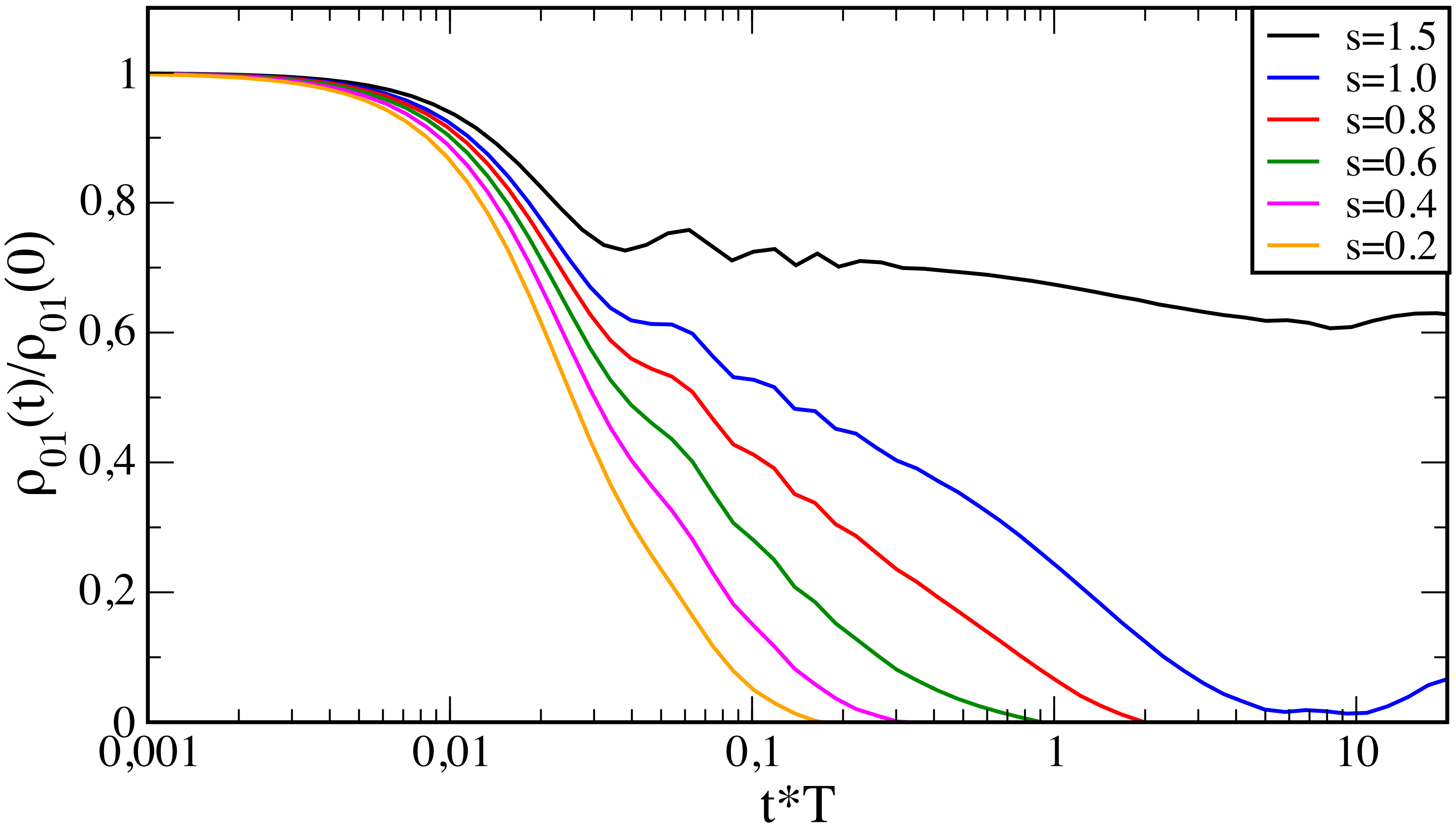
RG concept upside down:
discarded states contain information on the real-time evolution

FBA, A. Schiller, PRL **95**, 196801 (2005)
FBA, A. Schiller, PRB **74**, 245113 (2006)

spin-boson model: decoherence by dephasing

time-dependend NRG



$$H = \frac{\Delta}{2}\sigma_x + \sigma_z \sum_q \lambda_q (b_q^\dagger + b_q) + \sum_q \omega_q b_q^\dagger b_q$$

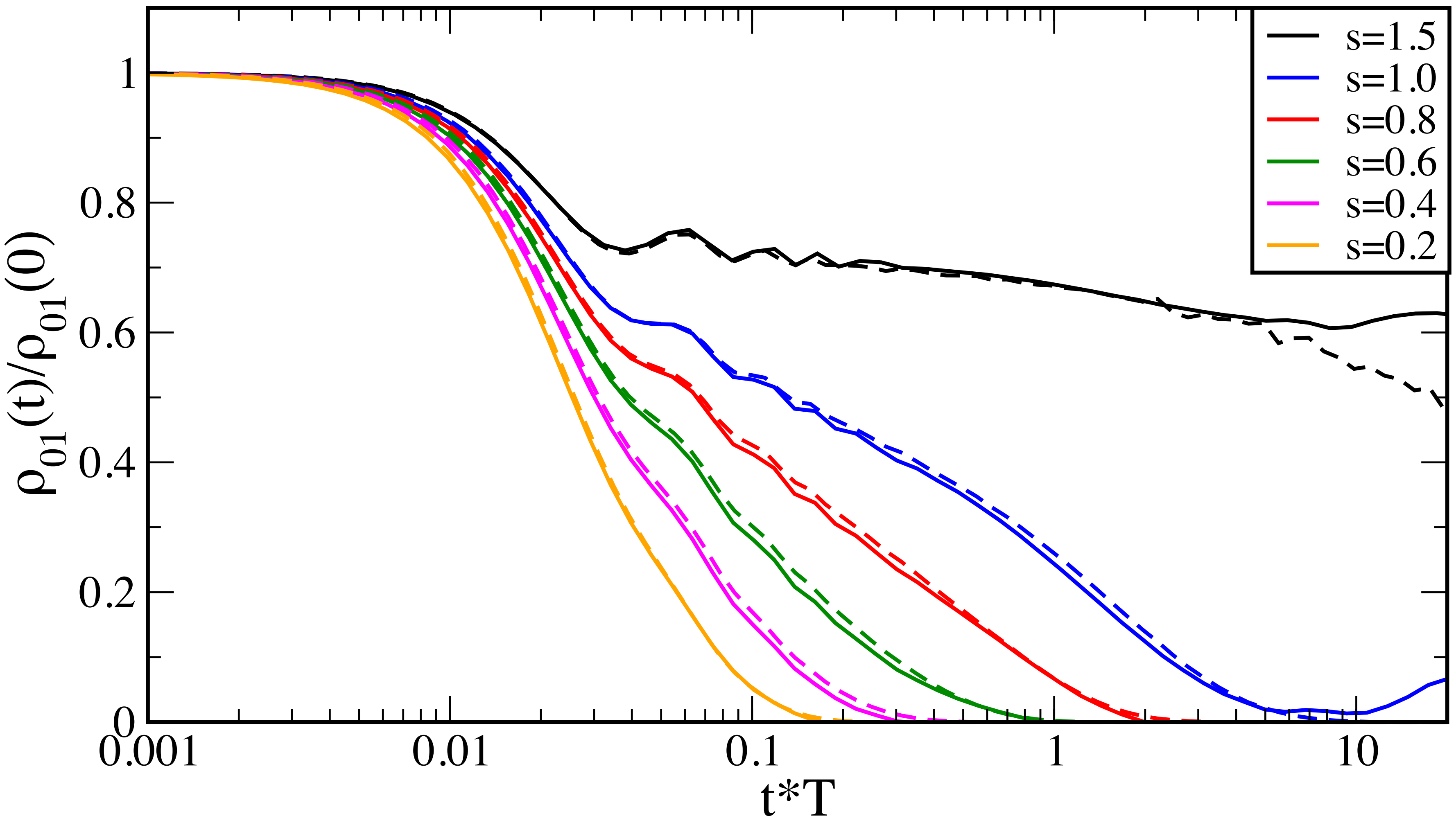
Δ=0

FBA, A. Schiller, PRL **95**, 196801 (2005)

FBA, A. Schiller, PRB **74**, 245113 (2006)

spin-boson model: decoherence by dephasing

time-dependend NRG plus analytic solution

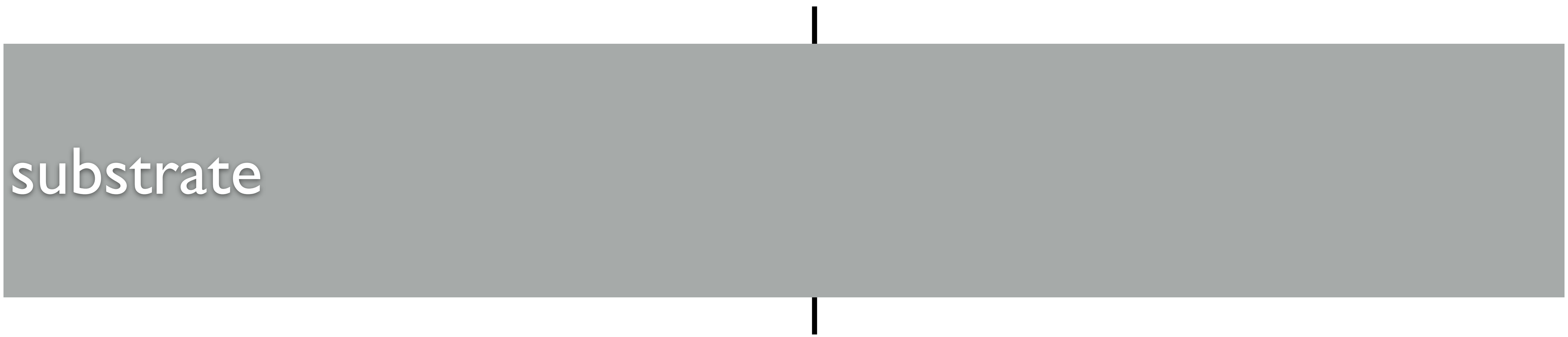


exact solution and TD-NRG: excellent agreement

FBA und A. Schiller, PRB **74,** 245113 (2006)

3. Spatial correlations: mapping to a two-impurity Kondo Problem

mapping of the Kondo problem



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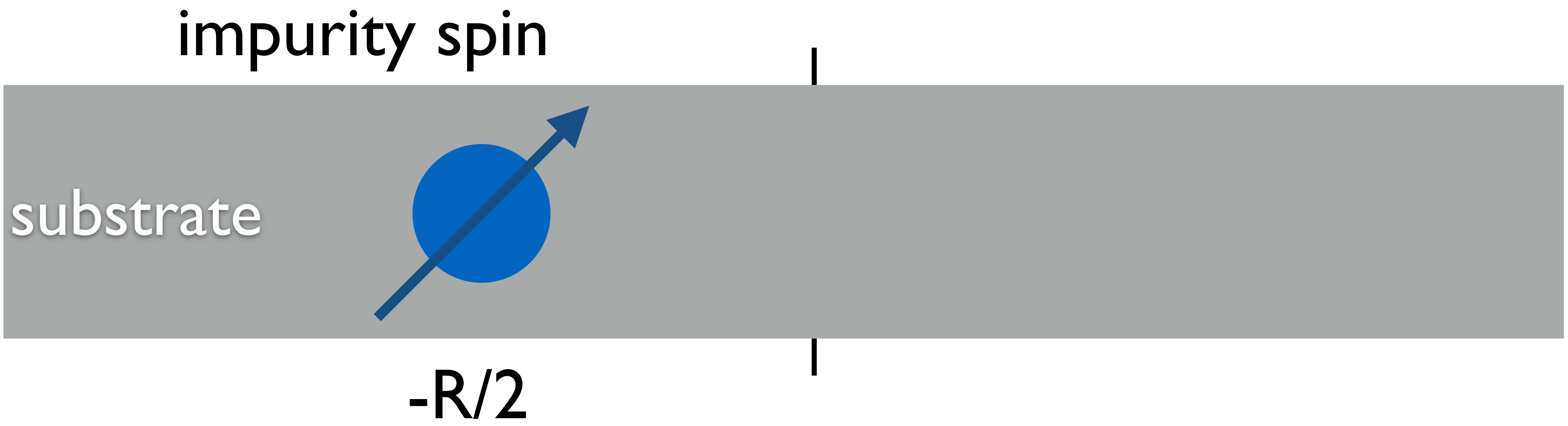

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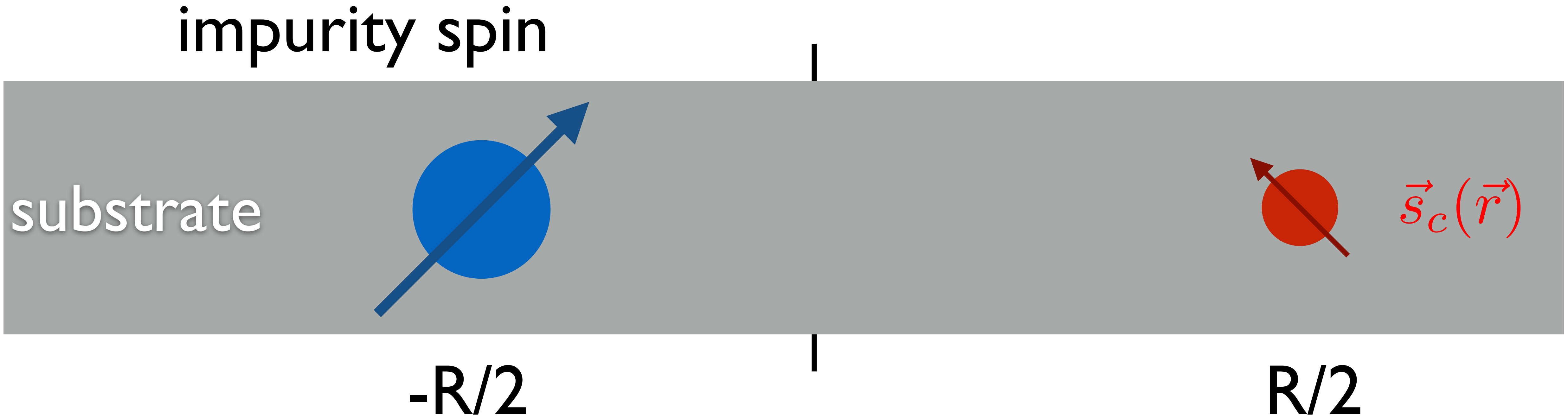

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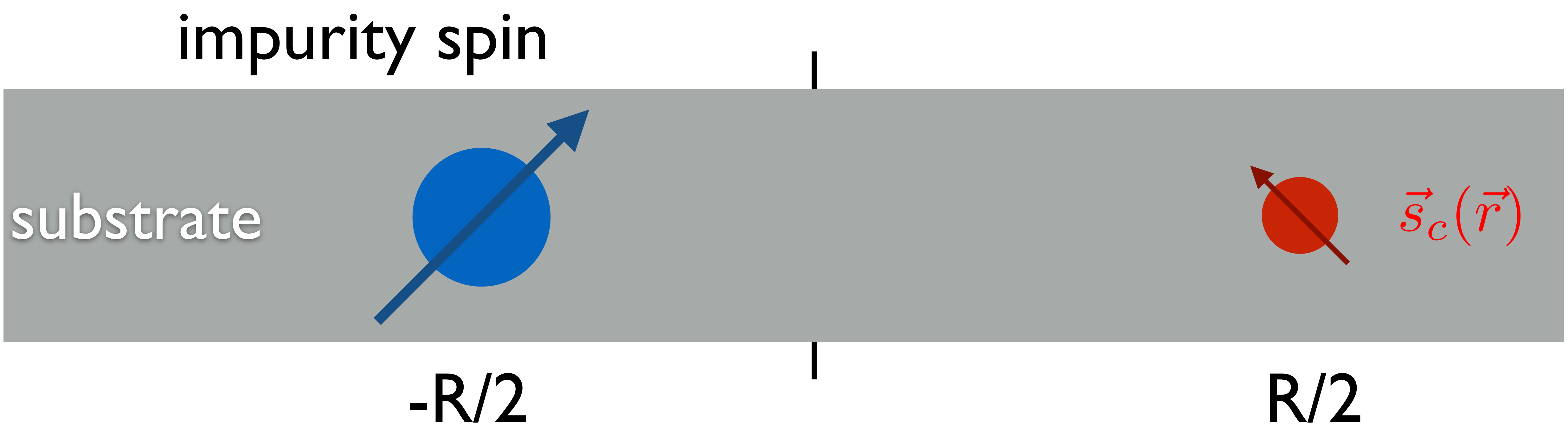
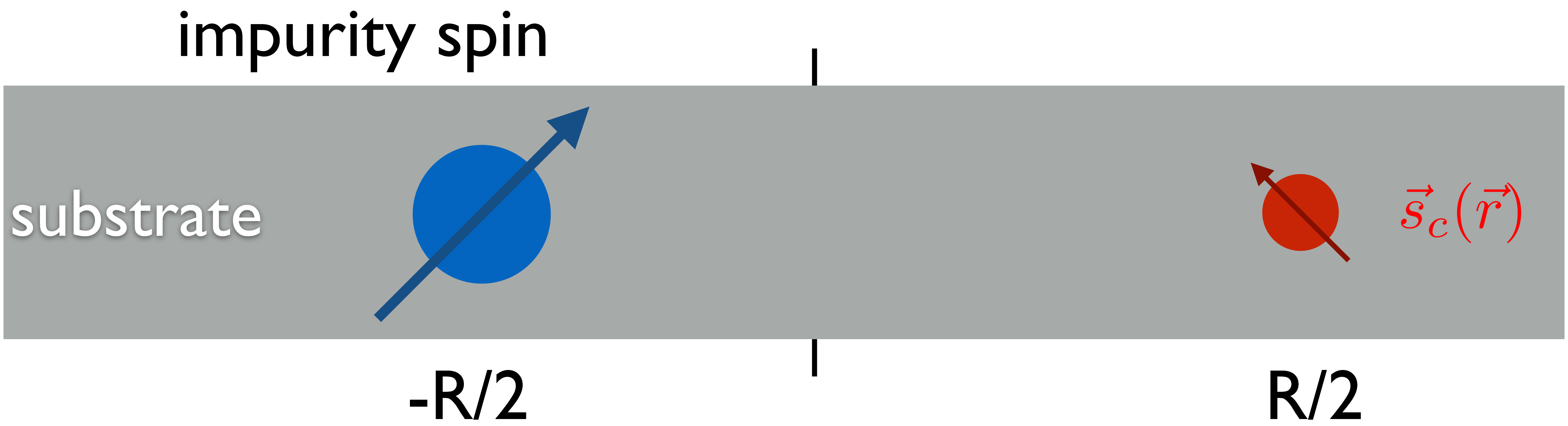


correlation function: $\chi(R,t) = \langle \vec{S}_{\rm imp} \vec{s}_{\rm c}(\vec{r}) \rangle (t)$

mapping of the Kondo problem



correlation function: $\chi(R,t) = \langle \vec{S}_{\mathrm{imp}} \vec{s}_{\mathrm{c}}(\vec{r}) \rangle (t)$

Borda, PRB 2007,
Jones, Varma PRB 1987,
Lechtenberg, FBA 2014

correlation function: $\chi(R,t) = \langle \vec{S}_{\mathrm{imp}} \vec{s}_c(\vec{r}) \rangle (t)$

mirror symmetry: even and odd parity!

Borda, PRB 2007,
Jones, Varma PRB 1987,
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mapping of the Kondo problem

correlation function: $\chi(R,t) = \langle \vec{S}_{\rm imp} \vec{s}_{\rm c}(\vec{r}) \rangle (t)$

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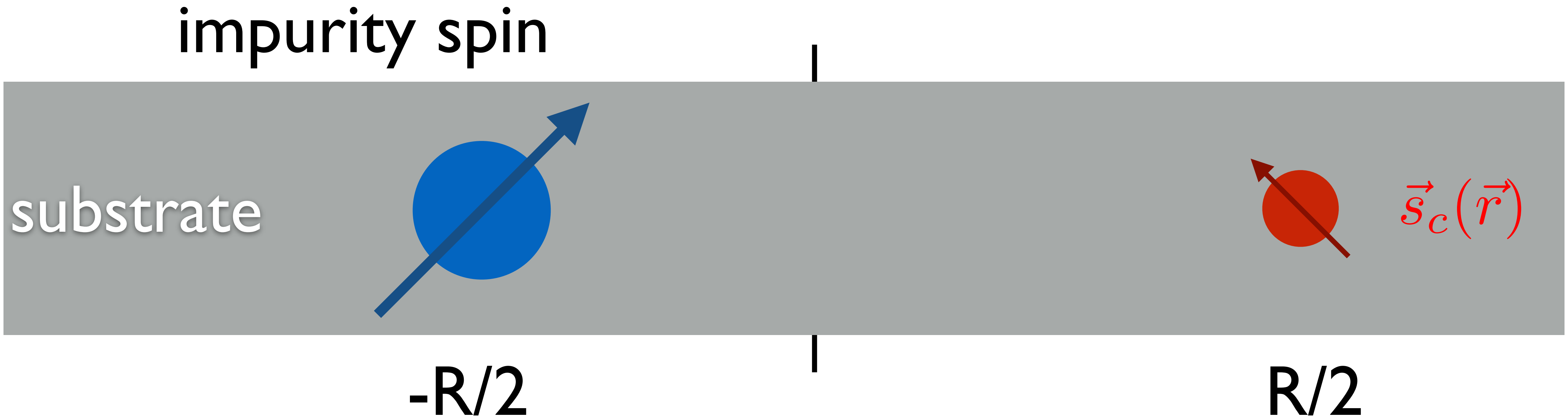
two band,
two impurity model

Borda, PRB 2007,
Jones, Varma PRB 1987,
Lechtenberg, FBA 2014

mapping of the Kondo problem



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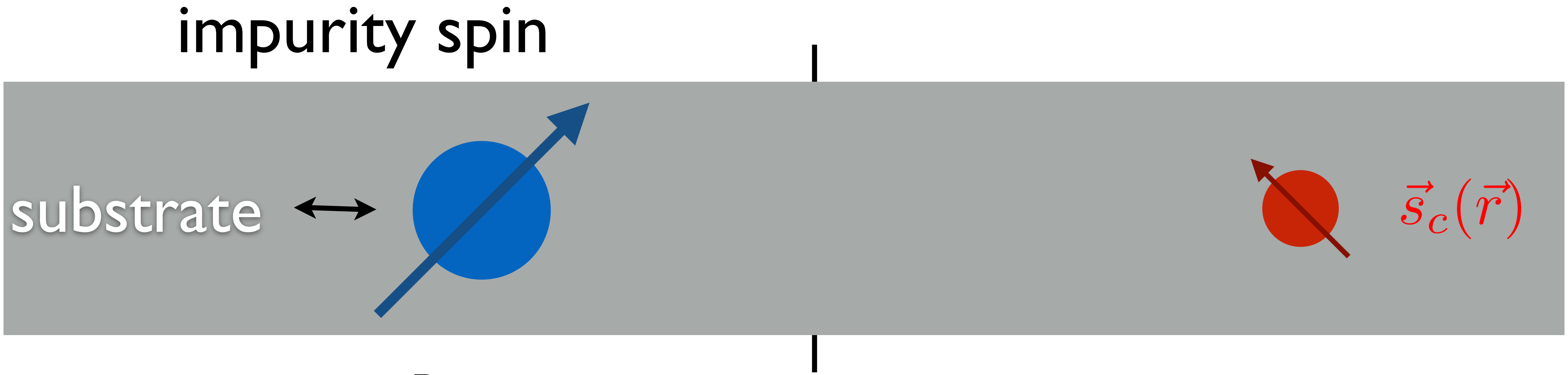
$$\psi_e(\varepsilon) = \frac{1}{\sqrt{2N_e(\varepsilon)}} \left(\psi(\frac{\vec{R}}{2}) + \psi(-\frac{\vec{R}}{2}) \right)$$

$$\psi_o(\varepsilon) = \frac{1}{\sqrt{2N_o(\varepsilon)}} \left(\psi(\frac{\vec{R}}{2}) - \psi(-\frac{\vec{R}}{2}) \right)$$

two band,
two impurity model

Borda, PRB 2007,
Jones, Varma PRB 1987,
Lechtenberg, FBA 2014

mapping of the Kondo problem



$$H = \sum_\sigma \sum_{\alpha=e,o} \int_{-D}^{D} d\varepsilon\, \varepsilon\, c^\dagger_{\varepsilon\sigma,\alpha} c_{\varepsilon\sigma,\alpha}$$

$$+ \frac{J}{8} \sum_{\sigma\sigma'} \left(\bar{N}_e(R) f^\dagger_{0\sigma,e} + \bar{N}_o(R) f^\dagger_{0\sigma,o} \right) [\underline{\vec{\sigma}}]_{\sigma\sigma'} \left(\bar{N}_e(R) f_{0\sigma,e} + \bar{N}_o(R) f_{0\sigma,o} \right) \vec{S}_{\text{imp}}$$

Borda, PRB 2007,
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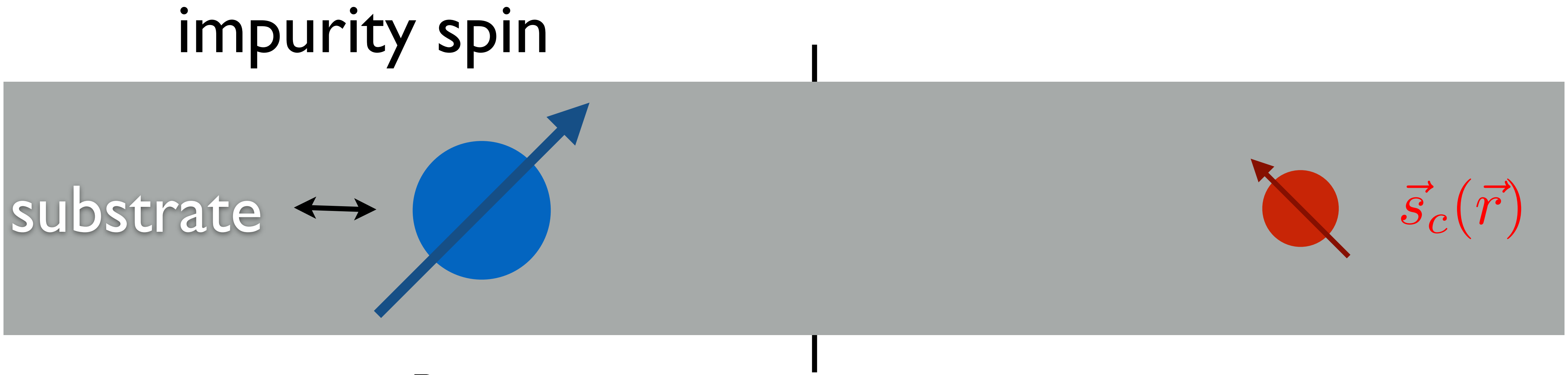
mapping of the Kondo problem



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$$\vec{s}(\frac{\vec{R}}{2}) = \frac{1}{8V_u} \sum_{\sigma\sigma'} \left(\bar{N}_e(R) f^\dagger_{0\sigma,e} - \bar{N}_o(R) f^\dagger_{0\sigma,o} \right) [\underline{\vec{\sigma}}]_{\sigma\sigma'} \left(\bar{N}_e(R) f_{0\sigma,e} - \bar{N}_o(R) f_{0\sigma,o} \right)$$

Borda, PRB 2007,
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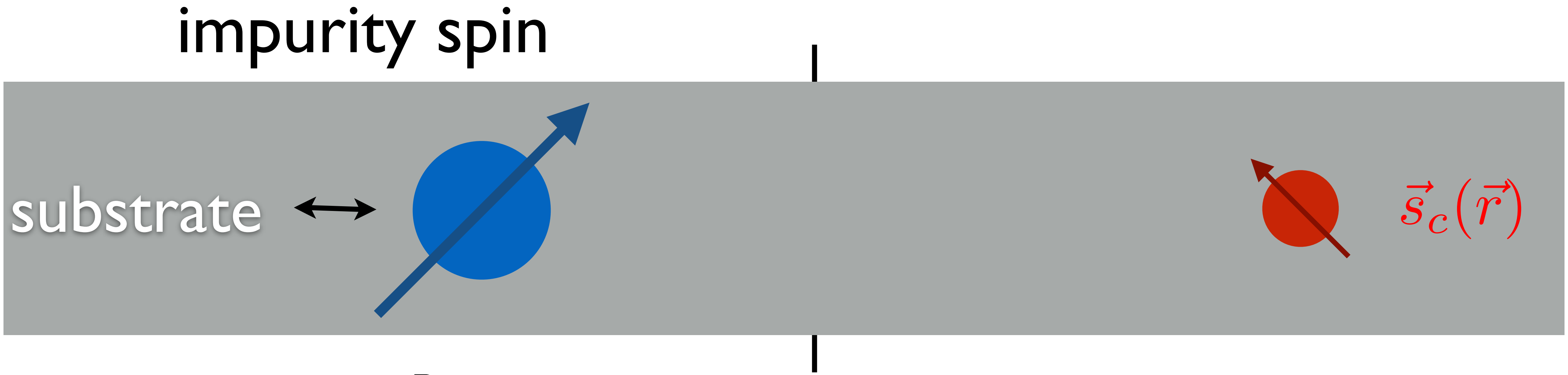

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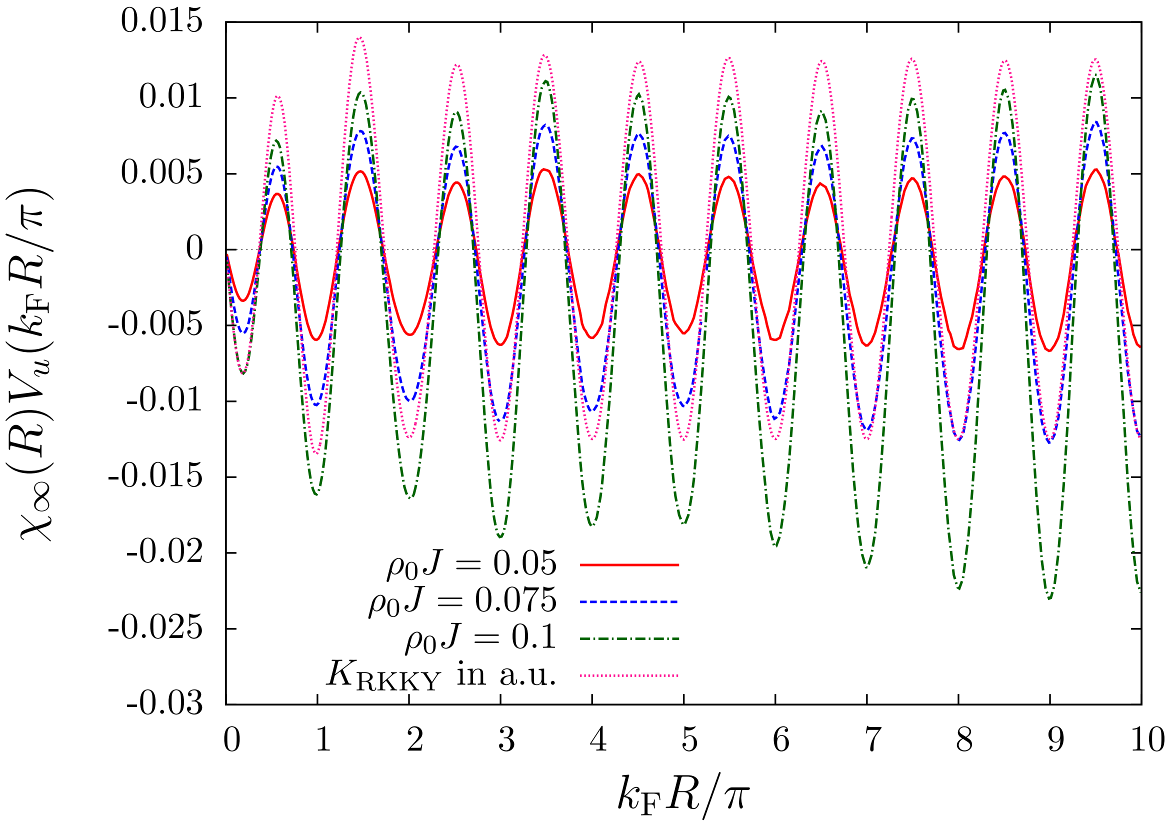
for each distance R one independent two band NRG calculation

Borda, PRB 2007,
Jones, Varma PRB 1987,
Lechtenberg, FBA 2014

4. Results

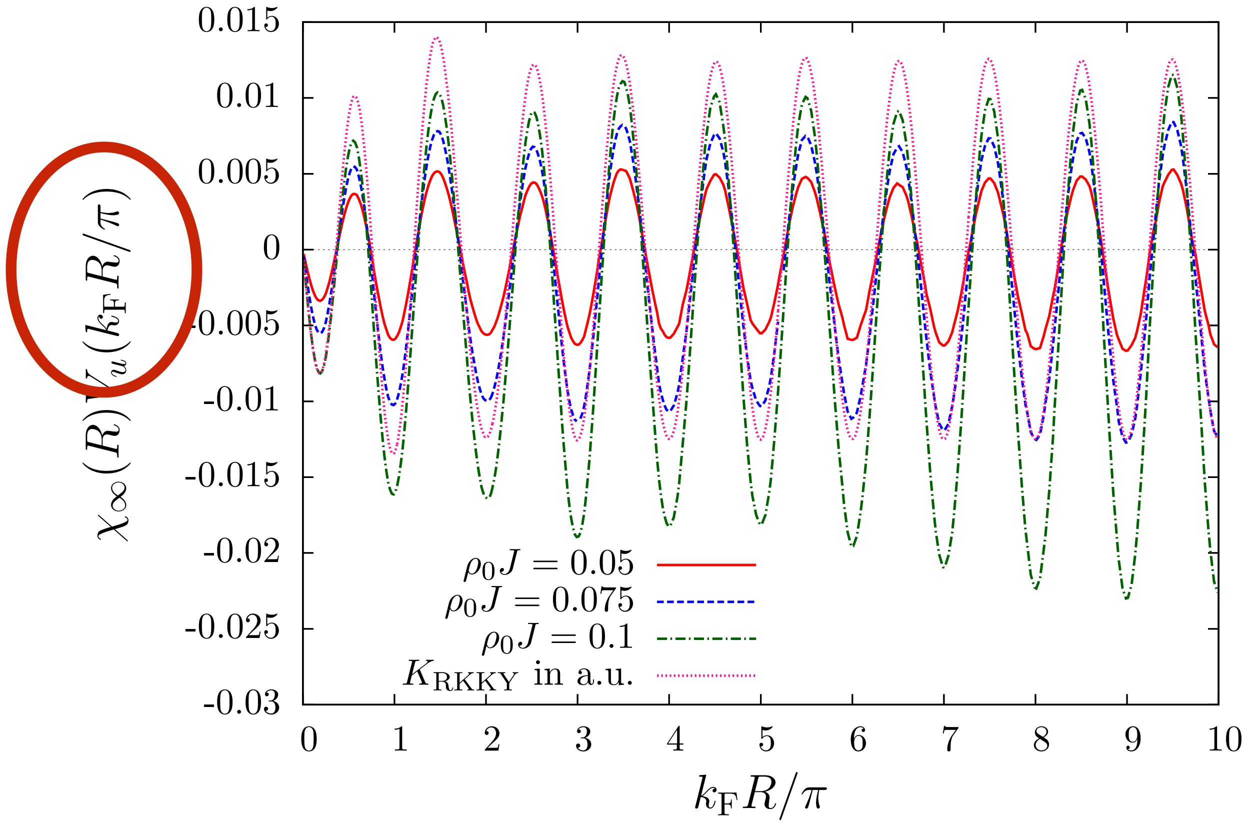
equilibrium: antiferromagnetic coupling



1D:

Lechtenberg, FBA arXiv:1402.1028

equilibrium: antiferromagnetic coupling



1D: 1/R

Lechtenberg, FBA arXiv:1402.1028

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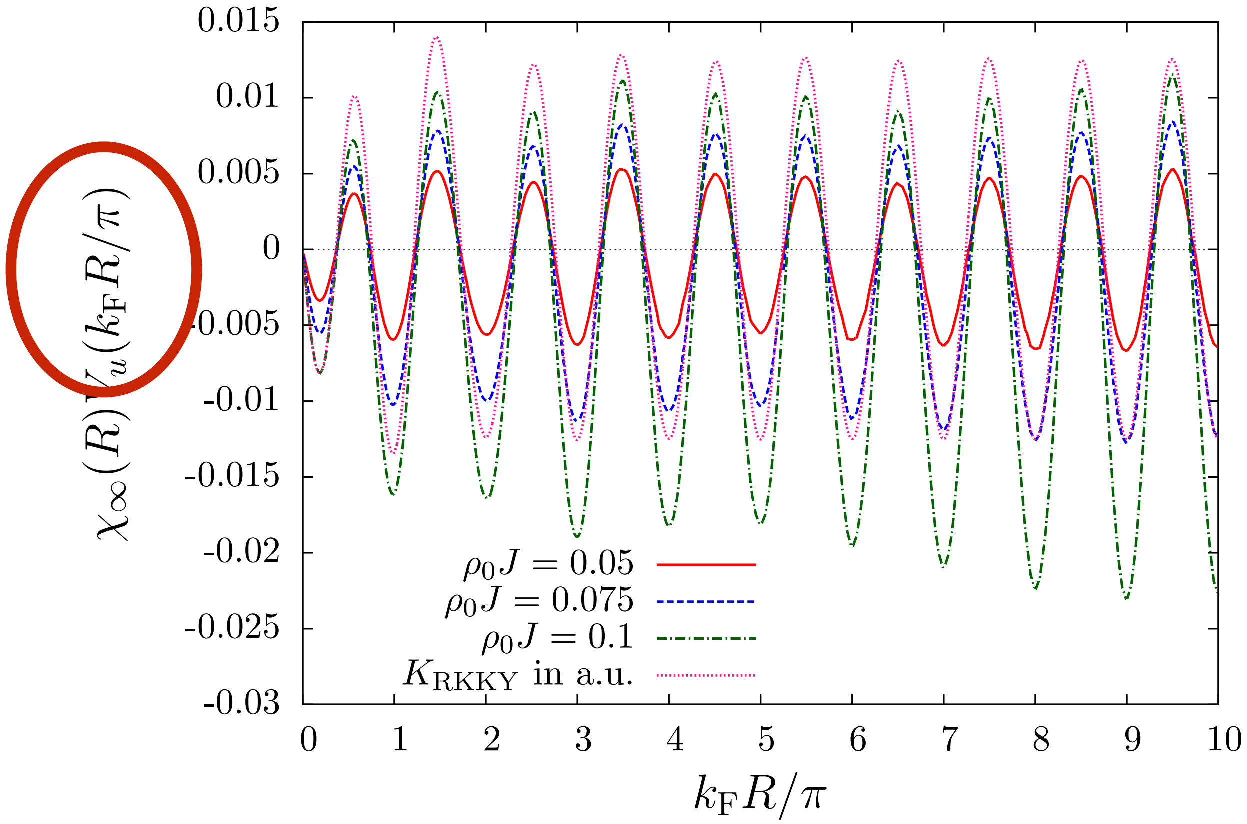
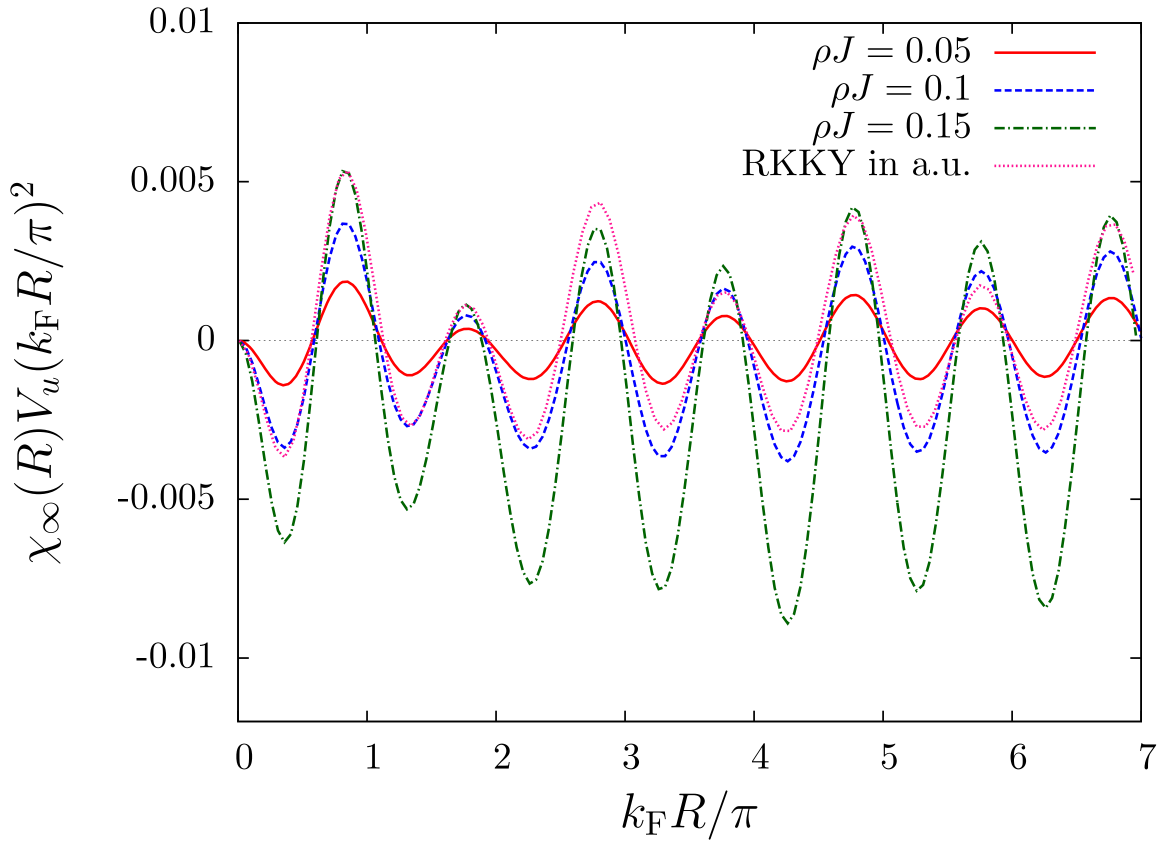


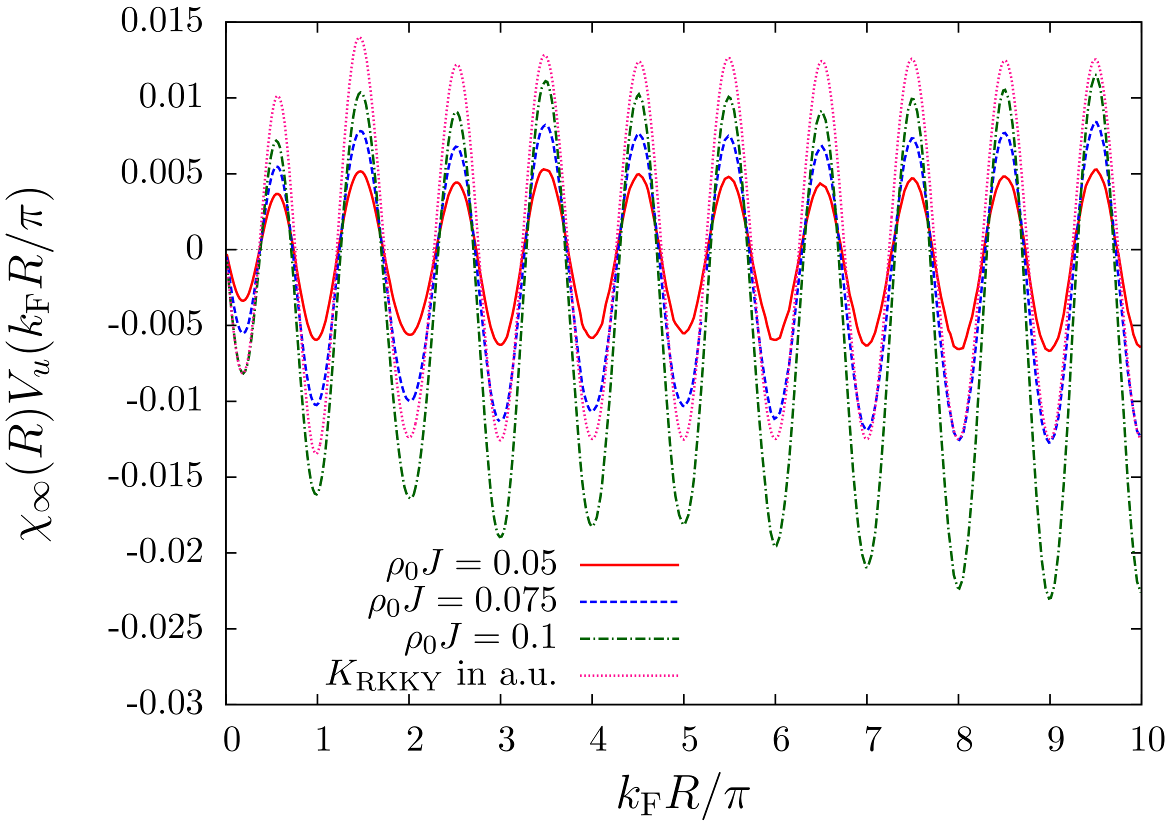


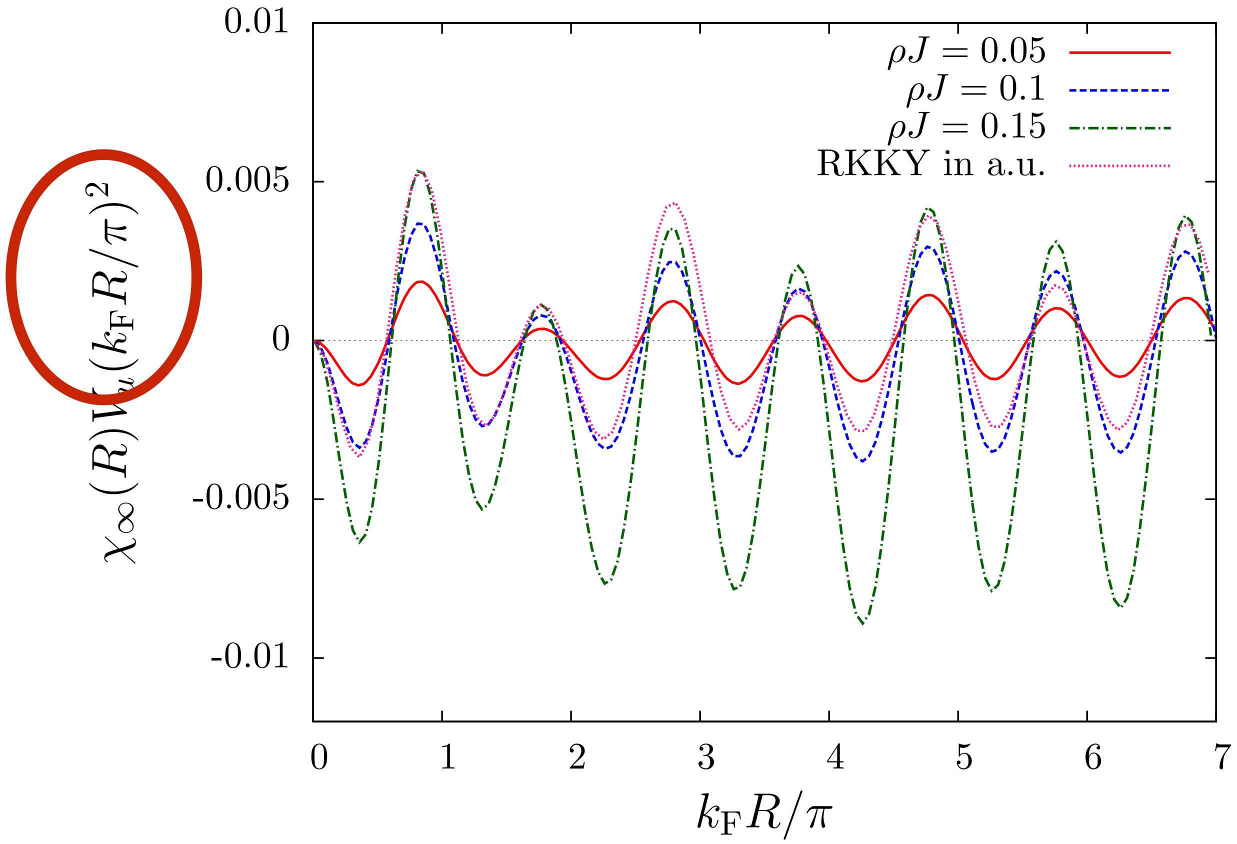
1D: 1/R

2D:

Lechtenberg, FBA arXiv:1402.1028

equilibrium: antiferromagnetic coupling

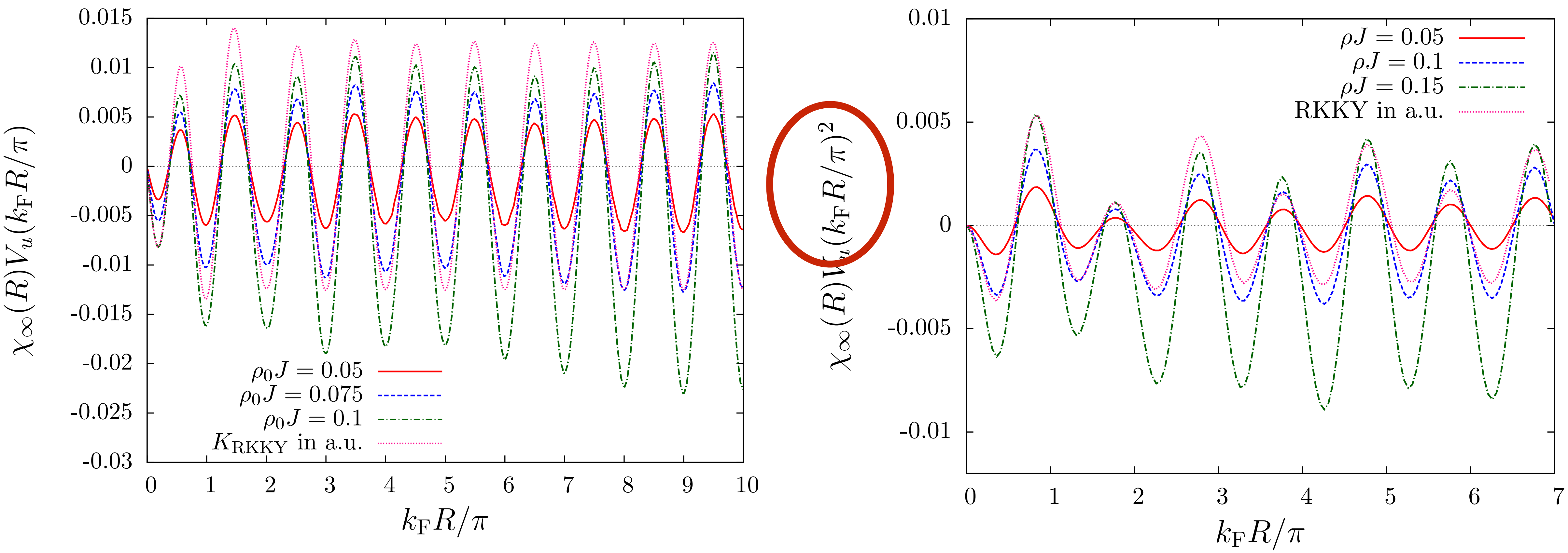




1D: 1/R

2D: $1/R^2$

equilibrium: antiferromagnetic coupling



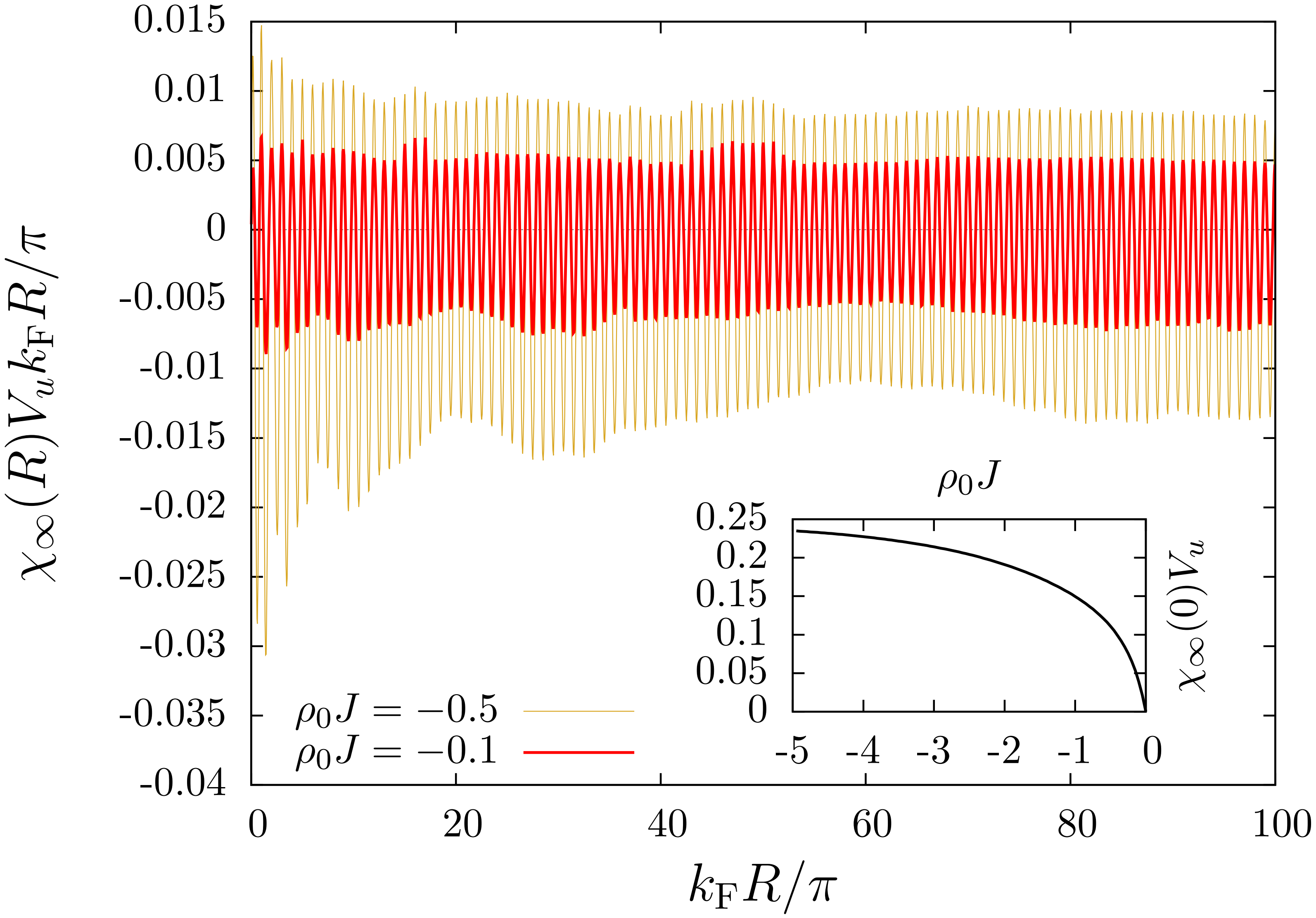
1D: 1/R

2D: $1/R^2$

$$\int_0^\infty dr r^{d-1} \chi_\infty(R) = -\frac{3}{4}$$

Lechtenberg, FBA arXiv:1402.1028

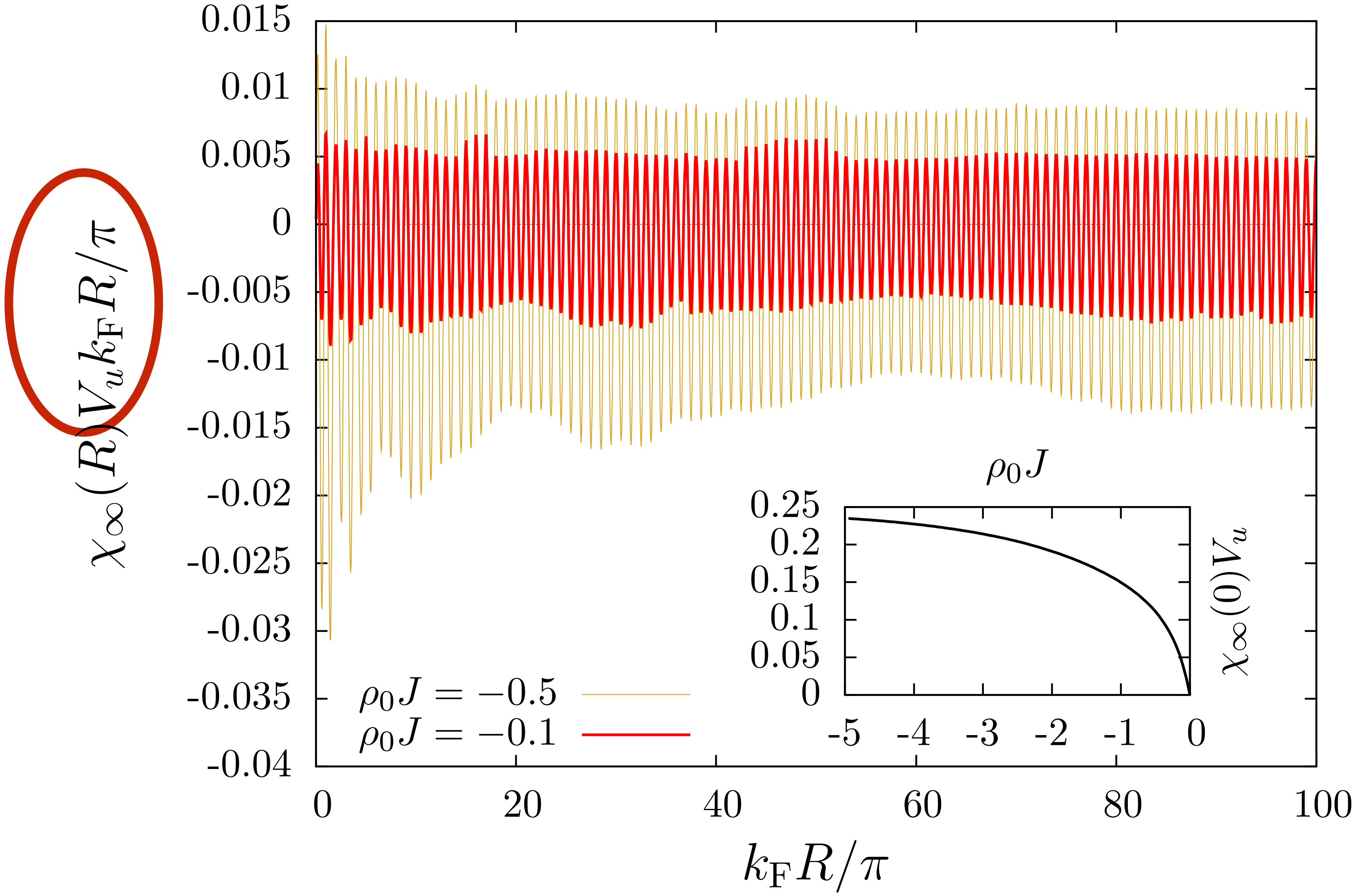
equilibrium: ferromagnetic coupling



$$\int_0^\infty dr r^{d-1} \chi_\infty(R) = 0$$

 Lechtenberg, FBA arXiv:1402.1028

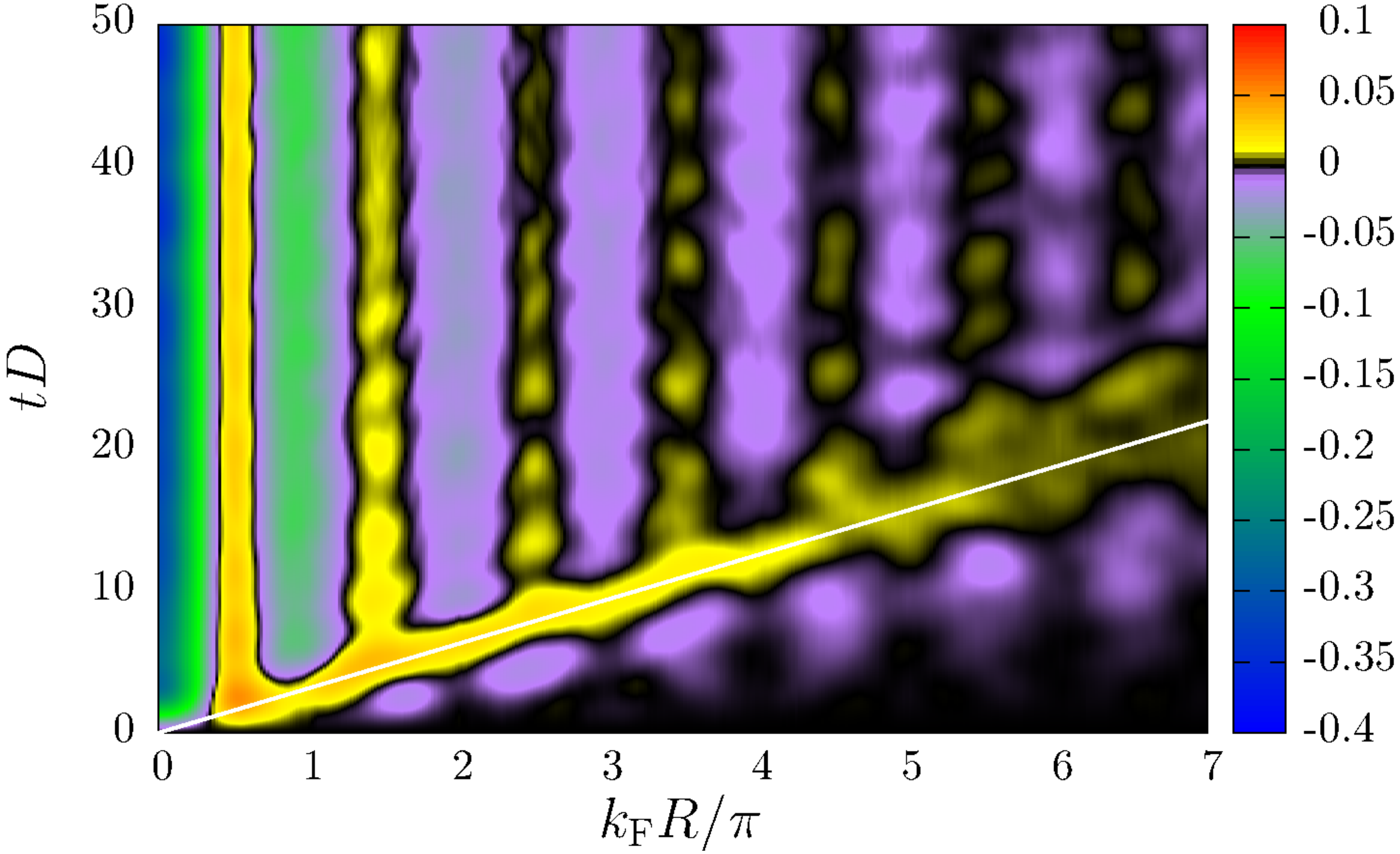
equilibrium: ferromagnetic coupling



$$\int_0^\infty dr r^{d-1} \chi_\infty(R) = 0$$

 Lechtenberg, FBA arXiv:1402.1028

non-equilibrium dynamics

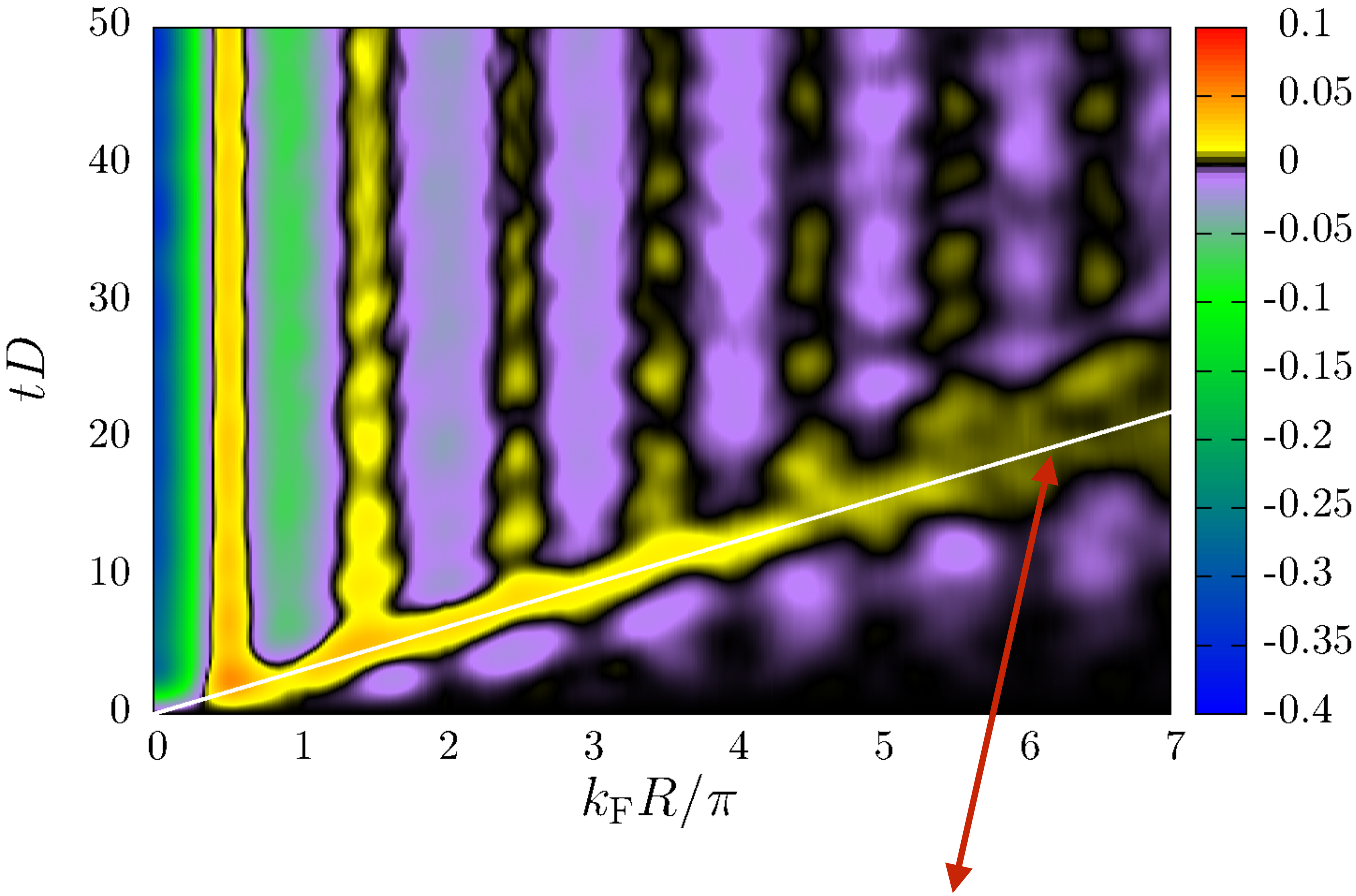


$$\chi(R,t) = \langle \vec{S}_{\rm imp} \vec{s}_{\rm c}(\vec{r}) \rangle (t)$$

$$\rho_0 J = 0.3$$

Lechtenberg, FBA arXiv:1402.1028

non-equilibrium dynamics



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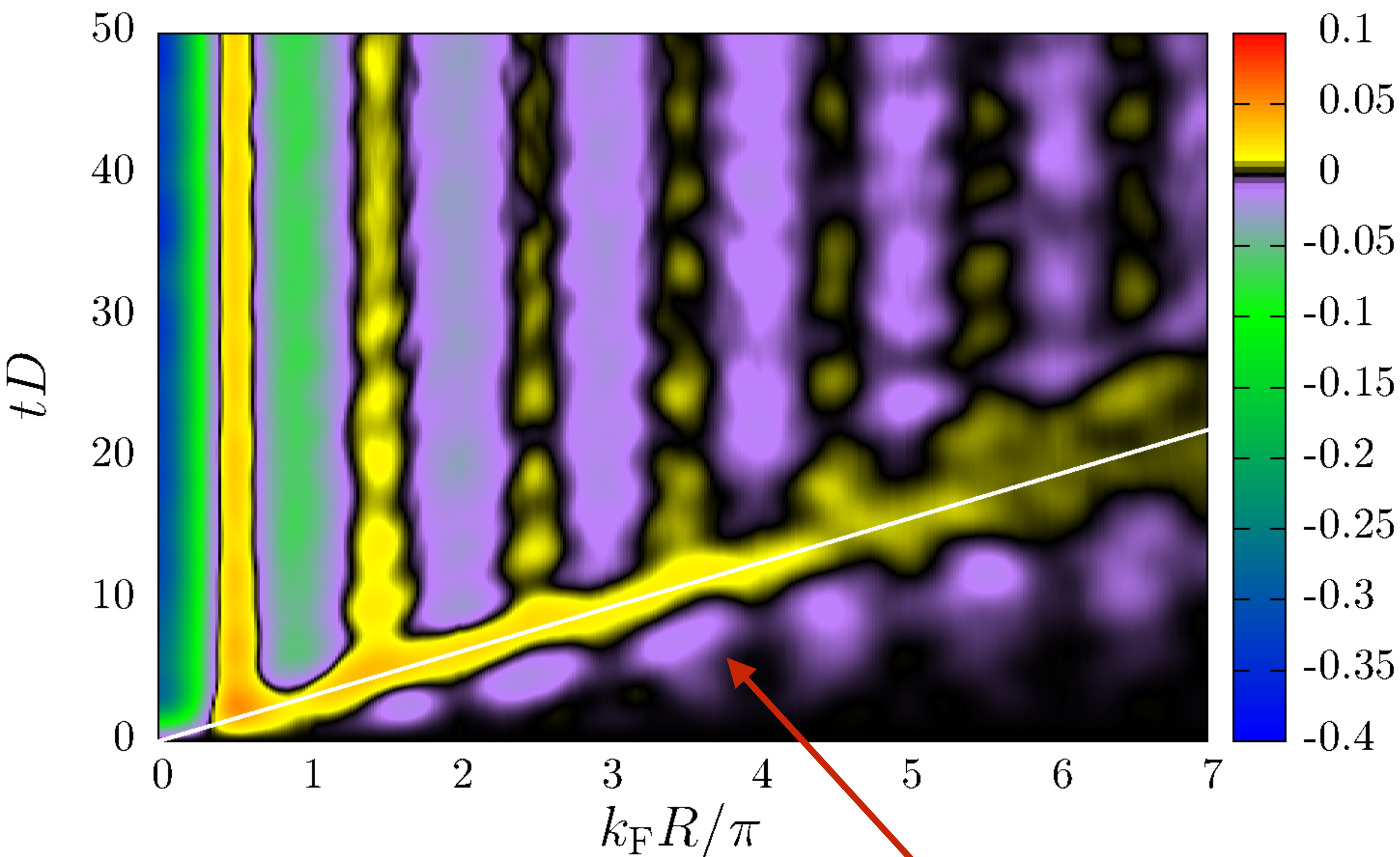
- "light-cone" physics $R=v_F t$

Lechtenberg, FBA arXiv:1402.1028



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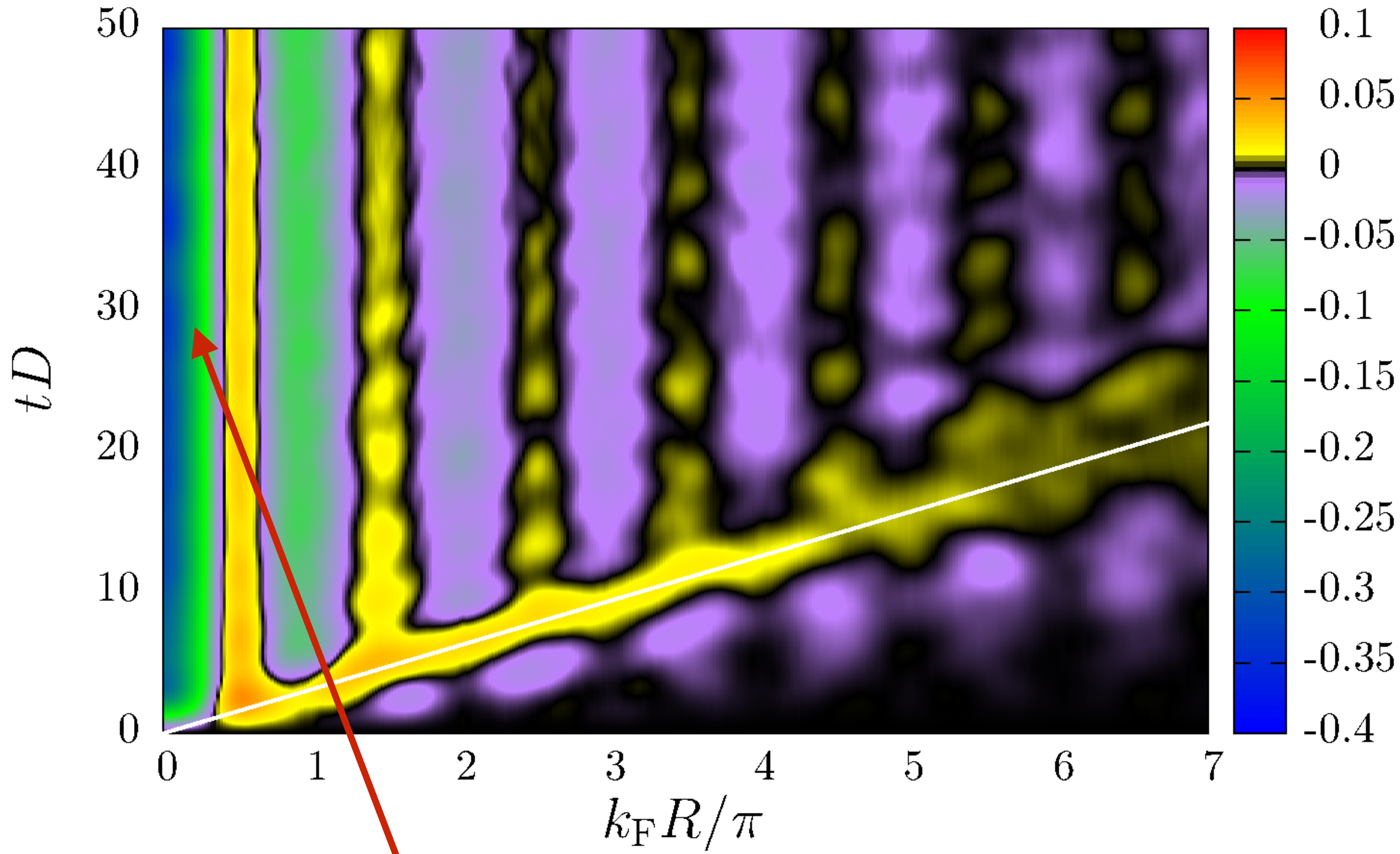
- “light-cone” physics $R=v_F t$
- surprice: buildup of correlations outside the light-cone

non-equilibrium dynamics



$$\chi(R,t) = \langle \vec{S}_{\mathrm{imp}} \vec{s}_{\mathrm{c}}(\vec{r}) \rangle(t)$$

$$\rho_0 J = 0.3$$

- “light-cone” physics $R=v_F t$
- surprice: buildup of correlations outside the light-cone
- fast short time scale and thermalisation inside the light-cone

perturbation theory

$$\rho^I(t) = \rho_0 + i\int_0^t \left[\rho_0, H_K^I(t_1)\right] dt_1 - \int_0^t \int_0^{t_1} \left[\left[\rho_0, H_K^I(t_2)\right] H_K^I(t_1)\right] dt_2 dt_1 + O(J^2)$$

Lechtenberg, FBA arXiv:1402.1028

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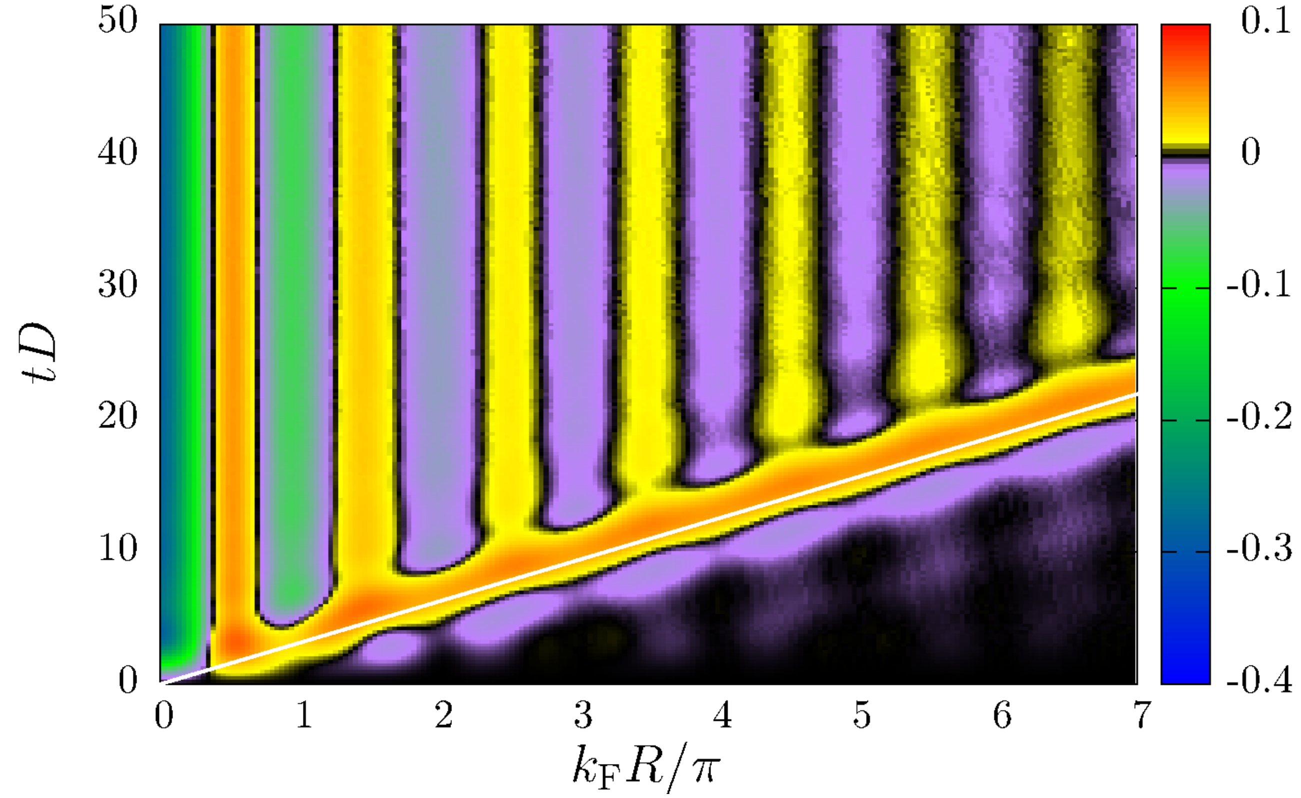

second order perturbation theory
no Kondo effect

Lechtenberg, FBA arXiv:1402.1028

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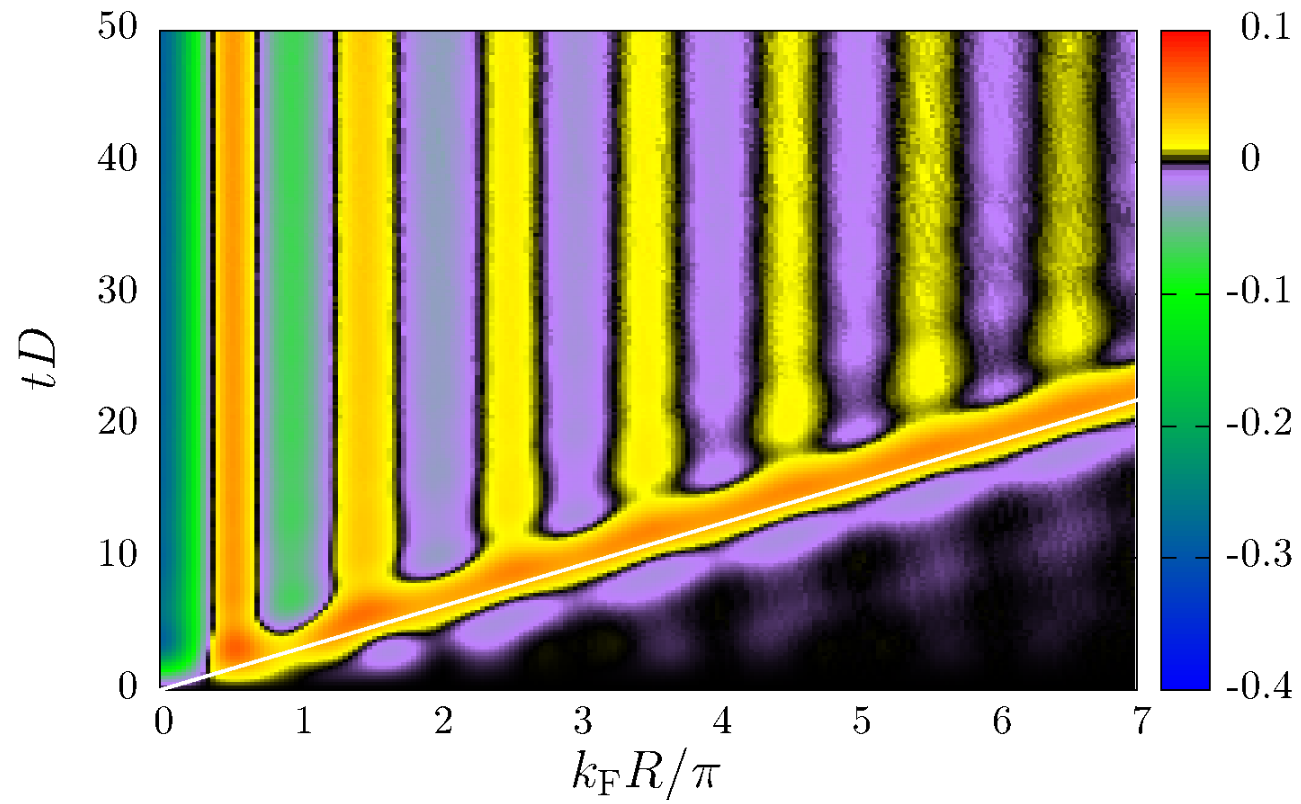

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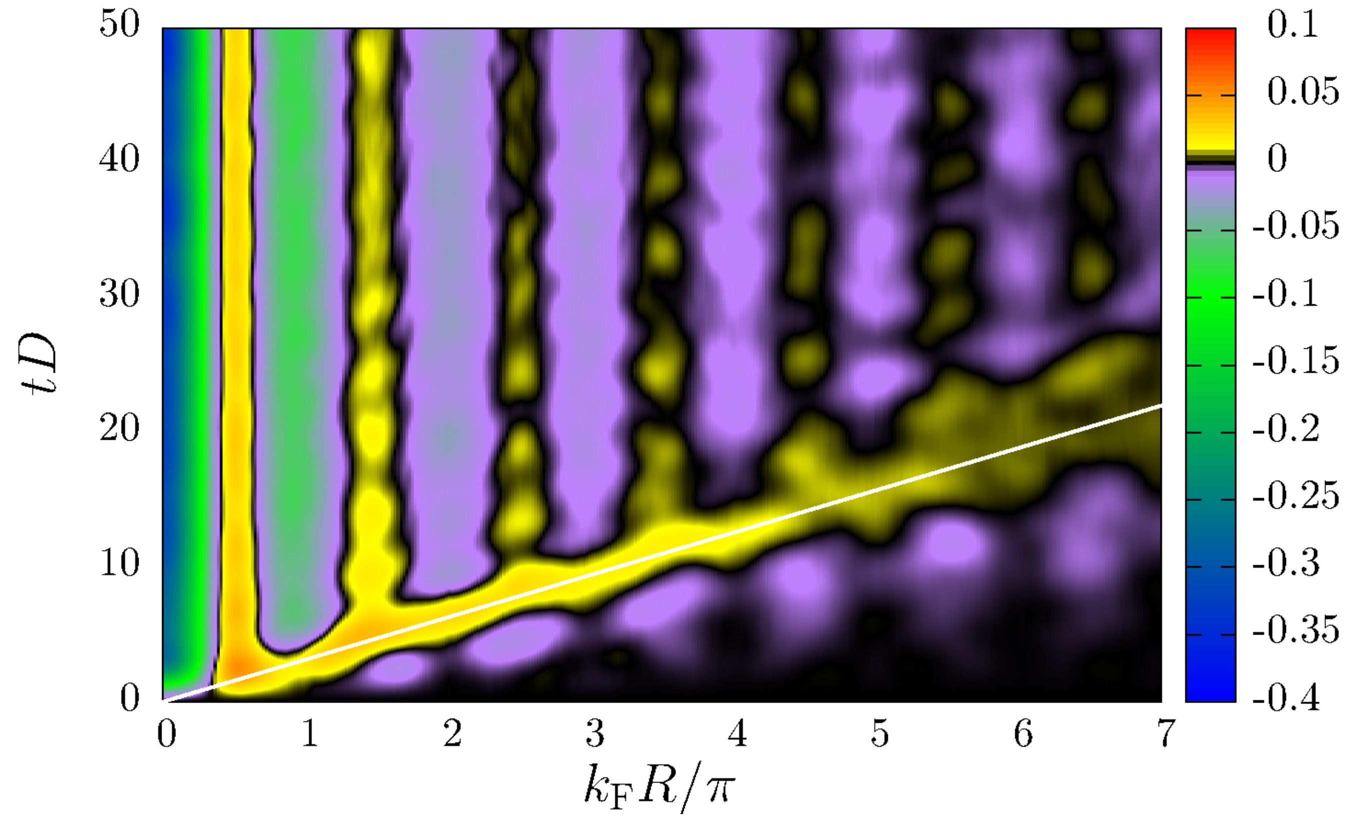

TD-NRG
Kondo effect included

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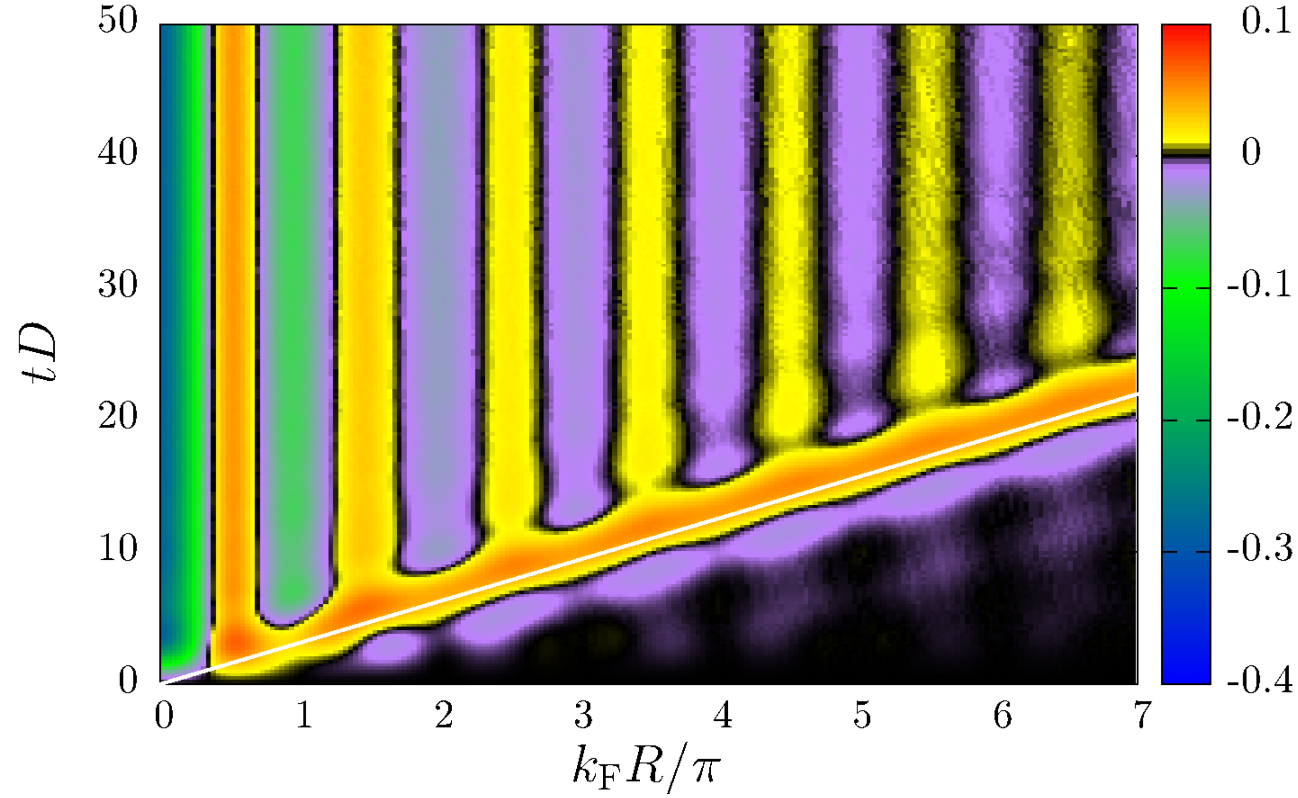

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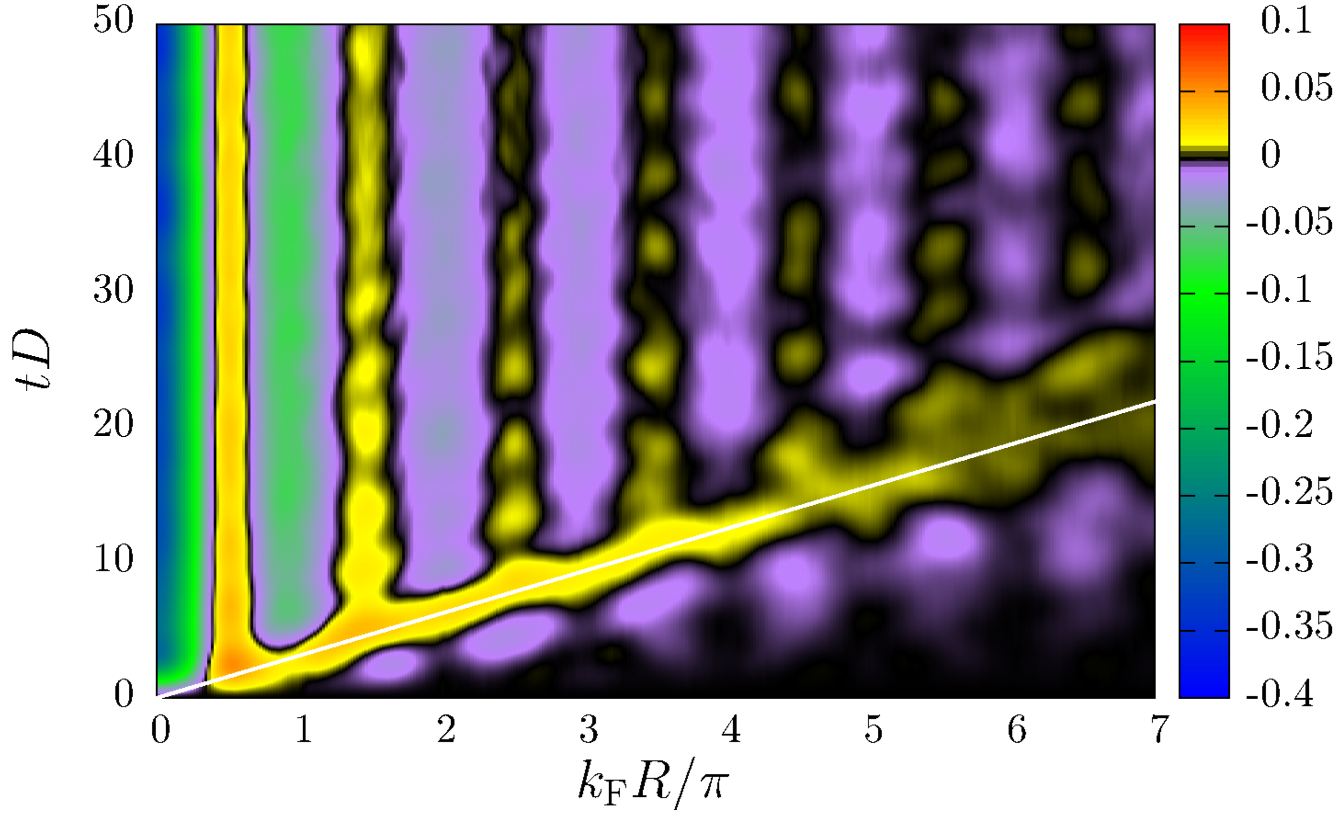

TD-NRG
Kondo effect included

qualitative very good agreement: correlations outside the light cone persist

Lechtenberg, FBA arXiv:1402.1028

correlations outside of the light cone?

Medvedyeva et al PRB 2013: intrinsic correlations of the Fermi sea

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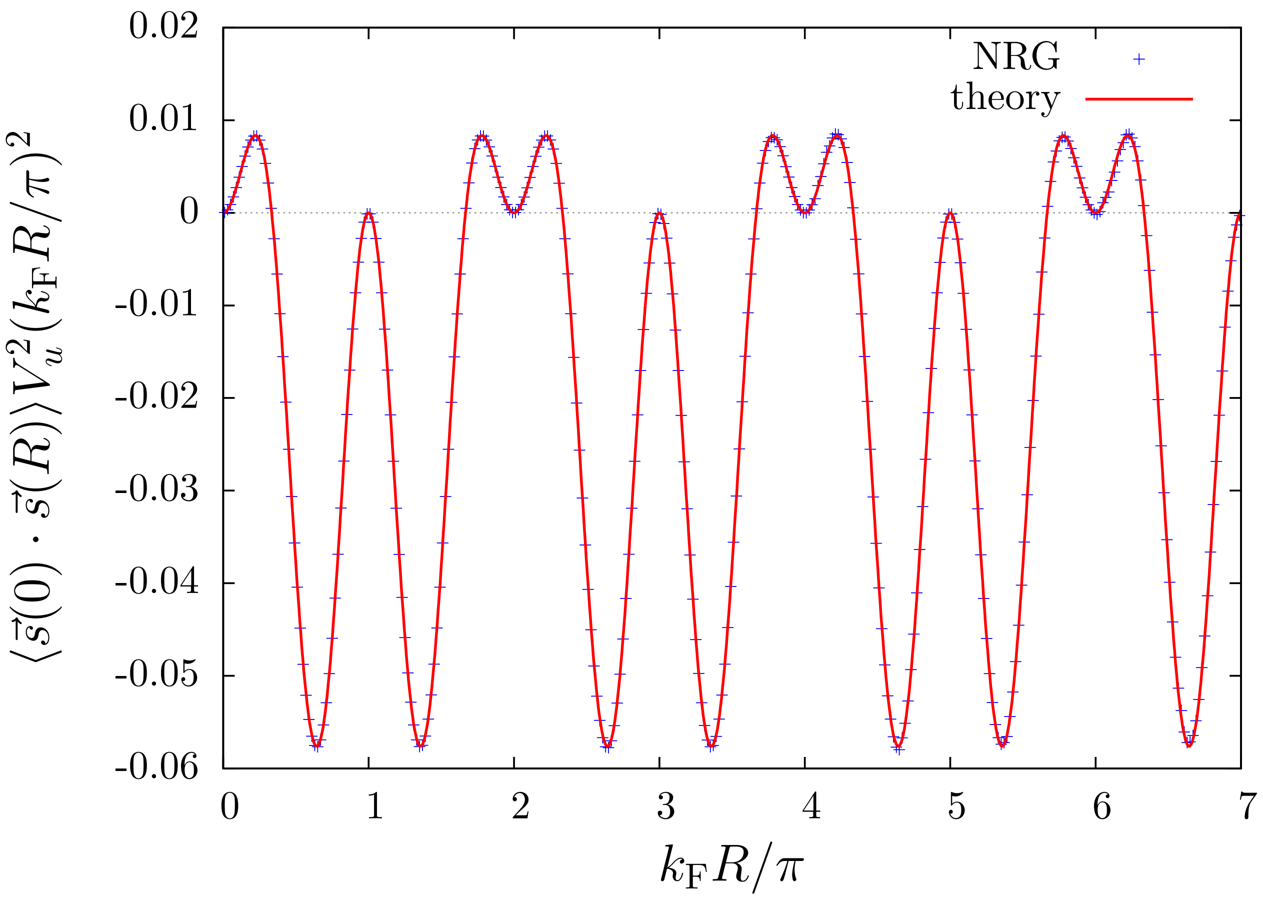

spatial spin-density correlation function: NRG vs analytic

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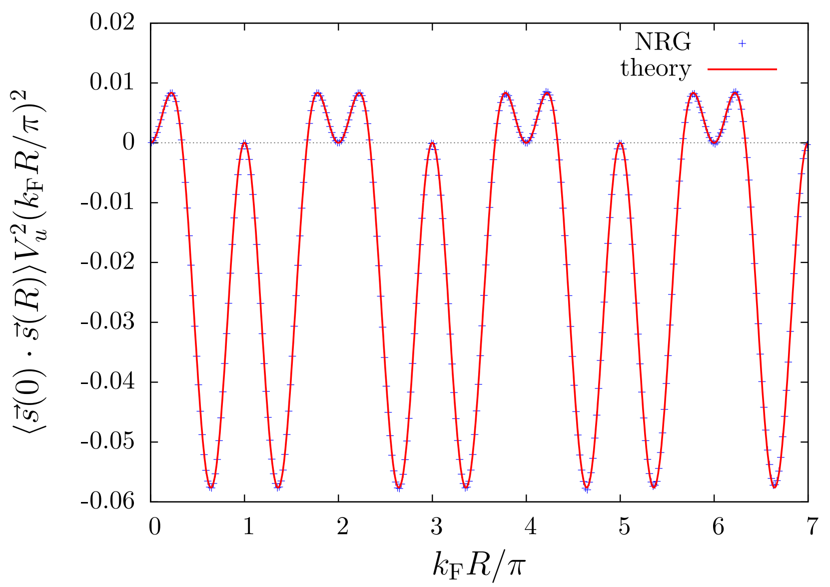

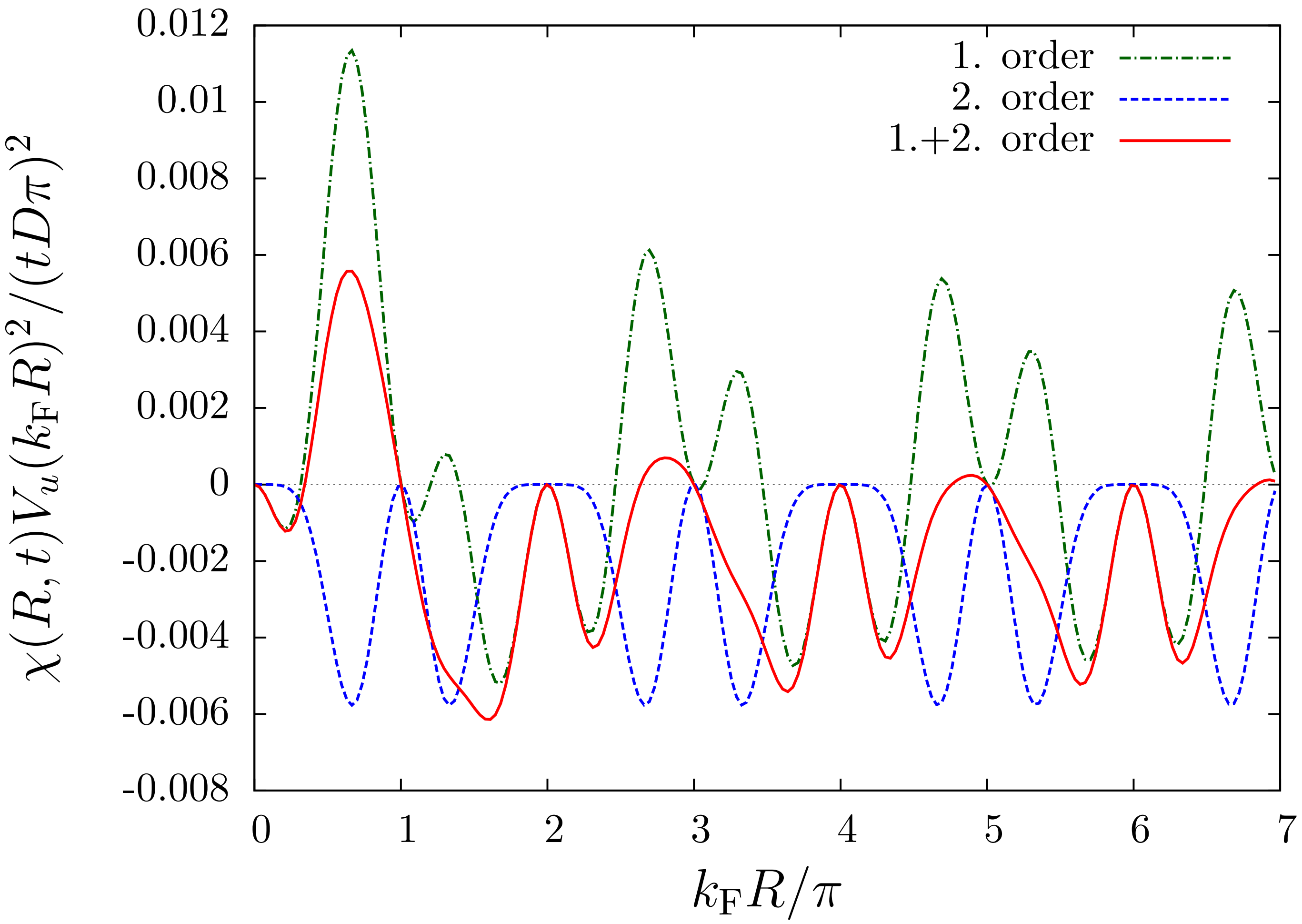

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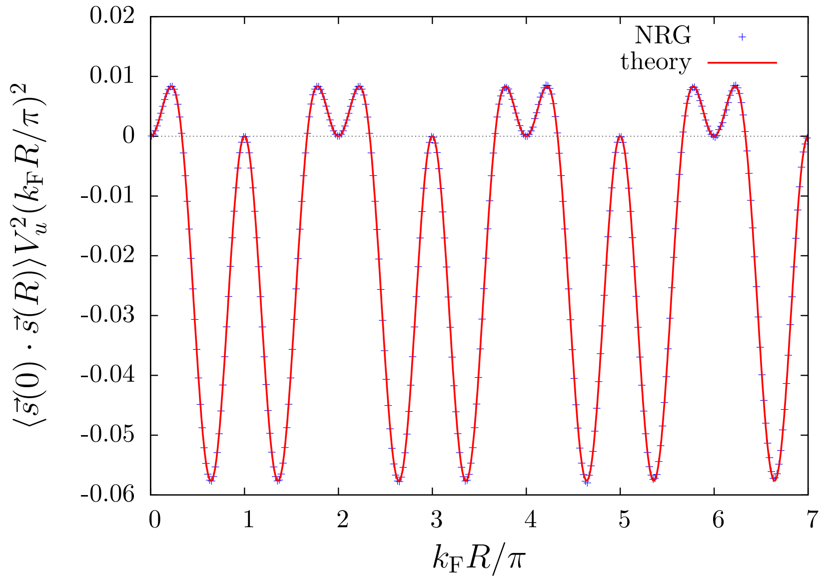

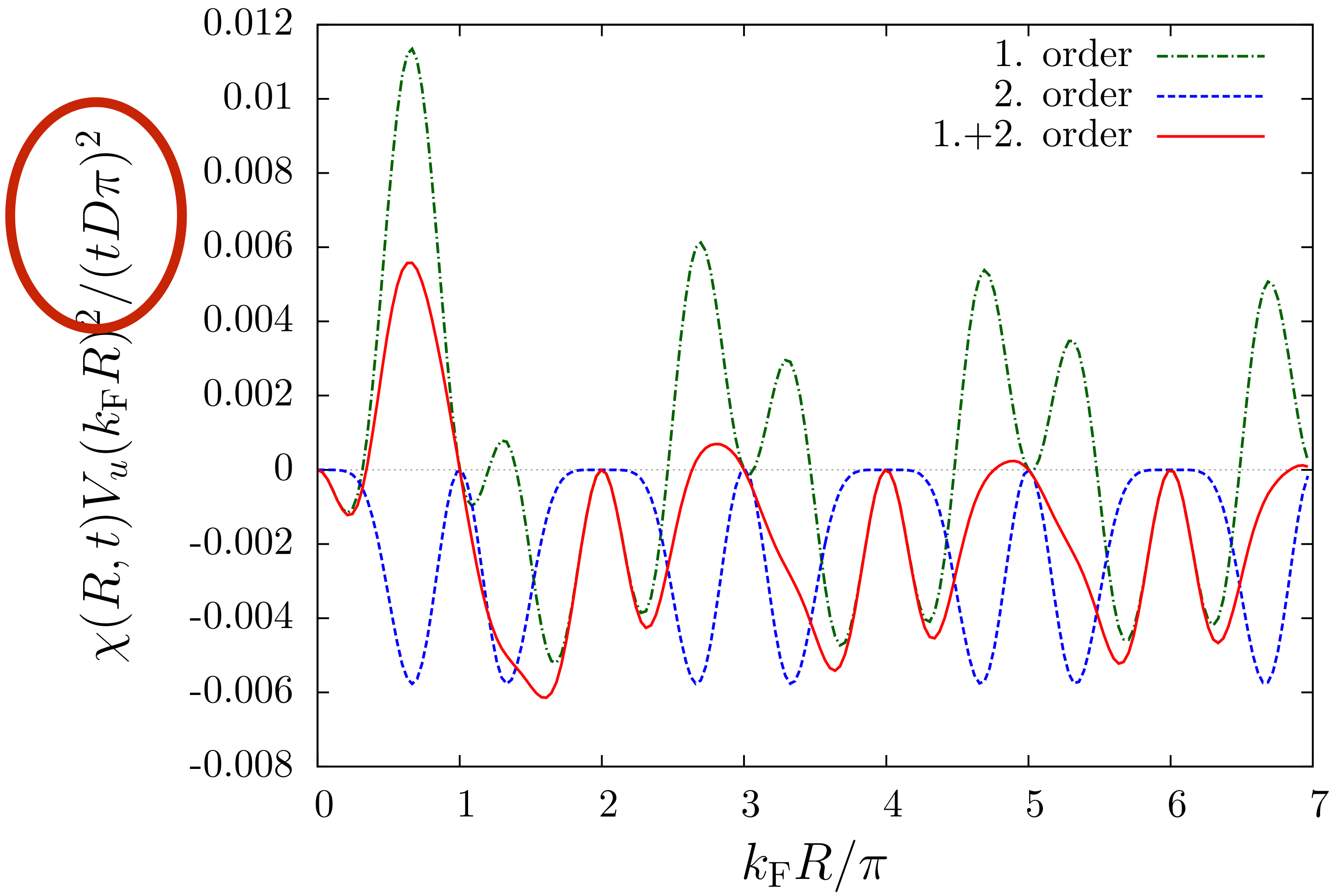

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- time scale 1/D

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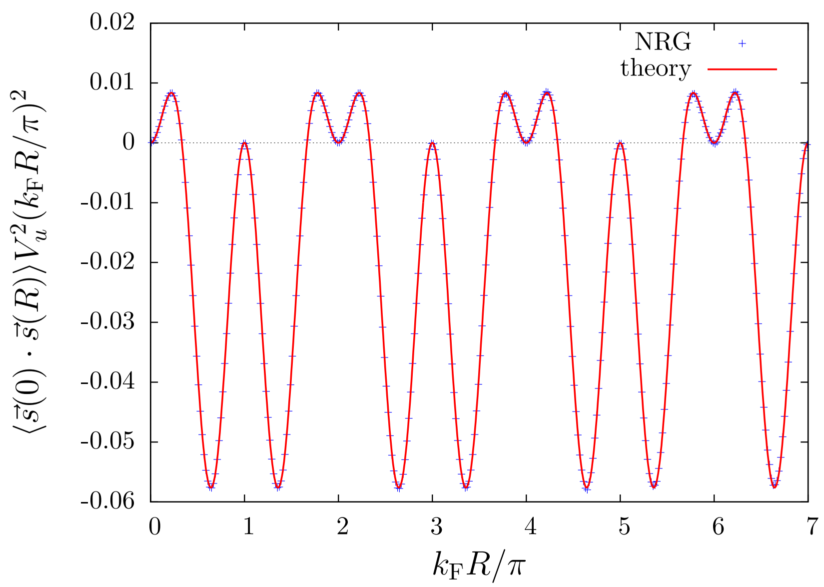

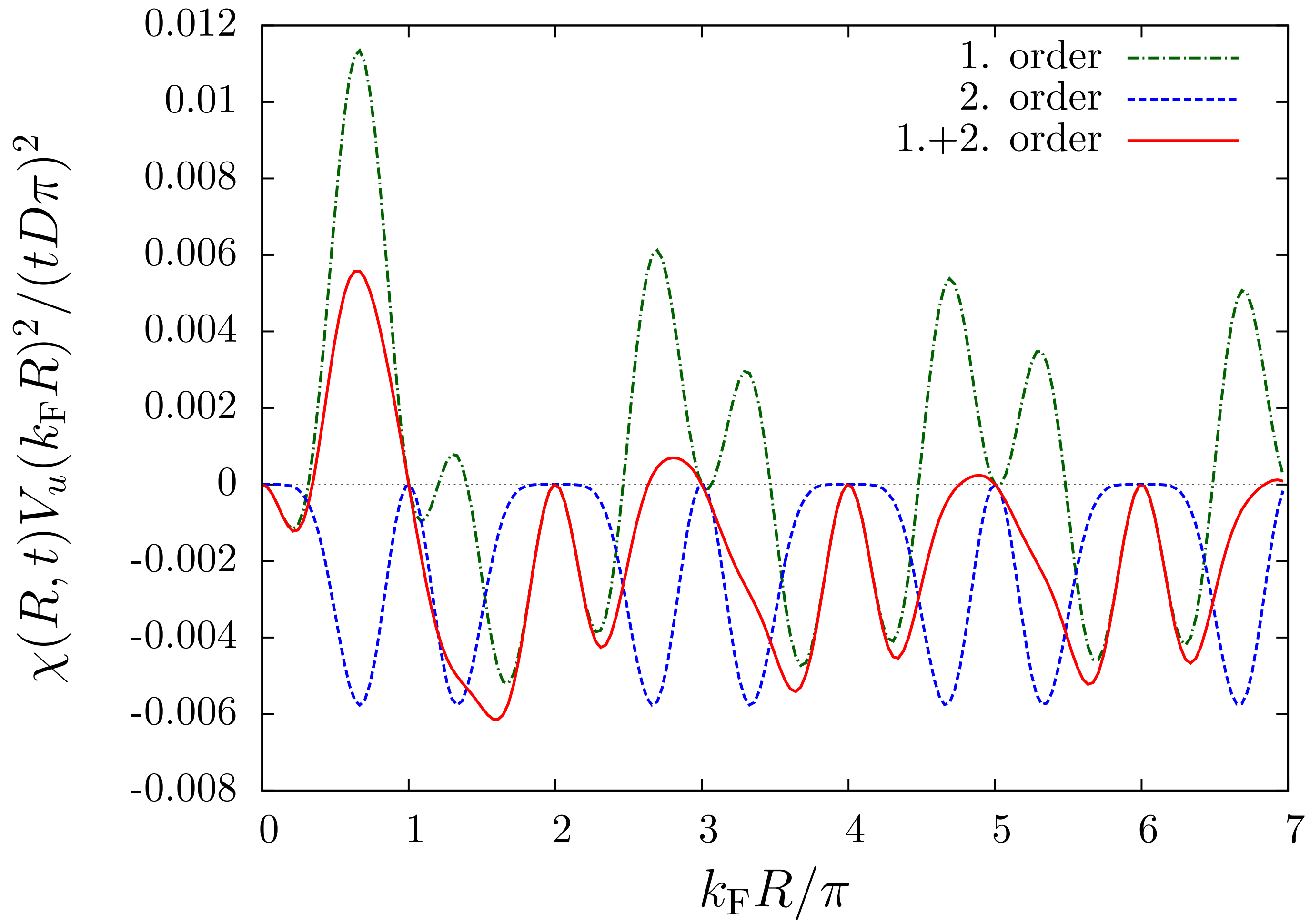

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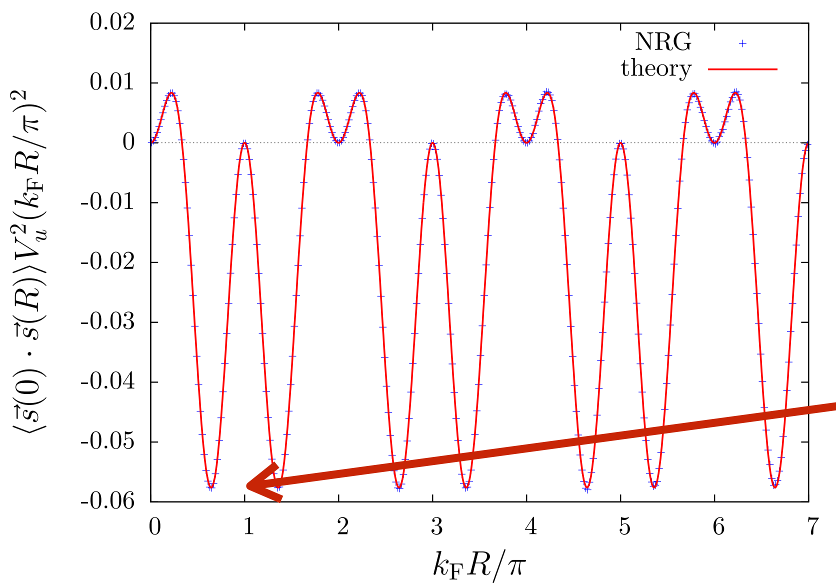

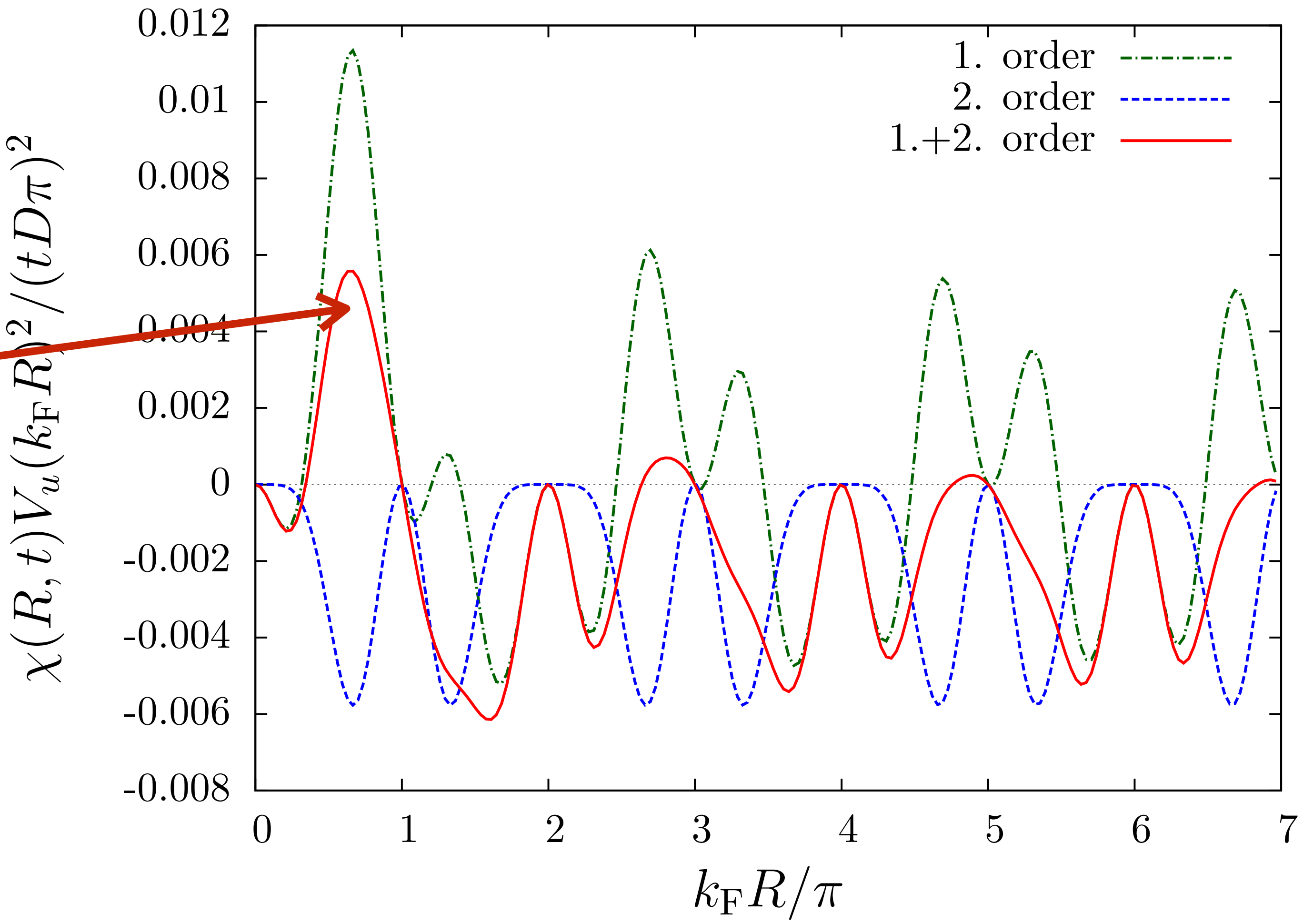

spatial spin-density correlation function: NRG vs analytic

perturbation theory

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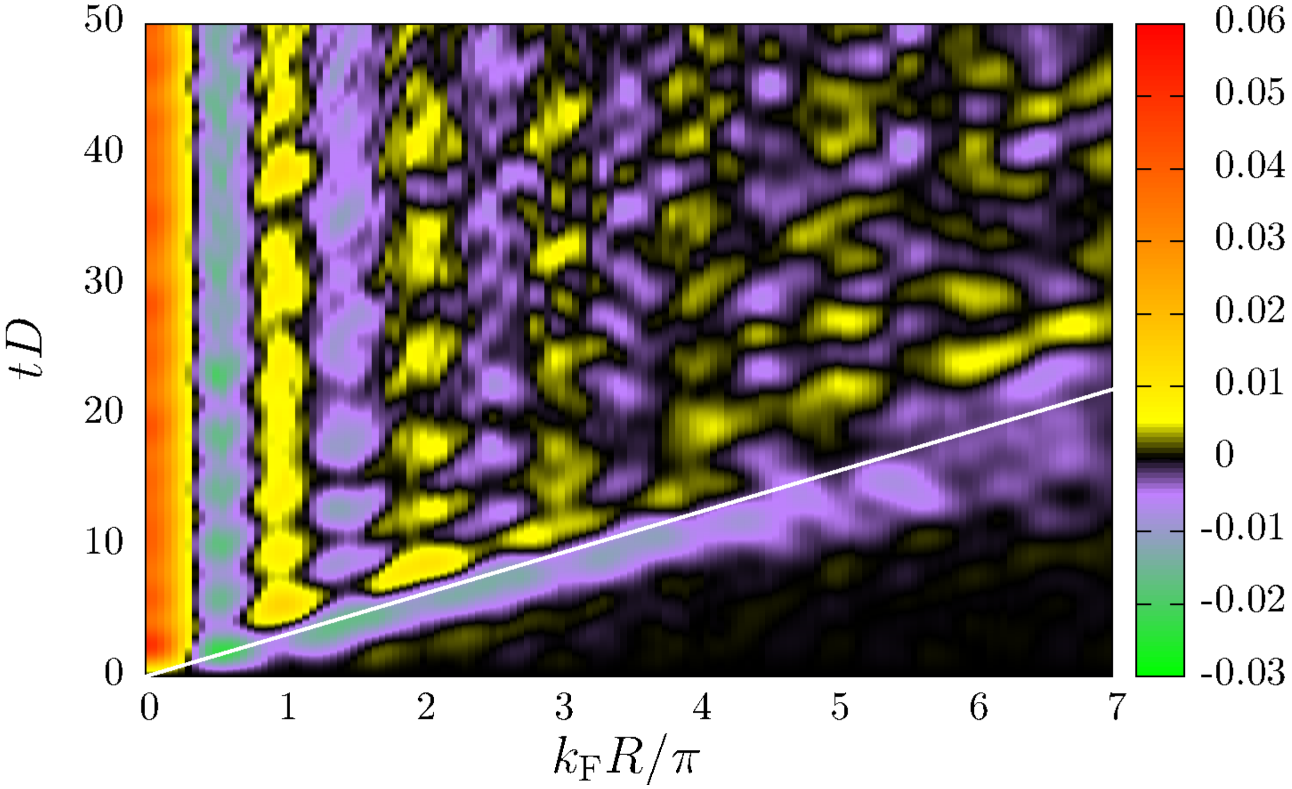
- maxima and minima coincide: AF coupling

$$\rho_0 J = -0.1$$



TD-NRG

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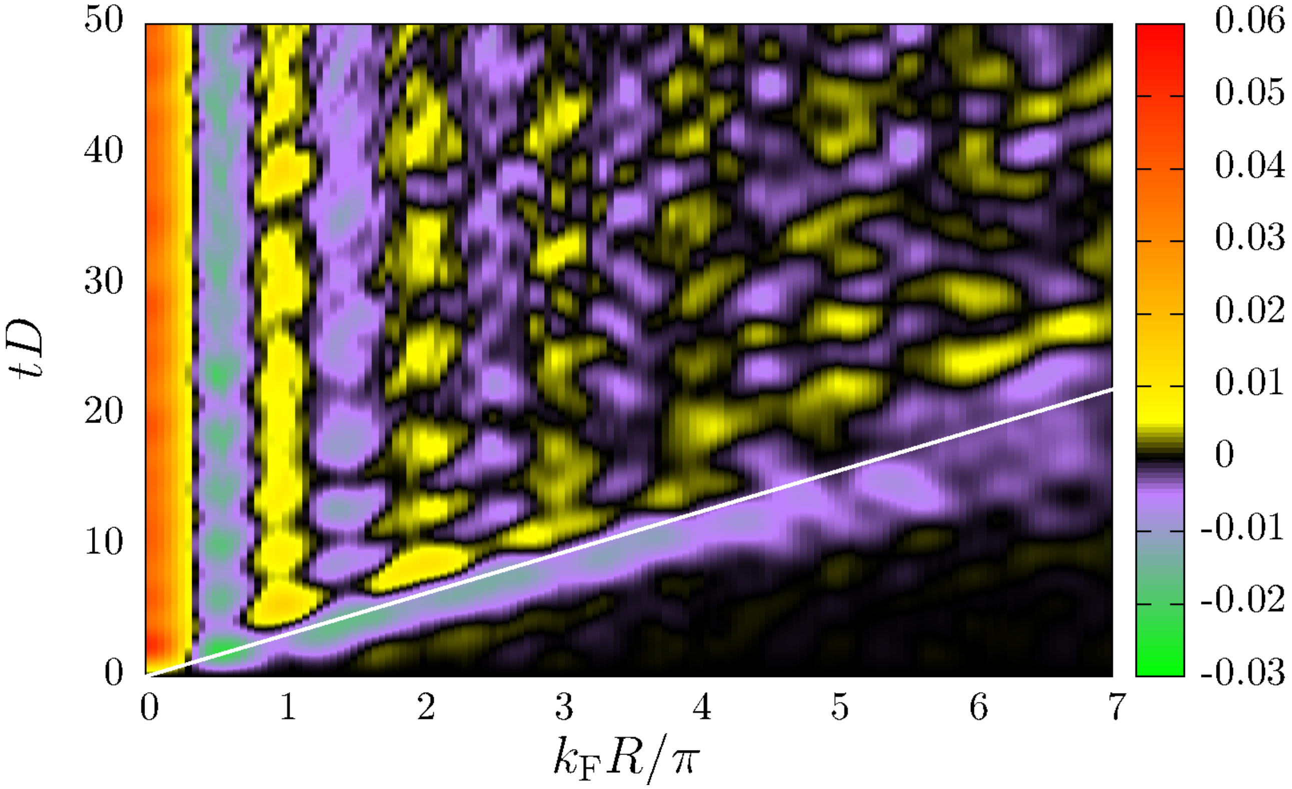
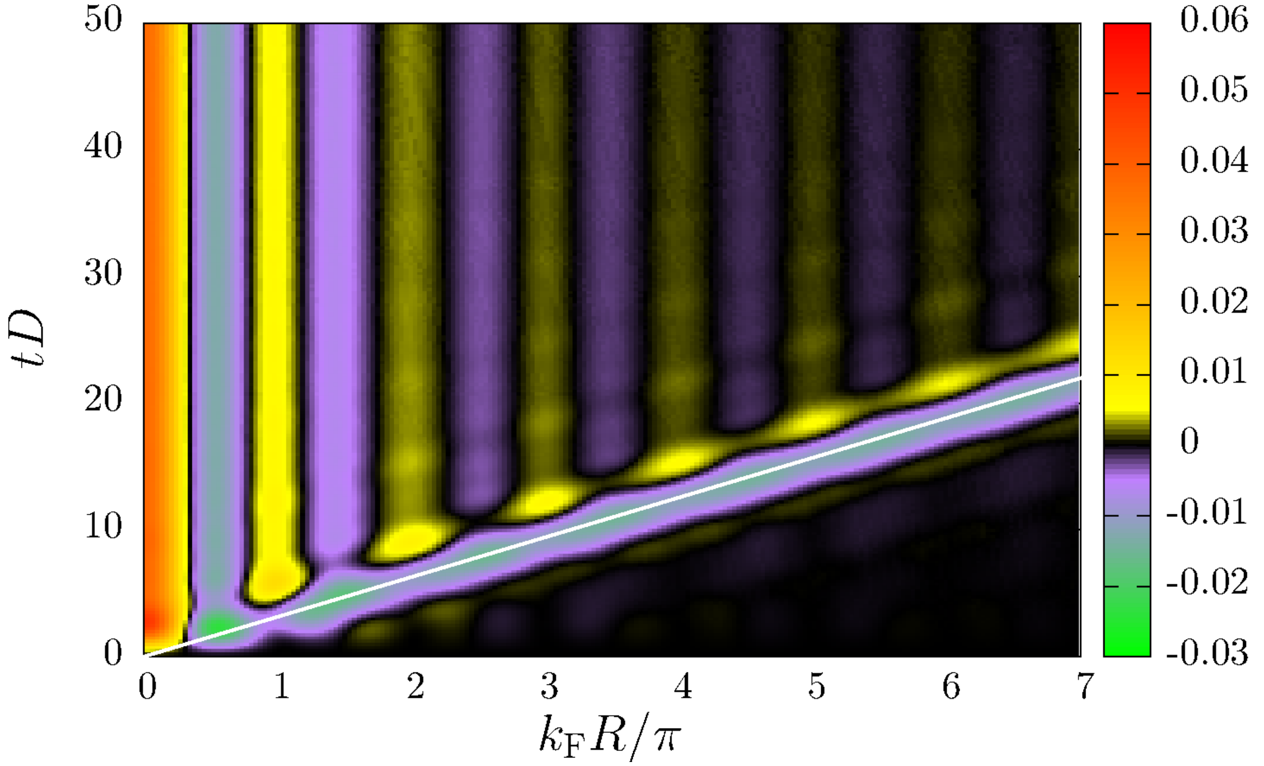


TD-NRG



second order perturbation theory

conclusion

- real-time dynamics of the spin-correlation $\chi(R,t)$ using the TD-NRG

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- outlook:
  - hybrid method: NRG+DMRG (Güttge, FBA, Schollwöck, Eidelstein, Schiller, PRB 87, 125115 (2013))
  - pulses: (Eidelstein, Schiller, Güttge, FBA, PRB 85, 075118 (2012))
  - general Hamiltonians by Costi and coworkers (PRB 2014)

Thank you for your attention!