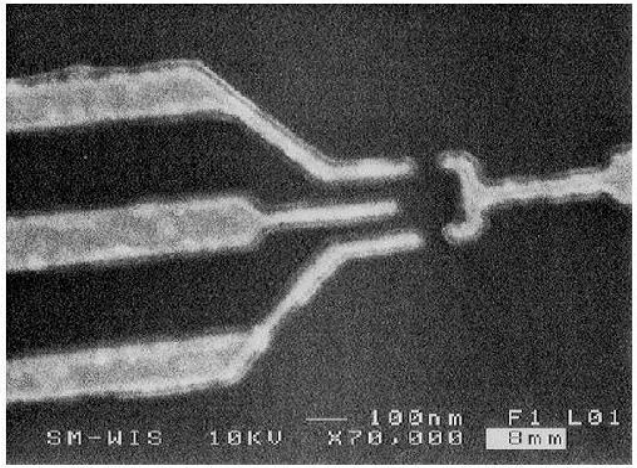
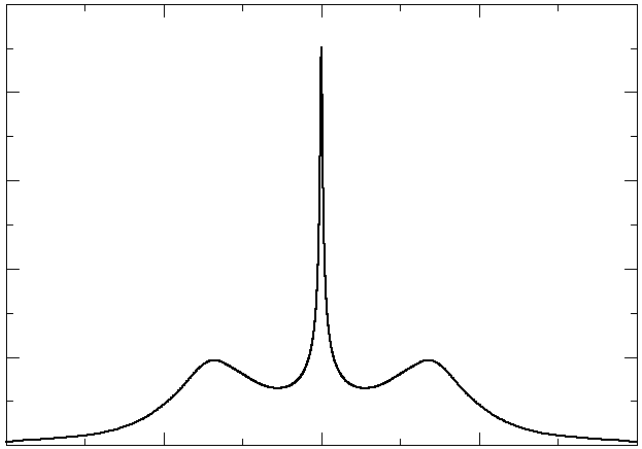
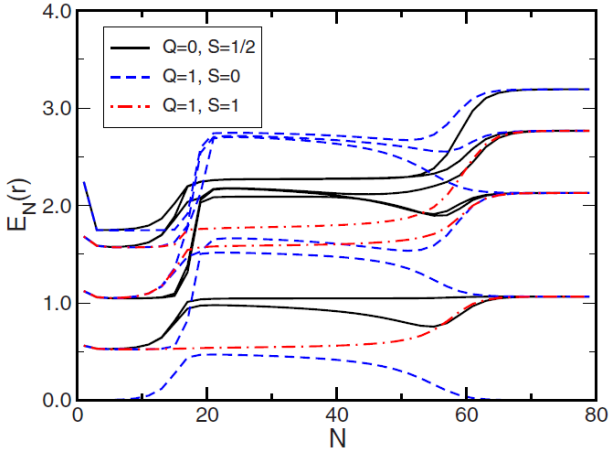
NUMERICAL METHODS FOR QUANTUM IMPURITY MODELS







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 3:
Wilson Chain and the RG in NRG.

March 2015

Andrew Mitchell, Utrecht University

Overview: Part 3

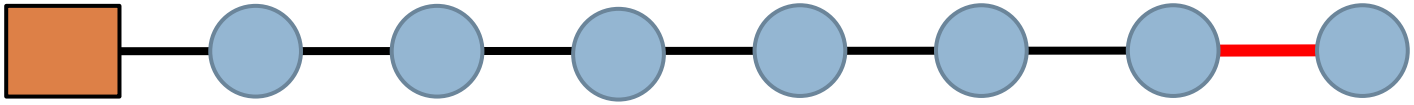
- **Particle in a box revisited**
- **The problem of truncation**

- **Linear discretization**
- **Logarithmic discretization**
- **The Wilson Chain**

- **Analytic structure: RG, flows, fixed points, scaling, universality**

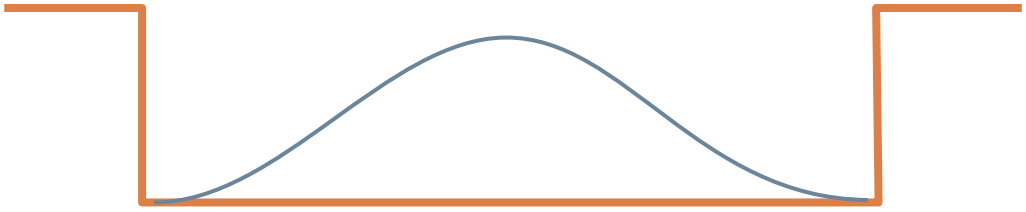
The problem of truncation…

- We wish to join two sub-systems into one large system.



- If we are only interested in the low-energy physics of the combined system, can we neglect the high-energy states of the two sub-systems?

- Consider simplest possible system: particle in a box!



Aside: particle in a box

- In the continuum: $H_{pb} = -\dfrac{\partial^2}{\partial x^2}$

with boundary conditions $\psi(0) = 0 = \psi(L)$

- On the lattice: $H^L_{pb} = t\sum_{r=0}^{L-1}\sum_{\sigma} c^\dagger_{r\sigma} c_{(r+1)\sigma} + \text{H.c.}$

(1d chain)

Hamiltonian conserves particle number and spin…

Consider only the 1-particle, spin-σ subspace

Aside: particle in a box

- Basis states:

$$|\sigma;-;-;-;\ldots\rangle$$
$$|-;\sigma;-;-;\ldots\rangle$$
$$|-;-;\sigma;-;\ldots\rangle$$
$$|-;-;-;\sigma;\ldots\rangle$$
$$\vdots$$

ie. single-particle states. Easy!

Aside: particle in a box

- Diagonalize *L*x*L* hopping matrix:

$$\begin{pmatrix} 0 & t & & \\ t & 0 & t & \\ & t & 0 & \ddots \\ & & \ddots & \ddots \end{pmatrix}$$

- Energy of states:

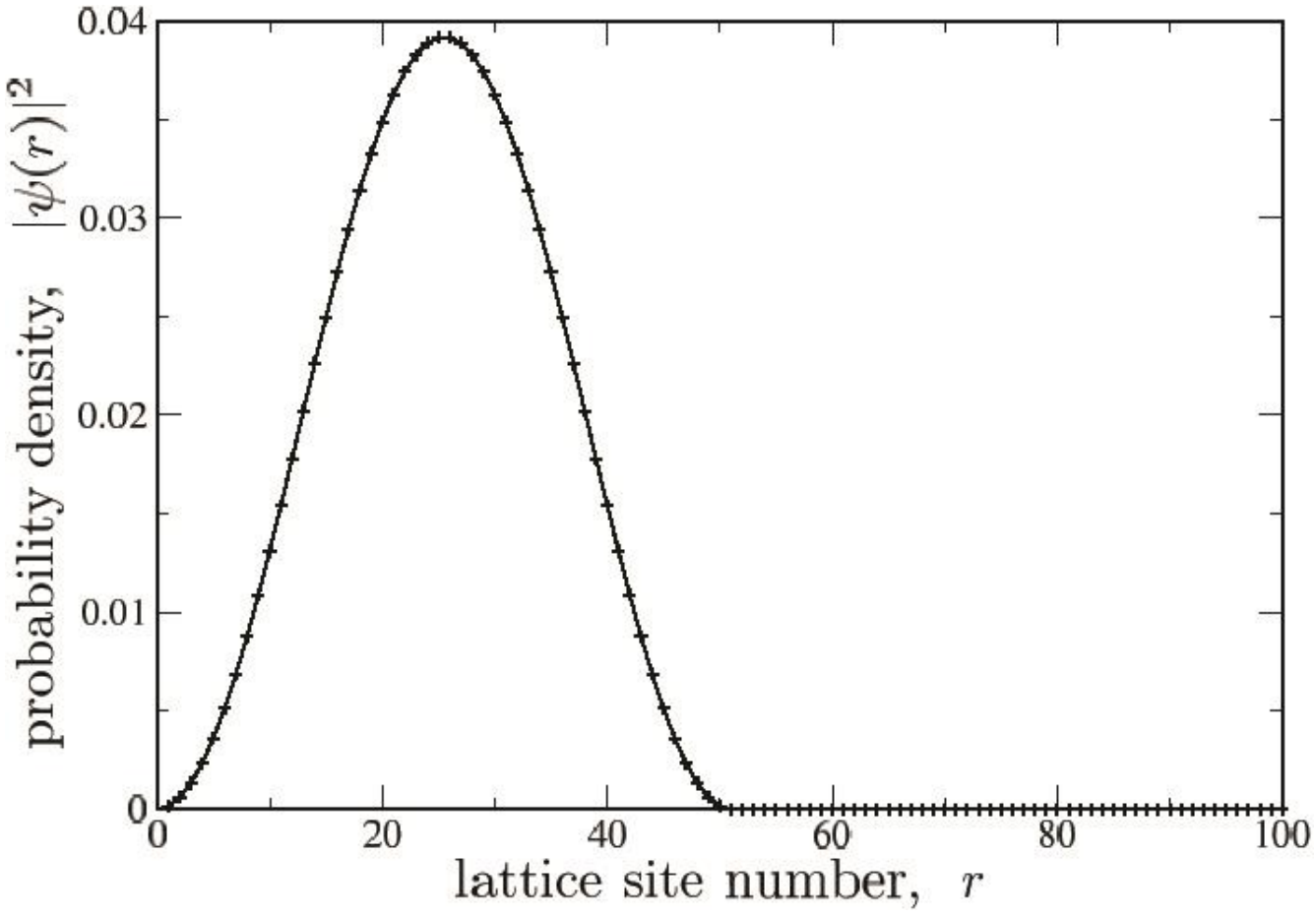
$$E_j = -2t\,\cos\left(\frac{j\pi}{L+1}\right)$$

- Eigenstates are particle-in-a-box wavefunctions

$$\psi_j = \sum_{r=1}^{L} U_j(r)\, c_{r\sigma}^{\dagger} |vac\rangle$$

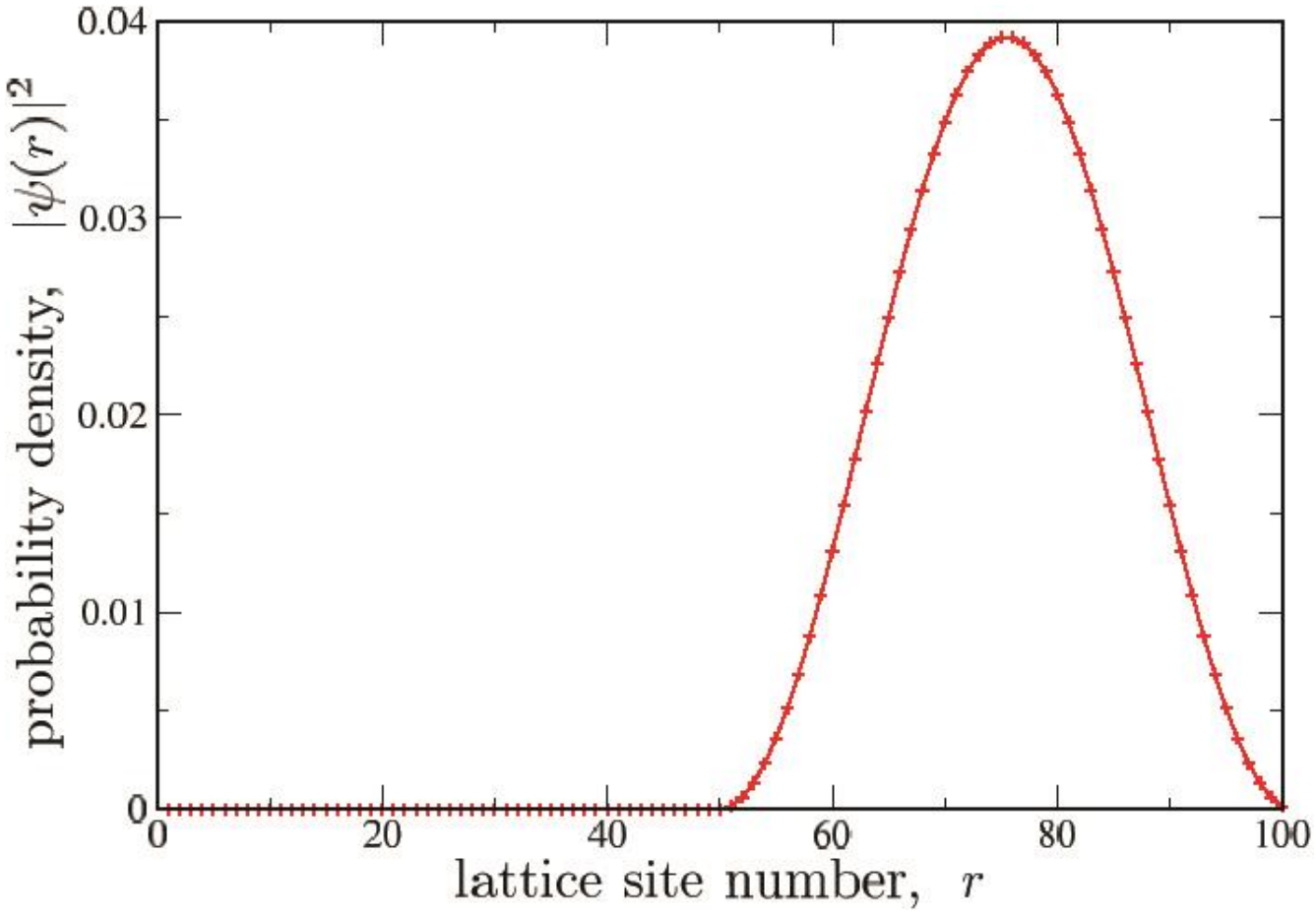
with coefficients $U_j(r) = \sqrt{\frac{2}{L+1}}\,\sin\left(\frac{jr\pi}{L+1}\right)$

Aside: particle in a box



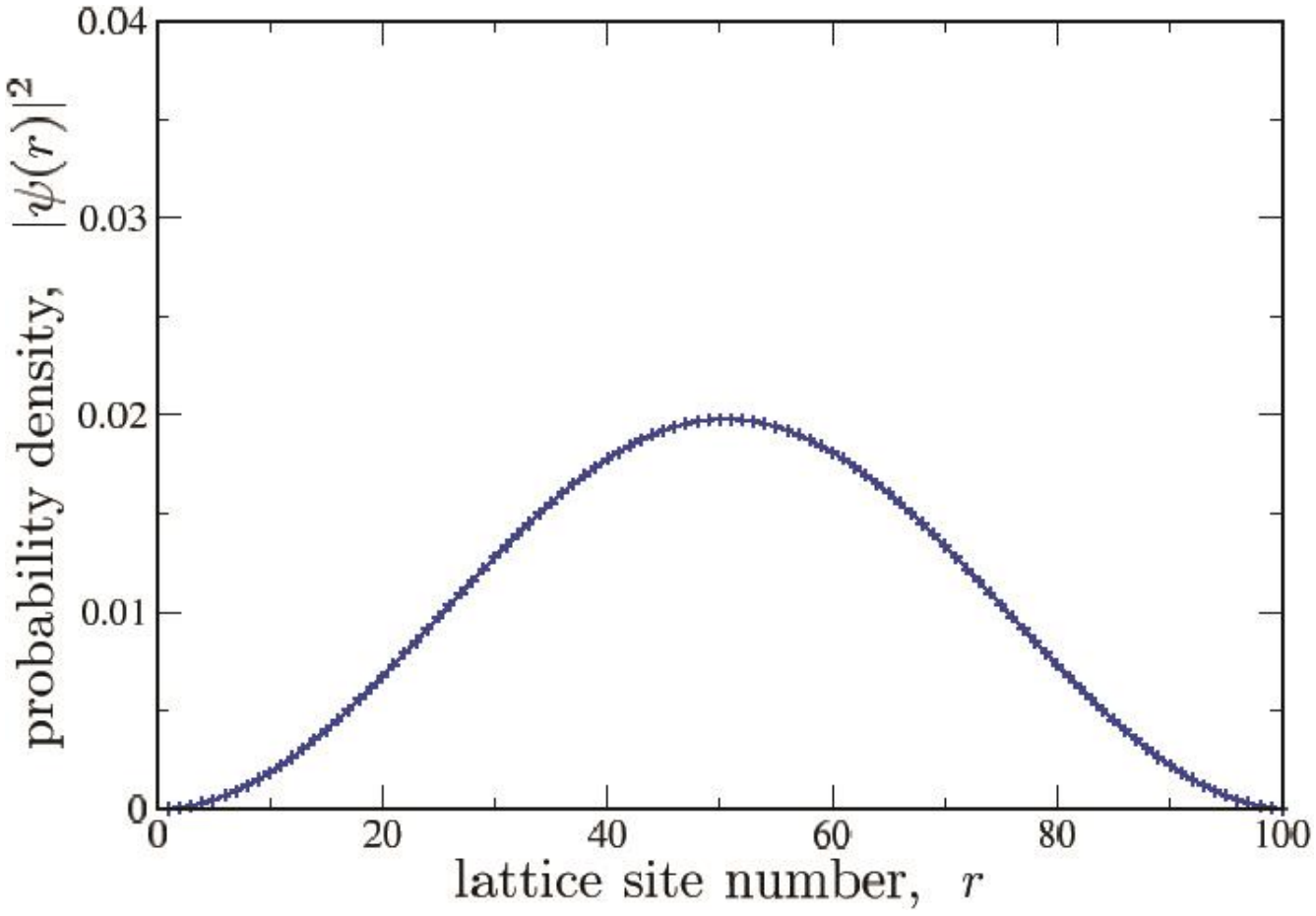
$L = 50$

Aside: particle in a box



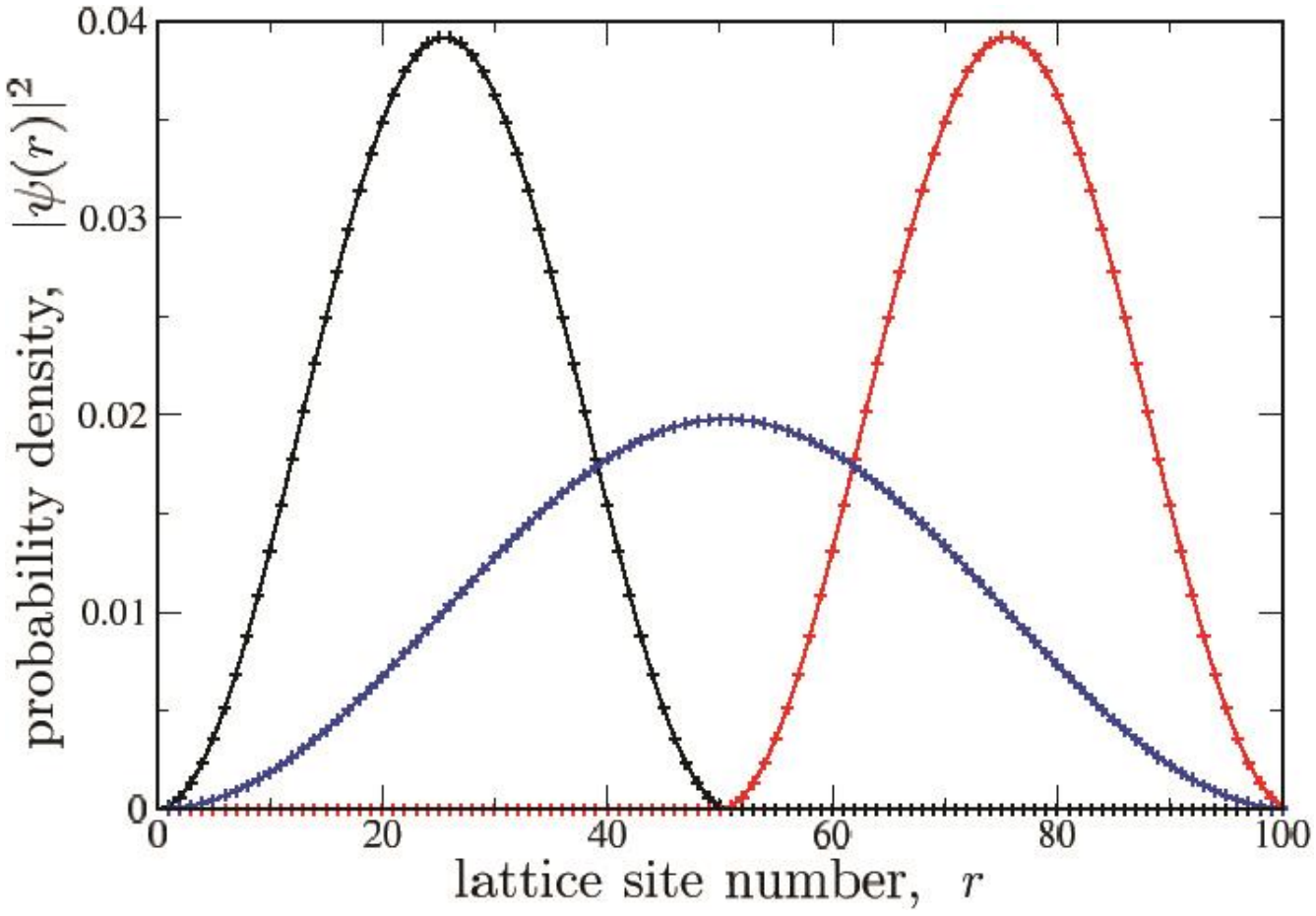
$L = 50$

Aside: particle in a box



$L = 100$

Aside: particle in a box



Aside: particle in a box

- Join two boxes together: $H = H_{box} + H_{join}$

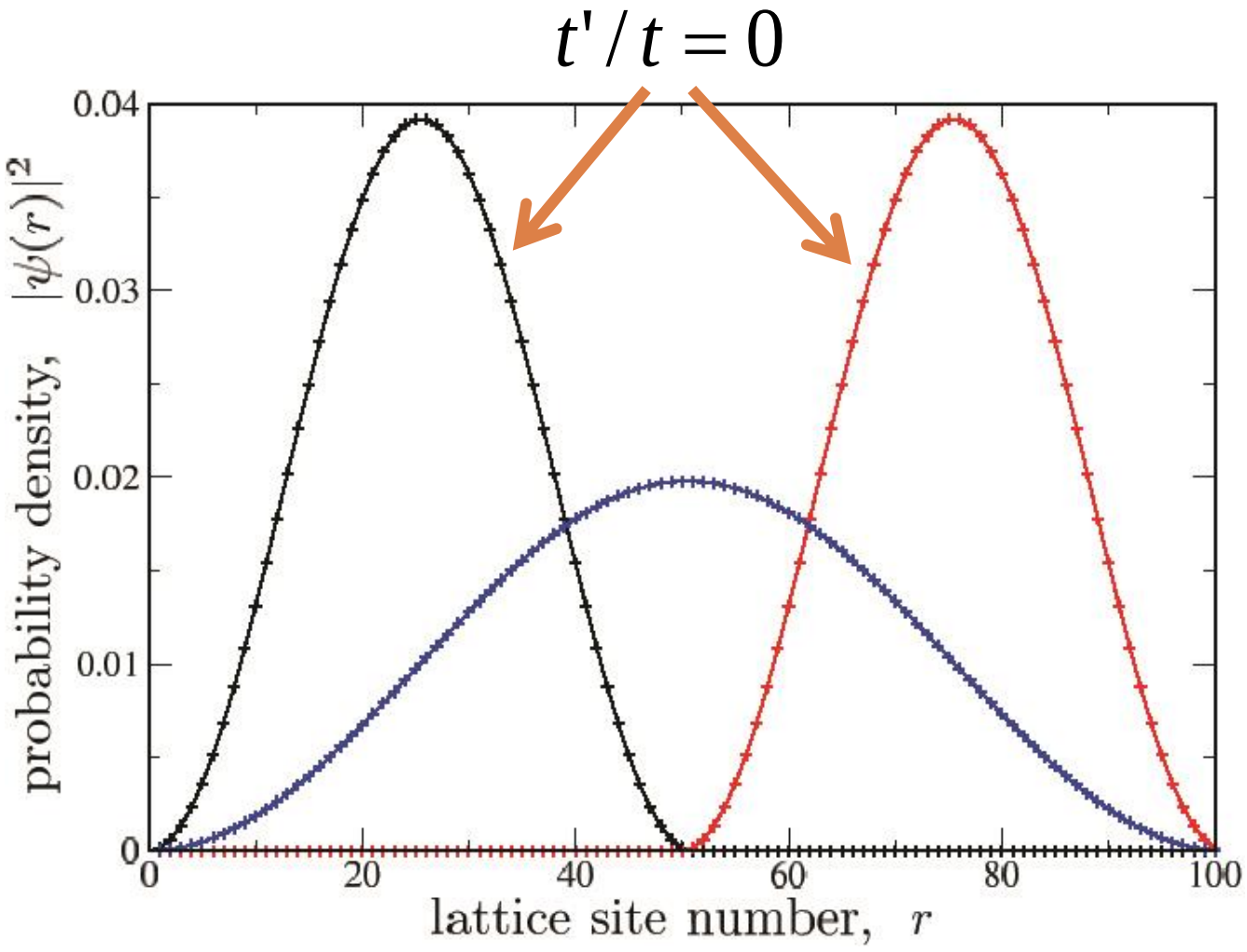
$$H_{box} = t \sum_{r=0}^{L/2-1} \sum_{\sigma} c^{\dagger}_{r\sigma} c_{(r+1)\sigma} + \text{H.c.}$$

$$+ t \sum_{r=L/2}^{L} \sum_{\sigma} c^{\dagger}_{r\sigma} c_{(r+1)\sigma} + \text{H.c.}$$

$$H_{join} = t' \sum_{\sigma} c^{\dagger}_{(L/2)\sigma} c_{(L/2+1)\sigma} + \text{H.c.}$$

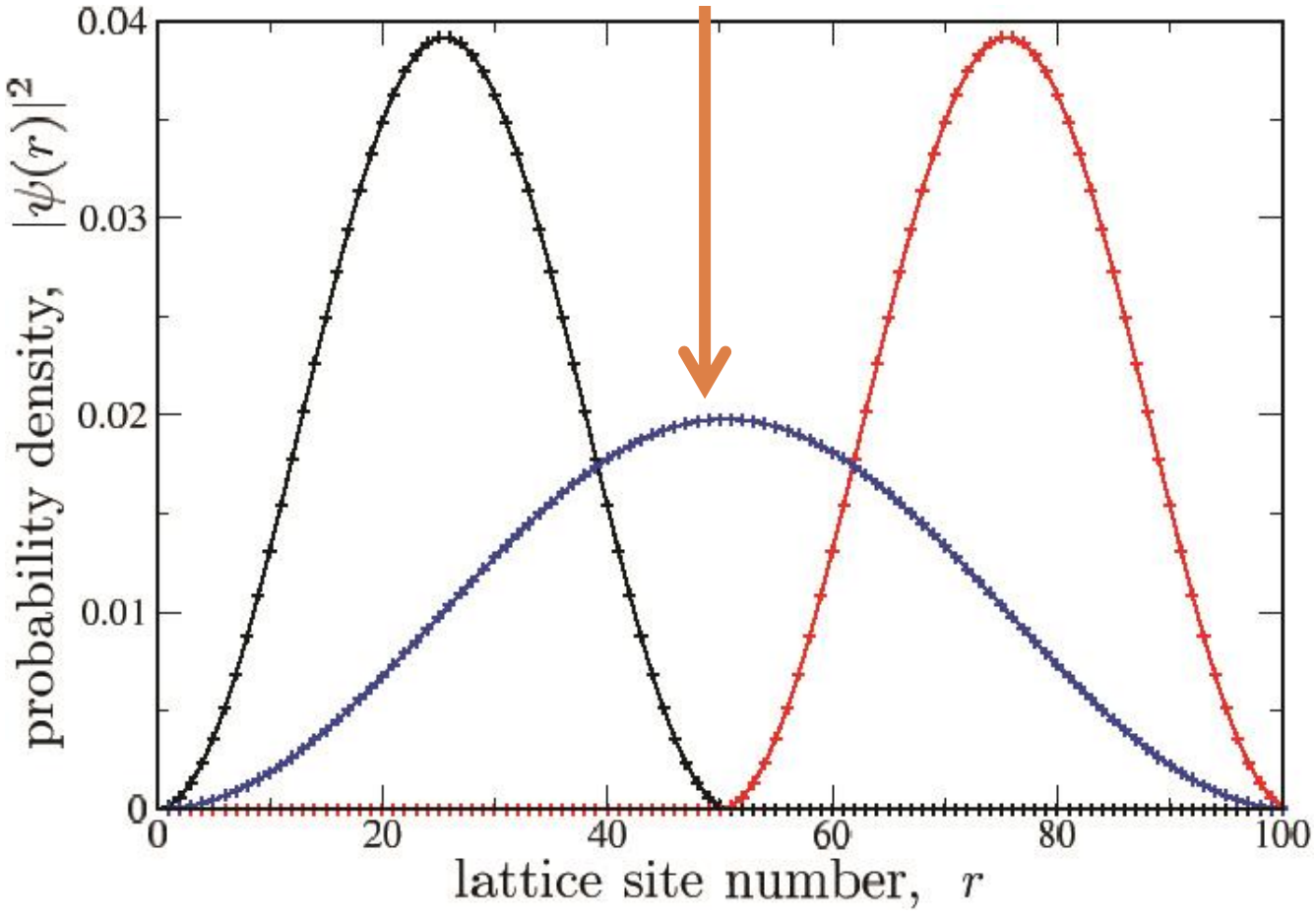
- For $t'/t = 1$, boundary condition mismatch!

Aside: particle in a box



Aside: particle in a box

$t'/t = 1$



$L = 100$

Aside: particle in a box

- This **boundary condition mismatch** means that low-energy states of a composite system cannot just be constructed from low-energy states of two sub-systems

  … in general

- Need to select states with the correct boundary conditions (ie, nodes in the right places)
  - **Motivation for development of DMRG**

- **But is there another way?** **A way that exploits RG?**

Aside: particle in a box

- Consider the **opposite** limit $t'/t \ll 1$
  Can now treat H_{join} perturbatively!

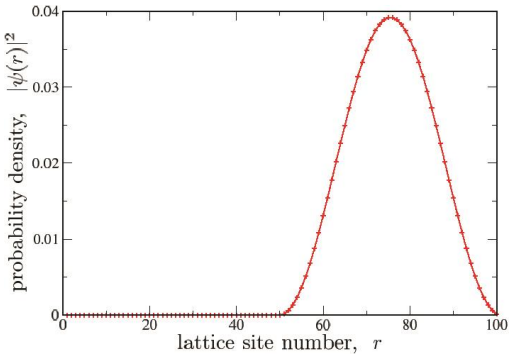
$$H^{eff} = \hat{\underline{1}}\, H_{box}\, \hat{\underline{1}} + \hat{\underline{1}}\, H_{join}\, \hat{\underline{1}} + \ldots$$

where $\hat{\underline{1}} = \sum_r |r\rangle\langle r|$ is the complete set of diagonal states of H_{box}

Aside: particle in a box

- When t' is the smallest energy scale of the problem, can project into the ground state manifold of H_{box}

$$\hat{1}_{gs} = \sum_{r=1,2} |gs;r\rangle\langle gs;r|$$



$$H^{eff} = \hat{1}_{gs} H_{box} \hat{1}_{gs} + \hat{1}_{gs} H_{join} \hat{1}_{gs} + \ldots$$

$$= \hat{1}_{gs} E_{gs} + t' \left[U_1(1)\right]^2 \sum_{r=1,2} |gs;r\rangle\langle gs;\bar{r}| + \ldots$$

Aside: particle in a box

- Ground state of composite (joined) system:

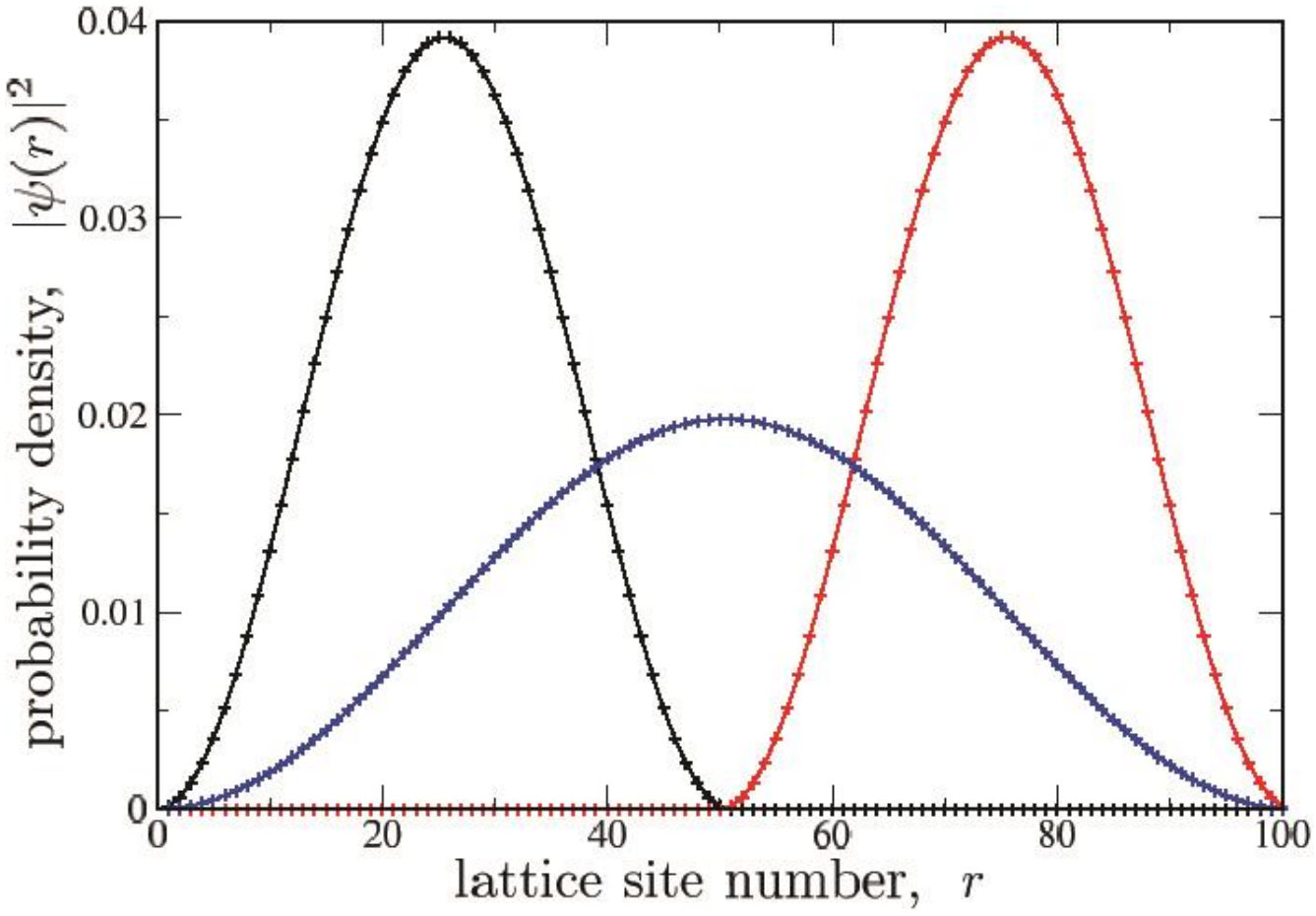
$$E_{gs}^{eff} = E_{gs} - t'\left[U_1(1)\right]^2$$

$$\psi_{gs}^{eff} = \frac{1}{\sqrt{2}}\left(\psi_1 - \psi_2\right)$$

- To first order: ground state of combined system can be constructed from ground states of sub-systems provided connecting terms are small.

Aside: particle in a box

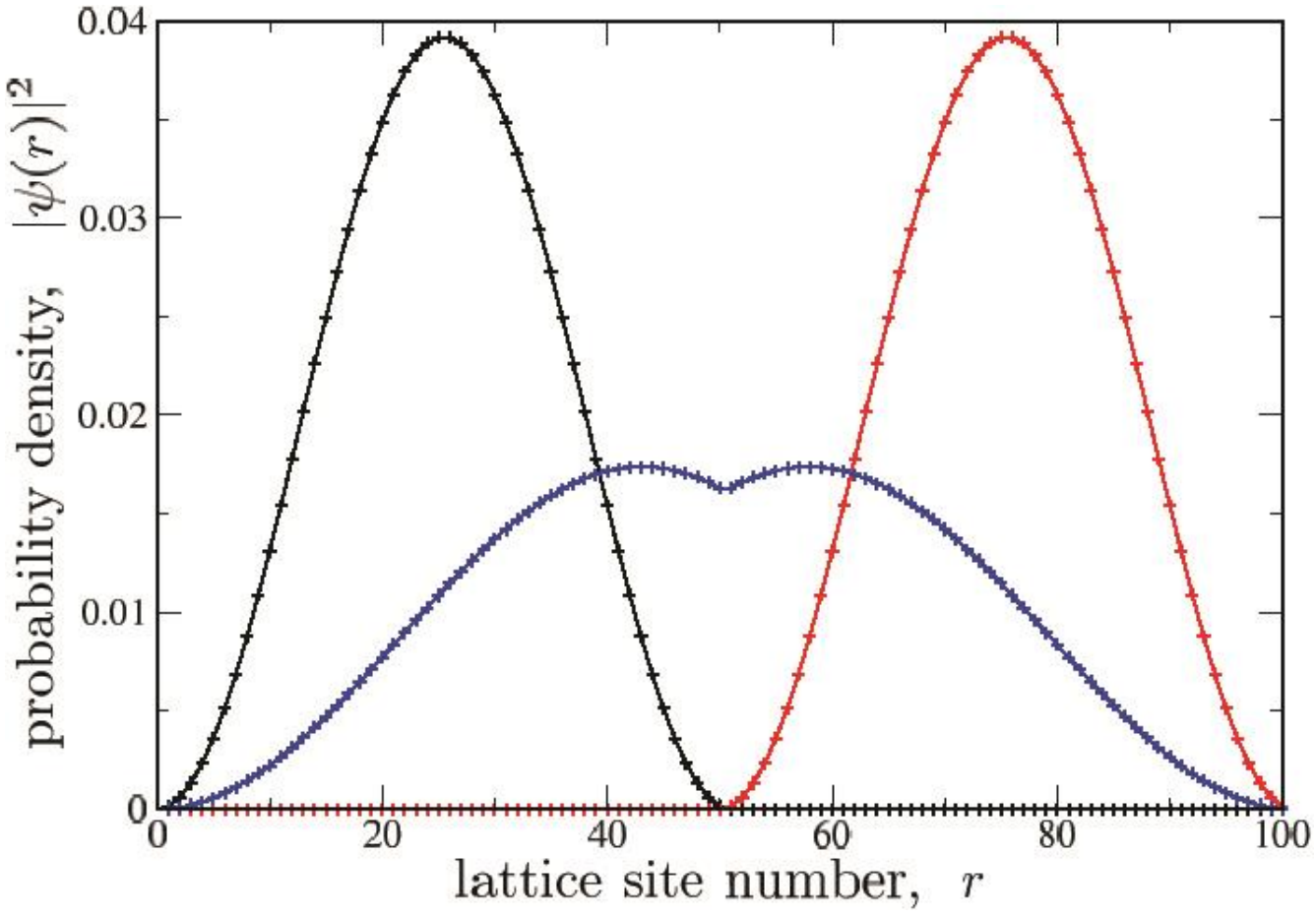
$t'/t = 1$



$L = 100$

Aside: particle in a box

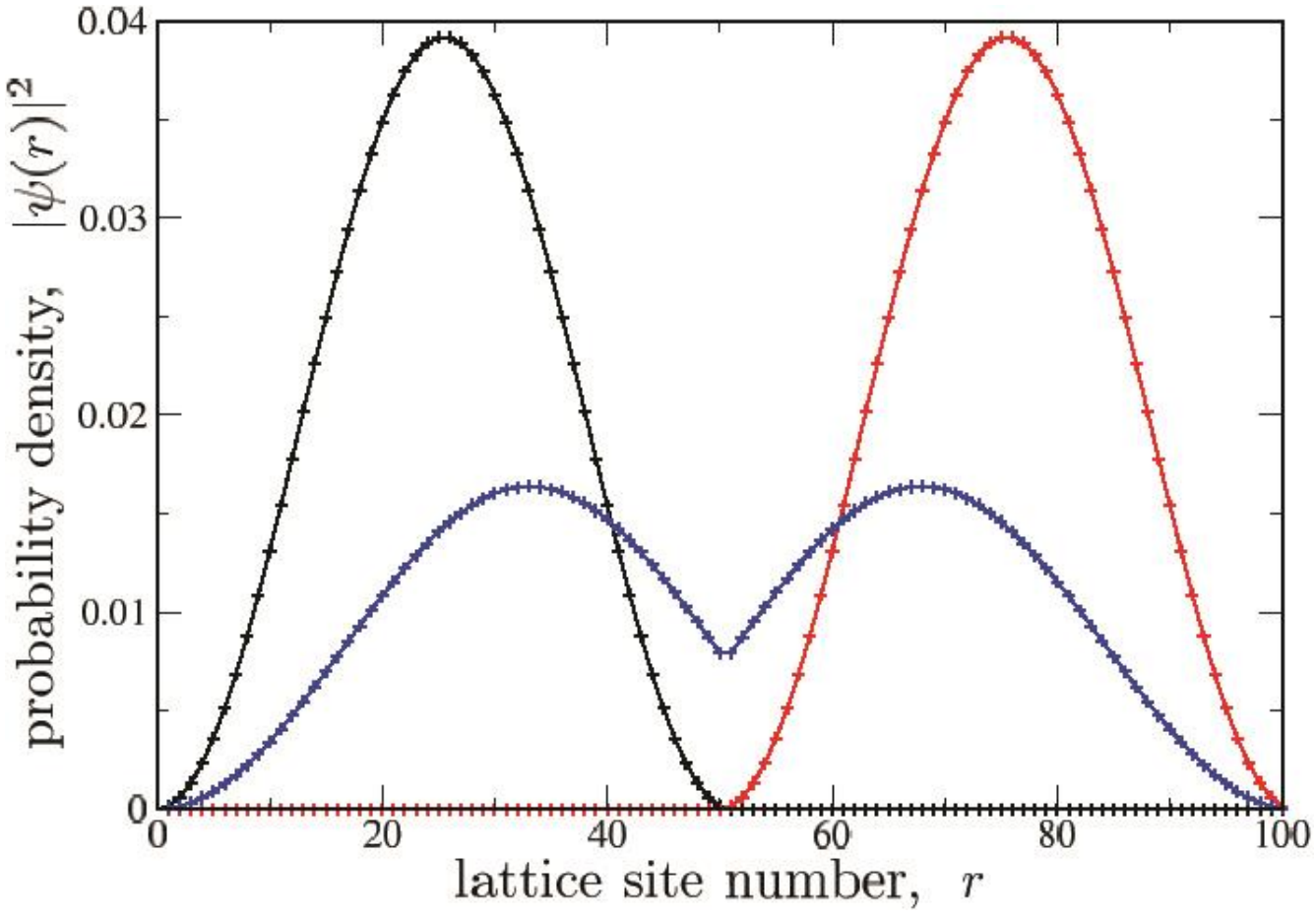
$t'/t = 0.99$



$L = 100$

Aside: particle in a box

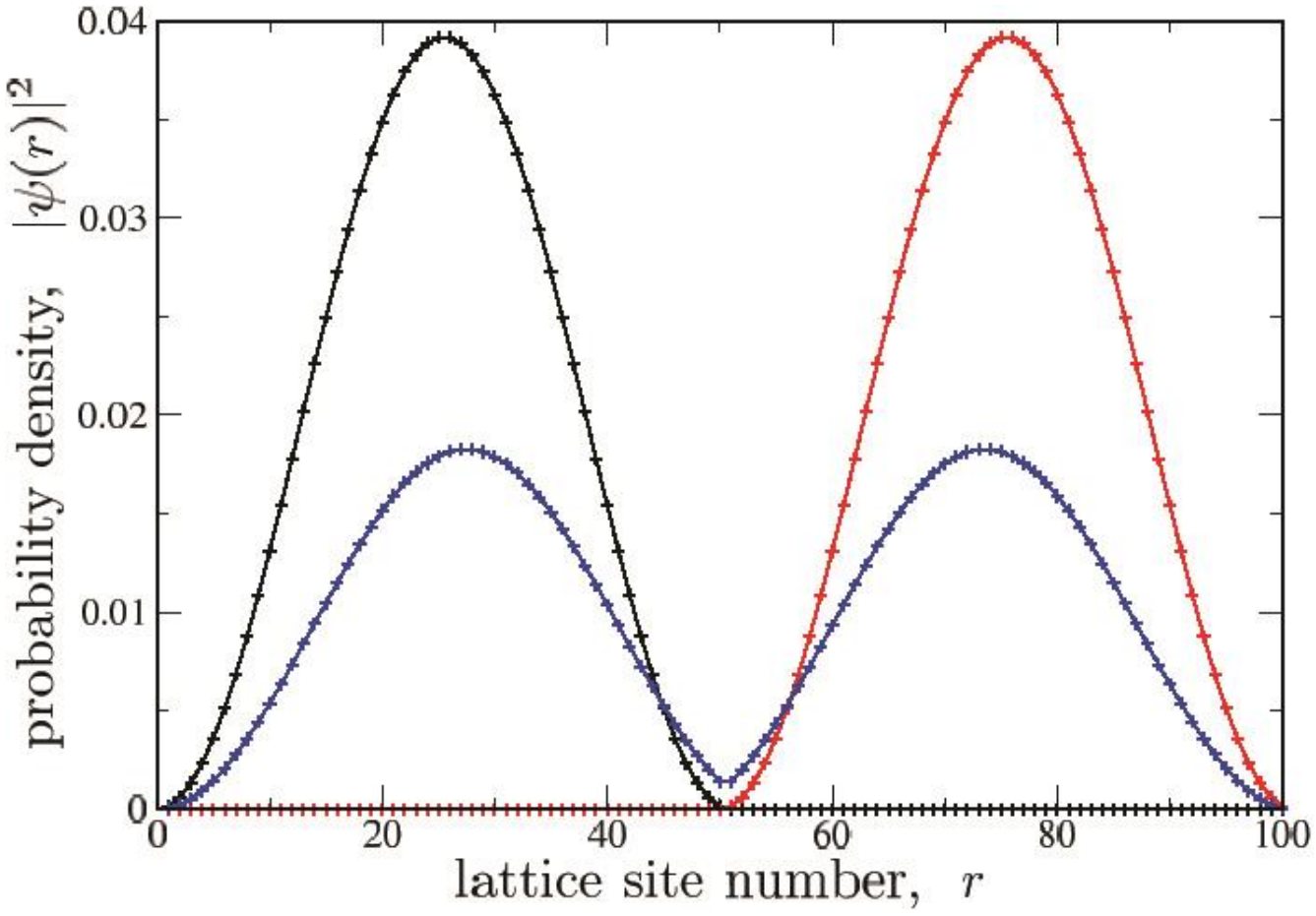
$t'/t = 0.95$



$L = 100$

Aside: particle in a box

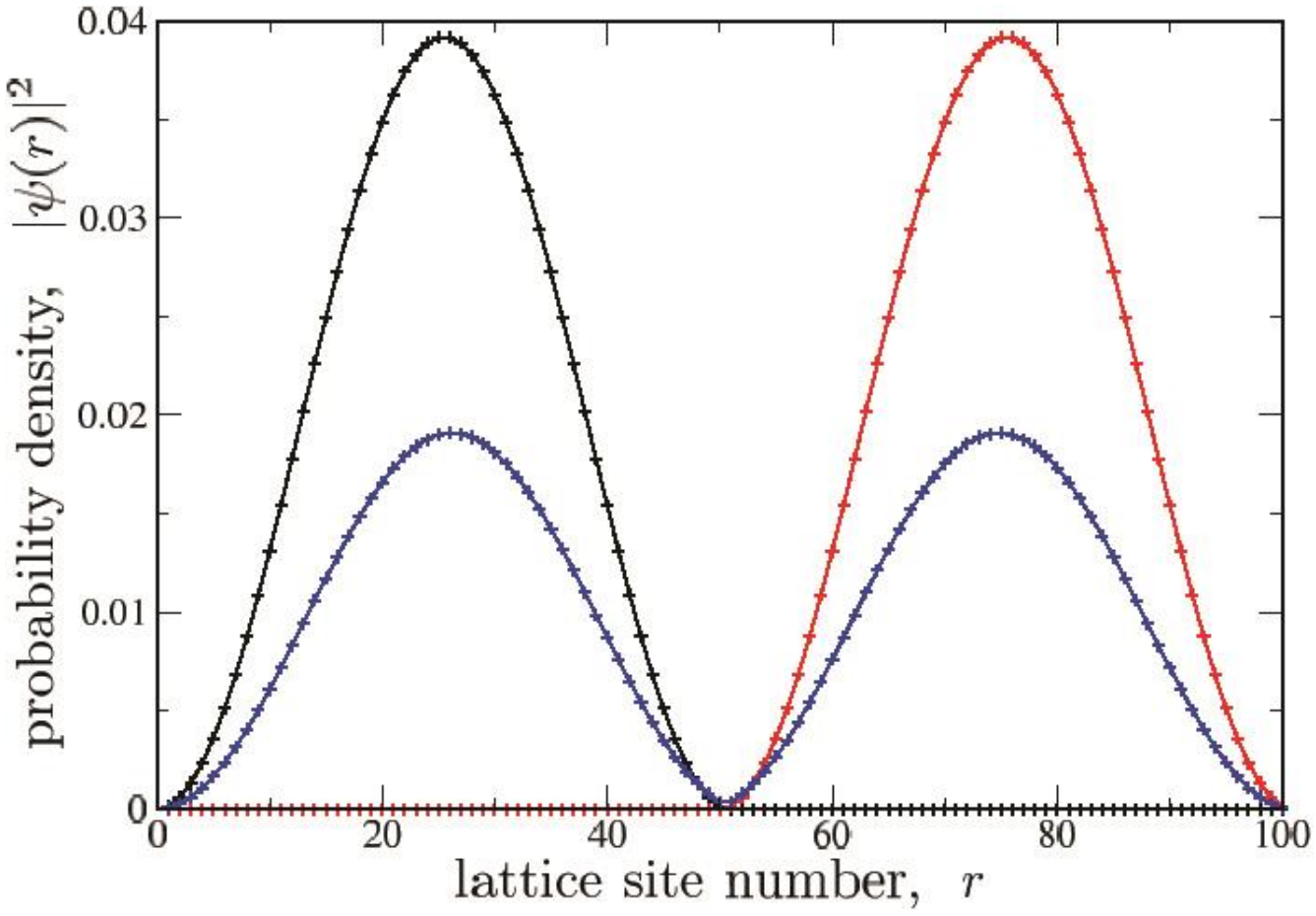
$t'/t = 0.8$



$L = 100$

Aside: particle in a box

$t'/t = 0.58$



$L = 100$

The Truncation Problem

- Back to iterative diagonalization and truncation!

- Philosophy in NRG:
  Ensure coupling to each added site is always **small**

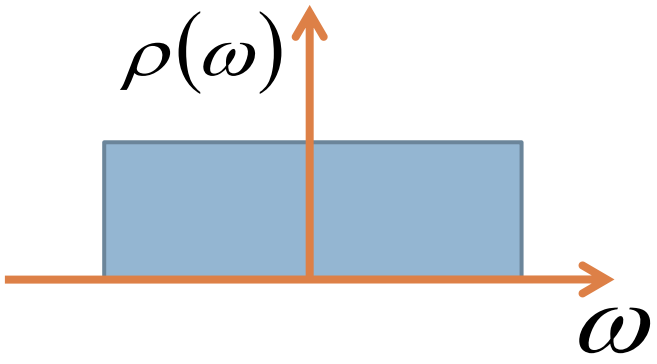
- In NRG, this is achieved by a **logarithmic discretization** of the conduction band.
  - Mapping to a 1d chain produces hoppings that **decrease exponentially** down the chain.

- Energy scale separation allows **truncation** at every step.

Discretization

- How does the discretization work in practice?
- We saw already that truncating the 1d chain representation is a type of discretization
- Another possibility: **discretize** the conduction electron **density of states**.
  - Replace the continuous spectrum by discretized poles

Linear Discretization



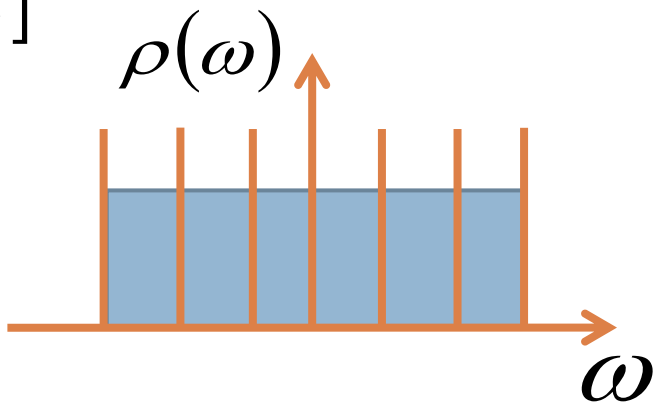
$$H_{host} = \sum_{k,\sigma} \varepsilon_k c^{\dagger}_{k,\sigma} c_{k,\sigma}$$

$$\rho(\omega) = \begin{cases} \frac{1}{2D} & : \ |\omega| \le D \\ 0 & : \ |\omega| > D \end{cases}$$

- Divide band up into *N* intervals, each of width $2D/N$

$$[P_0, P_1],\ [P_1, P_2],\ [P_2, P_3],\ \dots,\ [P_{N-1}, P_N]$$

$$P_n = D\left(-1 + 2n/N\right)$$



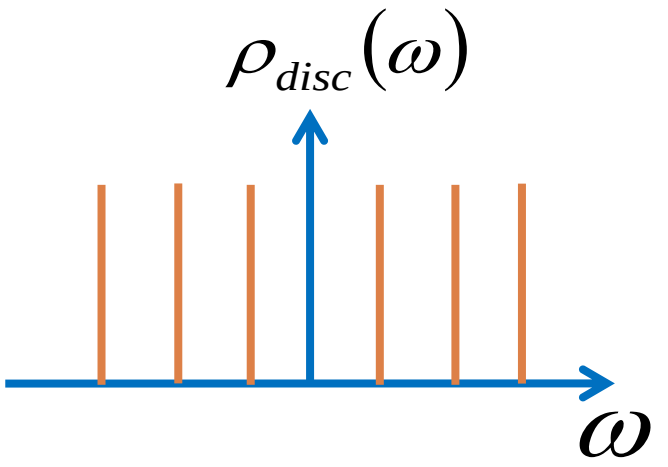
Linear Discretization

- Discretize the continuous spectrum by replacing with sum over delta-peaks:

$$\rho(\omega) \to \rho_{disc}(\omega) = \sum_{n=1}^{N} a_n \delta(\omega - \omega_n)$$

$$\omega_n = (P_{n-1} - P_n)/2$$

$$a_n = \int_{P_{n-1}}^{P_n} d\omega \ \rho(\omega) = \frac{(P_n - P_{n-1})}{2D} = \frac{1}{ND}$$



Logarithmic Discretization

- Logarithmic discretization of conduction band:

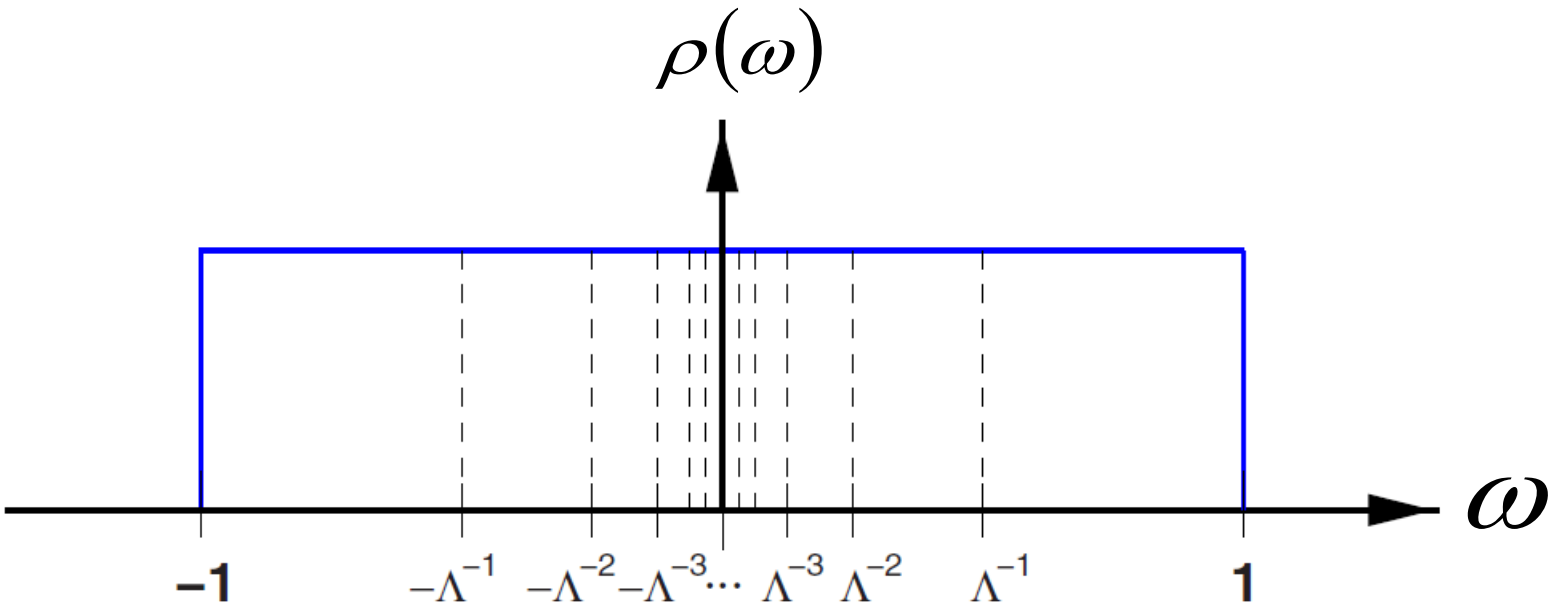
$$\rho(\omega) \to \rho_{disc}(\omega) = \sum_{n=1}^{N} a_n \delta(\omega - \omega_n)$$

  - Define intervals $P_n = \pm\Lambda^{-n}$ with $n = 0, 1, 2, 3, 4, \ldots$

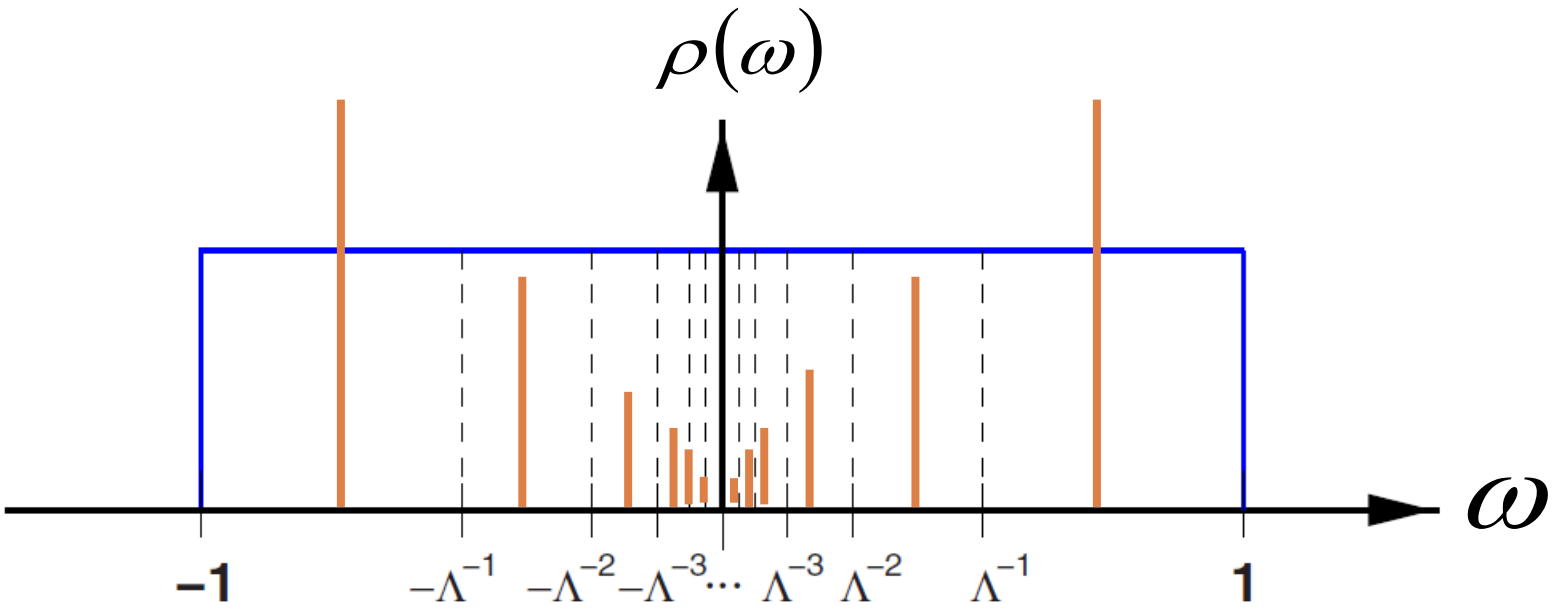
$$\omega_n \sim \pm\Lambda^{-n}$$

$$a_n = \int_{P_{n-1}}^{P_n} d\omega \ \rho(\omega) \sim \Lambda^{-n}$$

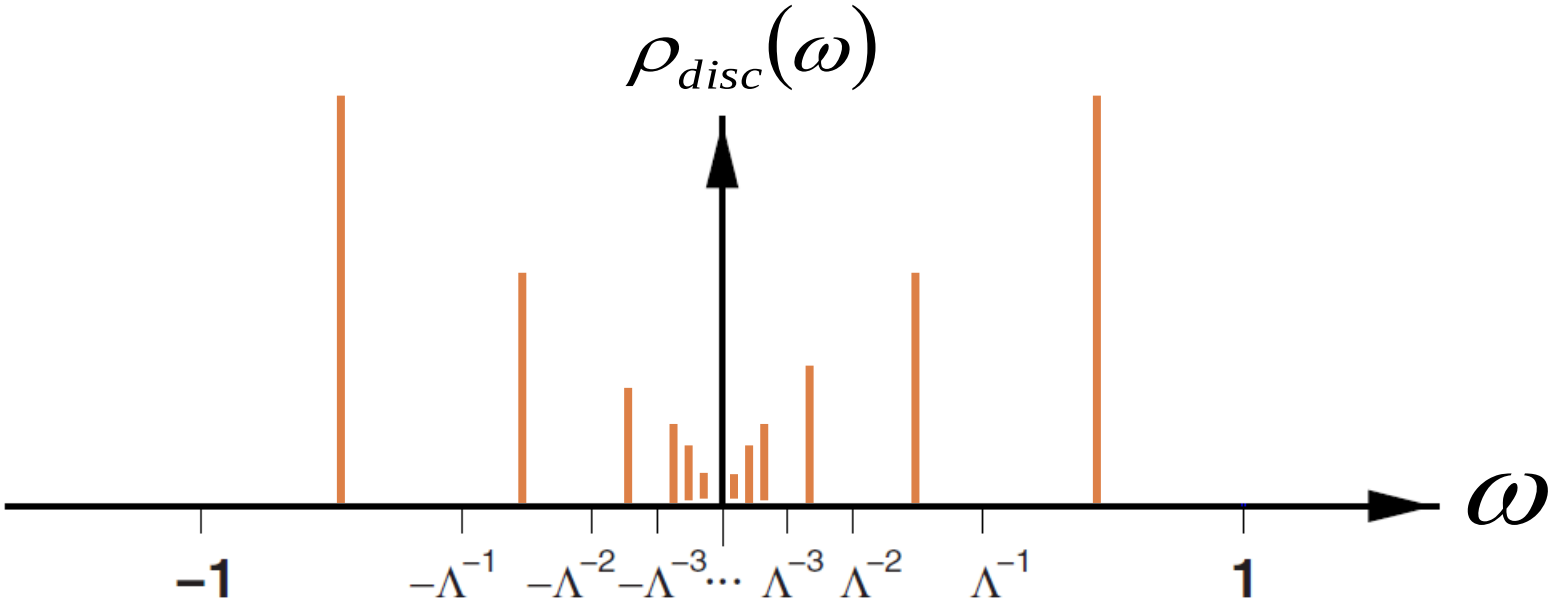
Logarithmic Discretization



Logarithmic Discretization

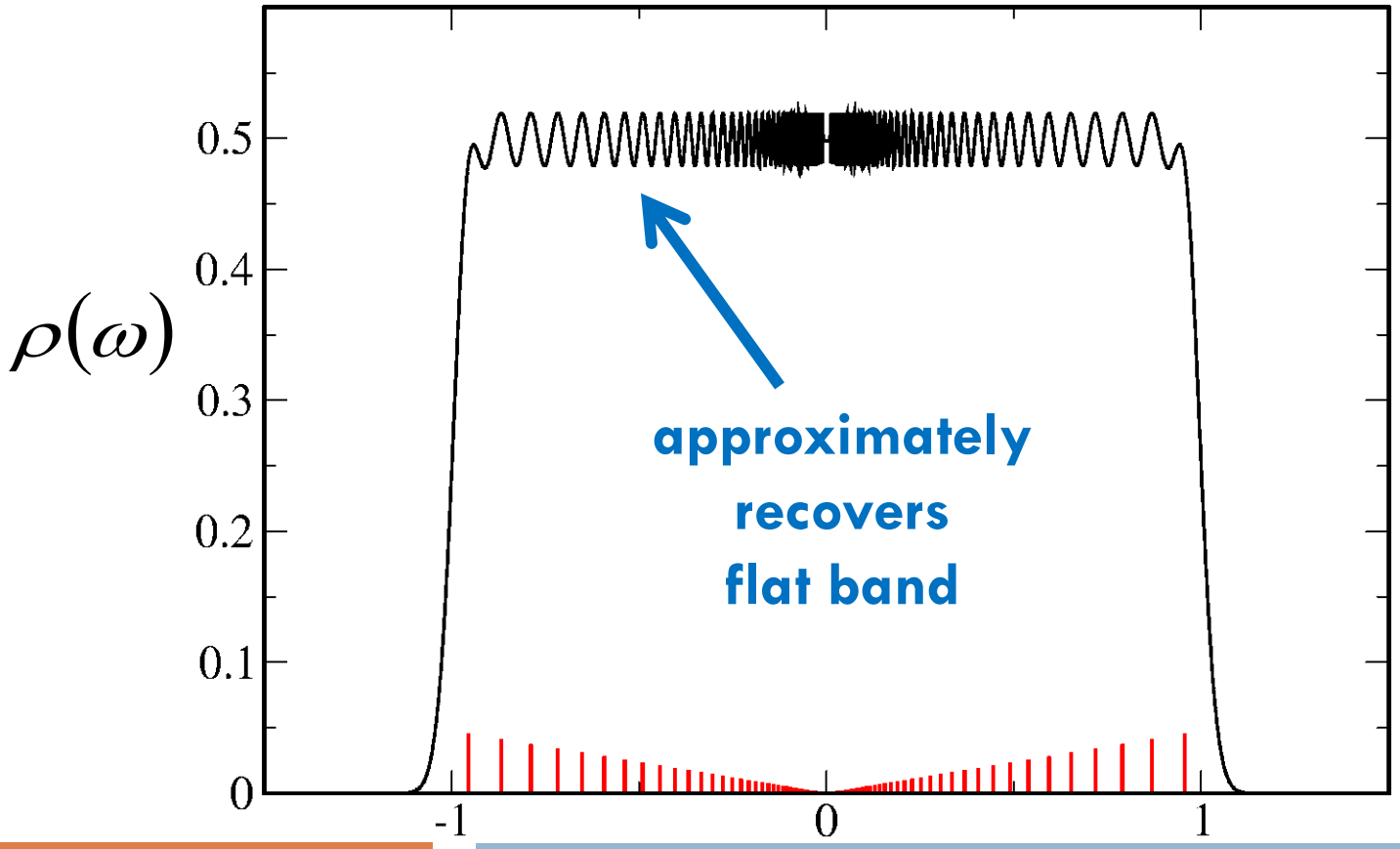


Logarithmic Discretization



Logarithmic Discretization

- Is this a good approximation to the true continuum?
  - Broaden the spectral poles into (log-) Gaussians to check:



Wilson's formulation

- Anderson Hamiltonian:

$$\mathcal{H}_A \equiv \sum_{\vec{k}} \epsilon_{\vec{k}} c^\dagger_{\vec{k}\mu} c_{\vec{k}\mu} + \epsilon_d c^\dagger_{d\mu} c_{d\mu} + U(c^\dagger_{d\uparrow} c_{d\uparrow})(c^\dagger_{d\downarrow} c_{d\downarrow}) + \sum_{\vec{k}} (V_{\vec{k}d} c^\dagger_{\vec{k}\mu} c_{d\mu} + V^*_{\vec{k}d} c^\dagger_{d\mu} c_{\vec{k}\mu})$$

- Conduction band assumed to be ***isotropic***:
  - $\epsilon_{\vec{k}}$ depends only on $|\vec{k}|$
  - $V_{\vec{k}d}$ depends only on $|\vec{k}|$
  - Impurity then just couples to the **s-wave states:**

$$\mathcal{H}_A = \int_{-D}^{D} \epsilon a^\dagger_{\epsilon\mu} a_{\epsilon\mu} d\epsilon + \epsilon_d c^\dagger_{d\mu} c_{d\mu} + U(c^\dagger_{d\uparrow} c_{d\uparrow})(c^\dagger_{d\downarrow} c_{d\downarrow}) + \int_{-D}^{D} d\epsilon [\rho(\epsilon)]^{1/2} [V_d(\epsilon) a^\dagger_{\epsilon\mu} c_{d\mu} + V^*_d(\epsilon) c^\dagger_{d\mu} a_{\epsilon\mu}]$$

Wilson's formulation

- Assume $\rho(\varepsilon) \equiv \rho$ and $V_d(\varepsilon) \equiv V_d$ are independent of energy (and write $k = \varepsilon / D$):

$$\mathcal{H}_A = D\left[\int_{-1}^{1} k a_{k\mu}^{\dagger} a_{k\mu}\, dk + \epsilon_d c_{d\mu}^{\dagger} c_{d\mu} + U(c_{d\uparrow}^{\dagger} c_{d\uparrow})(c_{d\downarrow}^{\dagger} c_{d\downarrow}) + \left(\frac{\Gamma}{\pi D}\right)^{1/2} \int_{-1}^{1} dk\, (a_{k\mu}^{\dagger} c_{d\mu} + c_{d\mu}^{\dagger} a_{k\mu})\right]$$

where

$$\Gamma \equiv \pi \rho V_d^2$$

Wilson's formulation

- Divide band into **logarithmic** intervals:

$$P_n = \pm\Lambda^{-n} \quad \text{with } n = 0, 1, 2, 3, 4, \ldots$$

- Set up a **Fourier series** in each interval:

$$\psi_{np}^{\pm}(k) \equiv \begin{cases} \dfrac{\Lambda^{n/2}}{(1-\Lambda^{-1})^{1/2}} e^{\pm i\omega_n pk} & \text{if } \Lambda^{-(n+1)} < \pm k < \Lambda^{-n} \\ 0 \quad \text{if } k \text{ is outside the above interval} \quad . \end{cases}$$

where, $\omega_n \equiv \dfrac{2\pi}{\Lambda^{-n} - \Lambda^{-(n+1)}} = \dfrac{2\pi\Lambda^n}{1-\Lambda^{-1}}$

Wilson's formulation

- Canonical transformation of operators in each interval:

$$a_{k\mu} = \sum_{np} \left[a_{np\mu} \psi^{+}_{np}(k) + b_{np\mu} \psi^{-}_{np}(k) \right] \;\; ;$$

$$a_{np\mu} \equiv \int_{-1}^{1} dk \; [\psi^{+}_{np}(k)]^* a_{k\mu}; \quad b_{np\mu} \equiv \int_{-1}^{1} dk \, [\psi^{-}_{np}(k)]^* a_{k\mu}$$

- Hybridization term of Hamiltonian:

$$\int_{-1}^{1} a_{k\mu} \, dk = (1 - \Lambda^{-1})^{1/2} \sum_{n} \Lambda^{-n/2} (a_{n0\mu} + b_{n0\mu})$$

  - Impurity **only couples to *p*=0** fundamental harmonic!

Wilson's formulation

- BUT: Conduction electron Hamiltonian:

$$\int_{-1}^{1} k a^{\dagger}_{k\mu} a_{k\mu}\, dk = \tfrac{1}{2}(1+\Lambda^{-1}) \sum_{np} \Lambda^{-n} (a^{\dagger}_{np\mu} a_{np\mu} - b^{\dagger}_{np\mu} b_{np\mu})$$
$$+ \frac{1-\Lambda^{-1}}{2\pi i} \sum_{n} \sum_{p \neq p'} \frac{\Lambda^{-n}}{p'-p} (a^{\dagger}_{np\mu} a_{np'\mu} - b^{\dagger}_{np\mu} b_{np'\mu}) \exp \frac{2\pi i (p'-p)}{1-\Lambda^{-1}}$$

  - $p \neq 0$ modes couple to impurity only **indirectly**, through the modes with $p = 0$

- Coupling between $p = 0$ and $p \neq 0$ modes controlled in the discretization parameter, and **vanish** as $\Lambda \to 1$

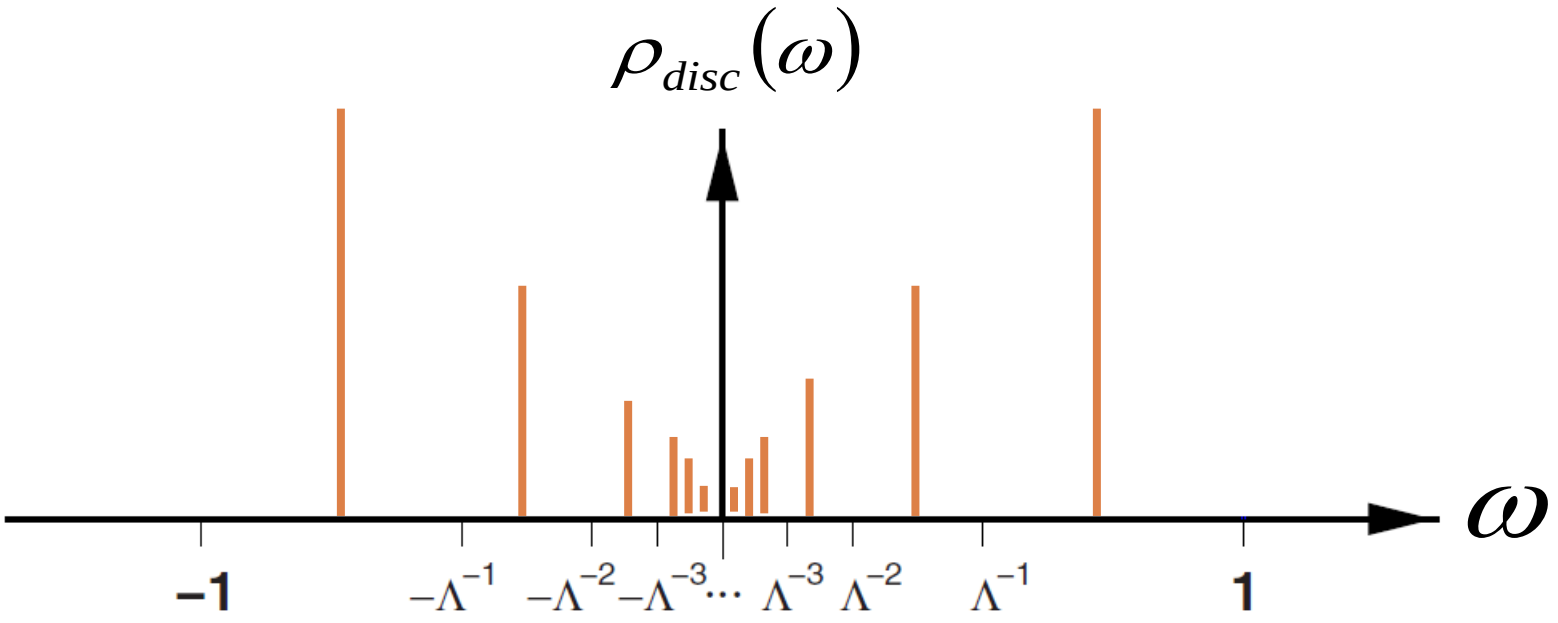
Wilson's formulation

- Keep only $p=0$ modes!

$$\frac{\mathcal{H}_A}{D} \cong \tfrac{1}{2}(1+\Lambda^{-1}) \sum_{n=0}^{\infty} \Lambda^{-n}(a^\dagger_{n\mu}a_{n\mu} - b^\dagger_{n\mu}b_{n\mu})$$
$$+ \frac{1}{D}\epsilon_d c^\dagger_{d\mu}c_{d\mu} + \frac{1}{D}U(c^\dagger_{d\uparrow}c_{d\uparrow})(c^\dagger_{d\downarrow}c_{d\downarrow})$$
$$+ \left(\frac{2\Gamma}{\pi D}\right)^{1/2}(f^\dagger_{0\mu}c_{d\mu} + c^\dagger_{d\mu}f_{0\mu})$$

where, $f_{0\mu} = \left[\tfrac{1}{2}(1-\Lambda^{-1})\right]^{1/2} \sum_{n=0}^{\infty} \Lambda^{-n/2}(a_{n\mu} + b_{n\mu})$

Logarithmic Discretization

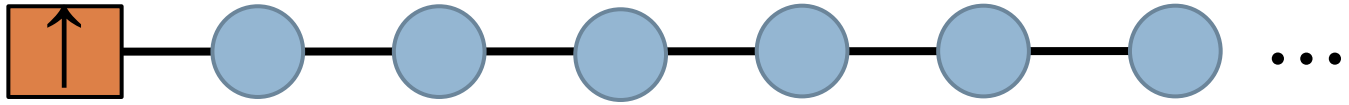


Logarithmic Discretization

- Low-energy excitations around Fermi level are **exponentially-well sampled**
  - needed to capture Kondo physics on the scale of T_K
- Treats physics on all energy scales on **equal footing**
  - Logarithmic divergences in perturbative treatment avoided by logarithmic discretization
- **But does this help?**
  - Continuous spectrum: uncountably infinite number of states
  - Discretized spectrum: countably infinite… but still infinite!

Mapping to 1d chain

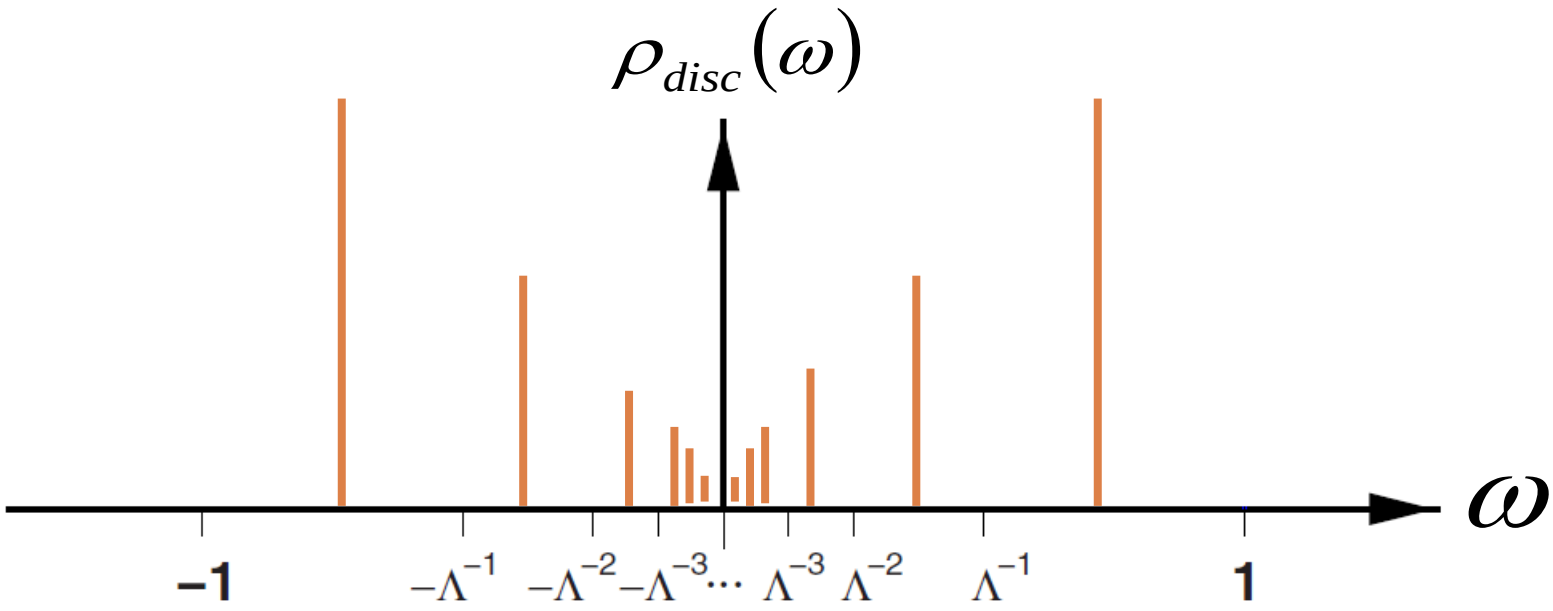
- The **Wilson Chain** is a 1d tight-binding chain, with the impurity located at one end:



impurity

'zero orbital' of the Wilson Chain: Local Density of States seen by the impurity is the logarithmically discretized host density of states, $\rho_{disc}(\omega)$

Wilson Chain



$$\rho_{disc}(\omega) = \sum_k |a_{0,k}|^2 \, \delta(\omega - \varepsilon_k)$$

$$\Rightarrow \quad H_{host}^{disc} = \sum_{k,\sigma} \varepsilon_k b_{k\sigma}^\dagger b_{k\sigma}$$

Wilson Chain

- But we don't want the diagonal representation!
  We need the **tridiagonal chain representation**

$$H_{host}^{disc} = \sum_{k,\sigma} \varepsilon_k b_{k\sigma}^{\dagger} b_{k\sigma} \quad \Rightarrow \quad \sum_{\sigma} \sum_{n} \left(h_n \; f_{n\sigma}^{\dagger} f_{(n+1)\sigma} + \text{H.c.} \right)$$

$$\sum_{\sigma} \vec{b}_{\sigma}^{\dagger} \underline{\underline{D}} \, \vec{b}_{\sigma} \quad \Rightarrow \quad \sum_{\sigma} \vec{f}_{\sigma}^{\dagger} \underline{\underline{W}} \, \vec{f}_{\sigma}$$

Wilson Chain

- But we don't want the diagonal representation!
  We need the **tridiagonal chain representation**

$$\begin{bmatrix} \varepsilon_1 & 0 & 0 & 0 \\ 0 & \varepsilon_2 & 0 & 0 \\ 0 & 0 & \varepsilon_3 & 0 \\ 0 & 0 & 0 & \varepsilon_4 \end{bmatrix} \Rightarrow \begin{bmatrix} e_1 & h_1 & 0 & 0 \\ h_1 & e_2 & h_2 & 0 \\ 0 & h_2 & e_3 & h_3 \\ 0 & 0 & h_3 & e_4 \end{bmatrix}$$

$$\underline{\underline{D}} \qquad\qquad \underline{\underline{W}}$$

Wilson Chain

- Tridiagonalize by **"Lanczos"** method
  - CONSTRAINT: **zero-orbital** of Wilson chain must have correct LDOS

$$\rho_{disc}(\omega) = \sum_k |a_{0,k}|^2 \, \delta(\omega - \varepsilon_k)$$

pole weights define the transformation for the zero-orbital, connected to the impurity

Lanczos starting vector: $|a_0\rangle$

Wilson Chain

- Tridiagonalize by **"Lanczos"** method:
  - **Starting ingredients:** diagonal host Hamiltonian and zero-orbital vector

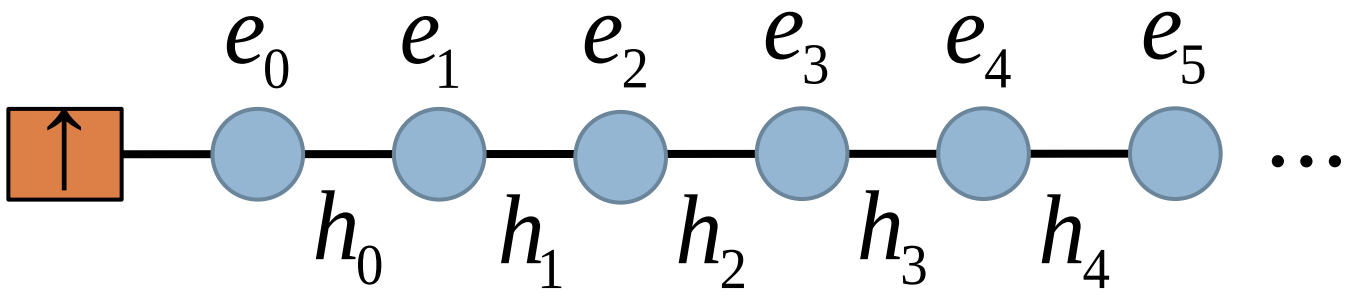
$$H_{host}^{disc} = \sum_{k,\sigma} \varepsilon_k b_{k\sigma}^{\dagger} b_{k\sigma} \qquad \left|a_0\right\rangle$$

- 1) Compute: $H\left|a_0\right\rangle = e_1\left|a_0\right\rangle + h_1\left|a_1\right\rangle$
- 2) Compute: $H\left|a_1\right\rangle = h_1\left|a_0\right\rangle + e_1\left|a_1\right\rangle + h_2\left|a_2\right\rangle$
- 3) At any step, only non-zero elements are:

$$\left\langle a_i\right|H\left|a_i\right\rangle = e_i \quad \text{and} \quad \left\langle a_i\right|H\left|a_{i-1}\right\rangle = h_i$$

Wilson Chain

- Tridiagonalize by **"Lanczos"** method:



- Wilson showed that the hoppings drop off exponentially down the chain, due to the logarithmic discretization:

$$h_n \sim \Lambda^{-n/2}$$

NRG

- **Iterative diagonalization** of Wilson chain

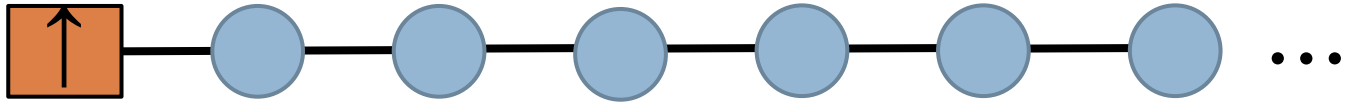
- **Truncation** of Hilbert space at each step
  - Throw away high lying states, keeping large but **fixed** number, N_s, states per iteration
  - Justified by the **energy-scale separation** going from iteration to iteration

- High-energy states discarded at one iteration do not affect low-energy states at later iterations

NRG: iterative procedure

- **Start from the impurity-zero orbital sub-system**
- **Apply recursion relation to add on extra sites**

$$H_{N+1} = \sqrt{\Lambda} H_N + \Lambda^{N/2} H_{N+1}^{join}$$

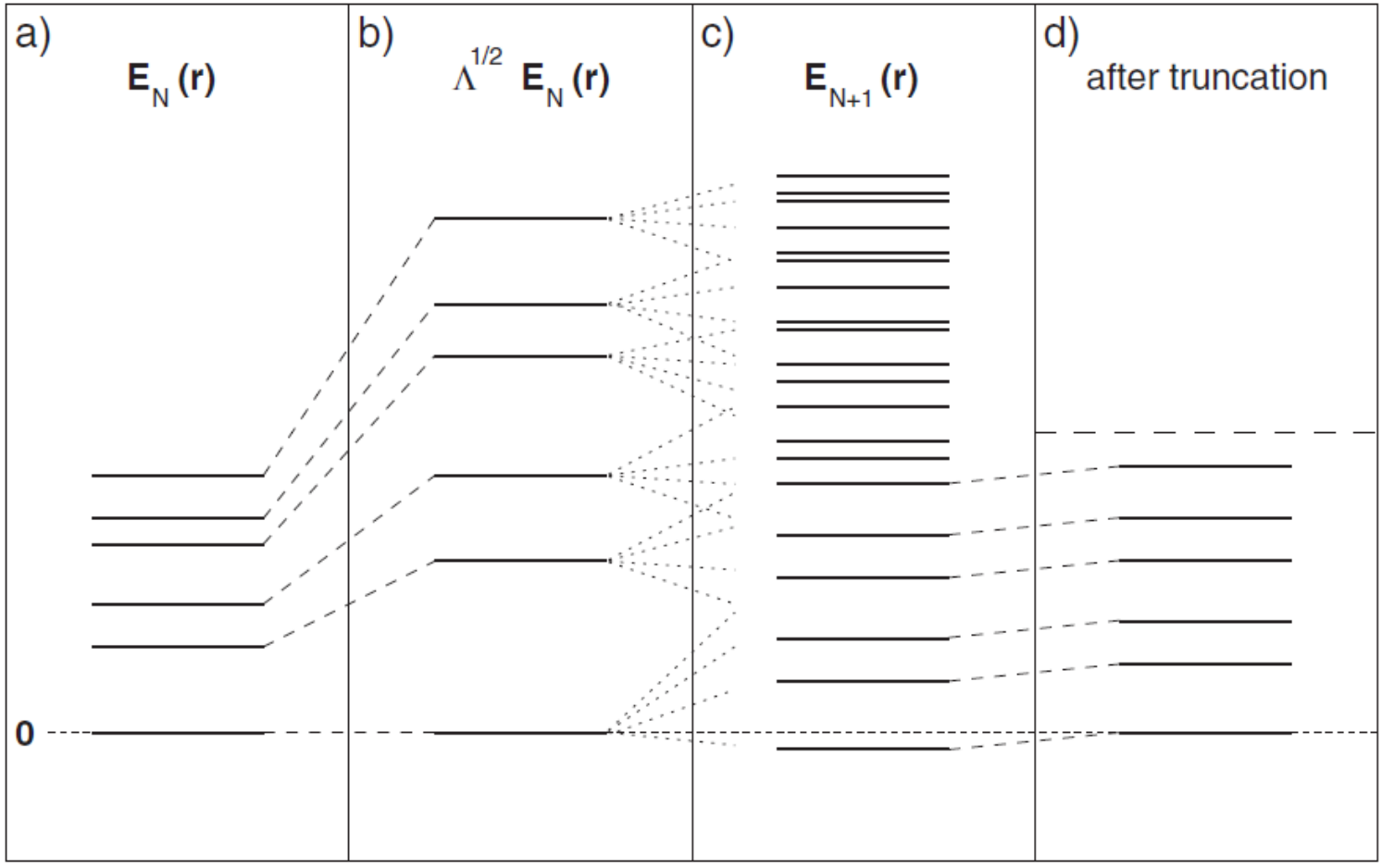


- **Full (discretized) Hamiltonian recovered as**

$$H = \lim_{N\to\infty} \Lambda^{-(N-1)/2} H_N$$

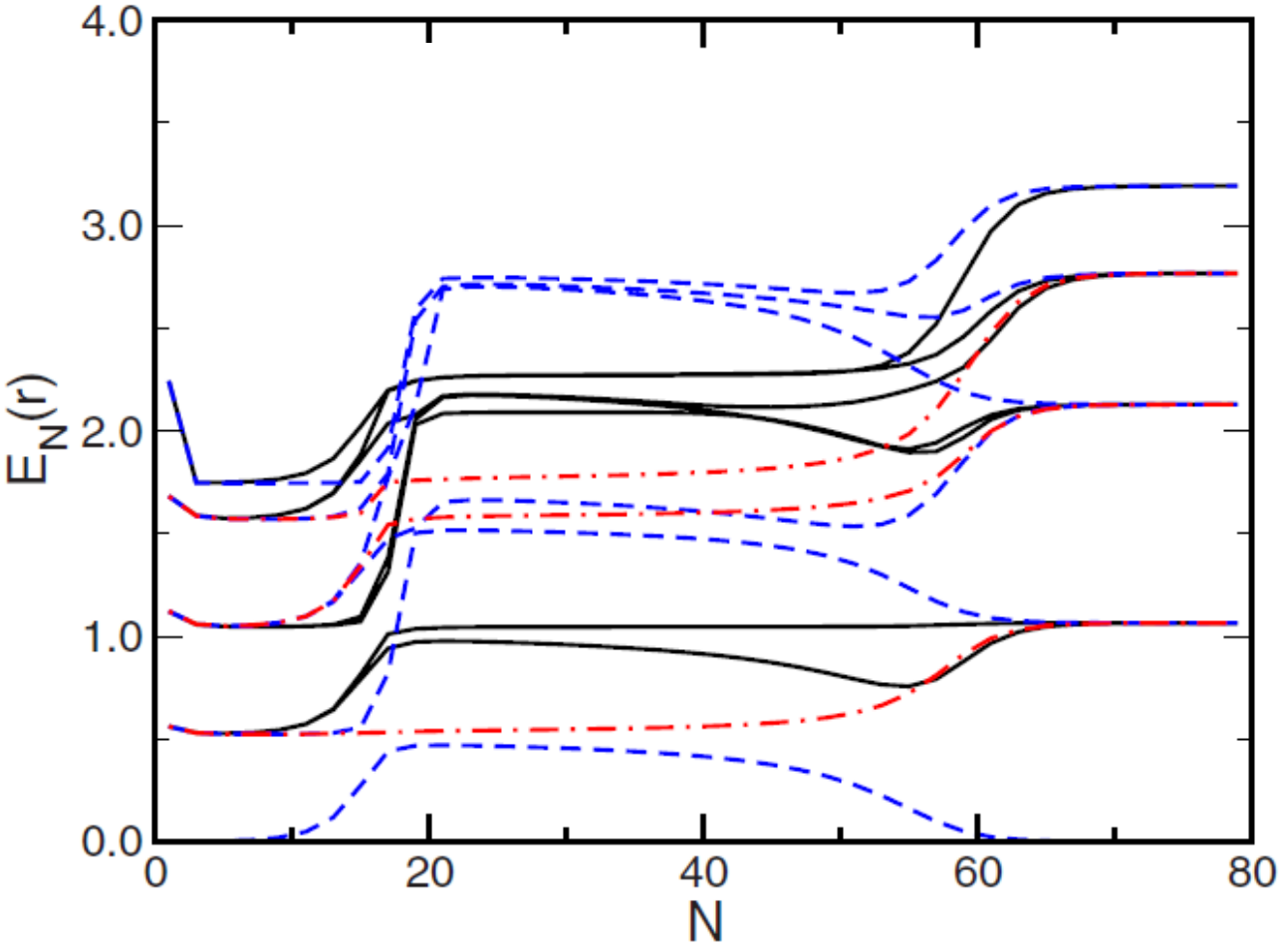
NRG: iterative procedure

- One iteration in NRG:



NRG: iterative procedure

- Flow of (rescaled) many-particle levels:



NRG: iterative procedure

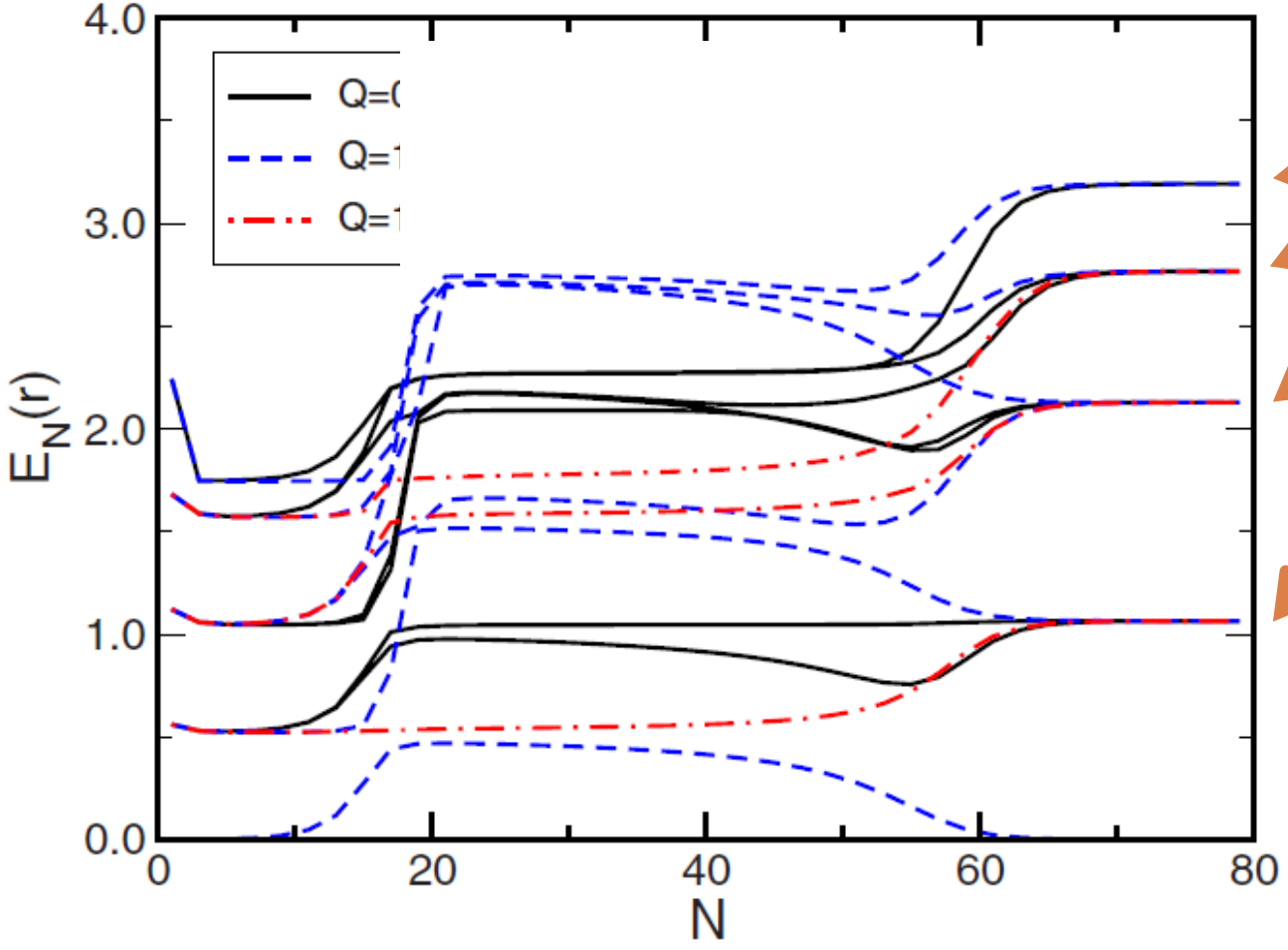
- Physics of the model at lower and lower energy scales is revealed as more Wilson chain orbitals are added

- Fixed number of states kept at each iteration, so no explosion of Hilbert space: linear scaling with N

- After a finite number of iterations (say N=100 for Λ=3), access ground state information
  - For the Kondo model:
    Strong coupling spin-singlet ground state
    Impurity screened by conduction electrons: Kondo effect!

NRG: iterative procedure

- Flow of (rescaled) many-particle levels:

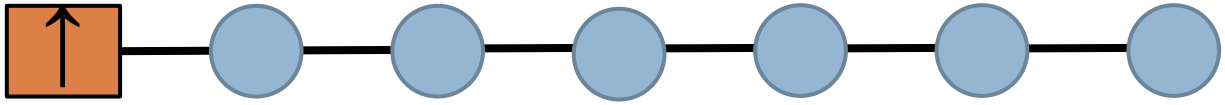


converged levels

Why?!

Analytic structure: the RG in NRG

- **View iterative construction of the Wilson chain…**



$$H_{N+1} = \sqrt{\Lambda} H_N + \Lambda^{N/2} H_{N+1}^{join}$$

… as an RG transformation:

$$H_{N+1} = \hat{R}\left(H_N\right)$$

The Renormalization Group

- The sequence of Hamiltonians, H_N , form a ***group***
- Application of the ***transformation***, $\hat{R}\left(H_N\right)$, generates a new member of the group, H_{N+1}
- ***Successive application*** of the transformation generates a characteristic ***RG flow*** through this Hamiltonian space
  - Flow starts from the 'initial' Hamiltonian (corresponding to the bare impurity with its original microscopic parameters)
  - At special points in the flow, physics can be understood in terms of the original model, but with **renormalized parameters.**

Fixed points

- **Fixed points** (FPs) of the RG transformation correspond to special cases where $H^* = \hat{R}\left(H^*\right)$

- A **fixed point Hamiltonian** is thus one that is invariant to the RG transformation, $H_N = H_{N+1} = H^*$

- Fixed point Hamiltonians often correspond to the original model, but with special **renormalized** values of the parameters (often 0 or infinity, but not always)

Fixed point stability

- Analyze behavior ***near*** to FPs:

$$H_N = H^* + \Delta H_N$$

- It follows from the RG transformation that:

$$\Delta H_{N+1} = \hat{R}\left(\Delta H_N\right)$$

- Does ΔH_N get larger or smaller with ***N*** ?
  - Construct possible perturbations to each FP consistent with model symmetries

$$\Delta H_N = \sum_i a_i \lambda_i^N \hat{O}_i$$

  - Can determine eigenvalue λ_i of the transformation $\hat{R}$ for operators $\hat{O}_i$ ***analytically***!

Fixed point stability

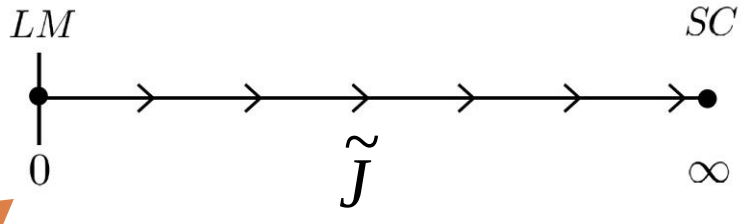
- Classify **perturbations** as **'relevant'** or **'irrelevant':**
  - A **'relevant'** perturbation **grows** under RG: $\lambda_i > 1$
  - An **'irrelevant'** perturbation **diminishes** under RG: $\lambda_i < 1$

- Classify **fixed points** as **'stable'** or **'unstable':**
  - A **'stable'** FP has **no relevant perturbations**
    - RG flow **'attracted'** to the FP
  - An **'unstable'** FP has **at least one** relevant perturbation
    - RG flow **'repelled'** by the FP

RG Flow

- RG flow between fixed points
  - Repelled by unstable FPs; attracted by stable FPs
  - Seen in many-particle energies and physical quantities
  - Schematically represented by RG flow diagram

Kondo model:



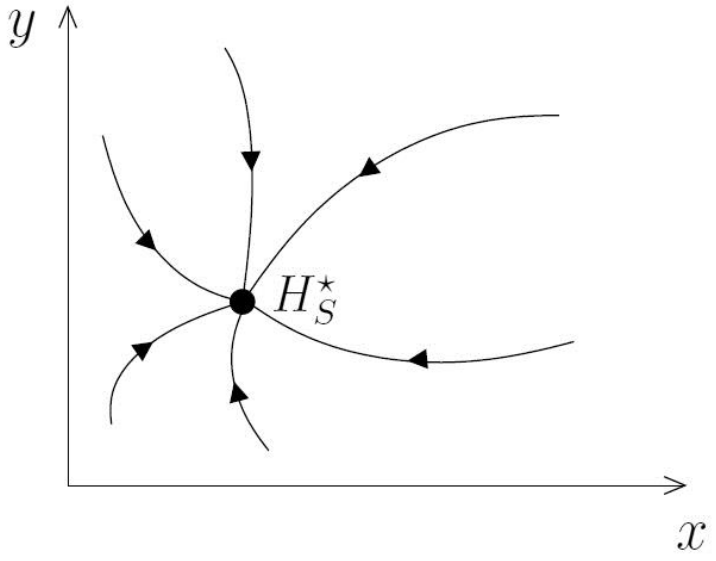
Unstable FP: 'Local Moment'

***Effective* renormalized coupling**

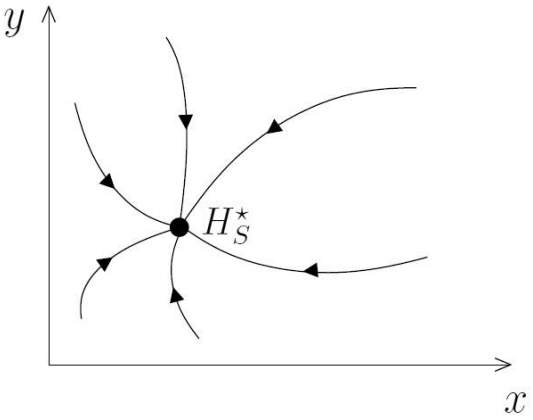
Stable FP: 'Strong Coupling'

RG Flow

- Number, character and stability of FPs determined by the specific RG transformation and symmetries
- RG flow (trajectory) determined by starting parameters of bare model



Universality

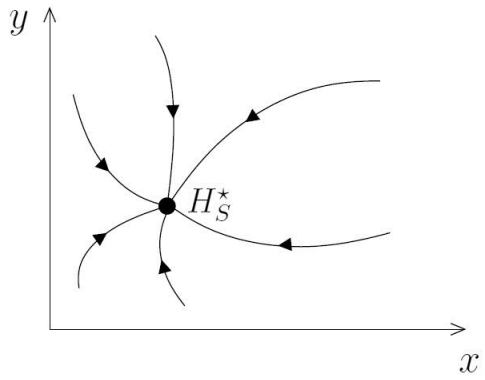


- **One stable FP:**
  - **Single ground state!**
  - For **any** starting parameters, always end up at the **same FP** (although path to reach the stable FP might be different)

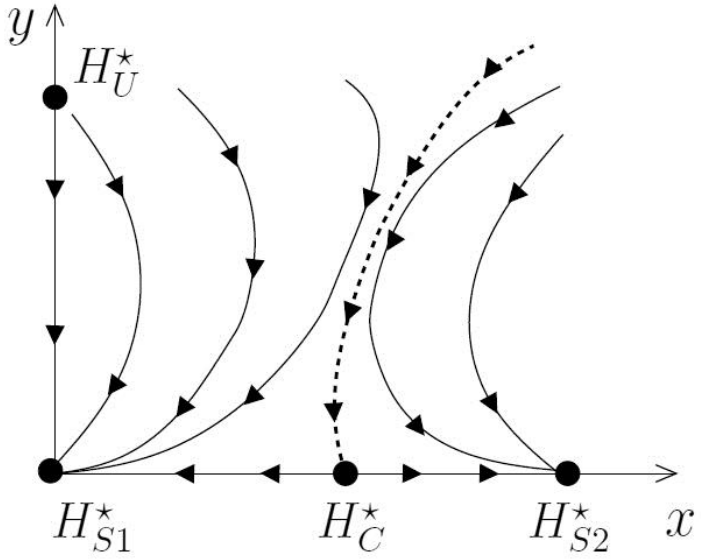
- **Universality**
  - Irrespective of the details of a model, or its bare parameters, two systems with the **same stable fixed point have the same ground state and low-energy physics**
  - RG flow between two fixed points is **universal**, and characterized only by a single crossover energy scale (for example, T_K for the Kondo model)
  - Physical quantities for different systems are described by a single **universal curve**, when rescaled in terms of T/T_K or ω/T_K

Critical phenomena

- **One stable FP:**
  - **Single ground state!**



- **Two stable FPs:**
  - **Two** possible ground states
  - **Starting parameters** determine RG trajectory and ultimately which stable FP is reached
  - **Quantum phase transition!**



Fixed point properties

- How to determine fixed points?
- What are their properties?
- Are they stable?

- Free Wilson Chain is invariant under the RG transformation…

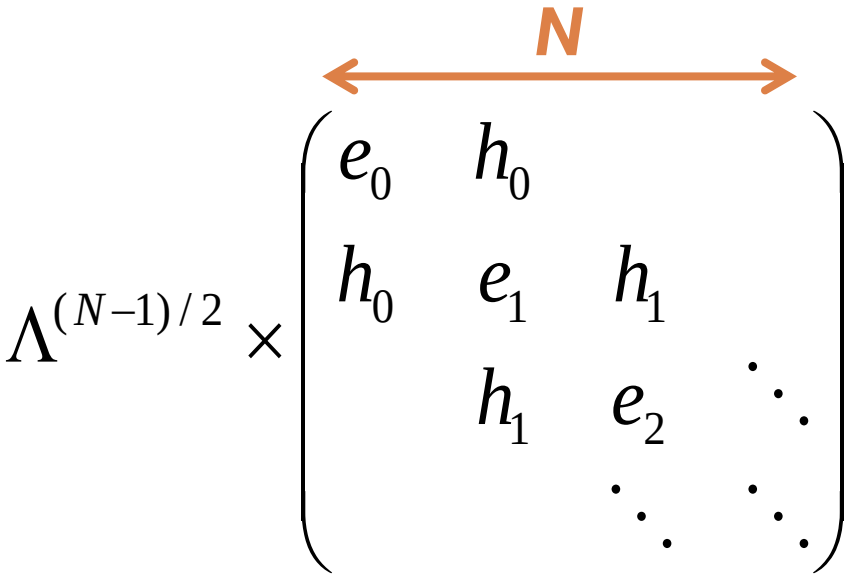
$$H_{host} = \hat{R}^2\left(H_{host}\right)$$

Fixed point properties

- Free Wilson Chain (no impurity):

$$H_N^{WC} = \Lambda^{(N-1)/2} \sum_{\sigma} \sum_{n=0}^{N} e_n \, f_{n\sigma}^{\dagger} f_{n\sigma} + \sum_{n=0}^{N-1} \left(h_n \, f_{n\sigma}^{\dagger} f_{(n+1)\sigma} + \text{H.c.} \right)$$

- Represented by tridiagonal matrix

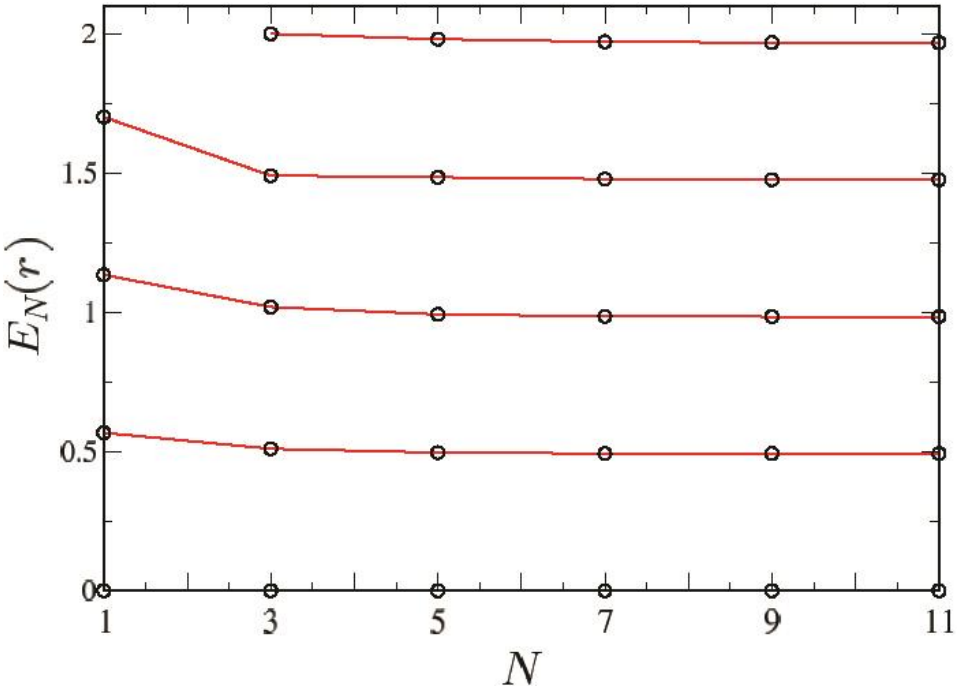


Diagonalize matrix to obtain single-particle levels:

$$H_N^{WC} = \sum_{k,\sigma} \varepsilon_k \, b_{k\sigma}^{\dagger} b_{k\sigma}$$

Fixed point properties

- Fill up single-particle levels up to the Fermi level (in accordance with Pauli principle)
- Construct many-particle excitations above ground state
- **Rapid convergence** with Wilson Chain length: adding more sites does not change levels!



- **Free Wilson chain is a FP of the RG transformation!**

Fixed point properties

- Anderson Impurity Model: reminder
  - Bare Hamiltonian:

$$H = \varepsilon\left(\hat{n}^{\uparrow}_{imp} + \hat{n}^{\downarrow}_{imp}\right) + U\left(\hat{n}^{\uparrow}_{imp}\hat{n}^{\downarrow}_{imp}\right) + \sum_{k,\sigma}\varepsilon_k \hat{n}^{\sigma}_{k} + V\sum_{k,\sigma}\left(d^{\dagger}_{\sigma}c_{k,\sigma} + \text{H.c.}\right)$$

Isolated impurity H_{imp}

$$\hat{n}^{\sigma}_{imp} = d^{\dagger}_{\sigma}d_{\sigma}$$

Isolated conduction band H_{host}

$$\hat{n}^{\sigma}_{k} = c^{\dagger}_{k,\sigma}c_{k,\sigma}$$

Hybridization H_{hyb}

discretize to give Wilson Chain

Fixed point properties

- Anderson Impurity Model: reminder
  - Bare Hamiltonian:

$$H = \varepsilon\left(\hat{n}^{\uparrow}_{imp} + \hat{n}^{\downarrow}_{imp}\right) + U\left(\hat{n}^{\uparrow}_{imp}\hat{n}^{\downarrow}_{imp}\right) + \sum_{k,\sigma}\varepsilon_k \hat{n}^{\sigma}_{k} + V\sum_{k,\sigma}\left(d^{\dagger}_{\sigma}c_{k,\sigma} + \text{H.c.}\right)$$

  - FPs Hamiltonians are of the same form, but with renormalized parameters:
    - **Free Orbital (FO) FP (high *T*)**

$$H^{*}_{FO} = H \quad \text{with} \quad V^{*}_{FO} = 0;\ U^{*}_{FO} = 0;\ \varepsilon^{*}_{FO} = 0$$

    - **Free Wilson chain with a single decoupled impurity SITE**

Fixed point properties

- Anderson Impurity Model: reminder
  - Bare Hamiltonian:

$$H = \varepsilon\left(\hat{n}^{\uparrow}_{imp} + \hat{n}^{\downarrow}_{imp}\right) + U\left(\hat{n}^{\uparrow}_{imp}\hat{n}^{\downarrow}_{imp}\right) + \sum_{k,\sigma}\varepsilon_k \hat{n}^{\sigma}_{k} + V\sum_{k,\sigma}\left(d^{\dagger}_{\sigma}c_{k,\sigma} + \text{H.c.}\right)$$

  - FPs Hamiltonians are of the same form, but with renormalized parameters:
    - **Local Moment (LM) FP** **(*T* ~ *U* : recall Schrieffer-Wolff)**

$$H^{*}_{LM} = H \quad \text{with} \quad V^{*}_{LM} = 0;\ U^{*}_{LM} = \infty;\ \varepsilon^{*}_{LM} = -U^{*}_{LM}/2$$

    - **Free Wilson chain with a single decoupled impurity SPIN**

Fixed point properties

- Anderson Impurity Model: reminder
  - Bare Hamiltonian:

$$H = \varepsilon\left(\hat{n}^{\uparrow}_{imp} + \hat{n}^{\downarrow}_{imp}\right) + U\left(\hat{n}^{\uparrow}_{imp}\hat{n}^{\downarrow}_{imp}\right) + \sum_{k,\sigma}\varepsilon_k \hat{n}^{\sigma}_{k} + V\sum_{k,\sigma}\left(d^{\dagger}_{\sigma}c_{k,\sigma} + \text{H.c.}\right)$$

  - FPs Hamiltonians are of the same form, but with renormalized parameters:
    - **Strong Coupling (SC) FP (low temperature… $T \ll T_K$)**

$$H^{*}_{SC} = H \quad \text{with} \quad \left(V^{*}_{SC}\right)^2 / U^{*}_{SC} = \infty; \quad \varepsilon^{*}_{SC} = -U^{*}_{SC}/2$$

    - **Free Wilson chain with 'zero-orbital' removed**

FO fixed point analysis

- Anderson Impurity Model
  - Near the FO FP:

$$H_N^{FO} = H_{FO}^{*} + \Delta H_N^{FO}$$

$$\Delta H_N^{FO} = \sum_i a_i \, \lambda_i^N \, \hat{O}_i$$

$$\hat{O}_1 = \left(d_\sigma^\dagger d_\sigma - 1\right)^2$$

$$\hat{O}_2 = \left(d_\sigma^\dagger f_{0,\sigma} + f_{0,\sigma}^\dagger d_\sigma\right)$$

relevant

FO FP unstable!

LM fixed point analysis

- Anderson Impurity Model
  - Near the LM FP:

$$H_N^{LM} = H_{LM}^{*} + \Delta H_N^{LM}$$

marginally relevant: LM FP unstable

$$\hat{O}_1 = \left(f_{0,\sigma}^{\dagger} \, \vec{\sigma} \, f_{0,\sigma'} \right) \cdot \vec{\tau}$$

$$H^{eff} = \Lambda^{(N-1)/2} \sum_{n=0}^{N-1} \sum_{\sigma} h_n \, f_{n\sigma}^{\dagger} f_{(n+1)\sigma} + \text{H.c.}$$

$$+ \tilde{J} \, \Lambda^{(N-1)/2} \left(f_{0,\sigma}^{\dagger} \, \vec{\sigma} \, f_{0,\sigma'} \right) \cdot \vec{\tau}$$

discretized form of Kondo model!

SC fixed point analysis

- Anderson Impurity Model
  - Near the SC FP:

$$H_N^{SC} = H_{SC}^{*} + \Delta H_N^{SC}$$

$$\hat{O}_1 = \left(f_{1,\sigma}^{\dagger} \; f_{2,\sigma} + f_{2,\sigma}^{\dagger} \; f_{1,\sigma} \right)$$

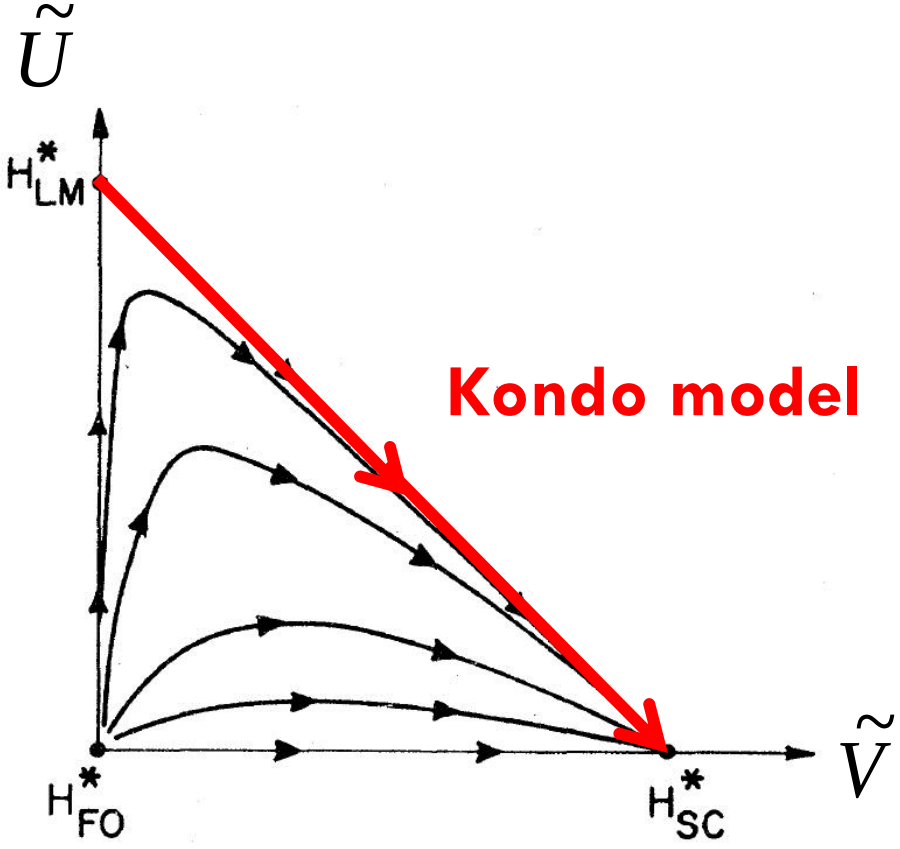
$$\hat{O}_2 = \left(f_{1,\sigma}^{\dagger} \; f_{1,\sigma} - 1 \right)^2$$

irrelevant

- **SC FP is 'stable'**
- **As *N* increases, get closer to SC FP**
- **MUST reach SC FP at low enough temperatures**
- ***T=0* ground state is described by SC FP: Kondo singlet**

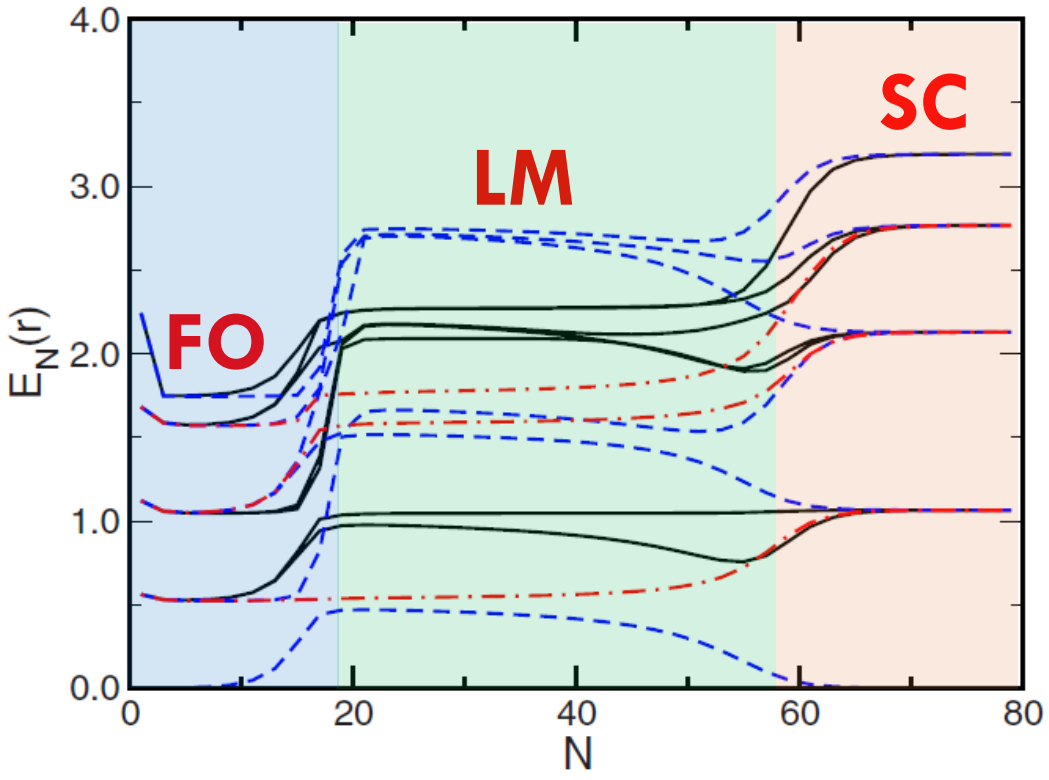
The Renormalization Group

- Anderson Impurity Model
  - Schematic RG flow diagram:



The Renormalization Group

- Anderson Impurity Model
  - RG flow of many-particle energies:



The Renormalization Group

- **RG flow also seen in physical quantities…**

… more in final part!