The Kondo Problem: Numerical renormalization group and the single-impurity Anderson Model

PHYS 4240: Solid State Physics

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22 April, 2025

Introduction

- In the 1930s, experiments revealed some interesting behavior in low-temperature measurements of the resistance of certain metals like Gold.
- The expectation was that the resistance decreases monotonically with temperature due to decreasing electron-phonon interactions.
- However, the observation was that a minimum was reached and the resistance started growing again at lower temperatures.

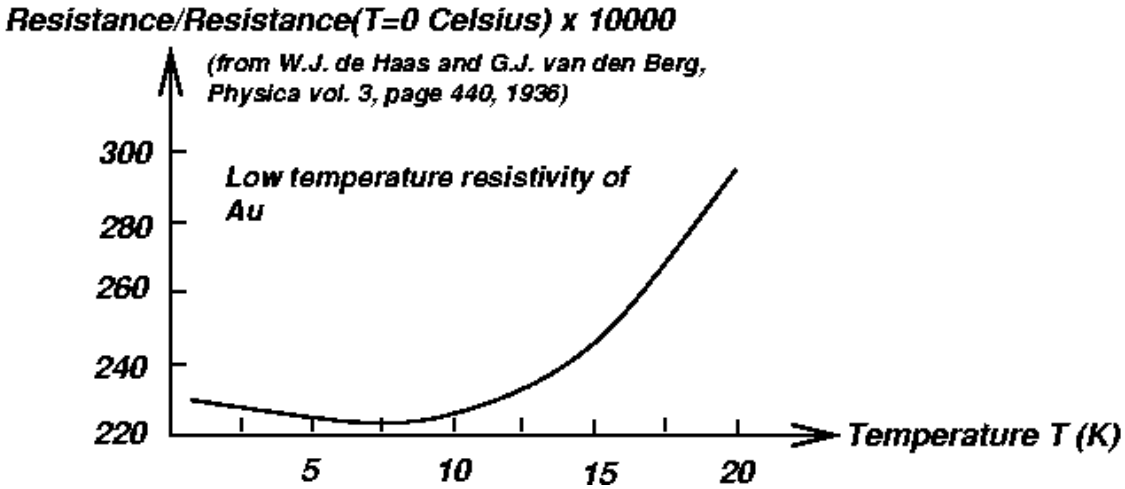


Figure: Figure created using measurements found in [1].

Kondo's Solution

- Eventually it became known that this was due to impurities within the metal.
- Jun Kondo then used perturbation theory on the spin-spin interaction between the impurity and the conduction electrons in the host metal:

$$H = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + J \sum_{\mathbf{k},\mathbf{k}',\alpha,\beta} c^{\dagger}_{\mathbf{k},\alpha} \boldsymbol{\sigma}_{\alpha,\beta} c_{\mathbf{k}',\beta} \cdot \mathbf{S}.$$

- This yielded corrections to the resistance that looked like

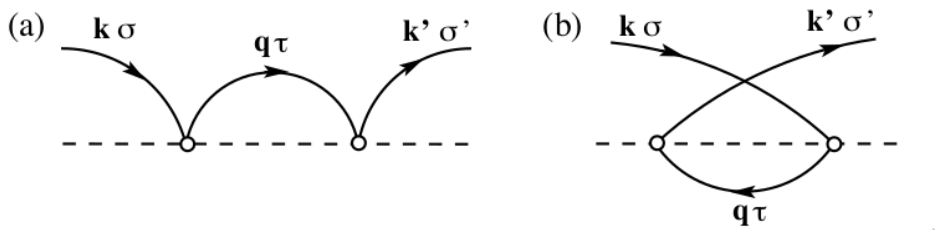
$$R(T) = aT^5 + c_{\text{imp}} R_0 - c_{\text{imp}} R_1 \log\left(\frac{k_B T}{D}\right).$$

- Yielded correct behavior *at* the minimum, but diverges for $T \to 0$.

Other Attempts at Solutions

- After this, a number more models were introduced, one in particular being Anderson's *Poor Man's Scaling* method [2].
- This method was effectively a renormalization group approach, but again failed at low temperatures.
- This was because subsequent renormalizations increased J to infinity, the parameter by which perturbation theory was applied later on.
- In 1975, Wilson [3] used the numerical renormalization group to approach the problem non-perturbatively, finally leading to accurate solutions in the low-energy regime.

Poor Man's Scaling



- One approach to this method is considering the scattering between electrons from an initial state $|\mathbf{k}\rangle$ to a final $|\mathbf{k}'\rangle$.
- We consider the so-called scattering T-matrix:

$$T_{\mathbf{k}',\mathbf{k}}(\omega) = V_{\mathbf{k}',\mathbf{k}} + V_{\mathbf{k}',\mathbf{q}} G_0(\omega, \mathbf{q}) T(\omega)$$

  where V is the Kondo exchange interaction $V \propto J$.
- By calculating this to second order in V, we are effectively renormalizing the interaction:

$$\hat{V} \to \hat{V}' = \hat{V} + \hat{V} \frac{1}{\omega - \hat{H}_0} \hat{V}$$

Poor Man's Scaling

- After some derivations, what we find is that the renormalization of the interactions look like $J_\alpha \to J_\alpha + \delta J_\alpha$ $(\alpha = \pm, z)$, with

$$\delta J_z = -J_\pm^2 \rho |\delta\Lambda| \left[\frac{1}{\omega - \Lambda + \epsilon_k} \frac{1}{\omega - \Lambda + \epsilon_{k'}} \right],$$
$$\delta J_\pm = -J_z J_\pm \rho |\delta\Lambda| \left[\frac{1}{\omega - \Lambda + \epsilon_k} \frac{1}{\omega - \Lambda + \epsilon_{k'}} \right]$$

- Leading to renormalization flow equations that go like

$$\frac{\mathrm{d}g_z}{\mathrm{d}\ln\Lambda} = -2g_\pm^2 + \mathcal{O}(g^3),$$
$$\frac{\mathrm{d}g_\pm}{\mathrm{d}\ln\Lambda} = -2g_z g_\pm + \mathcal{O}(g^3)$$

where gs are dimensionless couplings.

Variational Methods

- Variational methods can give us further qualitative understanding.
- We consider a filled Fermi sea of conduction electrons and a singly occupied d-orbital from the impurity.
- If the spins of a conduction electron and the d-orbital electron are the same, there are no important interactions, but if they are anti-parallel, virtual excitations may occur.
- A trial wavefunction representing this state is give by

$$|\psi_0\rangle = \left[\alpha_0 + \sum_{k<k_F,\sigma} \alpha_{\mathbf{k}} c^\dagger_{d,\sigma} c_{\mathbf{k},\sigma}\right] |0\rangle$$

- Importantly, this is representative of a singlet state formed between the d-orbital of the impurity and a conduction electron.

Variational Methods

- We now consider the variational energy functional

$$\tilde{E}[|\psi_0\rangle] = \frac{\langle\psi_0|H|\psi_0\rangle}{\langle\psi_0|\psi_0\rangle},$$

where we are considering the single-impurity Anderson Hamiltonian:

$$H = \epsilon_d n_d + U n_{d\uparrow} n_{d\downarrow} + \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k},\sigma} c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}$$
$$+ \sum_{\mathbf{k},\sigma} \left(V_{\mathbf{k}} c^\dagger_{\mathbf{k},\sigma} d_\sigma + V^*_{\mathbf{k}} d^\dagger_\sigma c_{\mathbf{k},\sigma} \right).$$

- All energies are measured relative to the Fermi surface.

Variational Methods

- By plugging H into the energy functional, we arrive at

$$\tilde{E} = 2 \sum_{k<k_F} \frac{|V_{\mathbf{k}}|^2}{\tilde{E} - \epsilon_d + \epsilon_{\mathbf{k}}}.$$

- Defining the binding energy $\Delta_K = \tilde{E} - \epsilon_d$, we find:

$$\epsilon_d + \Delta_K = 2 \sum_{k<k_F} \frac{|V_{\mathbf{k}}|^2}{\Delta_K - |\epsilon_{\mathbf{k}}|}.$$

- Converting to the continuum and letting $V_{\mathbf{k}} \to V$ (indep. of $\mathbf{k}$):

$$\epsilon_d + \Delta_K = 2\rho \int_0^{\epsilon_F} \mathrm{d}\epsilon \, \frac{-V^2}{\epsilon - \Delta_K} = -2\epsilon |V|^2 \ln\left(\frac{\epsilon_F}{|\Delta_K|}\right).$$

Variational Methods

- When the energy of the d-level (relative to the Fermi surface) is much larger than the binding energy, we find

$$\Delta_K = -\epsilon_F \exp\left[-\frac{1}{2\rho J}\right],$$

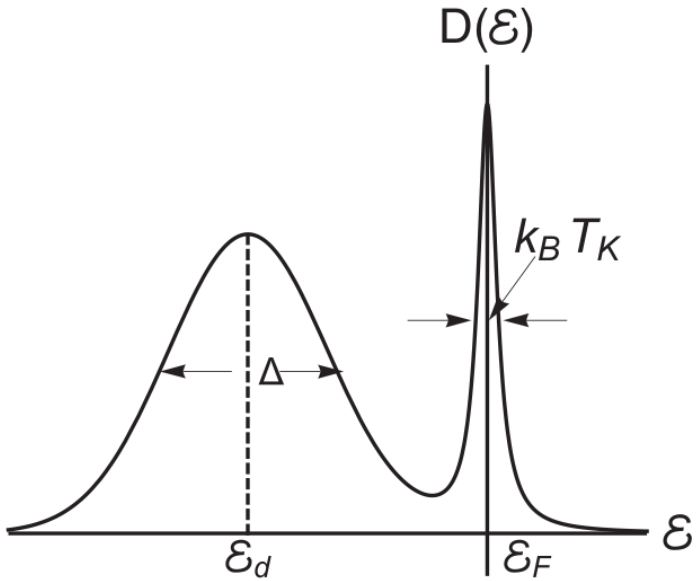
  where $J = V^2/\epsilon_d$ is defined as the coupling constant.
- Importantly, this is negative, indicating that the singlet state (represented by our original trial wavefunction) is the preferable and therefore likely state for this configuration.

Kondo Resonance

- We would expect, in the case of strong d-level on-site repulsion U, that $\langle n_d \rangle \approx 1$, or $1 - \langle n_d \rangle \approx 0$. What we find is

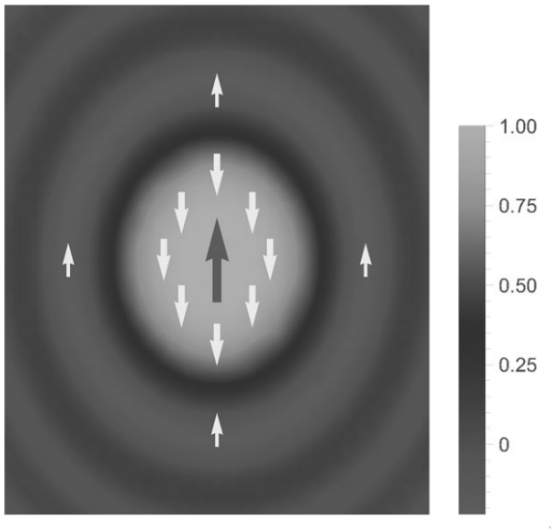
$$1 - \langle n_d \rangle \approx \frac{\pi \Delta_K}{2\Delta} \ll 1 \neq 0$$

- Because of a slightly less than unity d-level occupation, there is an excess of states in the Fermi surface.
- This observed increase in the density of states is what is called a **Kondo resonance**



Kondo Resonance

- This leads often to the picture of what is called the **Kondo cloud**



- Due to the increased density of states, there is also an increase (a maximum is achieved) for the scattering probability between the d-level impurity states and the conduction electrons.
- This manifests in the observation of increasing resistivity as $T \to 0$.

The Renormalization Group

- The renormalization group is a mapping of a Hamiltonian $H(\mathbf{K})$ with a set of parameters $\mathbf{K}$ to another with parameters $\mathbf{K}'$, valid at a new energy scale.

$$\mathcal{R}_\alpha[H(\mathbf{K})] = H(\mathbf{K}'), \quad \text{or} \quad \mathcal{R}_\alpha(\mathbf{K}) = \mathbf{K}'.$$

- The parameter α is the ratio of the energy scales; characterizes the "strength" of the transformation.
- Subsequent transformations form a *trajectory* in parameter space.

Fixed Points

- A **fixed point** is a set of params $\mathbf{K}^*$ that is invariant under the transformation:

$$\mathcal{R}(\mathbf{K}^*) = \mathbf{K}^*.$$

- We can linearize the transformation around this fixed point:

$$\mathcal{R}_\alpha(\mathbf{K}^* + \delta\mathbf{K}) = \mathbf{K}^* + \mathbf{L}^*_\alpha \delta\mathbf{K} + \mathcal{O}(\delta\mathbf{K}^2),$$

- Then we can express the mapping in terms of the eigenvectors/eigenvalues of $\mathbf{L}^*_\alpha$:

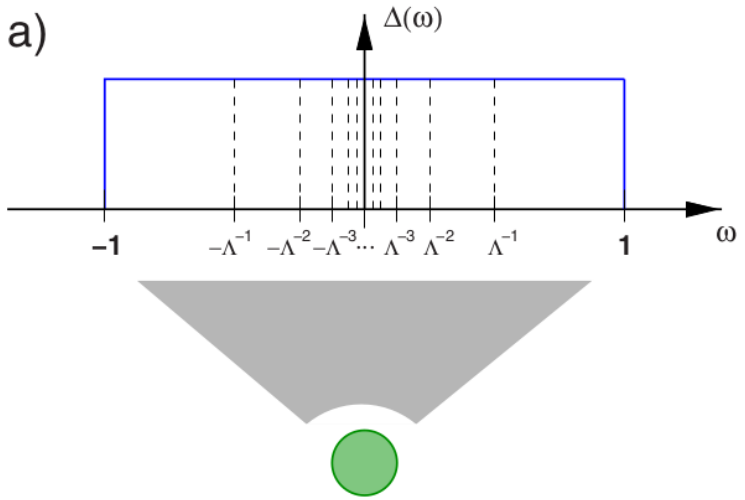
$$\mathcal{R}^m_\alpha(\mathbf{K}^* + \delta\mathbf{K}) = \mathbf{K}^* + \sum_n (\delta K)_n (\lambda^*_n)^m \mathbf{V}^*_n.$$

Fixed Points

- The point of doing this is so that we are able to effectively describe behavior *around* a fixed point using the effective Hamiltonian at that fixed point.
- We can make the connection from poor man's scaling results that the $J \to \infty$ / $T \to 0$ point is a fixed point.
- What we want to do is formalize our renormalization group transformations and determine the effective Hamiltonian for the $J \to \infty$ fixed point.
- We are then able to describe the behavior around the fixed point with this effective Hamiltonian and determine important quantities.
- In the trajectories/flows of our parameters, we also are able to recognize the transitions between fixed points.

The Numerical Renormalization Group (NRG)

The NRG is highly specialized per problem, but generally follows these steps:



1. Divide the energy spectrum into logarithmic bins via a parameter $\Lambda > 1$: we get intervals $[\Lambda^{-(n+1)}, \Lambda^{-n}]$, $[-\Lambda^{-n}, \Lambda^{-(n+1)}]$.

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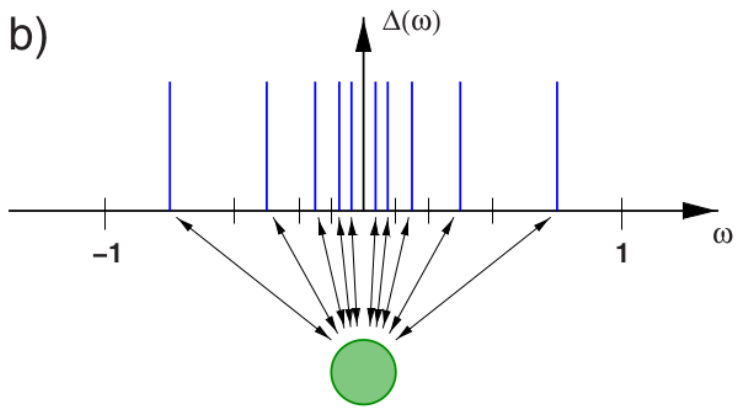

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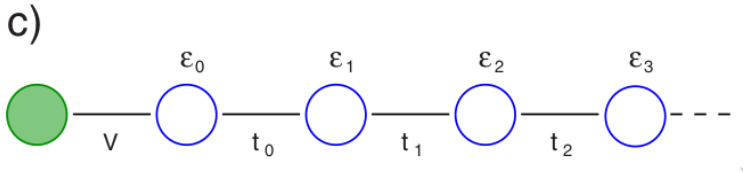

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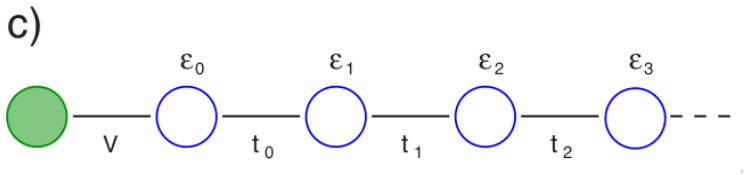

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2. Pick a single characteristic state from each interval.
3. Map these discrete states onto a semi-infinite chain, with the impurity placed at one end.
4. Iteratively diagonalize the resulting Hamiltonian, adding a site each iteration.

The NRG

- By logarithmically discretizing the energy spectrum, we arrive at the following relation for the hopping terms:

$$t_n = \Lambda^{-n/2} \frac{(1+\Lambda^{-1})(1-\Lambda^{-n-1})}{2\sqrt{1-\Lambda^{-2n-1}}\sqrt{1-\Lambda^{-2n-3}}}.$$

- We notice $t_n \propto 1/\sqrt{\Lambda}$, meaning that adding a term corresponds to accessing a new energy scale that is reduced by a factor of $\sqrt{\Lambda}$.
- This is the essence of the NRG.

Single-Impurity Anderson Model (SIAM)

- The SIAM considers that the impurity is represented by local moment formed via the Coulomb interaction U between the two electrons in the state.

$$H = \sum_{\sigma} \epsilon_d d_\sigma^\dagger d_\sigma + U d_\uparrow^\dagger d_\uparrow d_\downarrow^\dagger d_\downarrow + \sum_{k,\sigma} \epsilon_k c_{k,\sigma}^\dagger c_{k,\sigma} + \sum_{k,\sigma} V_k (d_\sigma^\dagger c_{k,\sigma} + \text{h.c.}).$$

- The ds are creation/annihilation operators for impurity states, cs are for conduction states, and V is the hybridization term.

Logarithmic Discretization

- Can bring the Hamiltonian to a quasi-continuous one:

$$H = H_{\text{imp}} + \sum_{\sigma} \int_{-1}^{1} \mathrm{d}\epsilon \; g(\epsilon) a^{\dagger}_{\epsilon,\sigma} a_{\epsilon,\sigma} + \sum_{\sigma} \int_{-1}^{1} \mathrm{d}\epsilon \; h(\epsilon)(d^{\dagger}_{\sigma} a_{\epsilon,\sigma} + \text{h.c.}).$$

- These new operators satisfy the standard fermionic anti-commutation relations:

$$\{a^{\dagger}_{\epsilon,\sigma}, a_{\epsilon'\sigma'}\} = \delta(\epsilon - \epsilon')\delta_{\sigma,\sigma'}.$$

- We can then discretize the model with points $x_n = \pm\Lambda^{-n}$, where $n = 0, 1, 2, \ldots$ and $\Lambda > 1$.

Logarithmic Discretization

- Inside each iterval, we define a new basis which are simply plane waves:

$$\psi^{\pm}_{np}(\epsilon) = \begin{cases} \frac{1}{\sqrt{d_n}} e^{\pm i\omega_n p\epsilon}, & \text{for } x_{n+1} < \epsilon < x_n, \text{ and} \\ 0 & \text{otherwise.} \end{cases}$$

  where $p \in \mathbb{Z}$ and $\omega_n = 2\pi/d_n$ is the characteristic frequency.
- Expanding our continuous a operators in terms of these (simply a Fourier expansion) we find:

$$a_{\epsilon\sigma} = \sum_{np} \left(a_{np\sigma}\psi^{+}_{np}(\epsilon) + b_{np\sigma}\psi^{-}_{np}(\epsilon) \right)$$

- Using these, our quasi-continuous Hamiltonian is now expanded in terms of logarithmically discretized creation/annihilation operators.

Mapping to semi-infinite chain

- With the Hamiltonian now logarithmically discretized, one can follow a tridiagonalization procedure in order to put it in the form of the semi-infinite chain (tight-binding form):

$$H = H_{\text{imp}} + \sqrt{\frac{\xi_0}{\pi}} \sum_{\sigma} (f_\sigma^\dagger c_{0,\sigma} + c_{0,\sigma}^\dagger f_\sigma) + \sum_{\sigma,n=0}^{\infty} \left[\epsilon_n c_{n,\sigma}^\dagger c_{n,\sigma} + t_n (c_{n,\sigma}^\dagger c_{n+1,\sigma} + c_{n+1,\sigma}^\dagger c_{n,\sigma}) \right].$$

- Assuming a particle-hole symmetric hybridization $\Delta(\omega) = \Delta(-\omega)$ and a k-independent hybridization term V, we have that $\epsilon_n = 0$ and $\sqrt{\xi_0/\pi} \to V$:

$$H = \epsilon_d n_d + U n_{d\uparrow} n_{d\downarrow} + V \sum_{\sigma} (d_\sigma^\dagger c_{0,\sigma} + c_{0,\sigma}^\dagger d_\sigma) + \sum_{\sigma,n=0}^{\infty} \left[t_n (c_{n,\sigma}^\dagger c_{n+1,\sigma} + c_{n+1,\sigma}^\dagger c_{n,\sigma}) \right].$$

Connection to the Renormalization Group

- Due to the choice of logarithmic binning, Wilson [3] calculated that the hopping terms decrease exponentially:

$$t_n = \Lambda^{-n/2} \frac{(1+\Lambda^{-1})(1-\Lambda^{-n-1})}{2\sqrt{1-\Lambda^{-2n-1}}\sqrt{1-\Lambda^{-2n-3}}}.$$

- Therefore, what we are doing by adding a site to the infinite chain is accessing an energy scale that is decreased by a factor of $\sqrt{\Lambda}$.
- In particular, we consider the main chain Hamiltonian is the limit of a sequence of Hamiltonians parameterized by N such that

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

where

$$H_N = \Lambda^{(N-1)/2}\Big[H_{\text{imp}} + V\sum_{\sigma}(f_\sigma^\dagger c_{0,\sigma} + c_{0,\sigma}^\dagger f_\sigma) + \sum_{\sigma,n=0}^{N-1} t_n(c_{n,\sigma}^\dagger c_{n+1,\sigma} + c_{n+1,\sigma}^\dagger c_{n,\sigma})\Big].$$

Connection to the Renormalization Group

- With this definition, we define recursion relations for subsequent Hamiltonians:

$$H_{N+1} = \sqrt{\Lambda} H_N + \Lambda^{N/2} \sum_\sigma t_N (c^\dagger_{N,\sigma} c_{N+1,\sigma} + c^\dagger_{N+1,\sigma} c_{N,\sigma}),$$

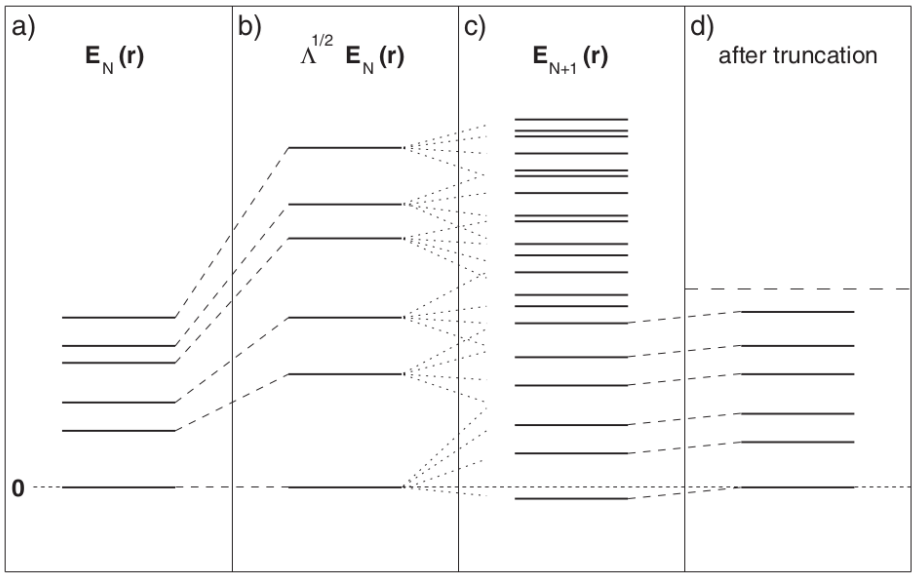
  with the initial given by

$$H_0 = \Lambda^{-1/2} \left[\sum_\sigma \epsilon_f f^\dagger_\sigma f_\sigma + U f^\dagger_\uparrow f_\uparrow f^\dagger_\downarrow f_\downarrow + V \sum_\sigma (f^\dagger_\sigma c_{0,\sigma} + c^\dagger_{0,\sigma} f_\sigma) \right].$$

- Therefore, what we have when going to H_N to H_{N+1} is a renormalization group transformation: $\mathcal{R}_\alpha[H_N] = H_{N+1}$, with α parameterized via $\sqrt{\Lambda}$.

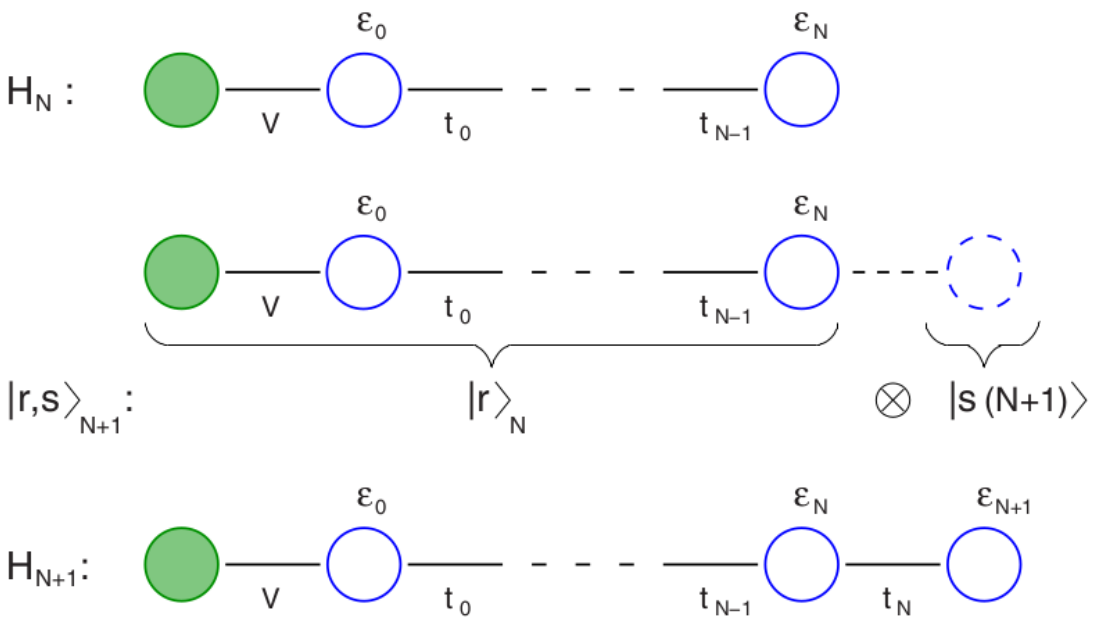
Iterative diagonalization of the semi-infinite chain

- As described, the procedure from here involves repeatedly adding sites to the chain and diagonalizing the resulting Hamiltonian.
- Due to the choice of basis, the dimensionality of the Hamiltonian increases exponentially each iteration.
- By sorting the energies and truncating them to keep only some fixed N_s lowest-lying energies, we remove the higher energy terms which have decreasing effect on the low energy behavior of the system.



Iterative diagonalization of the semi-infinite chain

- For this problem, we choose our basis to be the Fock basis consisting of four states: $|0\rangle$, $|\uparrow\rangle$, $|\downarrow\rangle$, and $|\uparrow\downarrow\rangle$ related to empty, single, or doubly-occupied states.
- Each iteration, we construct a new basis that is the outer product of the original bases $|r\rangle_N$ and the new basis $|s_{n+1}\rangle$.



Initial iteration

- For the initial iteration, we start by considering just the impurity and one conduction site; can construct the Hamiltonian in the combined Fock basis like so:

$$H = I_4 \otimes H_{\text{imp}} + H_{\text{hyb}},$$
$$H_{\text{hyb}} = V \sum_{\sigma} (c_{0,\sigma}^{\dagger} \otimes f_{\sigma} + c_{0,\sigma} \otimes f_{\sigma}^{\dagger}).$$

- With our choice of basis, we consider the form of the creation and annihilation operators (cs and fs are identical):

$$f_{\uparrow}^{\dagger} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}, \quad f_{\downarrow}^{\dagger} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

- The -1 is due to the fermionic nature of the operators.

Initial iteration

- With this, we are able to construct the (symmetrized) initial Hamiltonian

$$H_0 = \begin{pmatrix} \mathcal{H}_{\text{imp}} & Vf_\uparrow & Vf_\downarrow & 0 \\ Vf_\uparrow^\dagger & \mathcal{H}_{\text{imp}} & 0 & Vf_\downarrow \\ Vf_\downarrow^\dagger & 0 & \mathcal{H}_{\text{imp}} & -Vf_\uparrow \\ 0 & Vf_\downarrow^\dagger & -Vf_\uparrow^\dagger & \mathcal{H}_{\text{imp}} \end{pmatrix}$$

where $\mathcal{H}_{\text{imp}}$ represents the impurity occupation energies acting on the impurity subspace:

$$\mathcal{H}_{\text{imp}} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \epsilon_f & 0 & 0 \\ 0 & 0 & \epsilon_f & 0 \\ 0 & 0 & 0 & 2\epsilon_f + U \end{pmatrix}$$

Symmetries

- As mentioned before, the dimensionality of this Hamiltonian rapidly approaches being unfeasible to diagonalize.
- We can utilize symmetries, in particular S_z (twice the z-component of spin) and Q (charge with respect to half-filling)

$$S_z \to [0, 1, -1, 0], \quad Q \to [-1, 0, 0, 1]$$

- Since these are good quantum numbers, we can construct an operator combining them that commutes with the Hamiltonian.
- This effectively reduces the single matrix into several (significantly) smaller matrices corresponding to the states with the same eigenvalue of the new operator.

Subsequent Iterations

- Subsequent iterations increase the dimensionality by 4, but the structure of placing identities and the creation and annihilation operators remains largely the same, but instead with t_ns for the hopping parts.

$$t_n(c^\dagger_{n+1,\sigma} \otimes c_{n,\sigma} + c_{n+1,\sigma} \otimes c^\dagger_{n,\sigma})$$

- The diagonals are then the energies from the previous iteration.
- If $N > N_s$, we truncate the highest energy parts and keep the remaining N_s states.
- The energies are ordered and thus are the states, so we must rotate the operators:

$$f^\dagger_\sigma \to \mathbf{C}^\intercal_n f^\dagger_\sigma \mathbf{C}_n$$

- We also calculate thermodynamic quantities.

Calculation of Physical Quantities

- Each added site/iteration corresponds to a temperature T_N:

$$k_B T_N = \frac{1}{2}(1 + \Lambda^{-1})\Lambda^{-(N-1)/2}/\bar{\beta}.$$

- It turns out we can choose $\bar{\beta}$ to be in the range 0.5 to 1, from which we calculate the temperature for that particular iteration.
- This is because when evaluating things like the partition function, a low β requires higher energy terms, which we drop from the truncation scheme, and a higher β simply involves fewer terms leading to less accuracy.
- For each iteration, we determine this temperature, then determine additional physical quantities.

Calculation of Physical Quantities

- After determining the temperature, we can find the entropy, specific heat, and susceptibility:

$$S = \beta \langle H \rangle + \ln Z,$$
$$C = \beta^2(\langle H^2 \rangle - \langle H \rangle^2),$$
$$\chi_{\text{tot}} = \beta(\langle S_{\text{tot},z}^2 \rangle - \langle S_{\text{tot},z} \rangle^2).$$

- Here, the average of a quantity X is given by

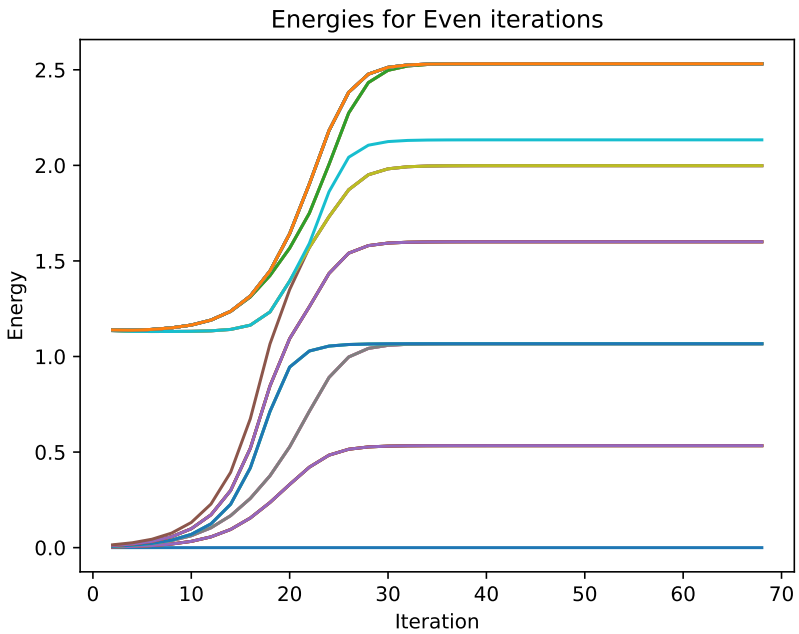
$$\langle X \rangle = \frac{1}{Z} \sum_i X_i e^{-\beta x_i},$$

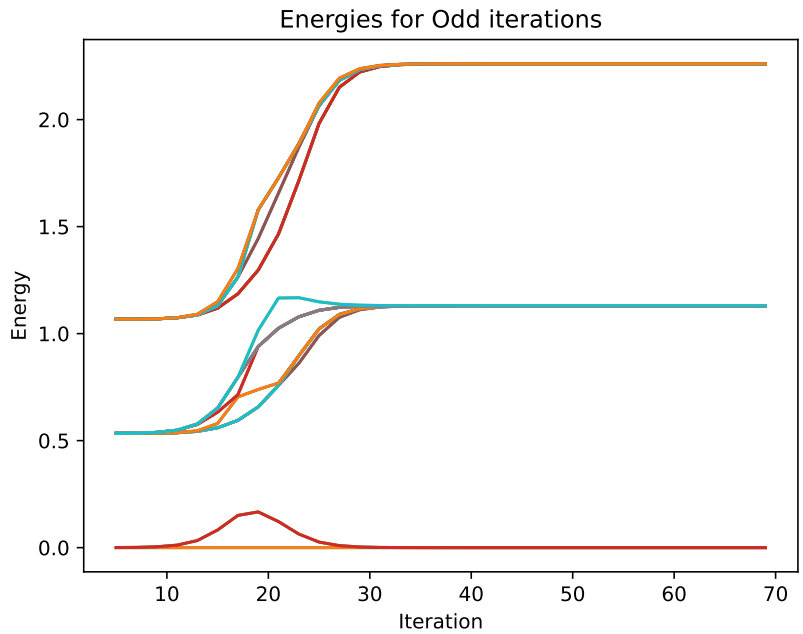
  with Z being the standard partition function.
- To get the contributions to these values of the impurity only, we subtract off from this value with the impurity the result from a simple fermionic chain (without the impurity).

Energy Flows

$N_s = 1000$, Λ=3.0, $N = 70$

$\epsilon_f = -0.5 \times 10^{-4}$, $U = -10^3$, $V = 4 \times 10^{-4}$





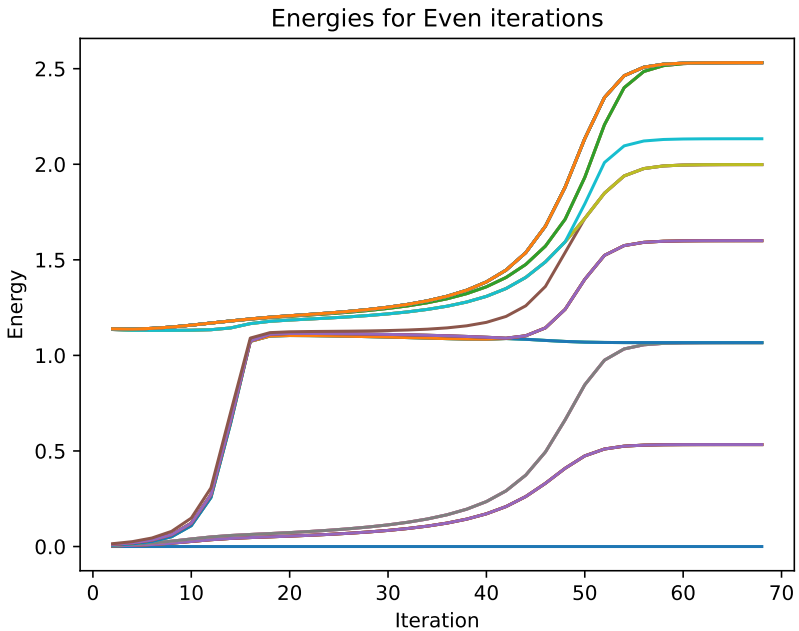
- We immediately notice that there is a crossover after a few iterations: this corresponds to the crossover between the $T \gg T_K$ fixed point and the $T \sim T_K$ fixed point, corresponding to a free moment and the strongly-coupled Kondo singlet

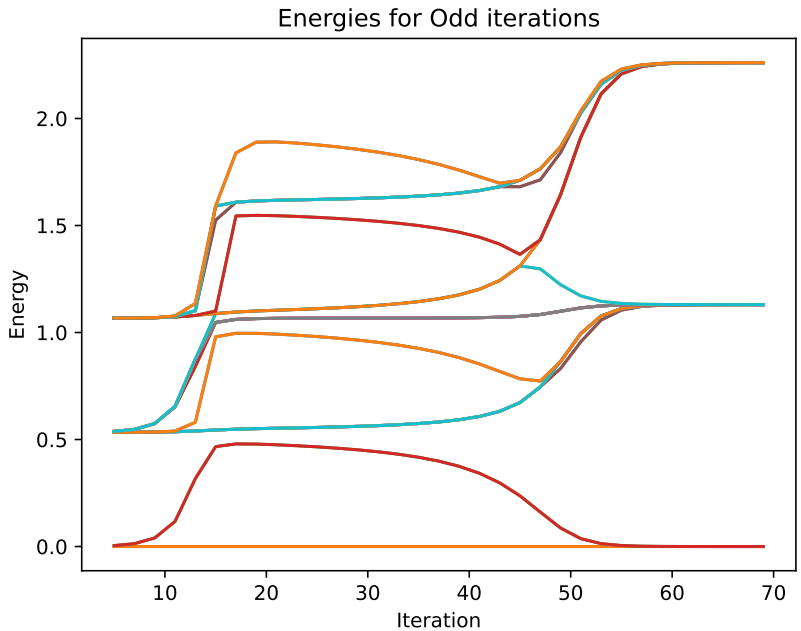
Energy Flows

$N_s = 1000$, Λ=3.0, $N = 70$

$\epsilon_f = -0.5 \times 10^{-3}$, $U = -10^2$, $V = 4 \times 10^{-4}$

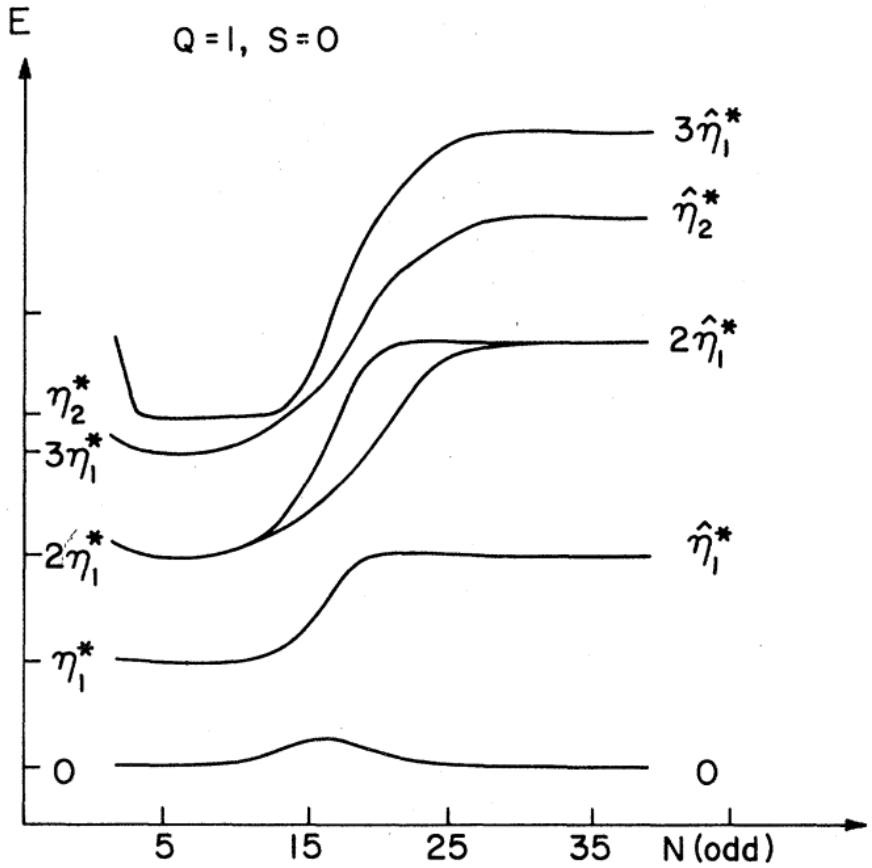
- Increasing U (and ϵ_d) by 10, we find that there is an intermediate fixed point corresponding to a weak coupling between a local moment and the conduction electrons.





Existing Results

- Some results were hard to directly compare; things like choice of $\bar{\beta}$ weren't clear from papers



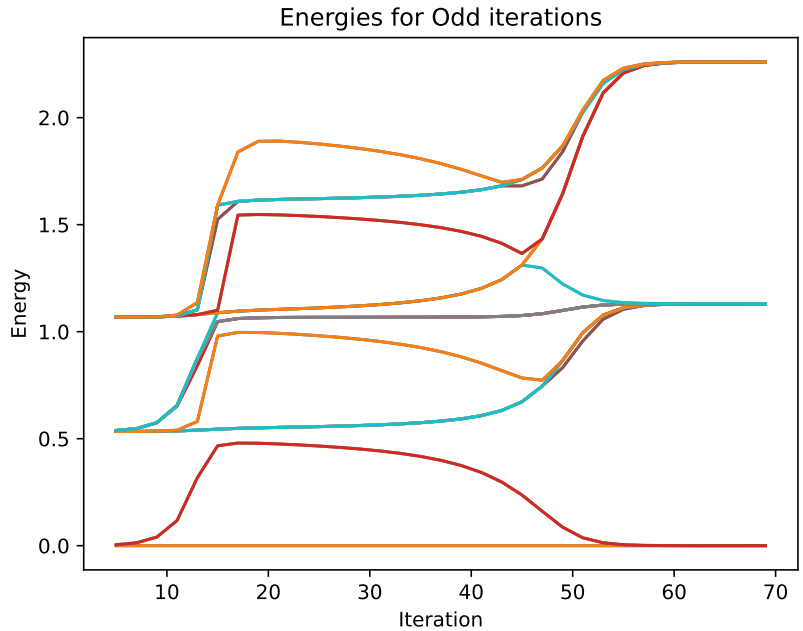


Figure: Left is from [4].

Impurity Contribution to Magnetic Susceptibility

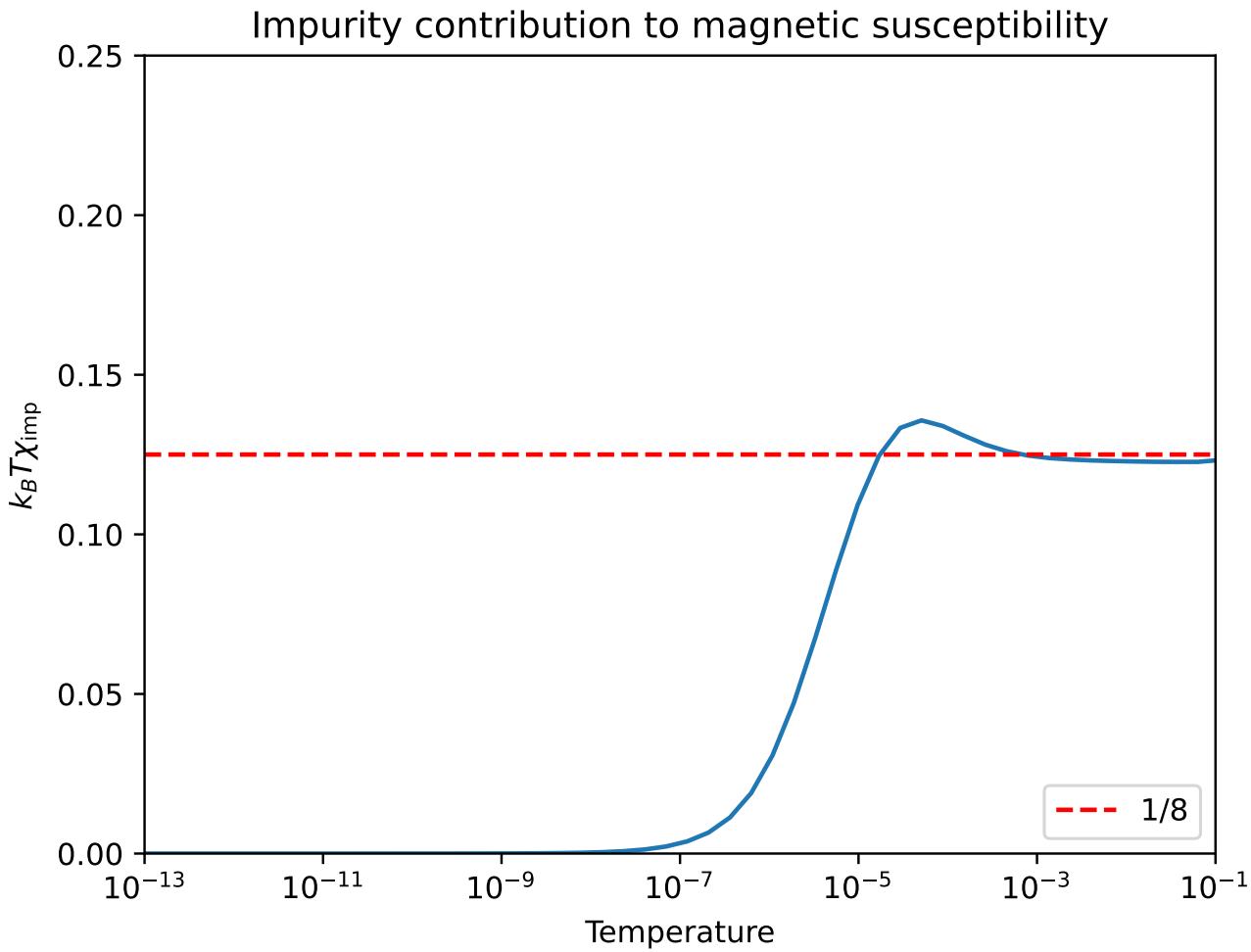
- The form of the susceptibility is as follows:

$$\chi_{\text{imp}}(T) = \frac{(g\mu_B)^2}{4k_B T[1+\exp(-U/2k_B T)]} \quad \text{with } g\mu_B \to 1,$$

$$4k_B T\chi_{\text{imp}} = \frac{1}{1+e^{-U/2k_B T}}.$$

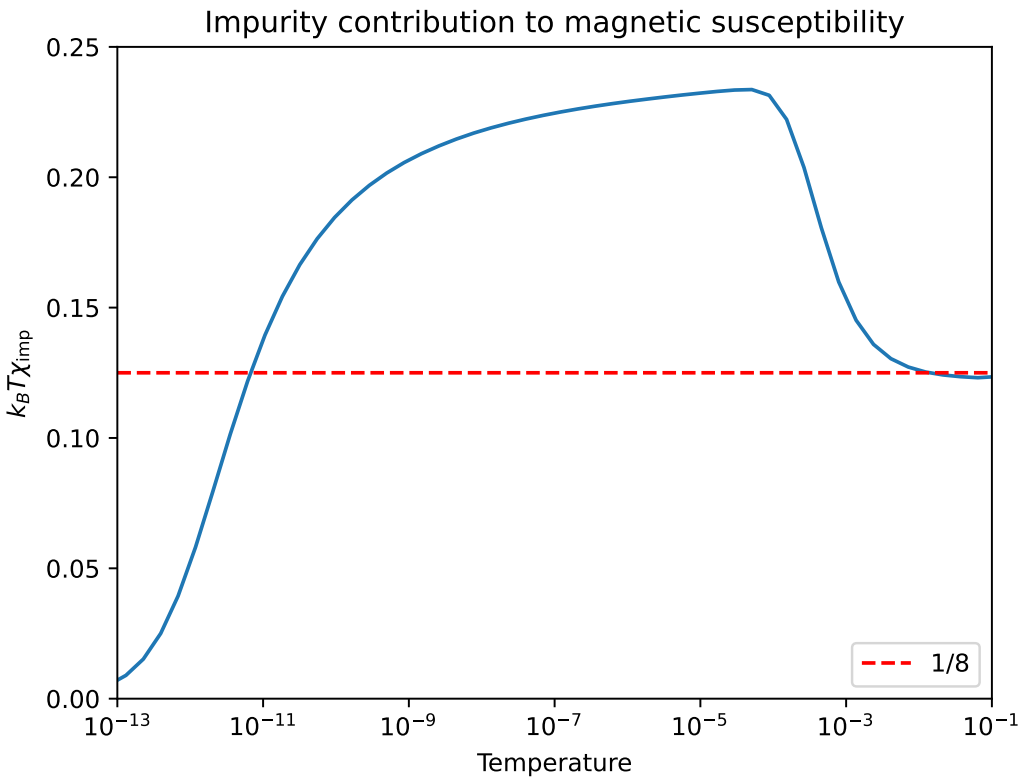
- If we take the onsite repulsion term U to be small enough, there is only one crossover region between two fixed points: the free moment and the strongly coupled Kondo singlet.
- From the above expression, we expect the free moment ($T \gg U$) to have $4k_B T\chi_{\text{imp}} = 1/8$.
- In the strong coupling limit, though, we expect for the local moment's spin to be entirely screened/compensated, giving no net addition to the susceptibility.

Impurity Contribution to Magnetic Susceptibility



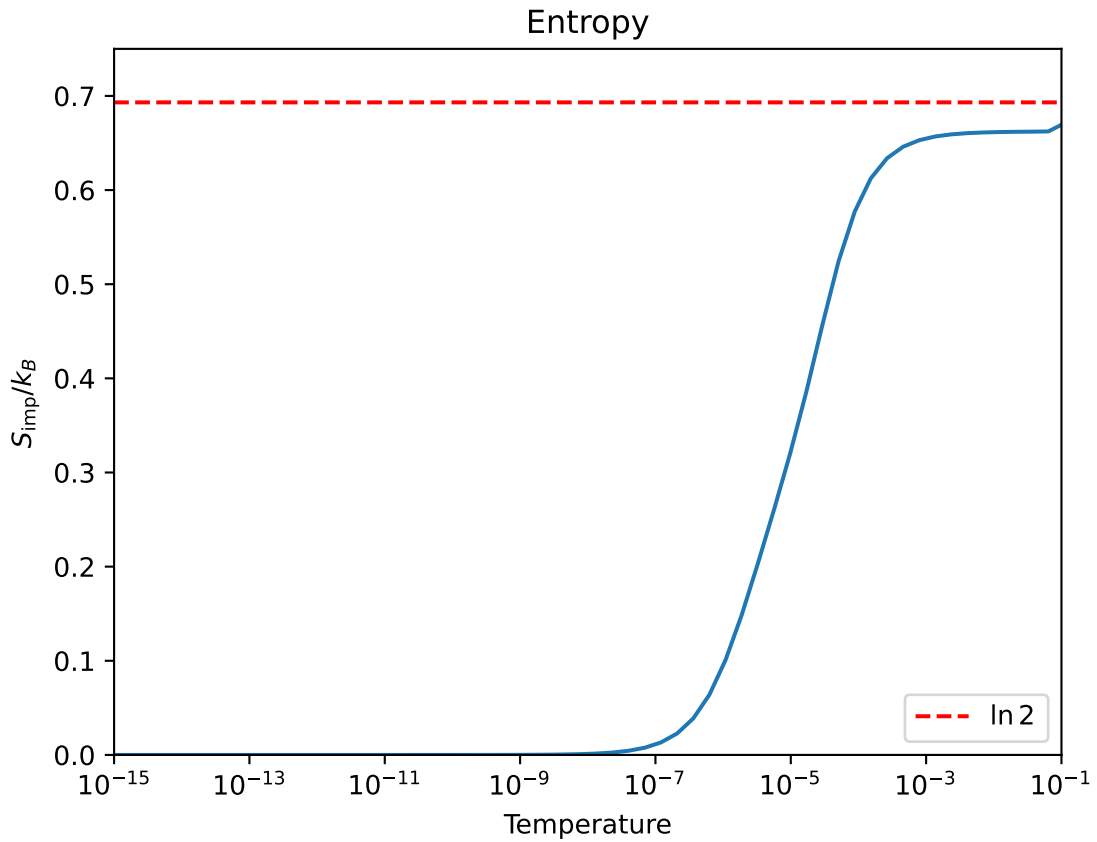
Impurity Contribution to Magnetic Susceptibility

- However, we can also have a case with a strong onsite repulsion U, in which there is an intermediate region characterized by a local moment weakly coupled to the conduction electrons.
- From the previous equation we would expect, for this region, that $4k_B T \chi_{\text{imp}} \approx 1/4$:



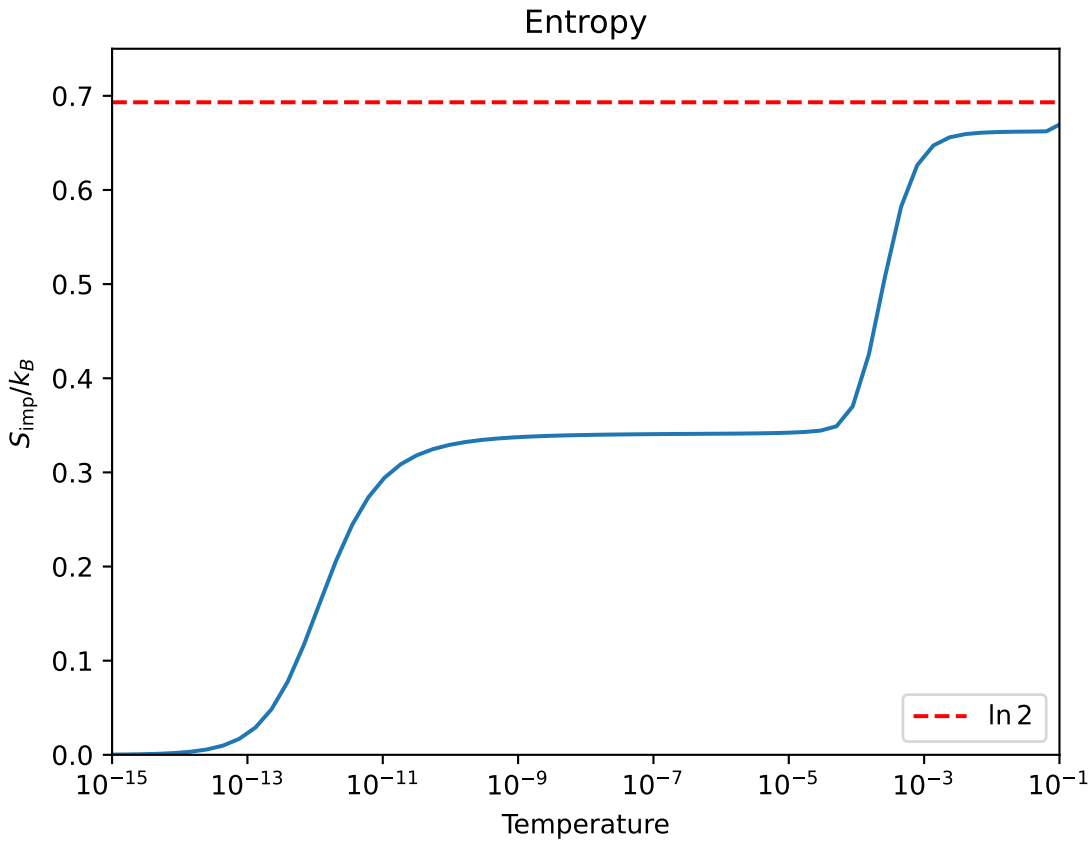
Impurity Contribution to Entropy

- Entropy is related to the logarithm of the multiplicity: $S = k_B \ln \Omega$.
- For the small U case, the Kondo singlet has a multiplicity of unity: $S = 0$, but in the free limit, the multiplicity is 2, leading to ordinary $S = k_B \ln 2$ behavior.



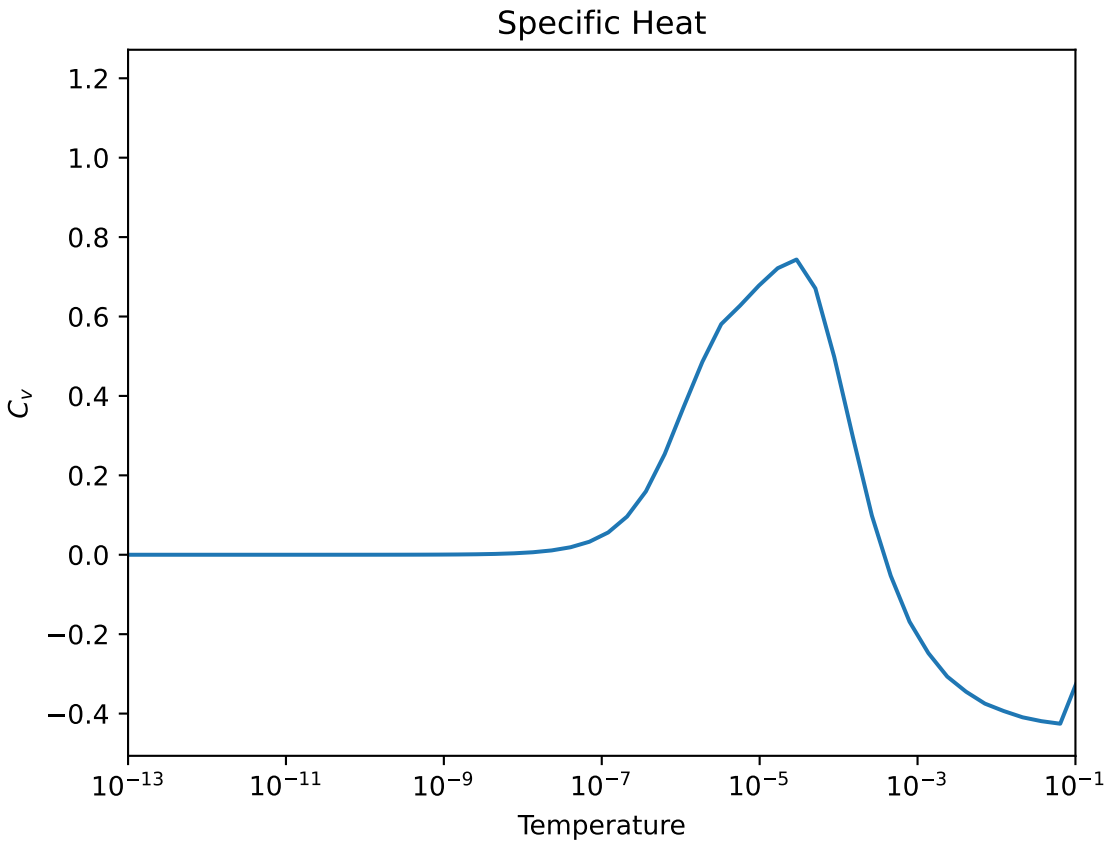
Impurity Contribution to Entropy

- As with the susceptibility, the large U case gives us three fixed points; in the weakly-coupled local moment region, the entropy takes on an intermediate value.



Impurity Contribution to Specific Heat

- In both U limits, the impurity's contribution to the specific heat vanishes for $T \ll T_K$ and $T \gg T_K$.
- Due to the increased density of states at T_K, there is also a peak here in the specific heat, with a second occuring in the large U limit.



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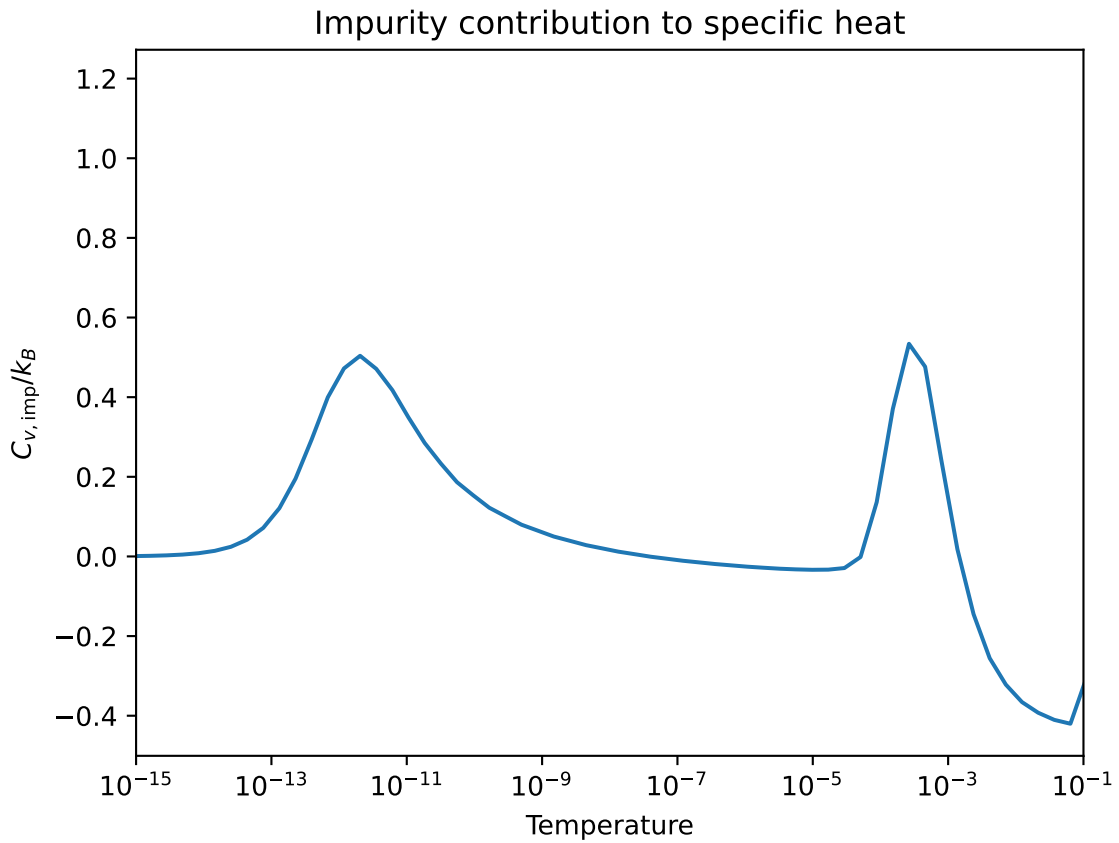

Conclusions

Conclusions

The Kondo problem and the NRG are hard!

Conclusions

- The Kondo problem was a good start at describing magnetic impurities.
- Variational/scaling methods helped reveal the qualitative behavior behind the phenomena, namely the formation of a strongly-bound Kondo singlet.
- The singlet led to an increased scattering probability within the metal, leading to the observed increase in low-temperature resistivity.
- The NRG was the first method that found success due to its non-perturbative nature and finally yielded accurate behavior at temperatures lower than the Kondo temperature.

References

[1] W. De Haas and G. Van Den Berg, "The electrical resistance of gold and silver at low temperatures," en, *Physica*, vol. 3, no. 6, pp. 440–449, Jun. 1936, ISSN: 00318914. DOI: 10.1016/S0031-8914(36)80009-3.

[2] P. W. Anderson, "A poor man's derivation of scaling laws for the kondo problem," *Journal of Physics C: Solid State Physics*, vol. 3, no. 12, pp. 2436–2441, Dec. 1970, ISSN: 0022-3719. DOI: 10.1088/0022-3719/3/12/008.

[3] K. G. Wilson, "The renormalization group: Critical phenomena and the kondo problem," en, *Reviews of Modern Physics*, vol. 47, no. 4, pp. 773–840, Oct. 1975, ISSN: 0034-6861. DOI: 10.1103/RevModPhys.47.773.

[4] H. Krishna-murthy, J. Wilkins, and K. Wilson, "Renormalization-group approach to the anderson model of dilute magnetic alloys. i. static properties for the symmetric case," en, *Physical Review B*, vol. 21, no. 3, pp. 1003–1043, Feb. 1980, ISSN:

Backup

Logarithmic Discretization

- The hybrization term looks like:

$$\int_{-1}^{1} \mathrm{d}\epsilon\ h(\epsilon) f_\sigma^\dagger a_{\epsilon,\sigma} = f_\sigma^\dagger \sum_{np} \Big[a_{np\sigma} \int_{x_{n+1}}^{x_n} \mathrm{d}\epsilon\ h(\epsilon)\psi_{np}^+(\epsilon) \tag{1}$$

$$+ b_{np\sigma} \int_{-x_n}^{-x_{n+1}} \mathrm{d}\epsilon\ h(\epsilon)\psi_{np}^-(\epsilon). \tag{2}$$

- By definition of $\psi_{np}^{\pm}(\epsilon)$, if we choose a constant hybridization $h(\epsilon) = h$, the integrals filter out the $p = 0$ state only:

$$h \int_{x_{n+1}}^{x_n} \mathrm{d}\epsilon\ \psi_{np}^+(\epsilon) = h\sqrt{d_n}\delta_{p,0}$$

- This corresponds to the fact that the impurity can only couple to the $p = 0$ state, so we drop the p index.

Logarithmic Discretization

- Defining a step hybridization $h(\epsilon) = h_n^{\pm}$ that is the average of $\Delta(\epsilon)$ in each interval, we find

$$\int_{-1}^{1} \mathrm{d}\epsilon \; h(\epsilon) f_\sigma^\dagger a_{\epsilon,\sigma} = \frac{1}{\sqrt{\pi}} f_\sigma^\dagger \sum_\sigma (\gamma_n^+ a_{n0p} + \gamma_n^- b_{n0p}), \tag{3}$$

$$(\gamma_n^+)^2 = \int_{x_{n+1}}^{x_n} \mathrm{d}\epsilon \; \Delta(\epsilon), \quad (\gamma_n^-)^2 = \int_{-x_n}^{-x_{n+1}} \mathrm{d}\epsilon \; \Delta(\epsilon) \tag{4}$$

- The conduction electron term, with all of this, turns into

$$\int_{-1}^{1} \mathrm{d}\epsilon \; h(\epsilon) a_{\epsilon,\sigma}^\dagger a_{\epsilon,\sigma} = \sum_{np} (\xi_n^+ a_{np\sigma}^\dagger a_{np\sigma} + \alpha_n^- b_{np\sigma}^\dagger b_{np\sigma}) \tag{5}$$

$$+ \sum_{n,p\neq p'} \left[\alpha_n^+(p,p') a_{np\sigma}^\dagger a_{np'\sigma} - \alpha_n^-(p,p') b_{np\sigma}^\dagger b_{np'\sigma} \right]. \tag{6}$$

Logarithmic Discretization

- The α prefactors are defined like so:

$$\alpha_n^{\pm}(p,p') = \frac{1-\Lambda^{-1}}{2\pi i}\frac{\Lambda^{-n}}{p'-p}\exp\left(\frac{2\pi i(p'-p)}{1-\Lambda^{-1}}\right).$$

- Before we found that the $p=0$ states are filtered out; here we consider $p \neq 0$ states as a perturbation to the $p=0$ part of the α terms, and drop them, leaving

$$\begin{aligned} H = H_{\text{imp}} &+ \sum_{n,\sigma}(\xi_n^+ a_{n,\sigma}^\dagger a_{n,\sigma} + \xi_n^- b_{n,\sigma}^\dagger b_{n,\sigma}) \\ &+ \frac{1}{\sqrt{\pi}}\sum_\sigma f_\sigma^\dagger \sum_n (\gamma_n^+ a_{n,\sigma} + \gamma_n^- b_{n,\sigma}) \\ &+ \frac{1}{\sqrt{\pi}}\sum_\sigma \left[\sum_n (\gamma_n^+ a_{n,\sigma}^\dagger + \gamma_n^- b_{n,\sigma}^\dagger)\right] f_\sigma . \end{aligned}$$

- This is finally the fully logarithmically discretized Hamiltonian.

Mapping to semi-infinite chain

- The next step is to map this Hamiltonian onto the semi-infinite chain, i.e. in a tight-binding form, with the impurity placed at one end.
- In this picture, the impurity only couples to the first conduction site, represented by creation/annihilation operators $c^{(\dagger)}_{0,\sigma}$, the form of which we can read off from the discretized Hamiltonian:

$$c_{0,\sigma} = \frac{1}{\sqrt{\xi_0}} \sum_n (\gamma_n^+ a_{n,\sigma} + \gamma_n^- b_{n,\sigma}),$$

- with

$$\xi_0 = \sum_n \left[(\gamma_n^+)^2 + (\gamma_n^-)^2 \right] = \int_{-1}^{1} \mathrm{d}\epsilon \, \Delta(\epsilon).$$