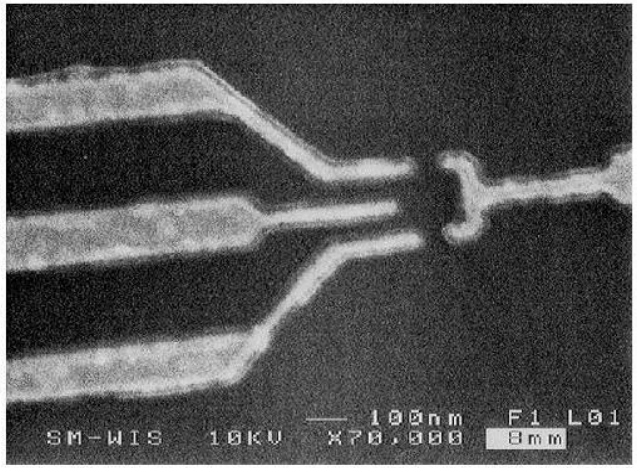
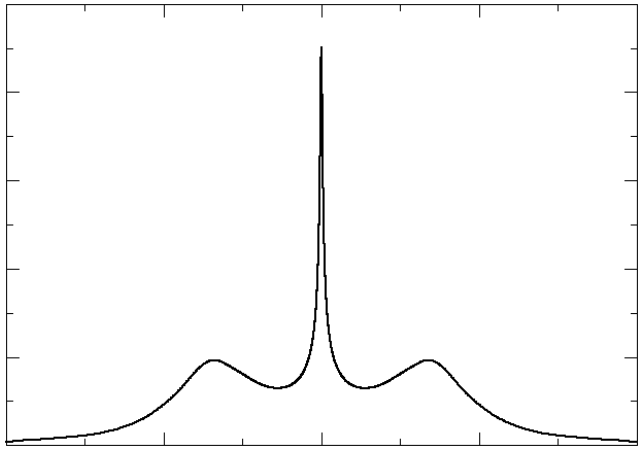
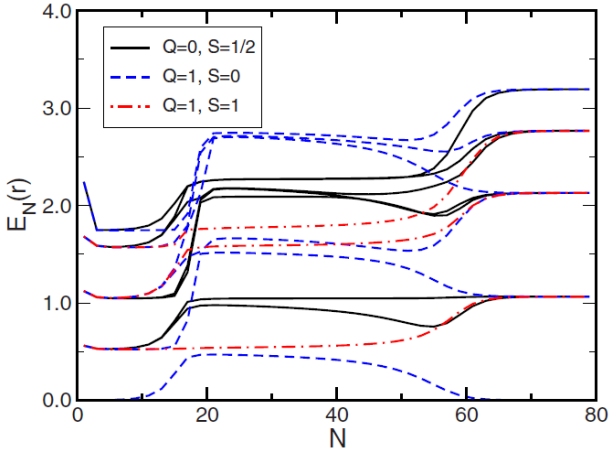
NUMERICAL METHODS FOR QUANTUM IMPURITY MODELS







http://www.staff.science.uu.nl/~mitch003/nrg.html

March 2015

Andrew Mitchell, Utrecht University

Quantum impurity problems

- **Part 1: Quantum impurity problems and theoretical background**
- **Part 2: Kondo effect and RG. 1d chain formulation and iterative diagonalization**
- **Part 3: Logarithmic discretization and truncation. The RG in NRG**
- **Part 4: Physical quantities. Results and discussion.**

NUMERICAL METHODS FOR QUANTUM IMPURITY MODELS

Part 2: Kondo effect and the Renormalization Group

March 2015

Andrew Mitchell, Utrecht University

Overview: Part 2

- **Kondo effect**
- **Perturbation theory**
- **Perturbative scaling**

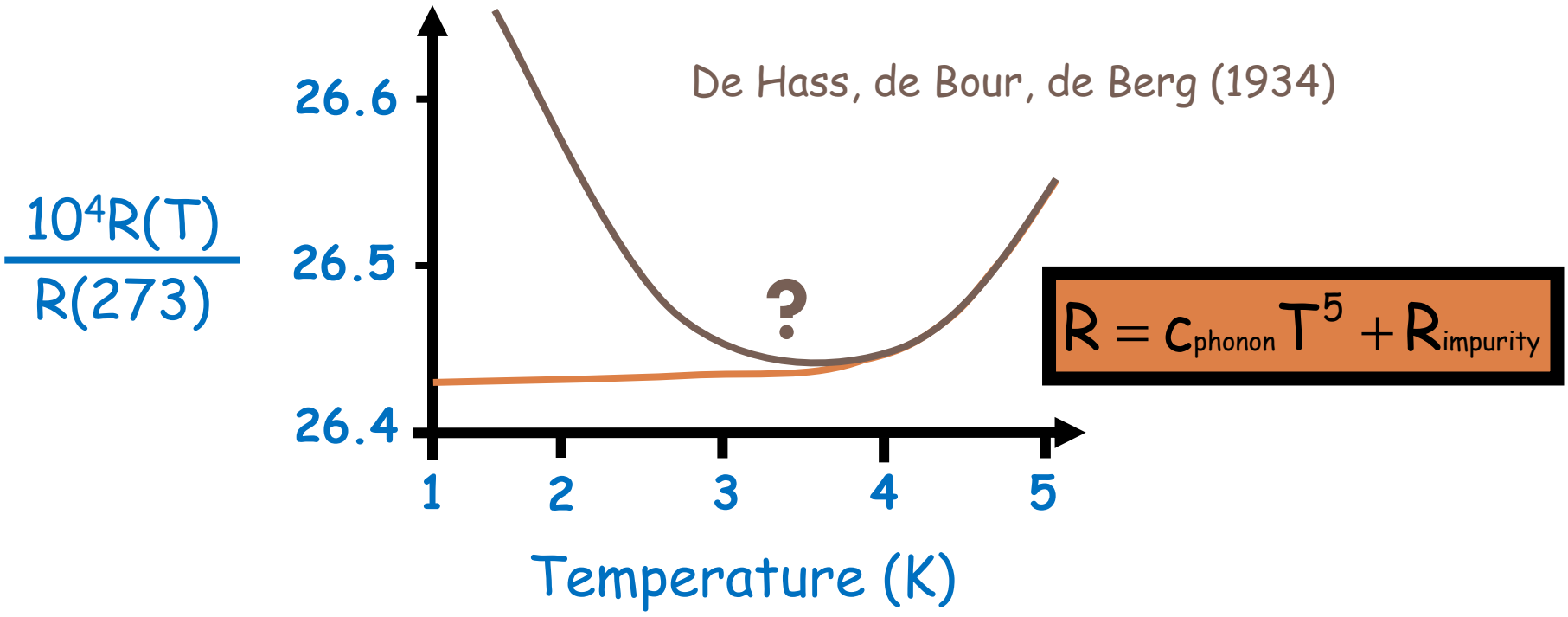
- **Mapping to 1d chain**

- **Iterative diagonalization**

Magnetic impurities

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

- **Resistance of metals:**
- **Experiments reveal low-temperature minimum**



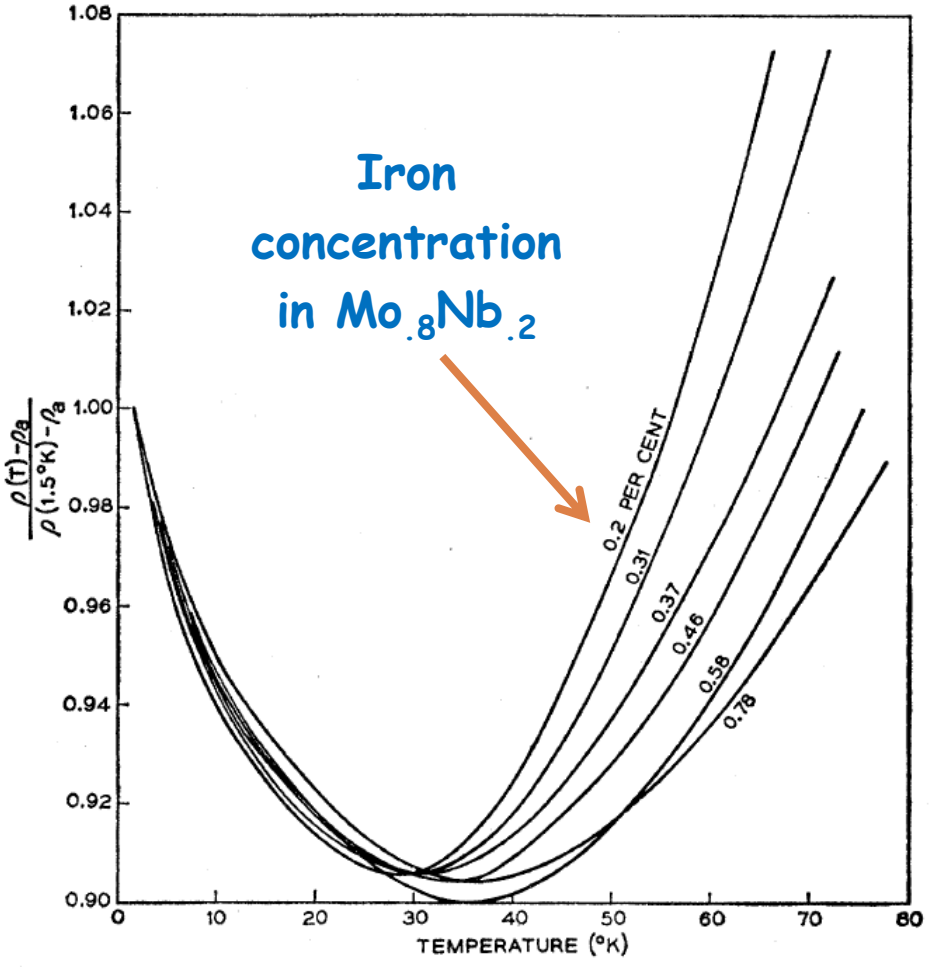
Magnetic impurities

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

- **Resistance minimum an *impurity* effect**

$$T_{min} \propto (c_{imp})^{1/5}$$

- **Conduction electrons scatter off impurities**

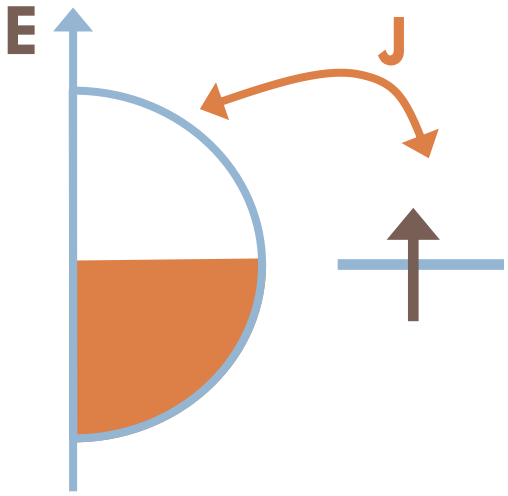


M. Sarachik et al. 1964

Recap: Kondo model

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

- **Scattering from magnetic impurities**
  - Single spin-½ impurity
  - Bath of non-interacting conduction electrons
  - AF Exchange coupling



$$H_K = H_{host} + J\,\vec{S}_{imp}\cdot\vec{s}_0$$

$$\sum_{k\sigma}\varepsilon_k c^\dagger_{k\sigma}c_{k\sigma}$$

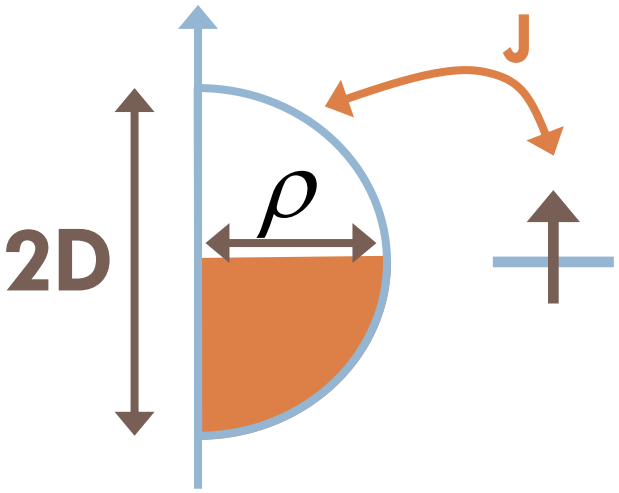
impurity spin-½

conduction electron spin density

The Kondo problem

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

- 3rd order perturbation theory in J:



$$R = c_{phonons} T^5 + R_{impurity} + c_{imp}\left[J^2 + \rho J^3 \mathrm{Log}\left(\frac{D}{T}\right)\right]$$

Resistance minimum ✓

$$T_{min} \propto (c_{imp})^{1/5}$$ ✓

The Kondo problem

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

- **Obviously: perturbation theory fails at low T:**

$$\rho J^3 \mathrm{Log}(D/T) > J^2 \rightarrow T_K = D\, e^{-1/\rho J}$$

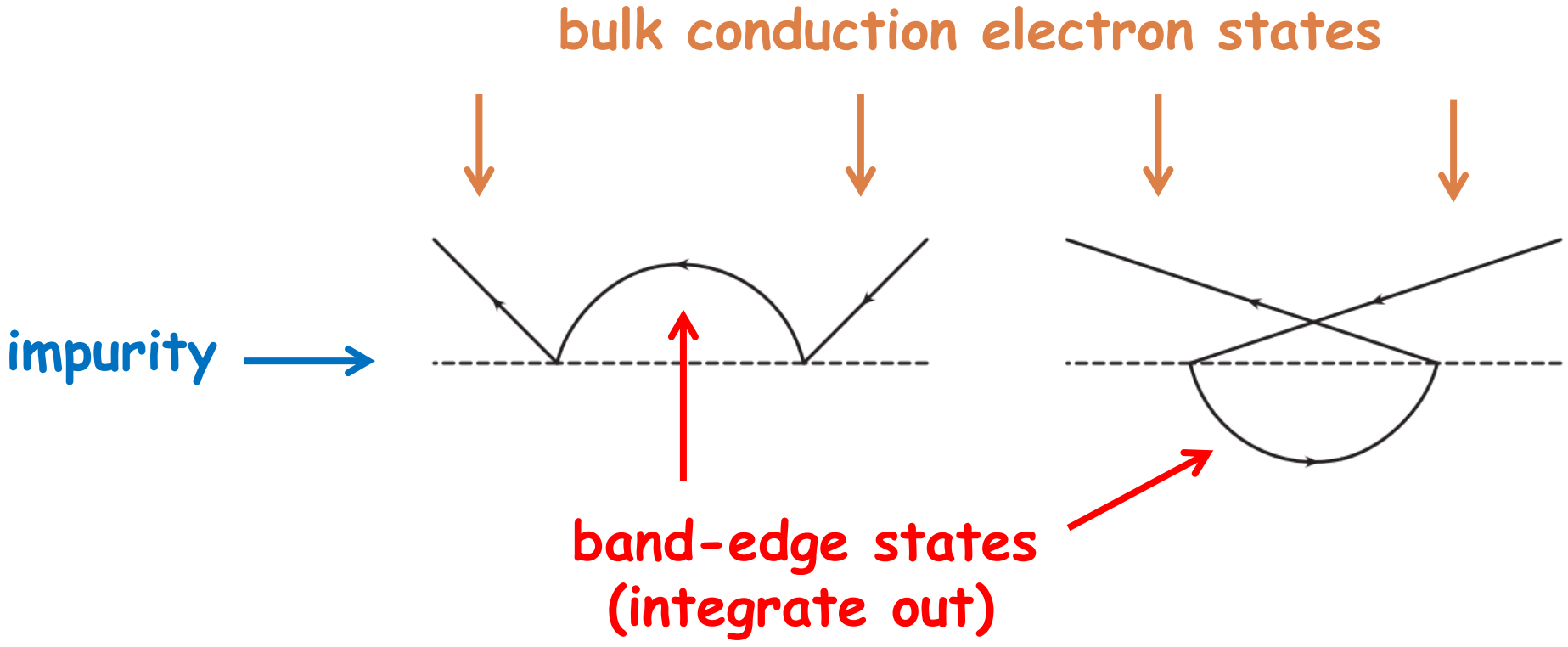
- **What happens below T_K?**

- **What is the ground state?**

Scaling and Renormalization

- **Look at physics at a lower energy scale**

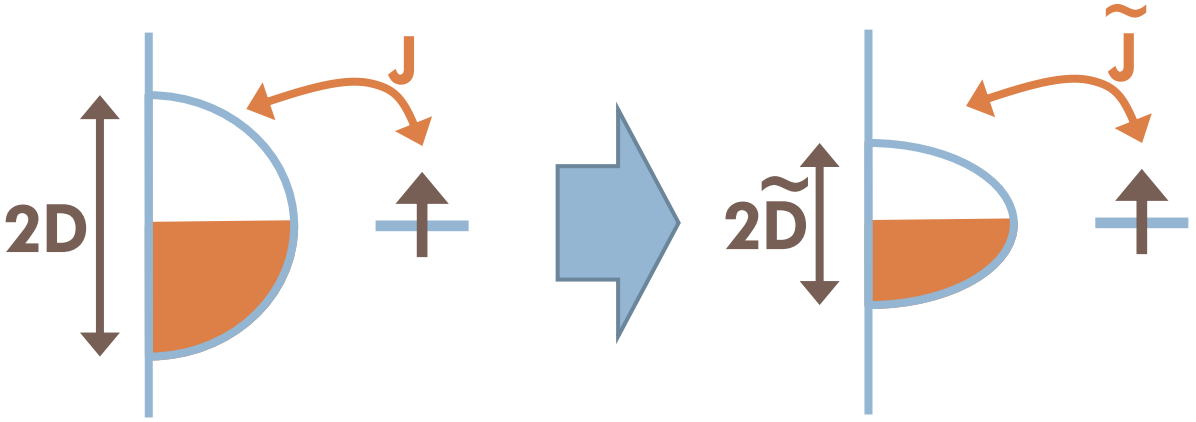
  P. W. Anderson, J. Phys. C 3, 2436 (1970)



Scaling and Renormalization

- **Map to a Kondo model of the same form**

  P. W. Anderson, J. Phys. C 3, 2436 (1970)



Consider a sequence of Hamiltonians with different effective (renormalized) parameters

Fixed points

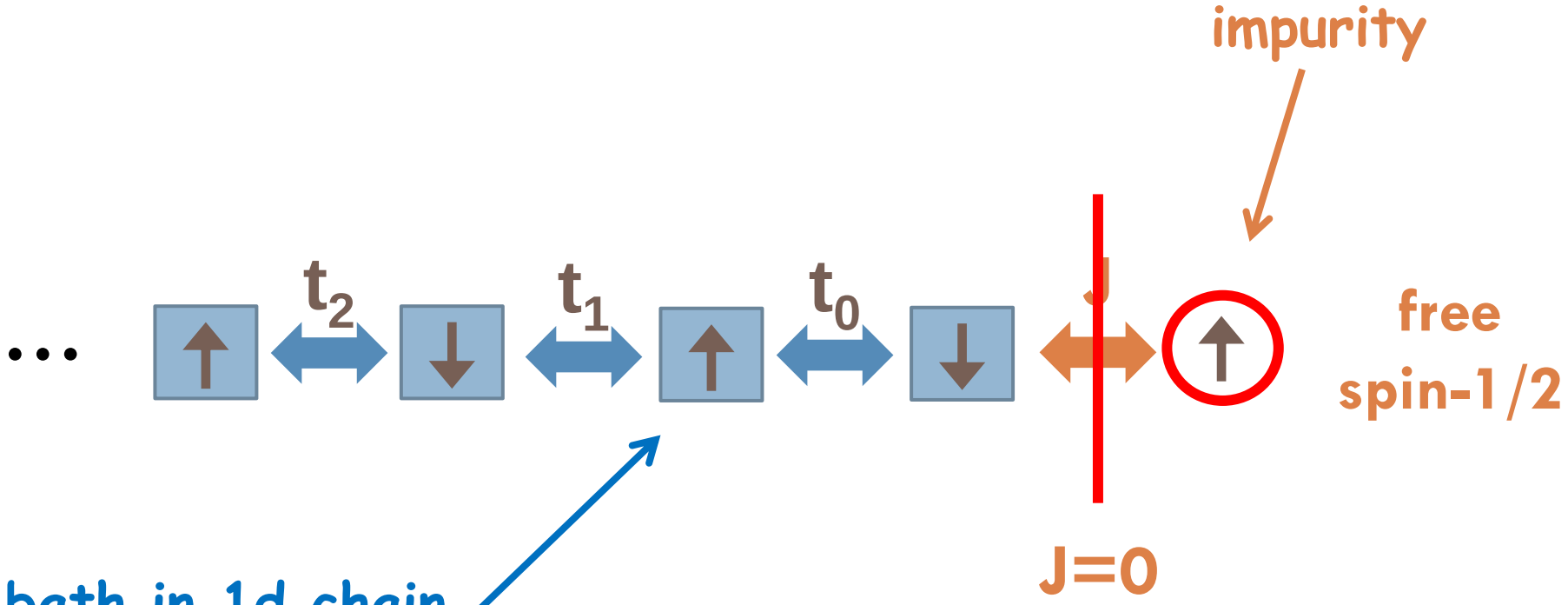
- **Special values of the parameters produce NO renormalization → "fixed points"**

- **Kondo model:**
  - **Local Moment (LM) fixed point: J=0**
  - **Strong coupling (SC) fixed point: J= ∞**

RG fixed points

see Alex Hewson's book
"The Kondo Problem..."
CUP (1997)

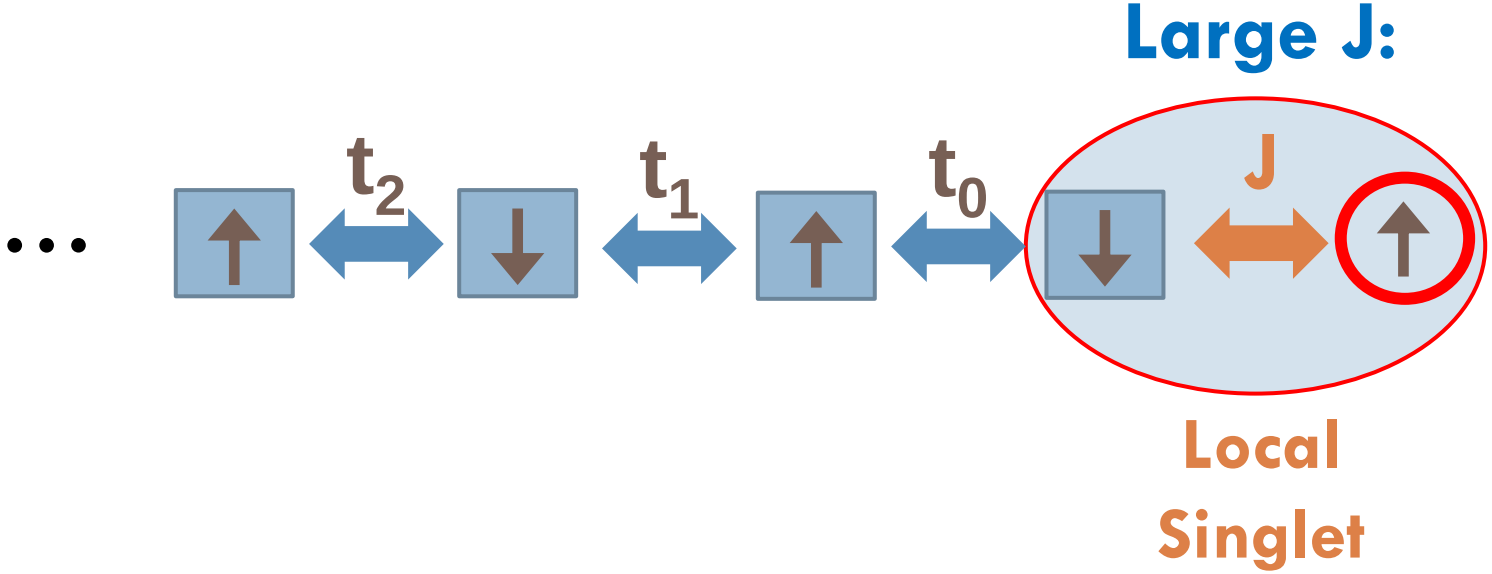
- **Small J: weak coupling**
  - **free impurity local moment**



RG fixed points

see Alex Hewson's book
"The Kondo Problem…"
CUP (1997)

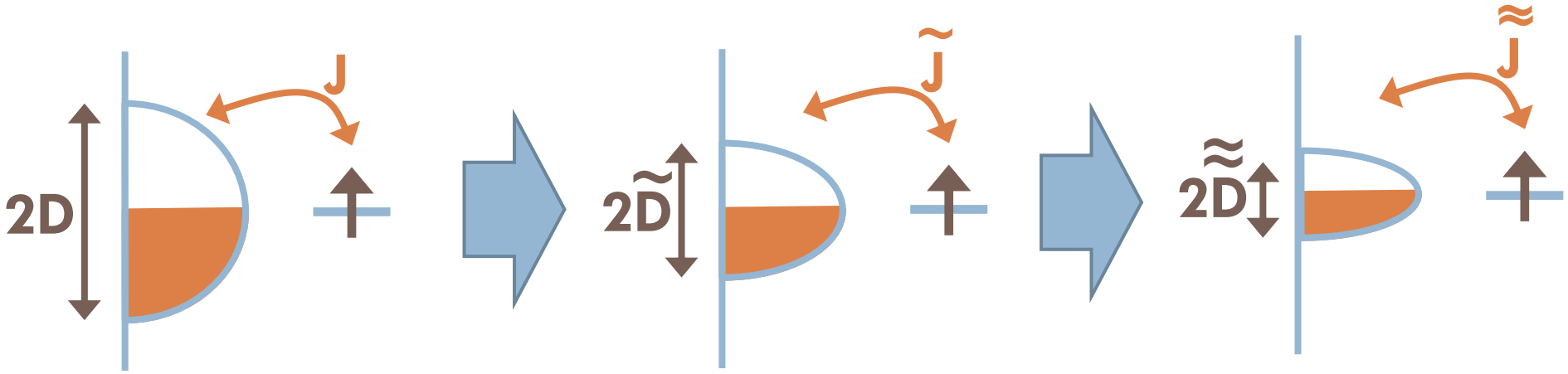
- **Large J: strong coupling state**
  - **Impurity forms spin-singlet with conduction electrons**



Scaling and Renormalization

- **Look at physics on successively lower energy scales**

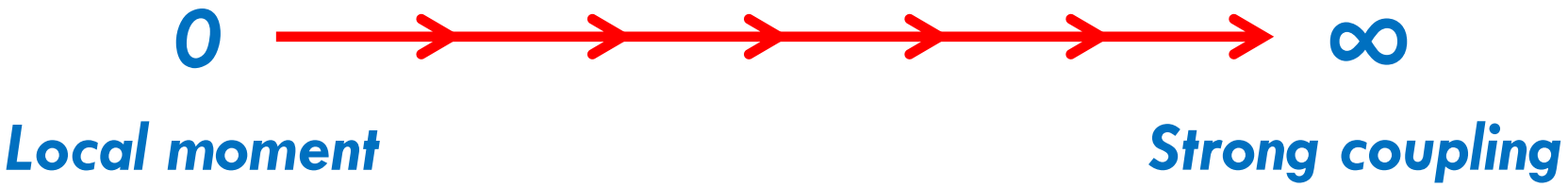
  P. W. Anderson, J. Phys. C 3, 2436 (1970)



$$\frac{\mathrm{d}\,\rho J}{\mathrm{d}\,\ln D} = -2(\rho J)^2 + \ldots \quad \Rightarrow \quad D\,e^{-1/\rho J} = \tilde{D}\,e^{-1/\rho \tilde{J}} \sim k_B T_K$$

Scaling and Renormalization

- **For (initially) weak coupling, perturbative scaling indicates that coupling J grows under RG**

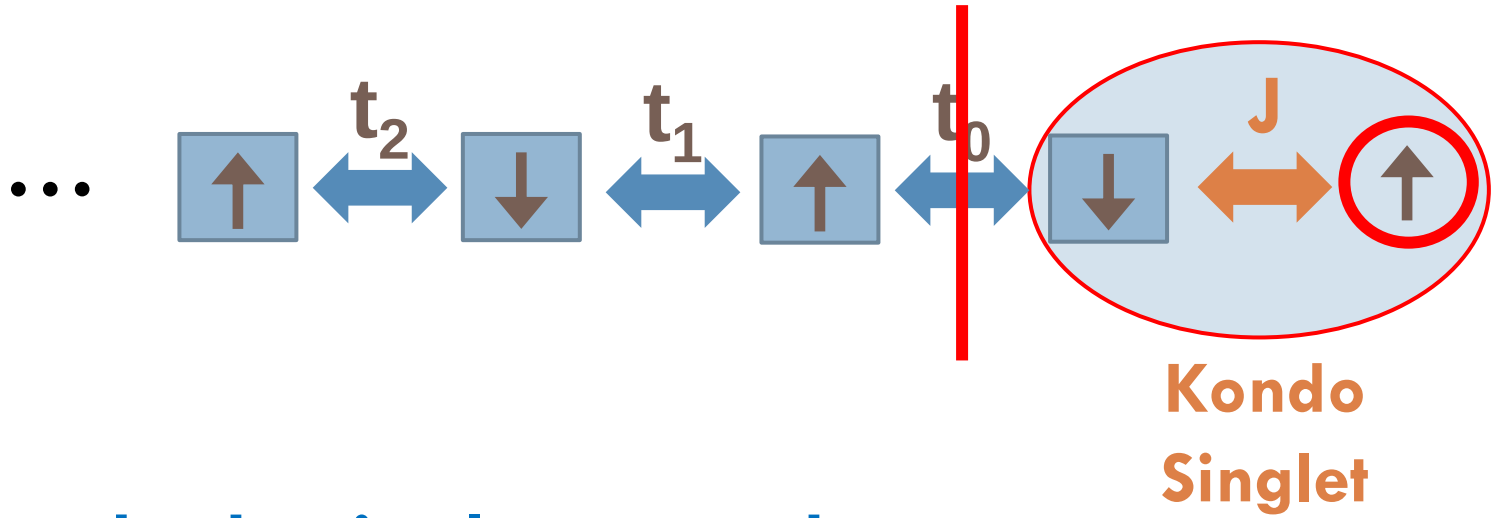


RG flow

see Alex Hewson's book
"The Kondo Problem…"
CUP (1997)

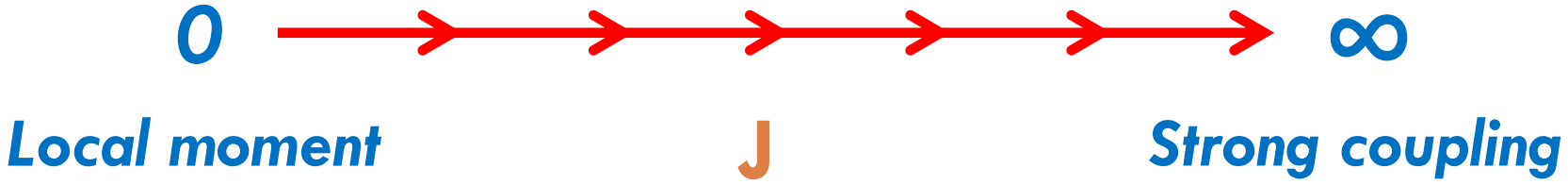
- So: when coupling is initially small…

  … it grows under RG and becomes large



many-body singlet ground state
(complicated real-space structure)

RG flow



BUT: analysis breaks down before $J \sim O(1)$

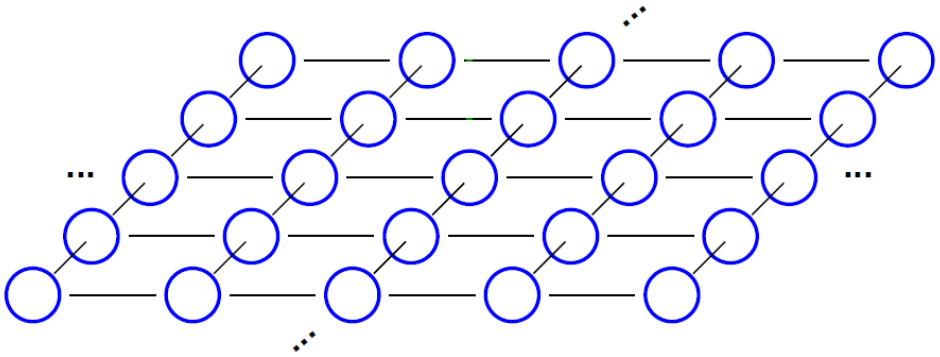
- **Need a non-perturbative approach!**
  - **Must be able to handle *large* energy scales: D, J etc.**
  - **… and *exponentially small* scales, T_K**
  - **Exploit *RG* character of the problem**

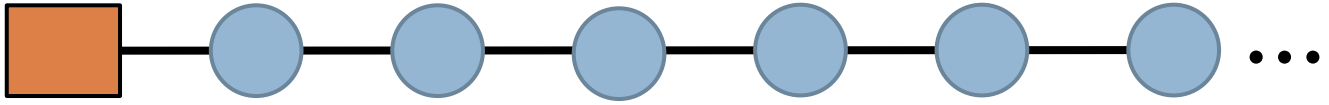
Numerical Renormalization Group

- **(very) brief description of NRG:**
  - **Logarithmic discretization of bath**
  - **Mapping to 1d chain**
  - **Iterative diagonalization**
  - **Successive Hilbert-space truncation**

NRG: preliminaries

- **1d chain representation**
  - **Any non-interacting system can be mapped to a 1d tight-binding chain: "Tridiagonalization"**



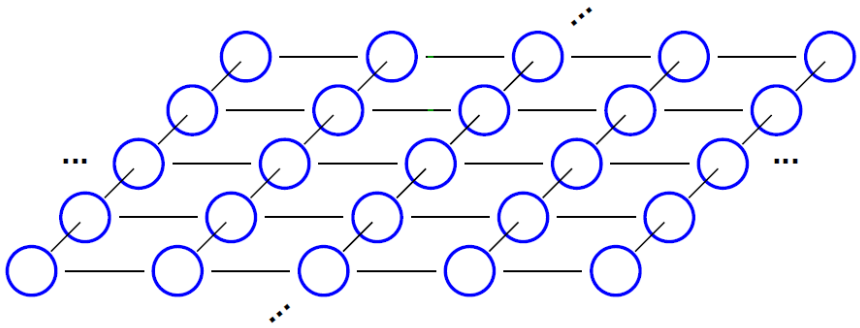


Recap: real-space representation

- **Host metal: non-interacting tight-binding model**

$$H_{host} = \sum_{\sigma} \sum_{<i,j>} t_{ij}\, c^{\dagger}_{i\sigma} c_{j\sigma}$$

$$\equiv \sum_{\sigma} \vec{c}^{\,\dagger}_{\sigma}\, \underline{\underline{T}}\, \vec{c}_{\sigma}$$



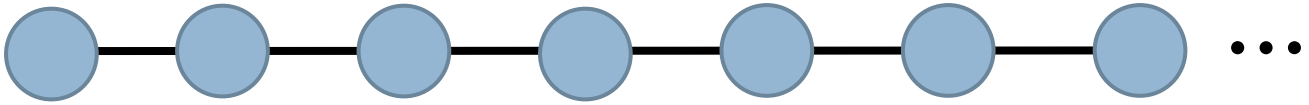
$$\vec{c}^{\,\dagger}_{\sigma} = \left(c^{\dagger}_{1\sigma},\ c^{\dagger}_{2\sigma},\ c^{\dagger}_{3\sigma},\ \ldots \right) \quad ; \quad \underline{\underline{T}} = \begin{bmatrix} t_{11} & t_{12} & \cdots \\ t^{*}_{12} & t_{22} & \\ \vdots & & \ddots \end{bmatrix}$$

Tridiagonal

- **Host metal: 1d chain representation**

$$H_{host} = \sum_{\sigma} \vec{c}^{\,\dagger}_{\sigma} \underline{\underline{T}}\, \vec{c}_{\sigma} = \sum_{\sigma} \vec{f}^{\,\dagger}_{\sigma} \underline{\underline{W}}\, \vec{f}_{\sigma}$$

$$= \sum_{\sigma} \sum_{n} e_n \, f^{\dagger}_{n\sigma} f_{n\sigma} + \left(h_n \, f^{\dagger}_{n\sigma} f_{(n+1)\sigma} + \text{H.c.} \right)$$



where, $\vec{f}_{\sigma} = \underline{\underline{S}}\, \vec{c}_{\sigma}$ **such that,** $\underline{\underline{W}} = \underline{\underline{S}}^{\dagger}\, \underline{\underline{T}}\, \underline{\underline{S}}$

Tridiagonal

$$H_{host} = \sum_{\sigma} \vec{c}^{\,\dagger}_{\sigma} \underline{\underline{T}} \vec{c}_{\sigma} = \sum_{\sigma} \vec{f}^{\,\dagger}_{\sigma} \underline{\underline{W}} \vec{f}_{\sigma}$$

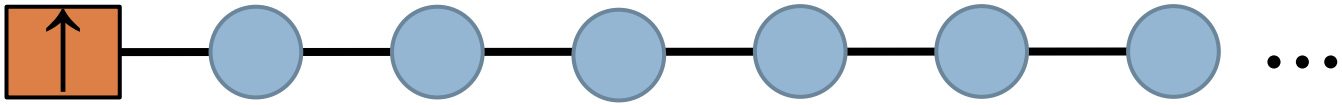
$$= \sum_{\sigma} \sum_{n} e_n \, f^{\dagger}_{n\sigma} f_{n\sigma} + \left(h_n \, f^{\dagger}_{n\sigma} f_{(n+1)\sigma} + \text{H.c.} \right)$$

$$\begin{bmatrix} t_{11} & t_{12} & t_{13} & t_{14} \\ t_{21} & t_{22} & t_{23} & t_{24} \\ t_{31} & t_{32} & t_{33} & t_{34} \\ t_{41} & t_{42} & t_{43} & t_{44} \end{bmatrix} \Rightarrow \begin{bmatrix} e_1 & h_1 & 0 & 0 \\ h_1 & e_2 & h_2 & 0 \\ 0 & h_2 & e_3 & h_3 \\ 0 & 0 & h_3 & e_4 \end{bmatrix}$$

$\underline{\underline{T}}$ $\qquad$ $\underline{\underline{W}}$

Impurity problem as a 1d chain

- **1d chain representation of impurity problem**



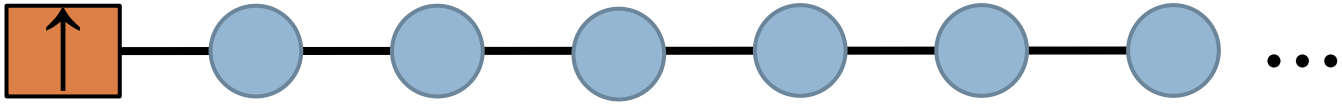
impurity

Choose 'zero-orbital' of the conduction electron chain to be the physical host orbital coupled to the impurity in real-space

$$f_{0\sigma} = c_{0\sigma} \quad \Rightarrow \quad \vec{s}_0 = \sum_{\sigma,\sigma'} f^{\dagger}_{0\sigma} \frac{\vec{\sigma}_{\sigma\sigma'}}{2} f_{0\sigma'}$$

Impurity problem as a 1d chain

- **1d chain representation of impurity problem**

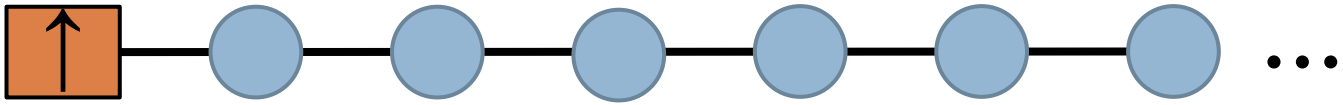


$$H_{Kondo} = H_{host} + H_{imp}$$

$$H_{imp} = J\,\vec{S}_{imp} \cdot \vec{s}_0$$

$$H_{host} = \sum_{\sigma}\sum_{n} e_n\, f^{\dagger}_{n\sigma} f_{n\sigma} + \left(h_n\, f^{\dagger}_{n\sigma} f_{(n+1)\sigma} + \text{H.c.} \right)$$

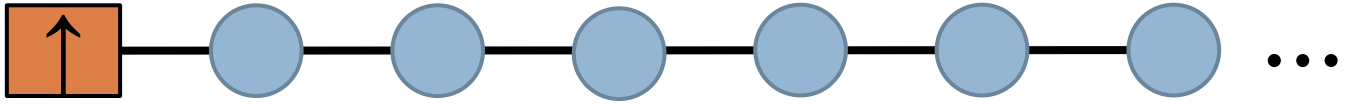
Impurity problem as a 1d chain



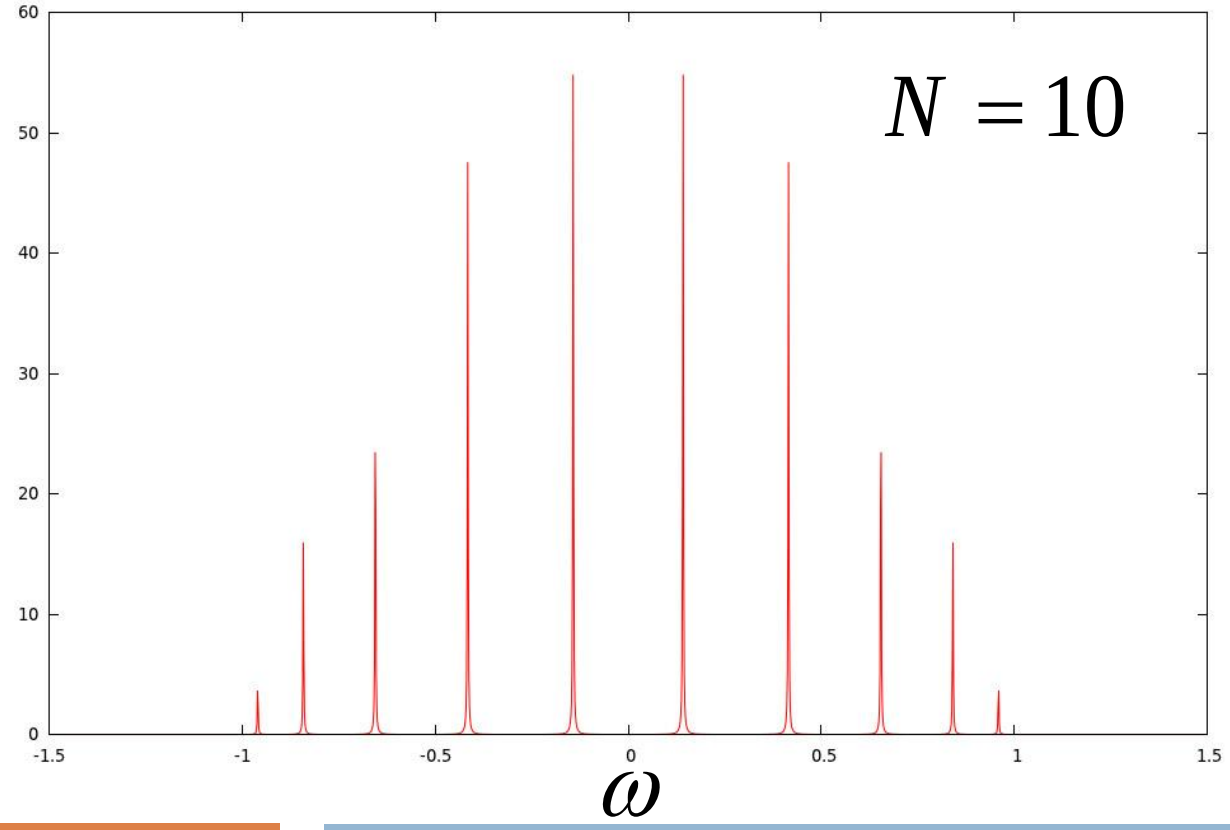
- **Idea: truncate chain?**
  - **Represent bath by the first N sites of the chain?**
  - **Then exact diagonalization of approximate model?**

Impurity problem as a 1d chain

Bath: 1d chain with constant hopping and onsite energies



$\rho_{0\sigma}(\omega)$

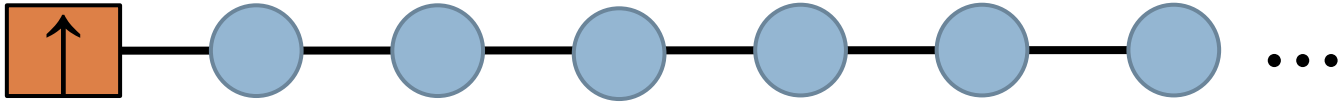


$$t_i \equiv t = \frac{1}{2}$$

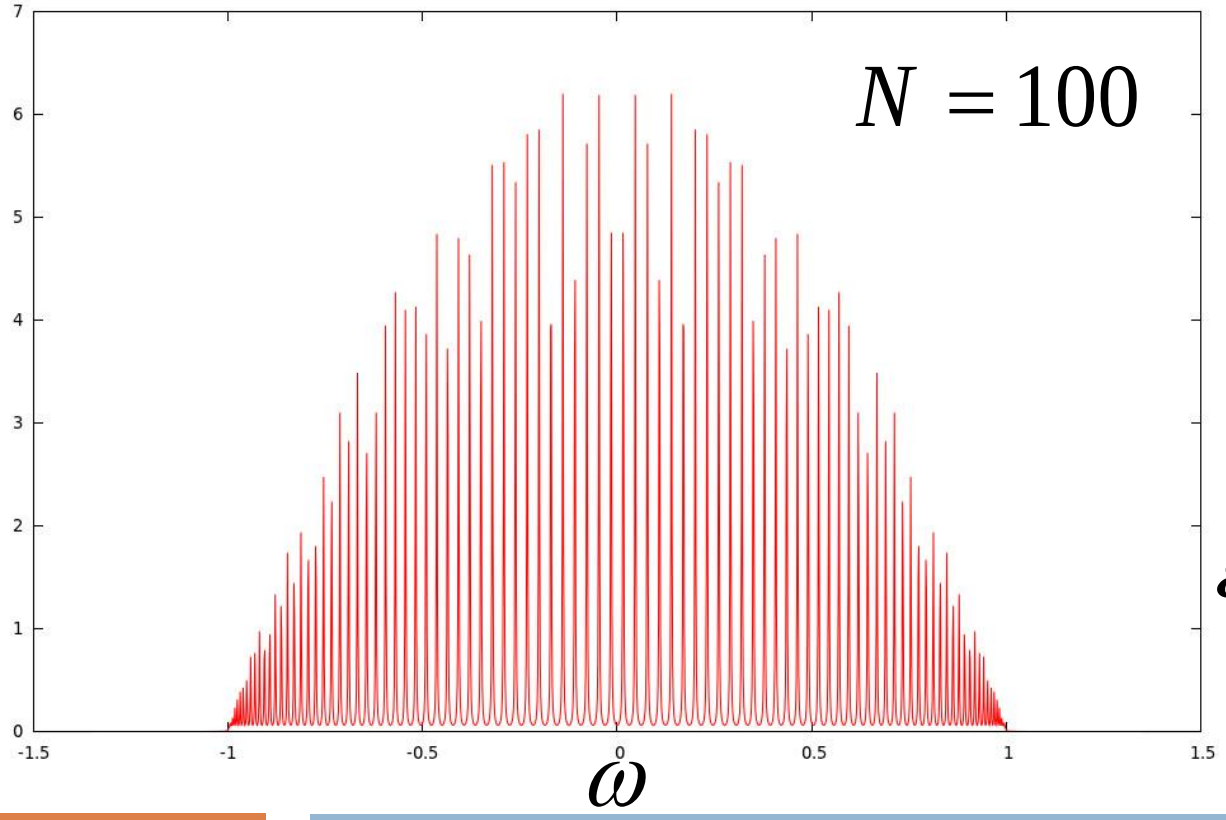
$$\varepsilon_i \equiv \varepsilon = 0$$

Impurity problem as a 1d chain

Bath: 1d chain with constant hopping and onsite energies



$\rho_{0\sigma}(\omega)$



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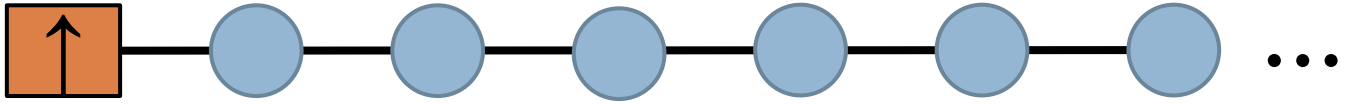
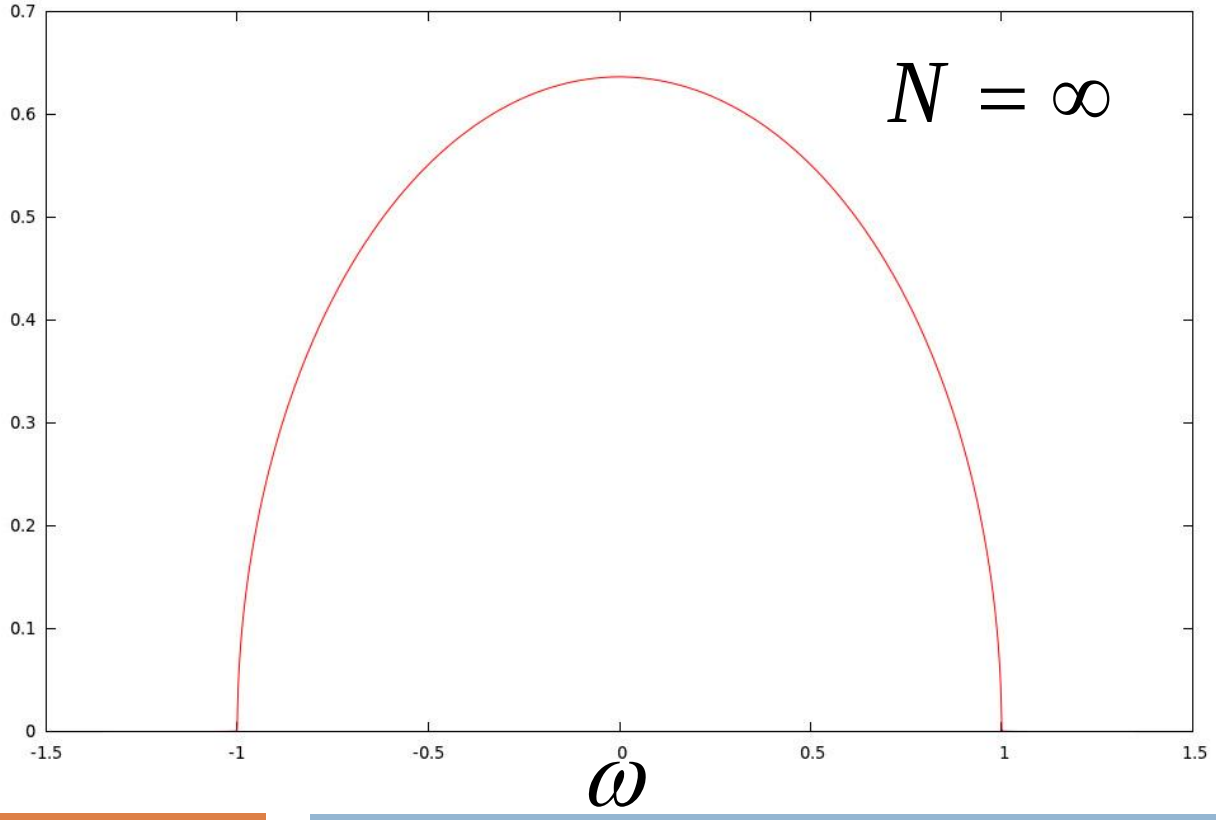
Impurity problem as a 1d chain

Bath: 1d chain with constant hopping and onsite energies



$\rho_{0\sigma}(\omega)$



$$t_i \equiv t = \frac{1}{2}$$

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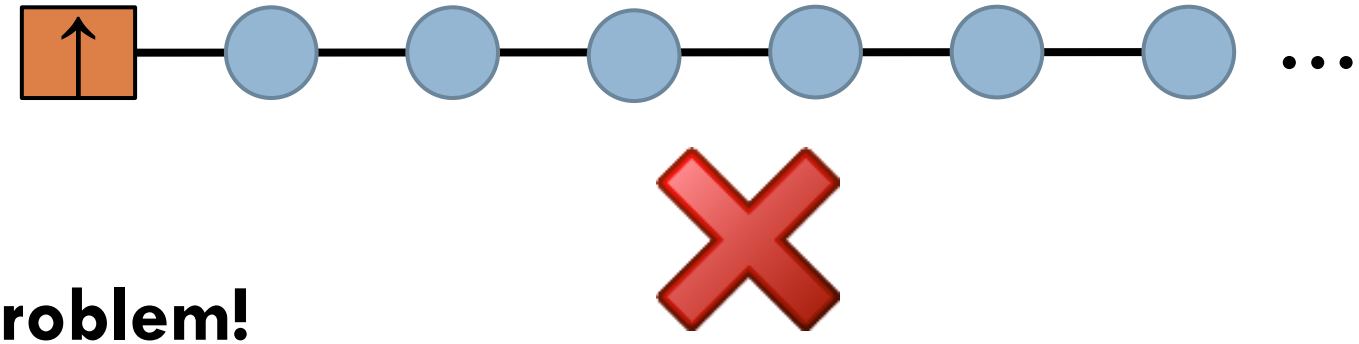
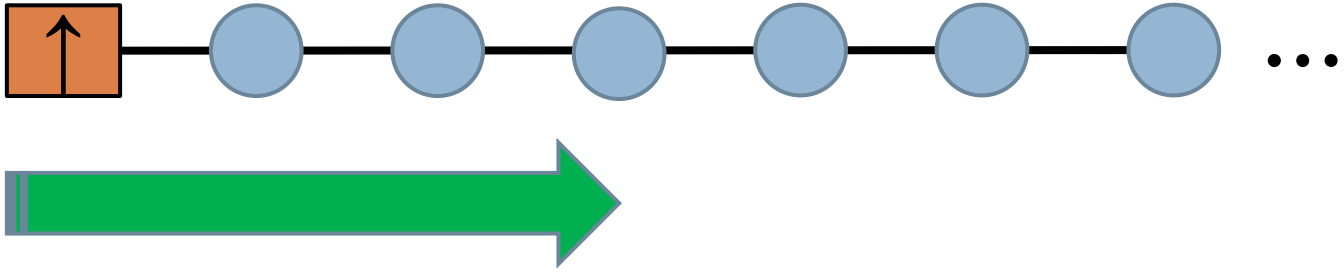
Impurity problem as a 1d chain



- **Problem!**
  - **Continuum limit not well-described by finite chain!**
  - **Spectrum has *N* poles for an *N*-site chain**
  - **Lowest energy scale resolved is of order** $\sim t / N$
  - **Unable to capture low-energy excitations around Fermi level, which are central to the Kondo effect**

Impurity problem as a 1d chain



- **Idea in NRG: diagonalize the chain iteratively**
  - **Throw away unimportant states at each step (successively truncate the Hilbert space)**
  - **Which states are unimportant?!**

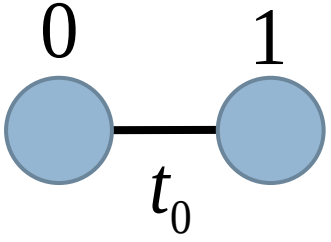
… more on that in next lecture!

Iterative diagonalization

- **Take the 'generic' tight-binding 1d chain**

$$H_N = \sum_{i=0}^{N-1} \sum_{\sigma} t_i c^{\dagger}_{i\sigma} c_{(i+1)\sigma} + \text{H.c.} \quad + \varepsilon_i c^{\dagger}_{i\sigma} c_{i\sigma}$$

- **Strategy: build up chain *successively* by adding on extra sites. Start by diagonalizing the dimer:**



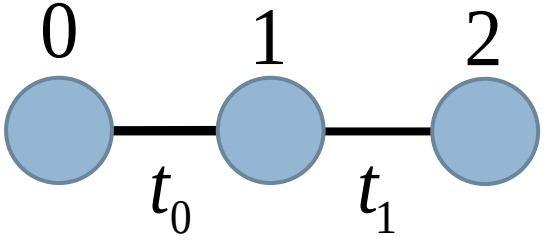
$$H_1 = \sum_{\sigma} t_0 c^{\dagger}_{0\sigma} c_{1\sigma} + \text{H.c.}$$

Iterative diagonalization

- **Take the 'generic' tight-binding 1d chain**

$$H_N = \sum_{i=0}^{N-1} \sum_{\sigma} t_i c^{\dagger}_{i\sigma} c_{(i+1)\sigma} + \text{H.c.}$$

- **Strategy: build up chain *successively* by adding on extra sites. Start by diagonalizing the dimer:**



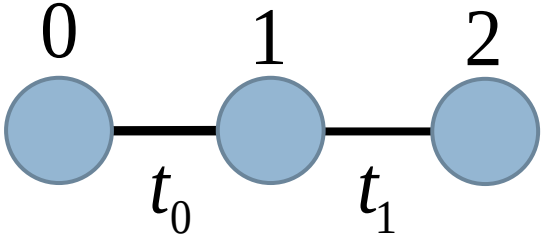
$$H_2 = \sum_{\sigma} t_0 c^{\dagger}_{0\sigma} c_{1\sigma} + t_1 c^{\dagger}_{1\sigma} c_{2\sigma} + \text{H.c.}$$

Iterative diagonalization

- **Take the 'generic' tight-binding 1d chain**

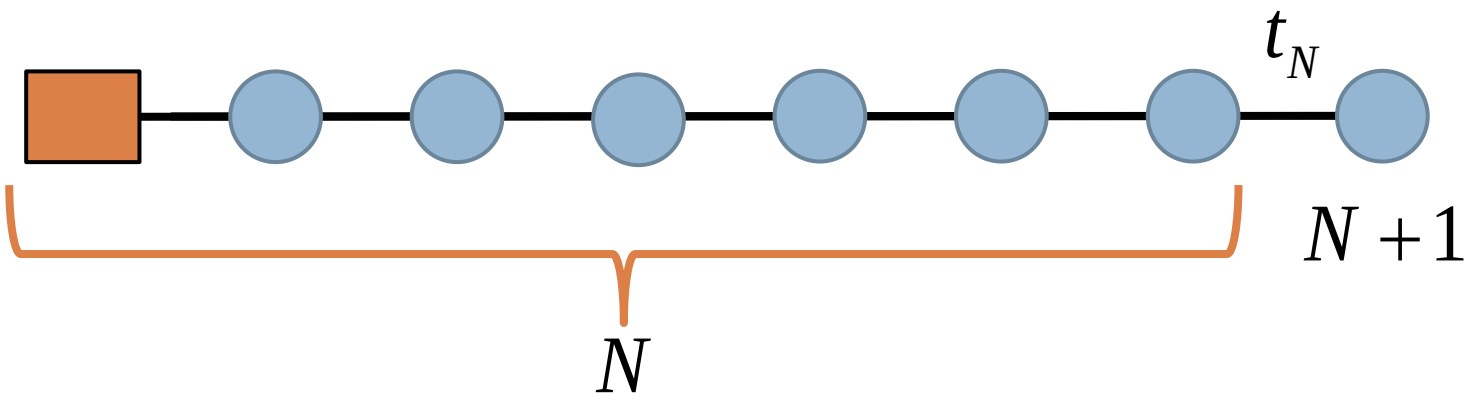
$$H_N = \sum_{i=0}^{N-1} \sum_{\sigma} t_i c^{\dagger}_{i\sigma} c_{(i+1)\sigma} + \text{H.c.}$$

- **Strategy: build up chain *successively* by adding on extra sites. Start by diagonalizing the dimer:**



$$H_2 = H_1 + \sum_{\sigma} t_1 c^{\dagger}_{1\sigma} c_{2\sigma} + \text{H.c.}$$

Iterative diagonalization



Recursion:

$$H_{N+1} = H_N + H^{hop}_{N+1}$$

$$H^{hop}_{N+1} = \sum_\sigma t_N c^\dagger_{N\sigma} c_{(N+1)\sigma} + \text{H.c.}$$

… same transformation for any *N* !

Iterative diagonalization

- Use the ***diagonal basis*** of iteration ***N*** and couple on an extra site. Then re-diagonalize.
- First, define matrix product states:

$$\left|N+1;k,r\right\rangle_{bs} = \left|N+1;k\right\rangle_{a} \otimes \left|N;r\right\rangle_{d}$$

Basis states for iteration N+1

Basis states for a single added site

Direct product

Diagonal states of previous iteration, N

Iterative diagonalization

- States of added site defined by:

$$\left|N+1;k=0\right\rangle_a = \left|-\right\rangle = \left|vac\right\rangle$$

$$\left|N+1;k=+1\right\rangle_a = \left|\uparrow\right\rangle = c^\dagger_{(N+1)\uparrow}\left|vac\right\rangle$$

$$\left|N+1;k=-1\right\rangle_a = \left|\downarrow\right\rangle = c^\dagger_{(N+1)\downarrow}\left|vac\right\rangle$$

$$\left|N+1;k=2\right\rangle_a = \left|\uparrow\downarrow\right\rangle = c^\dagger_{(N+1)\uparrow}c^\dagger_{(N+1)\downarrow}\left|vac\right\rangle$$

Iterative diagonalization

- Diagonalized states expressed as a linear combination of basis states:

$$\left|N+1;r\right\rangle_d = \sum_{k,r'} U^r_{N+1}(k,r')\left|N+1;k,r'\right\rangle_{bs}$$

Coefficients obtained by diagonalizing matrix H_{N+1}

Iterative diagonalization

- Construct Hamiltonian: $H_{N+1} = H_N + H_{N+1}^{hop}$
- Matrix elements:

$$ {}_{bs}\langle N+1;k,r|H_{N+1}|N+1;k',r'\rangle_{bs} $$

$$ = {}_{d}\langle N;r|_{a}\langle N+1;k|H_{N+1}|N+1;k'\rangle_{a}|N;r'\rangle_{d} $$

$$ = {}_{d}\langle N;r|_{a}\langle N+1;k|H_{N}|N+1;k'\rangle_{a}|N;r'\rangle_{d} $$

$$ + t_N \sum_{\sigma} {}_{d}\langle N;r|_{a}\langle N+1;k|c^{\dagger}_{N\sigma}c_{(N+1)\sigma}|N+1;k'\rangle_{a}|N;r'\rangle_{d} $$

Iterative diagonalization

$$
{}_d\langle N;r|{}_a\langle N+1;k|H_N|N+1;k'\rangle_a|N;r'\rangle_d
$$

$$
= {}_a\langle N+1;k|N+1;k'\rangle_a \times {}_d\langle N;r|H_N|N;r'\rangle_d
$$

$\delta_{kk'}$

$E_N(r)\ \delta_{rr'}$

Iterative diagonalization

$$t_N \sum_{\sigma} \; {}_d\langle N;r|_a \langle N+1;k| c^{\dagger}_{N\sigma} \; \hat{\underline{1}} \; c_{(N+1)\sigma} |N+1;k'\rangle_a |N;r'\rangle_d$$

insert complete set of basis states:

$$\hat{\underline{1}} = \sum_{k'',r''} |N+1;k''\rangle_a |N;r''\rangle_d \; {}_d\langle N;r''|_a \langle N+1;k''|$$

Iterative diagonalization

$$(-1)^{k''}\,{}_a\langle N+1;k\,|\,N+1;k''\rangle_a\;\; c^{\dagger}_{N\sigma}$$

$$t_N \sum_{\sigma} \sum_{\text{k", r"}} {}_d\langle N;r\,|_a\langle N+1;k\,|c^{\dagger}_{N\sigma}\,|\,N+1;k''\rangle_a|\,N;r''\rangle_d$$

$$\times\; {}_d\langle N;r''\,|_a\langle N+1;k''\,|c_{(N+1)\sigma}\,|\,N+1;k'\rangle_a|\,N;r'\rangle_d$$

Iterative diagonalization

$$\delta_{k,k''}\,(-1)^{k}\;\; c^{\dagger}_{N\sigma}$$

$$t_N \sum_{\sigma} \sum_{\mathrm{k''},\,\mathrm{r''}} {}_d\langle N;r|_a\langle N+1;k|c^{\dagger}_{N\sigma}|N+1;k''\rangle_a|N;r''\rangle_d$$

$$\times\ {}_d\langle N;r''|_a\langle N+1;k''|c_{(N+1)\sigma}|N+1;k'\rangle_a|N;r'\rangle_d$$

Iterative diagonalization

$$\delta_{k,k''}\ (-1)^k \times {}_d\langle N;r|\, c^\dagger_{N\sigma}\,|N;r''\rangle_d$$

$$t_N \sum_\sigma \sum_{\mathrm{k''},\,\mathrm{r''}} {}_d\langle N;r|_a\langle N+1;k|c^\dagger_{N\sigma}|N+1;k''\rangle_a|N;r''\rangle_d$$

$$\times\ {}_d\langle N;r''|_a\langle N+1;k''|c_{(N+1)\sigma}|N+1;k'\rangle_a|N;r'\rangle_d$$

Iterative diagonalization

$$\delta_{k,k''}\ (-1)^k \times {}_d\langle N;r|\, c^{\dagger}_{N\sigma}\,|N;r''\rangle_d$$

$$t_N \sum_{\sigma} \sum_{\mathrm{k''},\,\mathrm{r''}} {}_d\langle N;r|_a\langle N+1;k|c^{\dagger}_{N\sigma}|N+1;k''\rangle_a|N;r''\rangle_d$$

$$\times\ {}_d\langle N;r''|_a\langle N+1;k''|c_{(N+1)\sigma}|N+1;k'\rangle_a|N;r'\rangle_d$$

$$M^{\sigma}_{k'',k'}$$

Iterative diagonalization

$$\delta_{k,k''}\ (-1)^k \times {}_d\langle N;r|\, c^{\dagger}_{N\sigma}\,|N;r''\rangle_d$$

$$t_N \sum_{\sigma} \sum_{\mathrm{k''},\,\mathrm{r''}} {}_d\langle N;r|_a\langle N+1;k|c^{\dagger}_{N\sigma}|N+1;k''\rangle_a|N;r''\rangle_d$$

$$\times\ {}_d\langle N;r''|_a\langle N+1;k''|c_{(N+1)\sigma}|N+1;k'\rangle_a|N;r'\rangle_d$$

$$= {}_d\langle N;r''|N;r'\rangle_{\mathrm{d}}\ \ M^{\sigma}_{k'',k'}$$

Iterative diagonalization

$$\delta_{k,k''}\ (-1)^k \times {}_d\langle N;r|\, c^\dagger_{N\sigma}\,|N;r''\rangle_d$$

$$t_N \sum_\sigma \sum_{\mathrm{k''},\,\mathrm{r''}} {}_d\langle N;r|_a\langle N+1;k|c^\dagger_{N\sigma}|N+1;k''\rangle_a|N;r''\rangle_d$$

$$\times\ {}_d\langle N;r''|_a\langle N+1;k''|c_{(N+1)\sigma}|N+1;k'\rangle_a|N;r'\rangle_d$$

$$\delta_{r'',r'}\, M^\sigma_{k'',k'}$$

Iterative diagonalization

- Putting it all together:

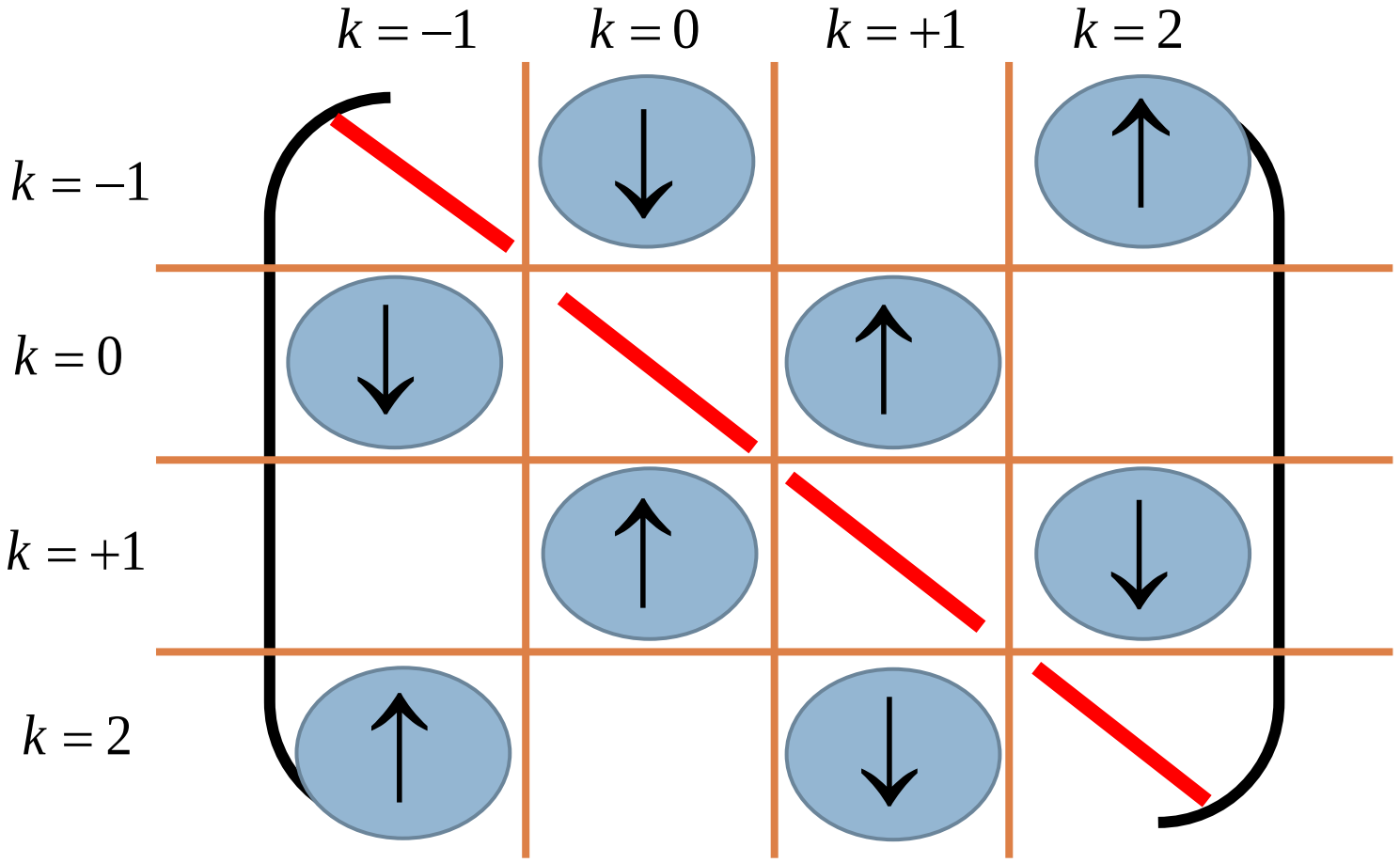
$$
{}_{bs}\left\langle N+1;k,r\left|H_{N+1}\right|N+1;k',r'\right\rangle_{bs}
$$

$$
=E_N(r)\ \delta_{rr'}\delta_{kk'}\ +\ t_N\sum_{\sigma}(-1)^k\ M^{\sigma}_{k,k'}\times\ {}_{d}\left\langle N;r\left|c^{\dagger}_{N\sigma}\right|N;r'\right\rangle_{d}
$$

- So: iterative diagonalization requires only:
  - Trivial matrix $M^{\sigma}_{k,k'}$ which is independent of N
  - Eigenenergies of previous iteration, $E_N(r)$
  - Matrix elements ${}_{d}\left\langle N;r\left|c^{\dagger}_{N\sigma}\right|N;r'\right\rangle_{d}$ between diagonal states of previous iteration

Iterative diagonalization

- Structure of Hamiltonian matrix:



Iterative diagonalization

- How to calculate non-trivial matrix elements?

- First, diagonalize Hamiltonian numerically:

$$\left|N+1;r\right\rangle_d = \sum_{\tilde{k},\tilde{r}} U^{r}_{N+1}(\tilde{k},\tilde{r}) \left|N+1;\tilde{k},\tilde{r}\right\rangle_{bs}$$

- For the next iteration, we'll need:

$${}_d\left\langle N+1;r\right| c^{\dagger}_{(N+1)\sigma} \left|N+1;r'\right\rangle_d = \sum_{\substack{\tilde{r},\tilde{k} \\ \tilde{r}',\tilde{k}'}} \left[U^{r}_{N+1}(\tilde{k},\tilde{r})\right]^{\dagger} U^{r'}_{N+1}(\tilde{k}',\tilde{r}') \times {}_{bs}\left\langle N+1;\tilde{k},\tilde{r}\right| c^{\dagger}_{(N+1)\sigma} \left|N+1;\tilde{k}',\tilde{r}'\right\rangle_{bs}$$

Iterative diagonalization

$$ {}_{bs}\left\langle N+1;\tilde{k},\tilde{r}\right| c^{\dagger}_{(N+1)\sigma}\left|N+1;\tilde{k}',\tilde{r}'\right\rangle_{bs} $$

$$ = {}_{d}\left\langle N;\tilde{r}\right|_{a}\left\langle N+1;\tilde{k}\right| c^{\dagger}_{(N+1)\sigma}\left|N+1;\tilde{k}'\right\rangle_{a}\left|N;\tilde{r}'\right\rangle_{d} $$

$$ \left[M^{\sigma}_{\tilde{k},\tilde{k}'}\right]^{\dagger} $$

$$ \delta_{\tilde{r},\tilde{r}'} $$

Iterative diagonalization

$$ {}_d\left\langle N+1; r \middle| c^{\dagger}_{(N+1)\sigma} \middle| N+1; r' \right\rangle_d = $$

$$ \sum_{\tilde{r},\tilde{k},\tilde{k}'} M^{\sigma}_{\tilde{k}',\tilde{k}} \left[U^{r}_{N+1}(\tilde{k},\tilde{r}) \right]^{\dagger} U^{r'}_{N+1}(\tilde{k}',\tilde{r}) $$

- **Starting at one end of the chain, we can couple on extra sites recursively, and iteratively diagonalize.**

Truncation

- **Obvious problem:** Hilbert space grows by a factor of 4 at each iteration (fermionic sites)
  - After only 10 sites have been added, Hamiltonian matrix in the many-particle basis is of dimension $10^6 \times 10^6$
  - Diagonalization time scales as cube of matrix dimension
  - **Disaster!**

- **Must stop after only a few steps: cannot access low-energy physics this way!**

Truncation

- **Exploit RG concept**
  (which we know is at the heart of quantum impurity problems, from perturbative scaling)

- **Idea in NRG:** **throw away high-energy states at each iteration, focusing on the low-energy physics at each step. Eventually determine ground state.**

- **How do to this?**

… solution next lecture!