

B 3 Numerical Renormalization Group for Quantum Impurities¹

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1 Introduction

This lecture deals with a particular implementation of the renormalization group (RG) idea: Wilson's non-perturbative numerical renormalization group (NRG) method for quantum impurity models[1]. This version of the NRG, which will be described in detail below, was originally developed in the context of the Kondo model of magnetic impurities (such as Fe or Mn) in non-magnetic metals (such as Cu, Au, Ag etc)². The Kondo model is defined by the Hamiltonian

$$H_{\text{KM}} = J\vec{S}\cdot\vec{s}_0 + \sum_{k\sigma} \varepsilon_{k\sigma} c_{k\sigma}^\dagger c_{k\sigma}, \quad (1)$$

and describes a localized impurity spin \vec{S} interacting antiferromagnetically ($J > 0$) with the conduction electrons of the host, via their spin-density \vec{s}_0 at the impurity site, see Sec. 2 for details. Unlike the case of non-magnetic impurities, or potential scatterers (see Lecture A5 by Mavropoulos), magnetic impurities have internal dynamical degrees of freedom which result in inelastic scattering of conduction electrons. This makes the Kondo problem, the scattering of electrons from magnetic impurities, a genuine many-body correlation problem. Wilson used the NRG to solve the many-body Hamiltonian (1) and demonstrated conclusively that a $S = 1/2$ magnetic impurity embedded in a non-magnetic metal has its magnetic moment completely screened by the surrounding conduction electrons, provided the temperature is sufficiently low, namely for $T \ll T_K$, where $T_K = \sqrt{JN_F}e^{-1/JN_F}$ is a dynamically generated low energy scale called the Kondo scale (see Sec. 2). This pioneering work established the formalism and gave a detailed analysis of the fixed points and thermodynamics of the Kondo model, and, later, also of the Anderson impurity model (see Sec. 2). The NRG has since been applied to many more quantum impurity models[2, 3, 4]. In addition, it has been extended to the calculation of equilibrium dynamical and transport properties [5, 6, 7, 8, 9, 10], e.g., dynamical susceptibilities, resistivities and thermopower or the conductance through quantum dots [11, 12], thereby making the NRG a useful tool for interpreting experiments which probe these quantities.

Two challenges for the NRG at present, are, (i), to extend it to more realistic multi-orbital and multi-channel models (e.g., for use in realistic modeling of materials), and, (ii), to extend it to the transient and non-equilibrium steady state response of quantum impurity systems. Recent progress and ideas in these two directions is outlined in Sec. 6.

The outline of this lecture is as follows: quantum impurity models are introduced in Sec. 2 and the Anderson impurity and Kondo models are described. The closely related spin-boson model is also briefly described (see also functional and real-time RG techniques in Lectures B7 and B5 by Meden and Schoeller, respectively). Wilson's NRG method is described in Sec. 3, and the calculation of physical properties is outlined in Sec. 4. In Sec. 5 we describe the recently introduced complete basis set and its use in constructing the full density matrix. Applications to thermodynamics and Green functions are given. An outline of some recent developments using the NRG is given in Sec. 6, and, Sec. 7 summarizes with possible future directions.

²Most readers will be familiar with the application of the renormalization group to critical phenomena and obtaining accurate values for critical exponents, see Appendix C. The NRG for quantum impurity models focuses on obtaining the complete spectrum of eigenvalues and eigenstates of such models on all energy scales and hence is more general in its aims, as will become clear in this Lecture

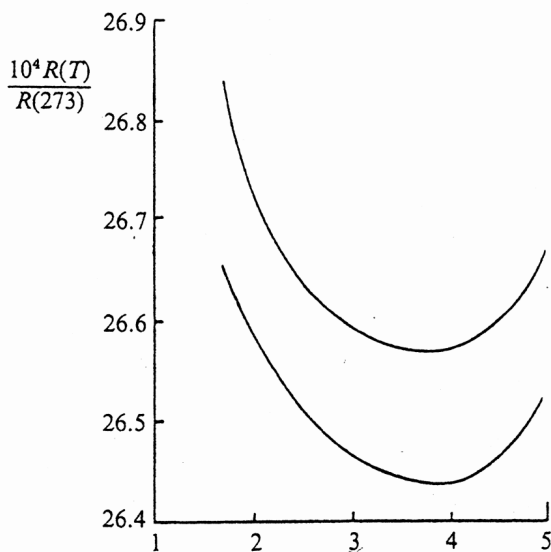


Fig. 1: Resistivity $R(T)$ versus temperature $T[K]$ of two samples of “pure” Au showing the first observation of the resistivity minimum [17]. The expected behaviour of $R(T)$ for a pure metal with weak static disorder is a T^5 term due to phonons and a saturation to a constant value, ρ_0 , at $T = 0$ due to static disorder. The former is seen in the experiment, but at low temperature an additional logarithmically increasing contribution is also found.

2 Quantum impurity models

Quantum impurity models describe systems where the many-body interaction (usually a Coulomb or exchange interaction) acts at one or only a few sites, the “impurity”, and the impurity is coupled to a large system, the bath, consisting of a macroscopically large number of non-interacting particles. These particles can be either bosons (e.g. phonons, magnons, photons, particle-hole pairs etc) or fermions (e.g. electrons in the conduction band, fermionic ^{40}K atoms in an optical lattice, etc). The “impurity” may be a real impurity, such as an Fe impurity (in Au), or a two-level atom (coupled to the electromagnetic field), or, just a confined region behaving like an artificial atom, as in the case of semiconductor quantum dots (coupled to leads). It may also simply represent the lowest two quantum mechanical states of a system with a double-well potential, as in the case of quantum tunneling between macroscopic fluxoid states in a superconducting quantum interference device, which can be used to realize a qubit for quantum computation. Two magnetic impurities in a non-magnetic metal at a distance R apart, interacting via the RKKY indirect exchange J_{RKKY} may also be regarded as a quantum impurity system [13]. Analogues of this in nanostructures, such as double quantum dots attached to leads also exist. The transfer of electrons between donor and acceptor molecules in photosynthesis and other biological processes may also be approximately described in terms of a two-state system coupled to environmental degrees of freedom (the solvent). Concrete models describing the above situations go under the names of (isotropic and anisotropic) single and multi-channel Kondo models, the Anderson impurity model and the dissipative two-state system [14, 15]. They describe a large number of physical systems of current experimental and theoretical interest. Quantum impurity models are also of relevance in the study of correlated lattice models, such as the Hubbard or Kondo lattice models, since the latter are often well approximated, via the dynamical mean field theory, by a local impurity model embedded in a medium which has to be determined self-consistently [16].

Historically, interest in quantum impurities arose when magnetic impurities were found to be present, albeit in very low concentrations, even in apparently very pure metals such as Au or Ag. In particular, measurements of the resistivity of Au as early as the 1930’s showed an unexpected minimum at low temperature (Fig. 1). The puzzle of the resistivity minimum was resolved by

Kondo in 1964, who showed that a small concentration c_{imp} of *magnetic* impurities modeled by Eq. (1) gives rise to an additional temperature dependent term in the resistivity of the form $\rho_K = -c_{\text{imp}} b \ln(T/D)$, which increases with decreasing temperature. The balance between the decreasing phonon contribution behaving as $\rho_{\text{phonon}} = aT^5$ and the increasing Kondo contribution gives rise to the observed resistivity minimum. The logarithmic contribution to the resistivity, found by Kondo in perturbation theory, cannot hold down to $T = 0$ as the total scattering remains finite in this limit (unitarity limit). Wilson's non-perturbative NRG provides a way to obtain the correct behaviour of the resistivity $\rho(T)$ from high temperatures through a crossover regime at $T \sim T_K$ all the way down to zero temperature [see Fig. 10 (a) showing the analogous quantity for a Kondo correlated quantum dot, the conductance $G(T)$].

The general form of the Hamiltonian for any quantum impurity system is given by

$$H = H_{\text{imp}} + H_{\text{int}} + H_{\text{bath}}, \quad (2)$$

where H_{imp} describes the impurity, a small quantum mechanical system with only a few degrees of freedom H_{bath} represents the bath, and H_{int} is the interaction between the two.

We next consider explicit examples which will appear in this and several other lectures.

Anderson and Kondo impurity models: linear chain form

The prototype model for strongly correlated systems is the single-band non-degenerate Anderson model [18, 19],

$$H_{AM} = \underbrace{\sum_{\sigma} \varepsilon_d n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow}}_{H_{\text{imp}}} + \underbrace{\sum_{k\sigma} V_{kd} (c_{k\sigma}^{\dagger} d_{\sigma} + d_{\sigma}^{\dagger} c_{k\sigma})}_{H_{\text{int}}} + \underbrace{\sum_{k\sigma} \epsilon_k c_{k\sigma}^{\dagger} c_{k\sigma}}_{H_{\text{bath}}}. \quad (3)$$

The first two terms describe the impurity, represented here by a non-degenerate s-level of energy ε_d (see Sec. 6 for generalizations). Electrons in the local level are subject to a Coulomb repulsion U which acts between spin-up and spin-down electrons. The local level hybridizes with the Bloch states of a non-interacting s-wave conduction band, the last term in H_{AM} , with amplitude V_{kd} . The properties of the model are determined by the hybridization function

$$\Delta(\omega) = \pi \sum_k |V_{kd}|^2 \delta(\omega - \varepsilon_k), \quad (4)$$

which, like the conduction density of states $\rho(\omega) = \sum_k \delta(\omega - \varepsilon_k)$, will in general be a complicated function of energy. In cases where the interest is in the very low energy physics, it is a good approximation to set $\Delta(\omega) \approx \Delta(\varepsilon_F) \equiv \Delta$. In applications to pseudogap systems [20] or to effective quantum impurities in dynamical mean field theory, the full frequency dependence has to be retained. In applications to quantum dots, the impurity is attached to two baths, the left and right leads, as shown in Fig. 2. The Anderson model also provides an approximate description of the the low temperature behaviour of nanoscale size (ca. 100nm or smaller) quantum dots exhibiting the Kondo effect, see Fig. 2.³

³Although such dots are attached to two baths (the left and right leads), for a single level on the dot, only the even combination of left and right lead states couples to the dot. When several levels on the dot are active in transport, one will have a two-channel multi-orbital Anderson model with intra- and inter-orbital Coulomb interactions playing a role (e.g. Hund's exchange).

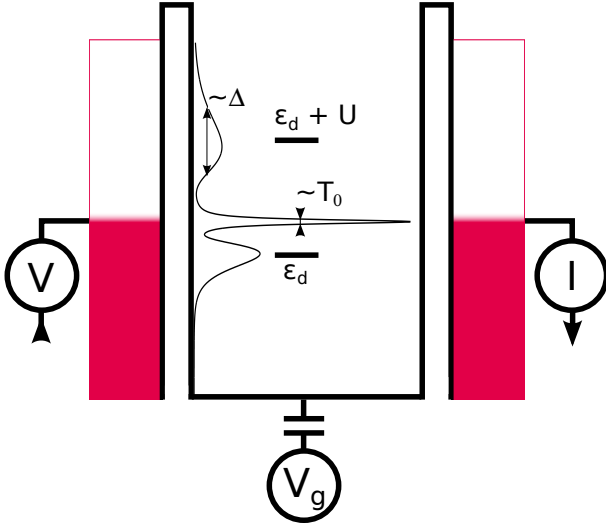


Fig. 2: A quantum dot with charging energy $U \gg \Delta$ and level energy ε_d connected to left/right leads $H_{\alpha=L/R} = \sum_k \epsilon_{k\alpha\sigma} c_{k\alpha\sigma}^\dagger c_{k\alpha\sigma}$ via tunnel barriers. The gate voltage $V_g \sim \varepsilon_d$ allows changing ε_d relative to ϵ_F and thereby the dot occupation n_d from $n_d = 1$ for $\varepsilon_d = -U/2$ (Kondo regime) to $n_d = 0$ through a mixed valence regime with $n_d \approx 0.5$ for $\varepsilon_d \approx 0$. [21]

Closely related to the Anderson model, is the Kondo model, which was briefly mentioned in the introduction. We write it's Hamiltonian as

$$H_{KM} = -g\mu_B B S_z + J \vec{S} \cdot \vec{s}_0 + \sum_{k\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma}, \quad (5)$$

where we included a magnetic field term $H_{\text{imp}} = -g\mu_B B S_z$ to indicate the impurity spin \vec{S} (taken here to be a $S = 1/2$ for simplicity), which interacts via an exchange interaction of strength J with the conduction electron spin-density $\vec{s}_0 = \sum_{\sigma\sigma'} f_{0\sigma}^+ \vec{\sigma}_{\sigma\sigma'} f_{0\sigma'}$ at the impurity site, where $f_{0\sigma} = \sum_k c_{k\sigma}$ the local Wannier state of the conduction electrons at the impurity site. The connection to the Anderson model can be established formally via a Schrieffer-Wolff transformation. In essence, provided $\varepsilon_d < 0$ and $\varepsilon_d + U > 0$ so that a single electron occupies the local level in the Anderson model, the physics of both models will be the same at low temperatures.⁴ In this case, one finds the correspondence $J = 2V^2 \left(\frac{1}{U+\varepsilon_d} - \frac{1}{\varepsilon_d} \right)$, which reduces to $8V^2/U$ for the symmetric case $\varepsilon_d = -U/2$ (see discussion of zero bandwidth limit below). For a numerical treatment of the Anderson and Kondo models, it is useful to reformulate them in the form of linear chain models [2, 3]. This will allow them to be iteratively diagonalized by a procedure to be described in Sec. 3. We carry this out for the Anderson model: first notice that the impurity state in the Anderson model hybridizes with a local Wannier state $|0\sigma\rangle = f_{0\sigma}^+ |\text{vac}\rangle$, with $|\text{vac}\rangle$ the vacuum state, and $f_{0\sigma}^+$ given by

$$V f_{0\sigma}^+ = \sum_k V_{kd} c_{k\sigma}^+. \quad (6)$$

The value of V follows from the normalization $\{f_{0\sigma}, f_{0\sigma}^+\} = 1$

$$V = \left(\sum_k |V_{kd}|^2 \right)^{1/2}. \quad (7)$$

Using the above local state one can apply the Lanczos procedure (Appendix B) for tridiagonalizing a Hermitian operator, such as H_{bath} , to obtain

$$H_{\text{bath}} = \sum_{k\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} \rightarrow \sum_{\sigma, n=0}^{\infty} [\epsilon_n f_{n\sigma}^+ f_{n\sigma} + t_n (f_{n\sigma}^+ f_{n+1\sigma} + H.c.)] \quad (8)$$

⁴Strictly speaking, one should also include a potential scattering term in the Kondo model, of the form $\sum_{kk'\sigma} V_{kk'}^{\text{pot}} c_{k\sigma}^\dagger c_{k'\sigma}$ for this to be true.

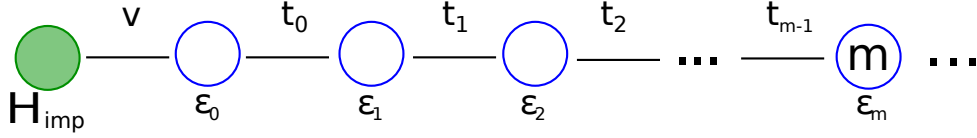


Fig. 3: The linear chain form of the Anderson model (9). $H_{\text{imp}} = \varepsilon_d n_d + U n_{d\uparrow} n_{d\downarrow}$. The “site energies” ε_n and “hoppings” t_n follow from $\Delta(\omega)$.

with site energies, ε_n , and hoppings, t_n , depending only on the dispersion ε_k and hybridization matrix elements V_{kd} through the hybridization function $\Delta(\omega)$ resulting in the linear chain form [2]

$$H_{AM} = \varepsilon_d n_d + U n_{d\uparrow} n_{d\downarrow} + V \sum_{\sigma} (f_{0\sigma}^+ d_{\sigma} + d_{\sigma}^+ f_{0\sigma}) + \sum_{\sigma, n=0}^{\infty} [\varepsilon_n f_{n\sigma}^+ f_{n\sigma} + t_n (f_{n\sigma}^+ f_{n+1\sigma} + f_{n+1\sigma}^+ f_{n\sigma})] \quad (9)$$

depicted in Fig. 3 (with $n_d \equiv \sum_{\sigma} n_{d\sigma}$). Although, formally, this model looks like the one-dimensional real-space models treated by the DMRG method[22, 23], the interpretation here is not in terms of electrons hopping on a one-dimensional lattice in real-space. Instead, as will become clearer in Sec. 3, each successive site added along the chain corresponds to adding lower energy degrees of freedom, measured relative to the Fermi level. By considering longer chains one can then access lower energies.

The same procedure can be used to reformulate any quantum impurity model in terms of an impurity site with local interactions attached to a one-dimensional chain of non-interacting sites. For example, the Kondo model (5) can be rewritten as

$$H_{KM} = -g\mu_B S_z + J \vec{S} \cdot \vec{s}_0 + \sum_{\sigma, n=0}^{\infty} [\varepsilon_n f_{n\sigma}^+ f_{n\sigma} + t_n (f_{n\sigma}^+ f_{n+1\sigma} + f_{n+1\sigma}^+ f_{n\sigma})] \quad (10)$$

A zeroth order (high energy) approximation to the spectrum of the Anderson model can be obtained by considering just the coupling of the $n = 0$ Wannier state to the impurity and neglecting all others (the zero-bandwidth limit),

$$H_{AM} \approx H_0 \equiv \varepsilon_d n_d + U n_{d\uparrow} n_{d\downarrow} + V \sum_{\sigma} (f_{0\sigma}^+ d_{\sigma} + d_{\sigma}^+ f_{0\sigma}) \quad (11)$$

There are 16 many-electron states $|n_d, n_0\rangle$, which can be classified by the conserved quantum numbers of total electron number N_{el} , total z-component of spin S_z^{tot} and total spin \vec{S} . Using these symmetries we can diagonalize the block matrices H_{N_{el}, S, S_z}^0 to obtain the many-body eigenstates $|N_{el}, S, S_z, r\rangle$ and the corresponding eigenvalues. For example, in the product basis $|n_d\rangle|n_0\rangle$, the Hamiltonian for $N_e = 1, S = 1/2, S_z = \pm 1/2$ is given by

$$H_{N_e=1, S=1/2, S_z=\pm 1/2} = \begin{pmatrix} \varepsilon_d & V \\ V & 0 \end{pmatrix}$$

with eigenvalues

$$E_{\pm} = (\varepsilon_d \pm \sqrt{\varepsilon_d^2 + 4V^2})/2$$

Proceeding similarly for the other Hilbert spaces (homework), we find that for the particle-hole symmetric case $\varepsilon_d = -U/2$ in the strong correlation limit $U \gg V^2$, the spectrum separates into two groups of states, one group of low energy states lying close to the (singlet) ground state with spacings $\mathcal{O}(V^2/U)$ and one group of high energy states lying at energies $\mathcal{O}(U/2)$ higher and also split by $\mathcal{O}(V^2/U)$. This limit corresponds to a singly occupied impurity level effectively behaving as a $S = 1/2$. In fact, the 8 lowest states correspond to those obtained from a zeroth order approximation to the spectrum of the Kondo model via

$$H_{KM} \approx H_0 \equiv J\vec{S} \cdot \vec{s}_0 = \frac{J}{2}[(\vec{S} + \vec{s}_0)^2 - \vec{S}^2 - \vec{s}_0^2]. \quad (12)$$

The Kondo model is therefore the low energy effective model of the Anderson model in the limit of strong correlations and single occupancy. By comparing the splitting of the two lowest levels in the Kondo model, the singlet and triplet states, with the corresponding splitting of the same levels in the Anderson model one finds the relation between the bare parameters of the models to be $J = 8V^2/U$, in agreement with the value obtained from the Schrieffer-Wolff transformation $J = 2V^2(\frac{1}{U+\varepsilon_d} - \frac{1}{\varepsilon_d})$ upon setting $\varepsilon_d = -U/2$ [24].

Within the above zeroth order approximation, $H \approx H_0$, of the Kondo (and Anderson) model, excitations are unrenormalized. The singlet-triplet excitation (splitting) takes the bare value J . The key ingredient of Wilson's NRG, to be discussed in the next section, is a *controlled procedure* for adding the remaining states $n = 1, 2, \dots$ neglected in the above zero bandwidth approximation. As we shall see in the calculation of dynamical quantities below, this leads to a drastic renormalization of the spin and single-particle excitations, such that the relevant excitations of the Kondo model are not on the bare scale J but on the Kondo scale $T_K = D(\rho J)^{1/2} \exp(-1/\rho J)$, where $\rho = 1/2D$ is the density of conduction states (e.g., see Fig. 7-8 in Sec. 3). One can interpret this large renormalization $J \rightarrow T_K$ as a renormalization of a bare tunneling amplitude (J) due to the dissipative effects of the bath of conduction electrons by a mapping of the Kondo model onto the dissipative two-state system (also called the spin-boson model). We introduce this briefly in the next subsection, partly to make the above connection, and partly to show that the linear chain representation, which is the starting point for NRG calculations, applies also to bosonic quantum impurity models. For a detailed discussion of the spin-boson model, and its real time dynamics, see lecture B5 by Schoeller.

Spin-boson model

The Hamiltonian of the spin-boson model is given by,

$$H_{\text{SB}} = \underbrace{-\frac{1}{2}\Delta_0\sigma_x + \frac{1}{2}\epsilon\sigma_z}_{H_{\text{imp}}} + \underbrace{\frac{1}{2}\sigma_z \sum_i \lambda_i (a_i + a_i^\dagger)}_{H_{\text{int}}} + \underbrace{\sum_i \omega_i (a_i^\dagger a_i + 1/2)}_{H_{\text{bath}}}. \quad (13)$$

The first term H_{imp} describes a two-level system with bias splitting ϵ and tunneling amplitude Δ_0 , and $\sigma_{i=x,y,z}$ are Pauli spin matrices. The third term, H_{bath} , is the environment and consists of an infinite set of harmonic oscillators ($i = 1, 2, \dots, \infty$) with $a_i(a_i^\dagger)$ the annihilation (creation) operators for a harmonic oscillator of frequency ω_i and $0 \leq \omega_i \leq \omega_c$, where ω_c is an upper cut-off frequency. The non-interacting density of states of the environment is denoted by $g(\omega) = \sum_i \delta(\omega - \omega_i)$ and is finite in the interval $[0, \omega_c]$ and zero otherwise. Finally, $H_{\text{int}} = \frac{1}{2}\sigma_z \sum_i \lambda_i (a_i + a_i^\dagger)$ describes the coupling of the two-state system co-ordinate

σ_z to the oscillators, with λ_i denoting the coupling strength to oscillator i . The function $\Gamma(\omega + i\delta) = \sum_i (\lambda_i/2)^2 / (\omega - \omega_i + i\delta) = \int d\omega' (\lambda(\omega')/2)^2 g(\omega') / (\omega - \omega' + i\delta)$ characterizes the system-environment interaction. It may be shown, that the Ohmic two-state system, specified by a spectral function $J(\omega) = -\frac{1}{\pi} \text{Im}\Gamma(\omega + i\delta) \sim \alpha\omega$ for $\omega \rightarrow 0$, where α is the dimensionless dissipation strength, is equivalent to the anisotropic Kondo model $H = \sum_{k\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \frac{J_\perp}{2} (S^+ s_0^- + S^- s_0^+) + J_\parallel S_z s_0^z + B S_z$, where J_\perp (J_\parallel) is the transverse (longitudinal) part of the Kondo exchange interaction and B is a local magnetic field. The correspondence is given by $\rho J_\perp = -\Delta_0/\omega_c$ and $\alpha = (1 + 2\delta/\pi)^2$ where $\delta = \arctan(-\pi\rho J_\parallel/4)$ and ρ is the density of states of the conduction electrons in the anisotropic Kondo model [25, 26, 14, 27, 15]. The low energy scale of the Ohmic two-state system is the renormalized tunneling amplitude Δ_r given by $\Delta_r/\omega_c = (\Delta_0/\omega_c)^{1/(1-\alpha)}$ and corresponds to the low energy Kondo scale T_K of the anisotropic Kondo model. This connection between the (anisotropic) Kondo and spin-boson models provides another viewpoint on the local dynamics of a Kondo spin in terms of tunneling and dissipation: T_K acquires the meaning of a renormalized tunneling amplitude, with frictional effects of the environment leading to a drastic renormalization of $J_\perp \rightarrow T_K$, particularly in the limit of strong dissipation $\alpha \rightarrow 1^-$, corresponding to the isotropic $J \ll 1$ limit of the Kondo model. Indeed, for $\alpha > 1$, the above correspondence states that $J_\parallel < 0$, which corresponds to the ferromagnetic sector of the Kondo model. Since in this limit, J_\perp is irrelevant [19, 24], it follows that T_K and hence Δ_r vanish for $\alpha > 1$, i.e., the frictional effects of the environment are so large for $\alpha > 1$ that quantum mechanical tunneling is destroyed at $T = 0$ and tunneling between the two states is possible only via thermal activation. Of interest also, is the transition from quantum coherent dynamics at weak dissipation $\alpha \ll 1$ to incoherent dynamics at strong dissipation $\alpha \rightarrow 1^-$, see lecture B5 by Schoeller.

For a numerical treatment using the NRG, one proceeds to re-formulate the model (13) in a linear chain form as in (9) and (10) for the Anderson and Kondo models. Thus, one uses the Lanczos procedure and applies H_{bath} repeatedly on the local bosonic orbital $\lambda b_0 = \sum_i \lambda_i a_i$ to tridiagonalize H_{bath} . The resulting linear chain model,

$$H_{\text{SB}} = \underbrace{-\frac{1}{2}\Delta_0\sigma_x + \frac{1}{2}\epsilon\sigma_z}_{H_{\text{imp}}} + \underbrace{\frac{1}{2}\sigma_z\lambda(b_0 + b_0^\dagger)}_{H_{\text{int}}} + \underbrace{\sum_{m=0}^{\infty} \epsilon_m b_m^\dagger b_m + t_m (b_m^\dagger b_{m+1} + b_{m+1}^\dagger b_m)}_{H_{\text{bath}}}, \quad (14)$$

may then be treated within NRG in a similar way to the treatment of the Anderson and Kondo models [28]. One difference, is that the number of bosons in the eigenstates of H_{SB} is arbitrary, requiring an additional approximation even at the first iteration for $H_0 = H_{\text{imp}} + \frac{1}{2}\sigma_z\lambda(b_0 + b_0^\dagger)$ to restrict the maximum number of bosons to n_b (typically 8 – 10).

3 Wilson's Numerical Renormalization Group Method

Wilson's formulation of the RG for the Kondo model is similar in spirit to Anderson's scaling method (see Hewson's book [24] or Ref. [19]). The main difference lies in the non-perturbative construction of the RG transformation using a numerical representation of the effective Hamiltonians. The scaling approach uses perturbation theory in the initially small dimensionless coupling (J/D) to construct such a transformation, but since J/D increases with decreasing energy scale this approach eventually becomes inaccurate. In the Wilson approach the RG transformation is perturbative only via a small parameter $\Lambda^{-1/2} < 1$ which is related to the momentum

rescaling factor $\Lambda > 1$. The accuracy of the transformation is the same at each step and is independent of the size of the running couplings. For this reason it gave the first correct description of the crossover from the weak coupling to the strong coupling regime of the Kondo model. The NRG procedure, described in detail below, involves three steps, illustrated in Fig. 4 (a)-(c) for the Anderson model.

Separation of scales and logarithmic discretization approximation

In the Kondo problem, as in other quantum impurity problems, the behaviour of the system changes qualitatively over many energy scales as it passes through a crossover between fixed points (e.g. from behaviour characteristic of a well defined magnetic moment at high temperature to behaviour characteristic of a Fermi liquid at temperatures below the crossover scale). In order to describe this crossover the idea is to separate out the many energy scales in the problem, which arise from the conduction band $[-D, +D]$, and to set up a procedure for treating each scale in turn. We saw in the previous section that it is always possible to rewrite a quantum impurity model in the form of a (semi-infinite) linear chain, see Fig. 3. Truncating this chain to include orbitals $n = 0, \dots, m$, we have

$$H_{AM} \approx H_m = \varepsilon_d n_d + U n_{d\uparrow} n_{d\downarrow} + V \sum_{\sigma} (f_{0\sigma}^+ d_{\sigma} + d_{\sigma}^+ f_{0\sigma}) + \sum_{\sigma, n=0}^m \epsilon_n f_{n\sigma}^+ f_{n\sigma} + \sum_{\sigma, n=0}^{m-1} t_n (f_{n\sigma}^+ f_{n+1\sigma} + f_{n+1\sigma}^+ f_{n\sigma}) \quad (15)$$

with the truncated Hamiltonians H_m satisfying the recursion relation

$$H_{m+1} = H_m + \sum_{\sigma} \epsilon_m f_{m\sigma}^{\dagger} f_{m\sigma} + t_m \sum_{\sigma} (f_{m\sigma}^+ f_{m+1\sigma} + f_{m+1\sigma}^+ f_{m\sigma}). \quad (16)$$

Hence, it appears that with this recursion relation, one can iteratively diagonalize the Anderson model starting from H_0 , which we diagonalized explicitly in the previous section. At some point, we will need to retain only the lowest many-body states of H_m since the Hilbert space grows as $4 \times 4^{m+1}$. The validity of this procedure then depends on whether the perturbation in Eq. 16, the last term involving t_m , is small, once we start neglecting some higher energy states.⁵ In practice, for a quasi-continuous band $H_{\text{bath}} = \sum_{k\sigma} c_{k\sigma}^{\dagger} c_{k\sigma} = \sum_{\sigma} \int_{-D}^{+D} \epsilon c_{\epsilon\sigma}^{\dagger} c_{\epsilon\sigma}$ the hoppings t_m do not decay with increasing m , and the above procedure breaks down after some iterations. For example, it can be easily shown that for a semi-elliptic density of states $\rho(\epsilon) = \frac{2}{\pi D^2} \sqrt{D^2 - \epsilon^2}$, that $t_m = D/2$ for all m (see Hewson's book[24]).

In order to have a working procedure, involving decreasing hoppings t_m along the chain, and at the same time achieve the energy scale separation described above, Wilson discretized the conduction band into positive and negative energy intervals, $D_n^+ = [\Lambda^{-(n+1)}, \Lambda^{-n}]$ and $D_n^- = [-\Lambda^{-n}, -\Lambda^{-(n+1)}]$, $n = 0, 1, \dots$, about the Fermi level $\epsilon_F = 0$ as shown in Fig. 4 a. The quasi-continuous band was then approximated by a discrete one by keeping only a single conduction state from each interval D_n^{\pm} ,

$$H_{\text{bath}} = \sum_{\sigma} \int_{-D}^{+D} \epsilon c_{\epsilon\sigma}^{\dagger} c_{\epsilon\sigma} \approx \sum_{n=0}^{\infty} (\varepsilon_{-n} c_{-n\sigma}^+ c_{-n\sigma} + \varepsilon_{+n} c_{+n\sigma}^+ c_{+n\sigma}) \quad (17)$$

⁵If we keep extending the system by one orbital at a time without neglecting any states, no error is made. The onsite term in ϵ_m is diagonal and shifts the low energy levels of H_m .

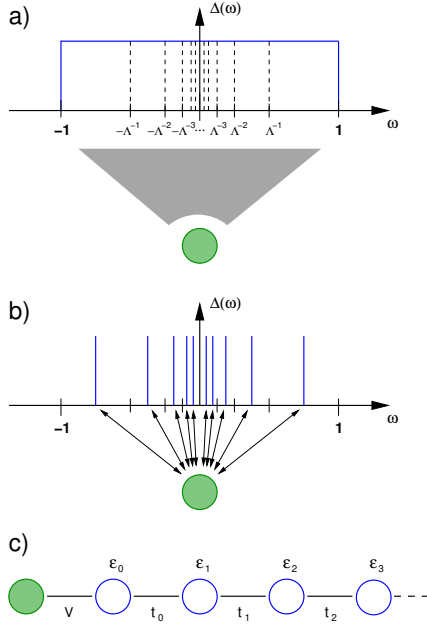


Fig. 4: Steps in the NRG procedure for an Anderson impurity (circle) coupled to a continuum of conduction states via a hybridization function $\Delta(\omega)$. (a) Logarithmic discretization of the continuum conduction band about the Fermi level $\epsilon_F = 0$ into discrete intervals $D_n^+ = [\Lambda^{-(n+1)}, \Lambda^{-n}]$ and $D_n^- = [-\Lambda^{-n}, -\Lambda^{-(n+1)}]$, $n = 0, 1, \dots$. (b) Within each discrete interval, choose the conduction state most localized on the impurity. (c) Transform logarithmically discretized model to linear chain form, with hoppings now decreasing along the chain and iteratively diagonalize.

with

$$\epsilon_{\pm n} = \pm \frac{1}{2} D (\Lambda^{-n} + \Lambda^{-(n+1)}) = \pm \frac{1}{2} D \Lambda^{-n} (1 + \Lambda^{-1}) \quad (18)$$

The states $c_{\pm n \sigma}^\dagger |vac\rangle$ appearing above are the states in each interval D_n^\pm which are most localized near the impurity [2], while the neglected states being orthogonal to these have their wavefunctions localized away from the impurity and are consequently less important (for a more detailed derivation and justification of the logarithmic discretization approximation see Appendix A). By formulating the Anderson model as a linear chain using the above logarithmically discretized conduction band, we obtain the same equations (15-16) as above, but, crucially, with hopping parameters t_m (and onsite energies ϵ_m) that now decay exponentially along the chain. For example, for a constant density of states $\rho(\omega) = 1/2D$ and constant hybridization function $\Delta(\omega) = \pi\rho(\omega)V^2 = \Delta_0$ and $\epsilon_F = 0$ one finds for $m = 0, 1, \dots$ [1]

$$\epsilon_m = 0, \quad (19)$$

$$t_m = \frac{1}{2} D (1 + \Lambda^{-1}) \Lambda^{-m/2} \xi_m, \quad (20)$$

$$\xi_m = \frac{1 - \Lambda^{-m-1}}{\sqrt{(1 - \Lambda^{-2m-1})(1 - \Lambda^{-2m-3})}}. \quad (21)$$

The ξ_m converge rapidly to 1 with increasing m and we may write $t_m \approx \frac{1}{2} D (1 + \Lambda^{-1}) \Lambda^{-m/2}$, so that the Anderson model in Eq. (9) becomes

$$\begin{aligned} H_{AM} = & \epsilon_d n_d + U n_{d\uparrow} n_{d\downarrow} + V \sum_{\sigma} (f_{0\sigma}^+ d_{\sigma} + d_{\sigma}^+ f_{0\sigma}) \\ & + \frac{1}{2} D (1 + \Lambda^{-1}) \sum_{\sigma, n=0}^{\infty} \Lambda^{-n/2} (f_{n\sigma}^+ f_{n+1\sigma} + f_{n+1\sigma}^+ f_{n\sigma}) \end{aligned} \quad (22)$$

This Hamiltonian provides a clear separation of the energy scales $\frac{1}{2}(1+\Lambda^{-1})\Lambda^{-n/2}$, $n = 1, 2, \dots$ in H and allows the diagonalization of the Hamiltonian in a sequence of controlled steps, each

step corresponding to adding an orbital $f_{n\sigma}$ which is a relative perturbation of strength $\Lambda^{-1/2} < 1$, thereby ensuring convergence of the method. This procedure is described in the following two subsections, where we henceforth restrict ourselves to a constant hybridization with hoppings $t_m \approx \frac{1}{2}D(1 + \Lambda^{-1})\Lambda^{-m/2}$. The procedure is easily generalized to any hybridization function $\Delta(\omega)$ with hoppings t_m decaying sufficiently fast along the chain.

Renormalization Group Transformation

A renormalization group transformation relating effective Hamiltonians on successive energy scales $\Lambda^{-n/2}$ and $\Lambda^{-(n+1)/2}$ can be set up as follows. First, H in (22) is truncated to H_m , whose lowest scale is $D_m = \frac{1}{2}D(1 + \Lambda^{-1})\Lambda^{-(m-1)/2}$. In order to look for fixed points we define rescaled Hamiltonians $\bar{H}_m \equiv H_m/D_m$ such that the lowest energy scale of \bar{H}_m is always of $\mathcal{O}(1)$:

$$\begin{aligned} \bar{H}_m &= \Lambda^{(m-1)/2} \left[\sum_{n=0}^{m-1} \Lambda^{-n/2} (f_{n\sigma}^+ f_{n+1\sigma} + f_{n+1\sigma}^+ f_{n\sigma}) \right. \\ &\quad \left. + \tilde{\varepsilon}_d n_d + \tilde{U} n_{d\uparrow} n_{d\downarrow} + \tilde{V} \sum_{\sigma} (f_{0\sigma}^+ d_{\sigma} + d_{\sigma}^+ f_{0\sigma}) \right], \end{aligned} \quad (23)$$

$$\tilde{\varepsilon}_d = \frac{\varepsilon_d}{\frac{1}{2}D(1 + \Lambda^{-1})}, \quad \tilde{V} = \frac{V}{\frac{1}{2}D(1 + \Lambda^{-1})}, \quad \tilde{U} = \frac{U}{\frac{1}{2}D(1 + \Lambda^{-1})}, \quad (24)$$

from which we can recover H as

$$H = \lim_{m \rightarrow \infty} \frac{1}{2}D(1 + \Lambda^{-1})\Lambda^{-(m-1)/2} \bar{H}_m. \quad (25)$$

The sequence of rescaled Hamiltonians \bar{H}_m satisfies the recursion relation

$$\bar{H}_{m+1} = \Lambda^{1/2} \bar{H}_m + (f_{m\sigma}^+ f_{m+1\sigma} + f_{m+1\sigma}^+ f_{m\sigma}), \quad (26)$$

and allows a RG transformation \mathcal{T} to be defined:

$$\bar{H}_{m+1} = \mathcal{T}[\bar{H}_m] \equiv \Lambda^{1/2} \bar{H}_m + (f_{m\sigma}^+ f_{m+1\sigma} + f_{m+1\sigma}^+ f_{m\sigma}) - \bar{E}_{G,m+1} \quad (27)$$

with $\bar{E}_{G,m+1}$ the ground state energy of \bar{H}_{m+1} . In fact \mathcal{T} defined in (27) does not have fixed points since it relates a Hamiltonian with an even number of orbitals to a Hamiltonian with an odd number of orbitals. The even/odd spectra do not match for the Kondo model. However, $\mathcal{R} = \mathcal{T}^2$, can be defined as the RG transformation and this will have fixed points, a set of even m fixed points and a set of odd m fixed points:

$$\bar{H}_{m+2} = \mathcal{R}[\bar{H}_m] \equiv \mathcal{T}^2[\bar{H}_m] \quad (28)$$

Iterative diagonalization scheme

The transformation R relates effective Hamiltonians $H_m = D_m \bar{H}_m$ and $H_{m+1} = D_{m+1} \bar{H}_{m+1}$ on decreasing scales $D_m > D_{m+1}$. It can be used to iteratively diagonalize the Anderson Hamiltonian by the following sequence of steps:

1. the local part

$$\bar{H}_0 = \Lambda^{-1/2} \left[\tilde{\varepsilon}_d n_d + \tilde{U} n_{d\uparrow} n_{d\downarrow} + \tilde{V} \sum_{\sigma} (f_{0\sigma}^{\dagger} d_{\sigma} + d_{\sigma}^{\dagger} f_{0\sigma}) \right], \quad (29)$$

which contains the many-body interactions, is diagonalized (the ‘‘zerth’’ order step described in Sec. 2),

2. assuming that \bar{H}_m has been diagonalized for some $m \geq 0$,

$$\bar{H}_m = \sum_q \bar{E}_q^m |q\rangle \langle q| \quad (30)$$

we add a ‘‘site’’ and use (27) to set up the matrix for \bar{H}_{m+1} within a product basis

$$|q, \alpha_{m+1}\rangle = |q\rangle_m |\alpha_{m+1}\rangle \quad (31)$$

consisting of the eigenstates $|q\rangle_m$ of \bar{H}_m and the 4 states $|\alpha_{m+1}\rangle$ of the next orbital along the chain (i.e. $|0\rangle, |\uparrow\rangle \equiv f_{m+1\uparrow}^{\dagger} |0\rangle, |\downarrow\rangle \equiv f_{m+1\downarrow}^{\dagger} |0\rangle$, and $|\uparrow\downarrow\rangle = f_{m+1\uparrow}^{\dagger} f_{m+1\downarrow}^{\dagger} |0\rangle$). The resulting matrix

$$\begin{aligned} \langle q, \alpha_{m+1} | \bar{H}_{m+1} | q', \alpha'_{m+1} \rangle &= \Lambda^{1/2} \delta_{\alpha_{m+1}, \alpha'_{m+1}} \delta_{q, q'} \bar{E}_q^m \\ &+ (-1)^{N_{e, q'} m} \langle q | f_{m\sigma}^{\dagger} | q' \rangle_m \langle \alpha_{m+1} | f_{m+1\sigma} | \alpha'_{m+1} \rangle \\ &+ (-1)^{N_{e, q} m} \langle \alpha_{m+1} | f_{m+1\sigma}^{\dagger} | \alpha'_{m+1} \rangle_m \langle q | f_{m\sigma} | q' \rangle_m, \end{aligned} \quad (32)$$

with $N_{e, q}, N_{e, q'}$ the number of electrons in $|q\rangle, |q'\rangle$ respectively, is diagonalized and the procedure is repeated for the next energy shell as depicted in Fig. 4 c. Since \bar{H}_m is already diagonalized, the off-diagonal matrix elements, involving ${}_m \langle q | f_{m\sigma}^{\dagger} | q' \rangle_m = {}_m \langle q' | f_{m\sigma} | q \rangle_m^{\dagger}$, can be expressed in terms of the known eigenstates of \bar{H}_m by using the unitary transformation relating the product states $|q\rangle_{m-1} |\alpha_m\rangle$ to the eigenstates $|q\rangle_m$ of \bar{H}_m ,

$$|q\rangle_m = \sum_{r, \alpha_m} U_m(r, \alpha_m, q) |q\rangle_{m-1} |\alpha_m\rangle, \quad (33)$$

where U_m is the matrix of eigenvectors of \bar{H}_m . (for explicit expressions of the resulting off-diagonal terms in Eq. (32) see [2]).

Equation (33) also shows that the NRG eigenstates have the form of so called matrix product states (MPS) [29], a feature of NRG shared also by the density matrix renormalization group method (DMRG) for one-dimensional quantum systems (see Appendix D for a comparison of NRG with this method). In order to see this, we introduce the notation $A_{q_m q_{m-1}}^{\alpha_m} \equiv U_m(q_{m-1}, \alpha_m, q_m)$ with $|q_m\rangle \equiv |q\rangle_m$ and repeatedly apply Eq. (33) to obtain

$$\begin{aligned} |q_m\rangle &= \sum_{q_{m-1}, \alpha_m} A_{q_{m-1} q_m}^{\alpha_m} |q_{m-1}\rangle |\alpha_m\rangle \\ &= \sum_{q_{m-1}, \alpha_m} A_{q_{m-1} q_m}^{\alpha_m} \left[\sum_{q_{m-2}, \alpha_{m-1}} A_{q_{m-2} q_{m-1}}^{\alpha_{m-1}} |q_{m-1}\rangle |\alpha_{m-1}\rangle \right] |\alpha_m\rangle \\ &= \sum_{q_{m_0}, \alpha_{m_0+1}, \dots, \alpha_m} (A^{\alpha_{m_0+1}} \dots A^{\alpha_m})_{q_{m_0} q_m} |\alpha_{m_0+1}\rangle \dots |\alpha_m\rangle, \end{aligned} \quad (34)$$

where $m_0 \geq 0$.

3. In order to reduce the size of the matrices that need to be diagonalized, one uses available symmetries, such as conservation of charge (electron number relative to half filling) $[Q_m, H_m] = 0$, with $Q_m = (n_d - 1) + \sum_{n=0}^m \sum_{\sigma} (f_{n\sigma}^{\dagger} f_{n\sigma} - 1/2)$, or conservation of total spin $[\vec{S}_m^2, H_m] = 0$. For multi-channel models, such as the three channel Kondo model, additional symmetries, such as $SU(3)$, may be used to significantly reduce the numerical effort [30, 31]. The use of symmetries, beyond the advantage of reducing the computational cost, also improves the accuracy of the calculations once one starts to neglect high energy states (see next subsection), since it avoids the possibility of splitting up degenerate states within a multiplet carrying the same conserved quantum numbers.

Truncation

In practice since the number of many-body states in \bar{H}_m grows as $4 \times 4^{m+1}$ it is not possible to retain all states after a given iteration $m = m_0$, where m_0 is typically 4 or 5 for single-channel models. For $m \geq m_0$ only the lowest 1000 or so states of \bar{H}_m are retained, we call these the kept states and denote them by $|k\rangle_m$, while the higher energy states neglected are denoted by $|l\rangle_m$, see Fig. 11 in Sec. 5. While only kept states are used to set up and diagonalize the sequence of Hamiltonians $\bar{H}_m, m = m_0, m_0 + 1, \dots$ up to a maximum chain size of length $m = N$, we shall see later that the discarded states $|l\rangle_m$ from each iteration $m \geq m_0$ prove to be very useful for calculating physical properties.

The truncation of the spectrum of \bar{H}_m restricts the range of eigenvalues in $H_m = D_m \bar{H}_m$ to be such that $0 \leq E_q^m \leq K D_m$ where $K = K(\Lambda)$ depends on Λ and the number of states retained. For 1000 states and $\Lambda = 3$, $K(\Lambda) \approx 10$. However, eigenvalues below D_m are only approximate eigenvalues of the infinite system H , since states with energies below D_m are calculated more accurately in subsequent iterations $m + 1, m + 2, \dots$. Therefore the part of the spectrum of H_m which is close to the spectrum of H is restricted to $D_m \leq E_q^m \leq K(\Lambda) D_m$. This allows the whole spectrum of H to be recovered by considering the spectra of the sequence of Hamiltonians $H_m, m = 0, 1, \dots$. In this way the many-body eigenvalues and eigenstates are obtained on all energy scales. Due to the smallness of the perturbation (of $\mathcal{O}(\Lambda^{-1/2}) < 1$) in adding an energy shell to go from H_m to H_{m+1} , the truncation of the high energy states turns out, in practice, to be a very good approximation.

Fixed Points

The analysis of fixed points is important to gain a conceptual understanding of the model and for accurate analytic calculations in the vicinity a fixed point [2].

From (28), a fixed point H^* of $\mathcal{R} = \mathcal{T}^2$ is defined by

$$H^* = \mathcal{R}[H^*]. \quad (35)$$

Proximity to a fixed point is identified by ranges of $m, m_1 \leq m \leq m_2$, where the energy levels \bar{E}_p^m of \bar{H}_m are approximately independent of m : $\bar{E}_p^m \approx \bar{E}_p$ for $m_1 \leq m \leq m_2$. A typical energy level flow diagram showing regions of m where the energy levels are approximately constant is shown in Fig. 5 (a) for the anisotropic Kondo model (AKM) [26]:

$$H_{AKM} = \sum_{k\sigma} \varepsilon_k c_{k\sigma}^{\dagger} c_{k\sigma} + \frac{J_{\perp}}{2} (S^+ f_{0\downarrow}^{\dagger} f_{0\uparrow} + S^- f_{0\uparrow}^{\dagger} f_{0\downarrow}) + \frac{J_{\parallel}}{2} S_z (f_{0\uparrow}^{\dagger} f_{0\uparrow} - f_{0\downarrow}^{\dagger} f_{0\downarrow}) \quad (36)$$

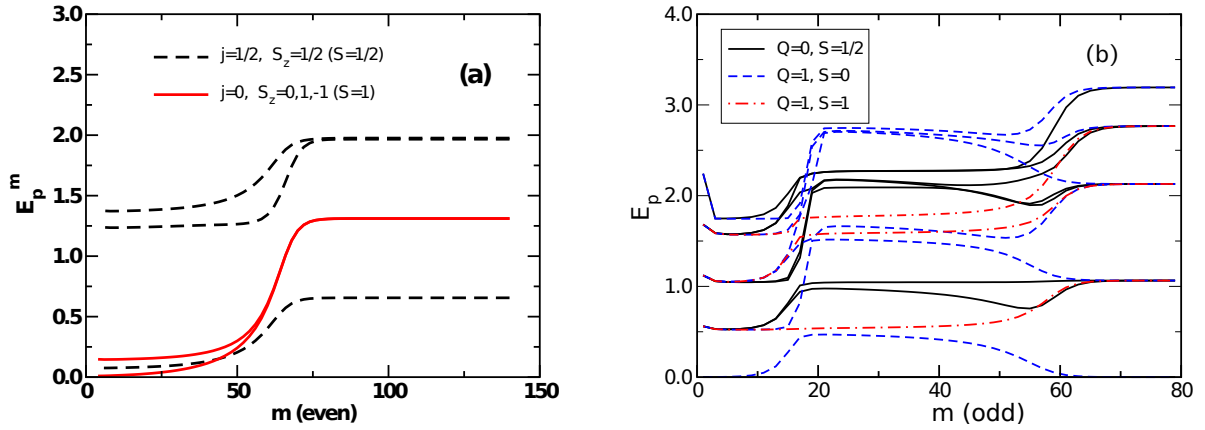


Fig. 5: (a) The lowest rescaled energy levels of the AKM for $J_{\parallel} = 0.443$ and $J_{\perp} = 0.01$. The states are labeled by conserved pseudospin j and total S_z (adapted from [26]). (b) The flow of the lowest many-body energy levels of the Anderson model for $\varepsilon_d = -U/2$, $U/\pi\Delta_0 = 12.66$, and $\Lambda = 2.5$. States are labeled by quantum numbers for total charge Q and total spin S (adapted from [4, 2]).

There is an unstable high energy fixed point (small m) and a stable low energy fixed point (large m). The low energy spectrum is identical to that of the isotropic Kondo model at the strong coupling fixed point $J = \infty$ in [1] (e.g. the lowest single particle excitations in Fig. 5 (a), $\eta_1 = 0.6555$, $\eta_2 = 1.976$ agree with the $\Lambda = 2$ results of the isotropic model in [1]). The crossover from the high energy to the low energy fixed point is associated with the Kondo scale T_K . Spin-rotational invariance, broken at high energies, is restored below this scale [e.g., the $j = 0$ states with $S_z = 0$ and $S_z = \pm 1$ become degenerate below T_K and can be classified by the same total spin S as indicated in Fig. 5 (a)]. In Fig. 5 (b) typical energy level flows for the symmetric Anderson impurity model $\varepsilon_d = -U/2$ in the strongly correlated Kondo regime are shown. Here, one sees three fixed points: an unstable free orbital fixed point for $m < 10$, a marginal fixed point for $10 < m < 50$ corresponding to formation of a local moment interacting weakly via the antiferromagnetic Kondo exchange with the conduction electrons. In this region, the effective Hamiltonian is essentially the Kondo model. Finally, for $m > 50$ there is a flow to the stable strong coupling fixed point, characterized by a fixed point spectrum obtained by setting $J = \infty$, i.e. the local spin and local conduction orbital are frozen out. The fixed point spectrum is then that of a free electron chain with one site removed, i.e., there is a crossover to an even m fixed point spectrum. The freezing out of the local spin, implies that inelastic scattering processes are blocked as $m \rightarrow \infty$ ($T \rightarrow 0$) and one obtains the picture of a renormalized Fermi liquid at low temperatures.

Analytic calculations can be carried out in the vicinity of these various fixed points by setting up effective Hamiltonians $H_{\text{eff}} = H^* + \sum_{\lambda} \omega_{\lambda} O_{\lambda}$, where the leading deviations O_{λ} about H^* can be obtained from general symmetry arguments. This allows, for example, thermodynamic properties to be calculated in a restricted range of temperatures, corresponding to the restricted range of m where \bar{H}_m can be described by a simple effective Hamiltonian H_{eff} . In this way Wil-

son could show that the ratio of the impurity susceptibility, χ_{imp} , and the impurity contribution to the linear coefficient of specific heat, γ_{imp} , at $T = 0$, is twice the value of a non-interacting Fermi liquid: $R = \frac{4\pi^2\chi_{\text{imp}}}{3\gamma_{\text{imp}}} = 2$. We refer the reader to the detailed description of such calculations in [1, 2], and we turn now to the numerical procedure for calculating thermodynamics, which can give results at all temperatures, including the crossover regions.

4 Calculation of physical properties

The ability of the method to yield thermodynamic, dynamic and transport properties makes it very useful for interpreting experimental results ⁶. We shall first describe the calculation of thermodynamics and dynamics using conventional approaches (without use of the complete basis set, but including reduced density matrices for dynamics) [2, 7, 8]. In Sec. 5 we shall then discuss more recent approaches using the complete basis set and full density matrix [33, 10] (this division, however, is somewhat arbitrary).

Thermodynamics: conventional approach

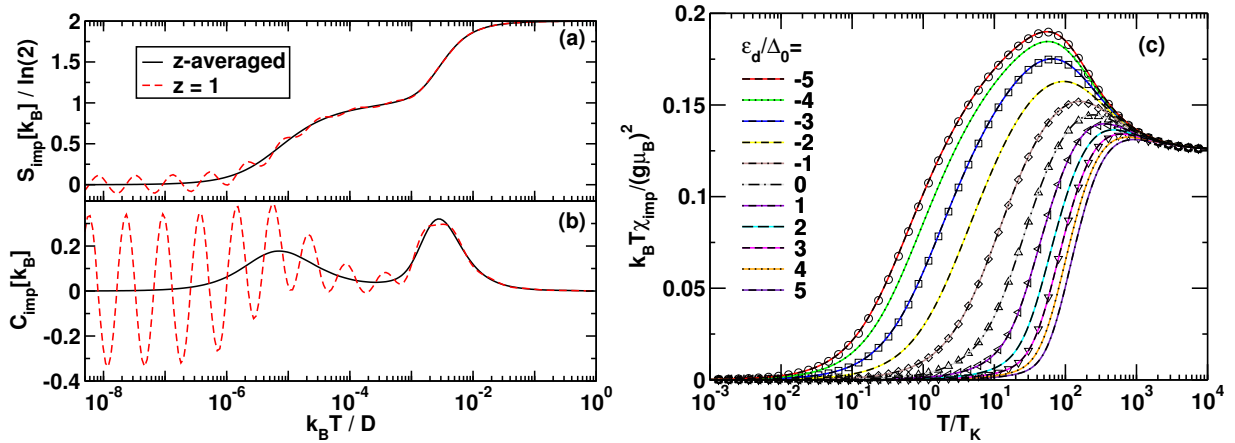


Fig. 6: Temperature dependence of, (a), the impurity entropy, $S_{\text{imp}}(T)$, and, (b), the impurity specific heat, $C_{\text{imp}}(T)$, for the symmetric Anderson model with $U/\Delta_0 = 12$ and $\Delta_0 = 0.001D$. The calculations are for $\Lambda = 4$, without z -averaging [$n_z = 1$, $z = 1$ (dashed lines)], and with z -averaging [$n_z = 2$, $z = 1/4, 3/4$ (solid lines)]. For $\Lambda = 4$ two z values suffice to eliminate the discretization oscillations[34]. (c) Impurity susceptibility, $\chi_{\text{imp}}(T)$, vs T/T_K for the asymmetric Anderson model with same parameters as above and several values of ϵ_d/Δ_0 with T_K for symmetric model. Broken lines: FDM approach. Solid lines: conventional approach. Symbols: Bethe ansatz (for selected values of $\epsilon_d/\Delta_0 = -5, -3, -1, 0, +1, +3$). NRG parameters: $\Lambda = 10$ with z -averaging [$n_z = 4$, $z = 1/8, 1/2, 3/8, 3/4$][35]

Suppose we have diagonalized exactly the Hamiltonian for a quantum impurity model such as the Kondo model and that we have all the many-body eigenvalues E_q and eigenstates $|q\rangle$:

$$H = \sum_q E_q |q\rangle \langle q| \equiv \sum_q E_q X_{qq}. \quad (37)$$

⁶Spatial correlations may also be investigated, see Ref. [32]

We can then calculate the partition function

$$Z(T) \equiv \text{Tr} e^{-H/k_B T} = \sum_q e^{-E_q/k_B T}, \quad (38)$$

and hence the thermodynamics via the impurity contribution to the free energy $F_{\text{imp}}(T) = -k_B T \ln Z/Z_c$, where $Z_c = \text{Tr} e^{-H_c/k_B T}$ is the the partition function for the non-interacting conduction electrons. In the NRG procedure we can only calculate the "shell partition functions" Z_m for the sequence of truncated Hamiltonians H_m :

$$Z_m(T) \equiv \text{Tr} e^{-H_m/k_B T} = \sum_q e^{-E_q^m/k_B T} = \sum_q e^{-D_m \bar{E}_q^m/k_B T} \quad (39)$$

We will have $Z_m(T) \approx Z(T)$ provided

1. we choose $k_B T = k_B T_m \ll E_{\text{max}}^m = D_m K(\Lambda)$ so that the contribution to the partition function from excited states $E_q^m > D_m K(\Lambda)$, not contained in Z_m , is negligible, and
2. the truncation error made in replacing H by H_m in equating (38) and (39) is small. This error has been estimated in [2] to be approximately $\Lambda^{-1} D_m/k_B T_m$.

Combining these two conditions requires that

$$\frac{1}{\Lambda} \ll \frac{k_B T_m}{D_m} \ll K(\Lambda). \quad (40)$$

The choice $k_B T = k_B T_m \approx D_m$ is reasonable and allows the thermodynamics to be calculated at a sequence of decreasing temperatures $k_B T_m \sim D_m, N = 0, 1, \dots$ from the truncated partition functions Z_m . The procedure yields essentially exact results. For small $\Lambda \lesssim 3$, the window for choosing the temperature T_m to satisfy Eq. 40 is small, and typically only one such temperature is used for each shell. For larger $\Lambda \gg 1$ one can use many temperatures $T_m^i, i = 1, \dots, n_T$ which satisfy the above condition, however, for large $\Lambda = 4 - 10$, discretization oscillations become important[36, 37]. This problem is overcome by averaging the results over several discretizations of the band, i.e. one carries out several calculations with discretizations of the band $\pm D, \pm D\Lambda^{-(1-z_k)}, \pm D\Lambda^{-(2-z_k)}, \dots$ and averages the results for several $z_k, k = 1, \dots, N_z$. Figure 6 (a)-(b) illustrates this for the entropy and specific heat of the Anderson model. In this way, the conventional approach can recover essentially exact results for thermodynamics. Fig. 6 (c) shows a comparison for the impurity static susceptibility of the Anderson impurity model

$$\chi_{\text{imp}}(T) = \frac{(g\mu_B)^2}{k_B T} \left[\frac{1}{Z} \text{Tr} (S_z^{\text{tot}})^2 e^{-H/k_B T} - \frac{1}{Z_c} \text{Tr} (S_{z,c}^{\text{tot}})^2 e^{-H_c/k_B T} \right]$$

to both Bethe-ansatz results and results obtained within the more recent full density matrix approach to be described below.

Dynamics: conventional approach without reduced density matrices

We consider now the application of the NRG method to the calculation of dynamic properties of quantum impurity models [38, 6, 7, 8]. For definiteness we consider the Anderson

impurity model and illustrate the procedure for the impurity spectral density $A_{d\sigma}(\omega, T) = -\frac{1}{\pi}\text{Im}G_{d\sigma}(\omega, T)$, with

$$G_{d\sigma}(\omega, T) = \int_{-\infty}^{+\infty} d(t-t') e^{i\omega(t-t')} G_{d\sigma}(t-t') \quad (41)$$

$$G_{d\sigma}(t-t') = -i\theta(t-t') \langle [d_{\sigma}(t), d_{\sigma}^{\dagger}(t')]_{+} \rangle_{\varrho} \quad (42)$$

with ϱ the density matrix of the system.

Suppose we have all the many-body eigenstates $|q\rangle$ and eigenvalues E_q of the Anderson impurity Hamiltonian H . Then the density matrix, $\varrho(T)$, of the full system at temperature $k_{\text{B}}T = 1/\beta$ can be written

$$\varrho(T) = \frac{1}{Z(T)} \sum_q e^{-\beta E_q} |q\rangle \langle q|, \quad (43)$$

and the impurity Green function can be written in the Lehmann representation as

$$G_{d\sigma}(\omega, T) = \frac{1}{Z(T)} \sum_{q,q'} |\langle q|d_{\sigma}|q'\rangle|^2 \frac{e^{-E_q/k_{\text{B}}T} + e^{-E_{q'}/k_{\text{B}}T}}{\omega - (E_{q'} - E_q)} \quad (44)$$

and the corresponding impurity spectral density $A_{d\sigma}$ as

$$A_{d\sigma}(\omega, T) = \frac{1}{Z(T)} \sum_{q,q'} |M_{q,q'}|^2 (e^{-E_q/k_{\text{B}}T} + e^{-E_{q'}/k_{\text{B}}T}) \delta(\omega - (E_{q'} - E_q)) \quad (45)$$

with $M_{q,q'} = \langle q|d_{\mu}|q'\rangle$.

Consider first the $T = 0$ case ($T > 0$ is described in the next section), then

$$A_{d\sigma}(\omega, T = 0) = \frac{1}{Z(0)} \sum_q |M_{q,0}|^2 \delta(\omega + (E_q - E_0)) + \frac{1}{Z(0)} \sum_{q'} |M_{0,q'}|^2 \delta(\omega - (E_{q'} - E_0)), \quad (46)$$

with $E_0 = 0$ the ground state energy. In order to evaluate this from the information which we actually obtain from an iterative diagonalization of H , we consider the impurity spectral densities corresponding to the sequence of Hamiltonians H_m , $m = 0, 1, \dots, N$,

$$A_{d\sigma}^m(\omega, T = 0) = \frac{1}{Z_m(0)} \sum_q |M_{q,0}^m|^2 \delta(\omega + E_q^m) + \frac{1}{Z_m(0)} \sum_{q'} |M_{0,q'}^m|^2 \delta(\omega - E_{q'}^m). \quad (47)$$

From the discussion on the spectrum of H_m in the previous section, it follows that the ground-state excitations of H_m which are representative of the infinite system H are those in the range $D_m \leq \omega \leq K(\Lambda)D_m$. Lower energy excitations and eigenstates are calculated more accurately at subsequent iterations, and higher energy excitations are not contained in H_m due to the elimination of the higher energy states at each m . Hence, for fixed m , we can approximately evaluate the spectral density at a characteristic frequency $\omega \approx \omega_m \equiv k_{\text{B}}T_m$ via

$$A_{d\sigma}(\omega, T = 0) \approx A_{d\sigma}^m(\omega, T = 0), \quad m = 0, 1, \dots, N. \quad (48)$$

In making this approximation, we are assuming that the matrix elements $M_{0,q'}^m$ of the finite system Hamiltonian are the same as those of the infinite system $M_{0,q'}$. This assumption fails, when an applied field strongly affects the groundstate and low lying excited states, thereby making

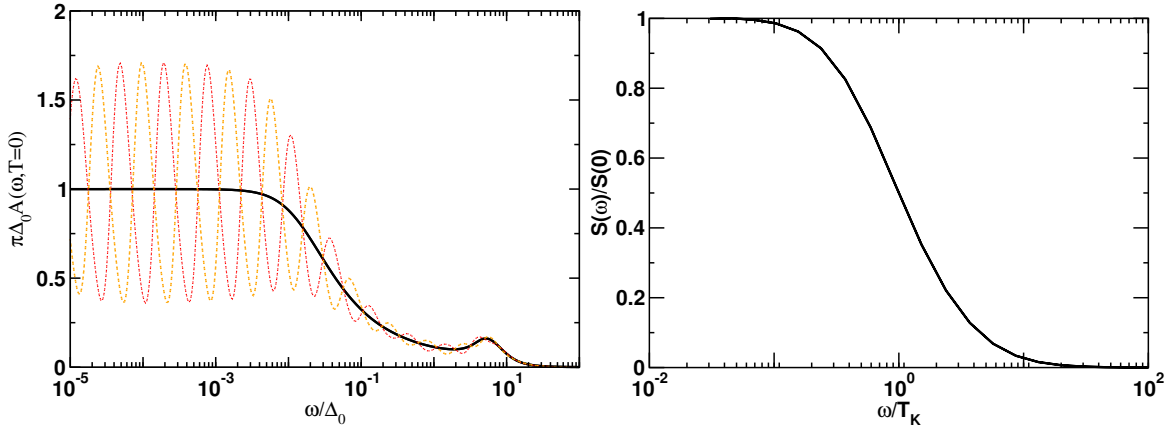


Fig. 7: (a) The impurity spectral density for the symmetric Anderson model for $U/\Delta_0 = 12$ at large $\Lambda = 10$ showing discretization oscillations for two values of z . Averaging over 8 z -values yields the smooth curve. (b). Longitudinal spin relaxation function $S(\omega)/S(0)$ versus ω/T_K for the isotropic Kondo model, showing that the spin relaxes incoherently.

also the matrix elements for the finite size system $M_{0,q}^m$ appreciably different to those of the infinite system. We shall come back to this point below, when we introduce the reduced density matrix approach to Green functions[8]. Returning to the calculation of spectral densities, a typical choice for the characteristic frequency to evaluate $A_{d\sigma}(\omega, 0)$ from $A_{d\sigma}^m(\omega, 0)$ is $\omega = 2\omega_m$ for $\Lambda = 2$. In this way $A_{d\sigma}(\omega, T = 0)$ can be calculated at a sequence of decreasing frequencies $\omega = 2\omega_m, m = 0, 1, \dots, N$ from the quantities $A_{d\sigma}^m$. In practice we are not interested in the discrete spectra $A_{d\sigma}^m(\omega) = \sum_q w_q^m \delta(\omega - E_q^m)$ of the Hamiltonians H_m but in continuous spectra which can be compared with experiment. Smooth spectra can be obtained from the discrete spectra by replacing the delta functions $\delta(\omega - E_q^m)$ by smooth distributions $P_m(\omega - E_q^m)$. A natural choice for the width η_m of P_m is D_m , the characteristic scale for the energy level structure of H_m . Two commonly used choices for P are the Gaussian and the Logarithmic Gaussian distributions [38, 7, 39]. More refined schemes also exist [40, 41] as well as different band discretizations to reduce artifacts close to band edges [42]. A peak of intrinsic width Γ at frequency Ω_0 will be well resolved by the above procedure provided that $\Omega_0 \ll \Gamma$, which is the case for the Kondo resonance and other low energy resonances. In the opposite case, the low (logarithmic) resolution at higher frequencies may be insufficient to resolve the intrinsic widths and heights of such peaks. Usually such higher frequency peaks are due to single-particle processes and can be adequately described by other methods (exceptions include interaction dominated features in the Ohmic two-state system, see below, and in strongly correlated lattice models in high dimensions [43, 16, 44, 45]). In both cases, $\Omega_0 \ll \Gamma$ and $\Omega_0 \gg \Gamma$, the positions and intensities of such peaks is given correctly. An alternative procedure for obtaining smooth spectra, which in principle resolves finite frequency peaks with the same resolution as the low energy peaks, has been proposed in [46] and uses the averaging over several band discretizations, described above for the thermodynamics. This procedure allows carrying out calculations for spectral functions at larger Λ . An example is shown in Fig. 7 (a) for the symmetric Anderson model. As in the thermodynamics, calculations of the dynamics at large $\Lambda \gg 1$ exhibit discretization oscillations, see Fig. 7 (a), which may be eliminated by averaging over several band discretizations.

How accurate is the NRG for dynamic properties? A good measure of the accuracy of the

procedure is given by the Friedel sum rule, a Fermi liquid relation which states that [24]

$$A_{d\sigma}(0) = \frac{1}{\pi\Delta_0} \sin^2(\pi n_d/2), \quad n_d = \int_{-\infty}^0 d\omega A_{d\sigma}(\omega) \quad (49)$$

From Fig. 7 (a), we find that $\pi\Delta_0 A_{d\sigma}(0, 0) = 1 \pm 10^{-3}$, i.e., the Friedel sum rule is satisfied to within 0.1% relative error. More important, however, is that this error remains small independent of the interaction strength $0 \leq U \leq \infty$. Two-particle Green functions and response functions, such as the longitudinal spin relaxation function,

$$S(\omega) = -\frac{1}{\pi} \frac{\text{Im}\chi_{zz}(\omega)}{\omega}, \quad \chi_{zz} = \langle\langle S_z; S_z \rangle\rangle,$$

of the Anderson impurity model and of the (anisotropic) Kondo model can also be calculated with comparable accuracy to single-particle spectral functions[26]. The spin relaxation function for the Kondo model is shown in Fig. 7 (b), and illustrates the statement made in Sec. 2, that the spin excitations of the Kondo model are drastically renormalized from the bare value of J down to the Kondo scale T_K due to the frictional effects of the environment.

The procedure for calculating finite temperature dynamical quantities, like $A_{d\sigma}(\omega, T)$, required as input for calculating transport properties, is similar to that for $T = 0$ dynamics described above [7]. The spectral density $A_{d\sigma}(\omega, T)$ at fixed temperature T is evaluated as above at frequencies $\omega \approx 2\omega_m, m = 0, 1, \dots, M \leq N$ until $2\omega_M$ becomes of order $k_B T$, i.e. $2\omega_M = \alpha k_B T$ with $\alpha \approx 1$. To calculate the spectral density at frequencies $\omega < k_B T$ a smaller ‘‘cluster’’ is used. This is done because when $k_B T$ is larger than the frequency at which the spectral density is being evaluated, it is the excited states of order $k_B T$ contained in previous clusters that are important and not the excitations very much below $k_B T$. This approach suffers from the same criticism as the $T = 0$ approach above, namely one is using a finite cluster H_m to approximate $M_{q',q} \approx M_{q',q}^m$ (and also $Z(T) \approx Z_m(T)$). In particular, for $\omega < k_B T$, the use of a small cluster of size $M < N$ does not capture the full information available, a deficiency which is corrected by the full density matrix approach. Nevertheless, this early approach gives remarkably good results for finite temperature spectra and transport properties[7].

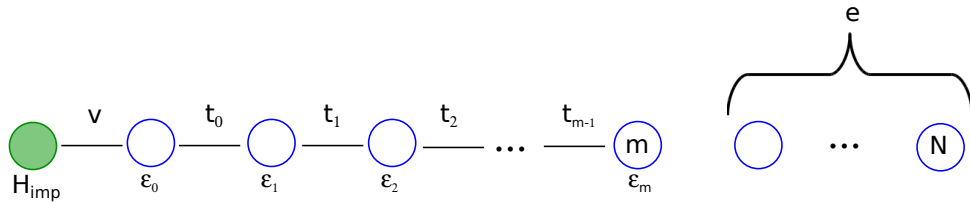


Fig. 8: The Hilbert space of H_m is supplemented with $N - m$ environment degrees of freedom $e = (\alpha_{m+1}, \dots, \alpha_N)$ [8].

Dynamics: conventional approach with reduced density matrices

A way of reducing finite size errors, inherent in the above approach to Green functions, has been proposed by Hofstetter [8], which we shall describe next. As mentioned above, there are situations when a small field can strongly polarize the low energy states of H_m , thereby strongly affecting the matrix elements $M_{q',q}^m$ and hence the spectra. For example, a magnetic

field $B \approx T_K$ in the Anderson model is sufficiently strong to polarize the groundstate such that $n_{d\uparrow} \approx 1$ and $n_{d\downarrow} \approx 0$ at $T \ll T_K$. In this case, the use of the canonical density matrix $\varrho(T) \approx \varrho_m(T) = \frac{1}{Z_m(T)} \sum_q e^{-\beta E_q^m} |q\rangle\langle q|$ in evaluating the spectra on scales $\omega_m \gg T_K$ can result in large errors. A solution to this is to use $\varrho_N(T) = \frac{1}{Z_N(T)} \sum_q |q\rangle e^{-\beta E_q^N} \langle q|$ for the longest chain diagonalized and to evaluate the Green functions on scales $\omega_m > \omega_N$ by tracing out intermediate degrees of freedom $e = (\alpha_{m+1}, \dots, \alpha_N)$ in ϱ_N . Since the longest chain H_N is close to the infinite system limit, this should provide a better description of the spectra, particularly at higher frequencies. In order to carry this procedure, the Hilbert space of each H_m is extended to that of H_N by adding the $N - m$ environment degrees of freedom e , see Fig. 8. Evaluating the reduced density matrix $\varrho_m^{\text{red}} = \text{Tr}_e[\varrho_N]$ appearing in Eq. (42) leads to a Lehmann representation for the spectral density at $T = 0$

$$A_{d\sigma}(\omega, T = 0) = \sum_{kk'} C_{kk'}^N M_{kk'}^N \delta(\omega - (E_\kappa^N - E_{\kappa'}^N)) \quad (50)$$

$$C_{kk'}^N = \sum_p \varrho_{pk'}^{\text{red}} M_{p\kappa}^N + \sum_p \varrho_{kp}^{\text{red}} M_{\kappa'p}^N \quad (51)$$

in place of (46). In Fig. 9 (a)-(b), we show a comparison of this approach with results from the

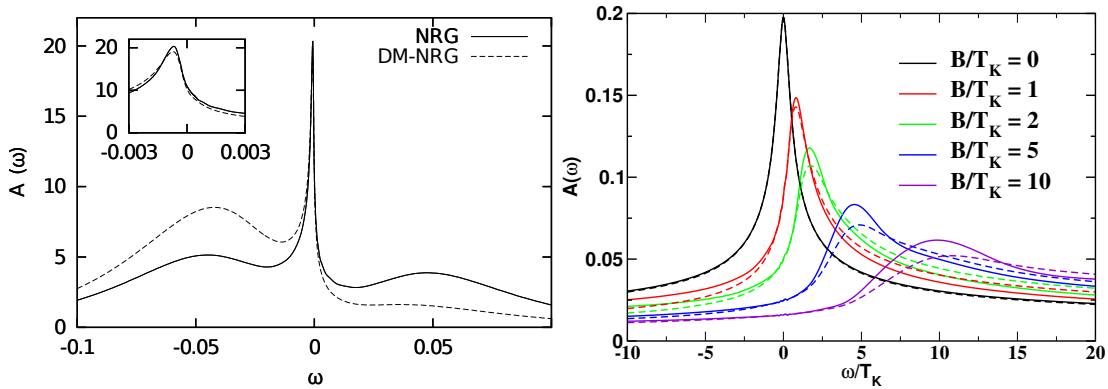


Fig. 9: Spin-up spectral density $A(\omega, T = 0)$ for, (a), the symmetric Anderson model, with $U/\Delta_0 = 10$, $\Delta_0 = 0.01$ and $B = \Delta_0/10$, with and without reduced density matrices (DM-NRG/NRG) [8], and, (b), for the Kondo model in several magnetic fields B , with and without reduced density matrices (dashed/solid lines, respectively) [12, 47], showing that the low energy Kondo resonance is sufficiently well captured in the conventional approach.

previous approach for the Anderson and Kondo models in a magnetic field. A field-induced rearrangement of spectral weight at $\omega \approx \varepsilon_d, \varepsilon_d + U$ is well captured by the reduced density matrix approach [Fig. 9 (a)]. The low energy Kondo resonance is less subject to finite size corrections, since this part of the spectrum is already calculated from sufficiently long chains, such that the corrections in using reduced density matrices are small [Fig. 9 (b)].

Transport properties

The transport properties of quantum impurity models, require knowledge of both the frequency and temperature dependence of the impurity spectral density, a topic which was addressed above. The linear response conductance, $G(T)$, and thermopower, $S(T)$, through a quantum dot described by the Anderson model, are given by the following expressions (see Lecture

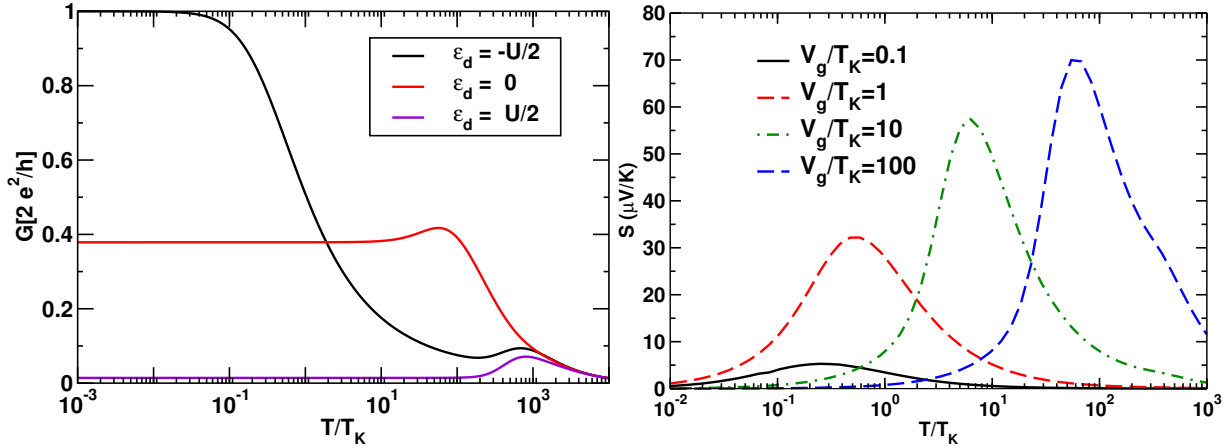


Fig. 10: (a) Linear conductance $G(T)$ versus T/T_K for $U/\Delta_0 = 16$ and several values of $\epsilon_d = -U/2, 0, +U/2$ using the approach of Yoshida et al. [48]. The resistivity of a Kondo impurity $\rho(T)$ is similar to $G(T)$ for the $\epsilon_d = -U/2$ curve. NRG parameters were for $\Lambda = 4$, $n_z = 2$ [49]. (b). Thermopower of a negative $U = -16\Delta_0$ quantum dot, exhibiting a large enhancement for gate voltages $V_g \geq T_K$ [50] (calculated within full density matrix approach to spectral functions).

B2 by Jakobs for non-equilibrium expressions)

$$G(T) = \frac{e^2}{h} \int d\omega \left(-\frac{\partial f}{\partial \omega} \right) \sum_{\sigma} \mathcal{T}_{\sigma}(\omega, T, B), \quad (52)$$

$$S(T) = -\frac{1}{|e|T} \frac{\int d\omega \omega (-\partial f / \partial \omega) \sum_{\sigma} \mathcal{T}_{\sigma}(\omega)}{\int d\omega (-\partial f / \partial \omega) \sum_{\sigma} \mathcal{T}_{\sigma}(\omega)}, \quad (53)$$

where the transmission function, $\mathcal{T}_{\sigma}(\omega, T)$, through a quantum dot symmetrically coupled to left and right leads is related to $A_{d\sigma}(\omega, T)$ via

$$\mathcal{T}_{\sigma}(\omega, T) = 2\pi\Delta_0 A_{d\sigma}(\omega T).$$

Note, that the discrete form of the spectral function may be directly substituted into the expressions for $G(T)$ and $S(T)$ above, without the necessity of broadening[48]. For the conductance, this leads to

$$G(T) = \frac{\gamma\beta}{Z} \sum_{\sigma} \sum_{m,n} |M_{mn}^{\sigma}|^2 \frac{1}{e^{\beta E_m} + e^{\beta E_n}}, \quad (54)$$

with $\gamma = 2\pi\Delta_0 \frac{e^2}{h}$. Results for the temperature dependence of the conductance of the Anderson model, using this procedure, are shown in Fig. 10 (a). Thermoelectric properties have also been investigated for quantum dots with repulsive onsite Coulomb interactions [51] and also for attractive onsite interactions [50]. The latter provide a mechanism for enhancing thermopower, as shown in Fig. 10 (b). The method gives uniformly accurate results at high and low temperatures, as well as correctly describing the crossover region $T \approx T_K$ (detailed comparisons of the resistivity of dilute magnetic impurities with known results at high and low temperature can be found [7]). These calculations, and similar resistivity calculations for dilute impurities, provide a quantitative interpretation of experiments for $S = 1/2$ realizations of the Kondo effect. They have also been extended using the full density matrix approach to describe the resistivity and dephasing rates of real Fe impurities in Au and Ag by using a 3-channel Kondo model[52, 31].

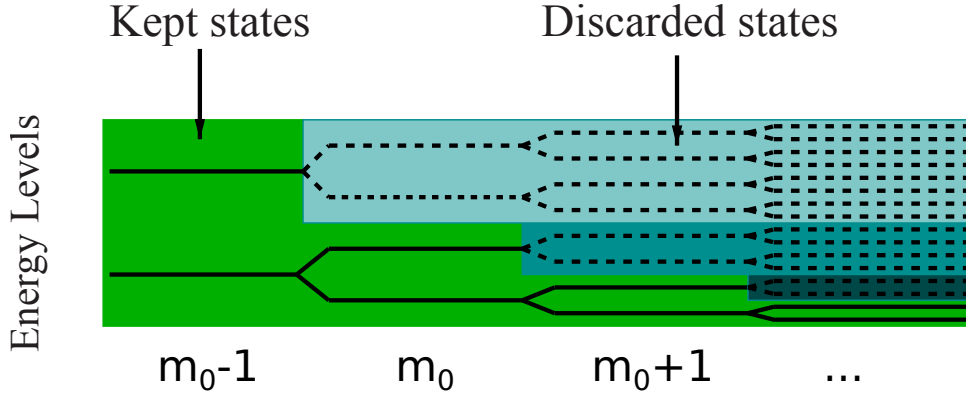


Fig. 11: For iterations $m < m_0$ all states are kept, while for $m \geq m_0$ only the lowest 1000 or so states generated are used to set up the Hamiltonian for the next iteration $m + 1$ (adapted from [54]).

5 Complete Basis Set and Full Density Matrix

We noted in Sec. 3, that at each m , the states generated, denoted $|qm\rangle$, are partitioned into the lowest energy retained states, denoted $|km\rangle$, and the high energy eliminated (or discarded) states, $|lm\rangle$. In order to avoid an exponential increase in the dimension of the Hilbert space, only the former are used to set up and diagonalize the Hamiltonian for the next iteration $m + 1$. The eliminated states, while not used in the iterative NRG procedure, may be used to set up a complete orthonormal basis set [33]. This complete basis set is very powerful and allows evaluating correlation functions $\langle A(t)B(0) \rangle$, transient quantities and even thermodynamic expressions in an unambiguous way, avoiding any possible double counting of excitations. Eliminated states from different iterations have no overlap, see Fig. 11, in contrast to the retained states. Hence, using the latter to carry out calculations of physical quantities restricts one to using excitations from a single shell only. However, for finite temperature Green functions and non-equilibrium quantities, multiple-shell contributions become important [53] and the complete basis set offers a way to evaluate these quantities [33].

The complete basis set is defined by the product states $|lem\rangle = |lm\rangle|e\rangle$, $m = m_0, \dots, N$, where m_0 is the first iteration at which truncation occurs, and $|e\rangle = |\alpha_{m+1}\rangle|\alpha_{m+2}\rangle \dots |\alpha_N\rangle$ are environment states at iteration m such that the product states $|lem\rangle$, for each $m = m_0, m_0 + 1, \dots, N$, reside in the same Fock space (that of the largest system diagonalized, $m = N$). By “e” we shall henceforth denote the collection $e = \{\alpha_{m+1} \dots \alpha_N\}$. The eliminated states satisfy the completeness relation [33, 55]

$$\sum_{m=m_0}^N \sum_{le} |lem\rangle \langle lem| = 1, \quad (55)$$

where for $m = N$ all states are counted as discarded (i.e. there are no kept states at iteration

$m = N$). We shall also use the following representations of this relation, [33, 55]

$$1 = 1_m^- + 1_m^+, \quad (56)$$

$$1_m^- = \sum_{m'=m_0}^m \sum_{l'e'} |l'e'm'\rangle \langle l'e'm'| \quad (57)$$

$$1_m^+ = \sum_{m'=m+1}^N \sum_{l'e'} |l'e'm'\rangle \langle l'e'm'| = \sum_{ke} |kem\rangle \langle kem|. \quad (58)$$

By using the complete basis set, we can construct the full density matrix FDM [10, 56],

$$\rho = \frac{1}{Z(T)} \sum_{m=m_0}^N \sum_{le} e^{-\beta E_l^m} |lem\rangle \langle lem|, \quad \text{Tr} \rho = 1 \Rightarrow \quad (59)$$

$$Z(T) = \sum_{m=m_0}^N 4^{N-m} \sum_l e^{-\beta E_l^m} \equiv \sum_{m=m_0}^N 4^{N-m} Z_m(T) \quad (60)$$

where $Z(T)$ is the partition function made up of the complete spectrum, i.e., it contains the eliminated states from all H_m , $m = m_0, m_0 + 1, \dots, N$. Consequently, it can be used to evaluate the impurity thermodynamics at arbitrary temperatures.

Consider the following density matrix for the m 'th shell (defined, however, in the Hilbert space of H_N),

$$\tilde{\rho}_m = \sum_{le} |lem\rangle \frac{e^{-\beta E_l^m}}{\tilde{Z}_m} \langle lem|. \quad (61)$$

Normalization $\text{Tr} [\tilde{\rho}_m] = 1$ implies that

$$1 = \sum_l \frac{e^{-\beta E_l^m}}{\tilde{Z}_m} 4^{N-m} = 4^{N-m} \frac{Z_m}{\tilde{Z}_m} \quad (62)$$

where $Z_m = \sum_l e^{-\beta E_l^m}$. Then the FDM can be written as a sum of weighted density matrices for shells $m = m_0, \dots, N$

$$\rho = \sum_{m=m_0}^N w_m \tilde{\rho}_m \quad (63)$$

$$w_m = 4^{N-m} \frac{Z_m}{Z}; \quad \sum_{m=m_0}^N w_m = 1 \quad (64)$$

Application to Thermodynamics

Substituting $\rho = \sum_m w_m \tilde{\rho}_m$ into the expression for the thermodynamic average $\langle \hat{O} \rangle$ of a local observable of the impurity (e.g., n_d or $n_{d\uparrow} n_{d\downarrow}$) and making use of the decomposition of unity Eq. (55), we have

$$\begin{aligned} \langle \hat{O} \rangle_\rho &= \text{Tr} [\rho \hat{O}] = \sum_{l'e'm'} \langle l'e'm'| \hat{O} \sum_{lem} w_m |lem\rangle \frac{e^{-\beta E_l^m}}{\tilde{Z}_m} \langle lem| l'e'm' \rangle \\ &= \sum_{lem} O_{ll}^m w_m \frac{e^{-\beta E_l^m}}{\tilde{Z}_m} = \sum_{lm} 4^{N-m} w_m O_{ll}^m \frac{e^{-\beta E_l^m}}{4^{N-m} Z_m} = \sum_{m=m_0, l}^N w_m O_{ll}^m \frac{e^{-\beta E_l^m}}{Z_m}, \end{aligned} \quad (65)$$

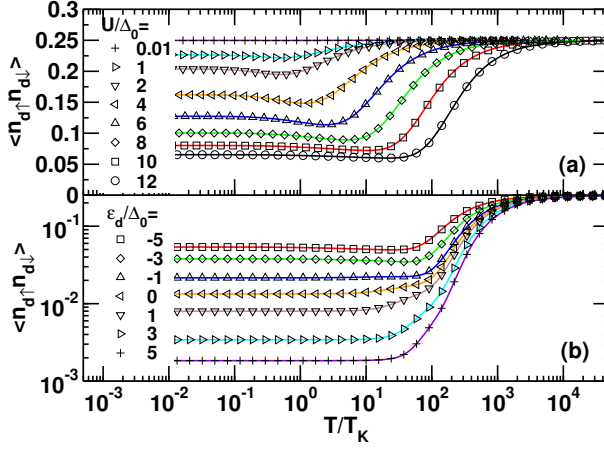


Fig. 12: Double occupancy $D_{\text{occ}} = \langle n_{d\uparrow} n_{d\downarrow} \rangle$ as a function of temperature T/T_K for, (a), the symmetric Anderson model at different U/Δ_0 , and, (b), for the asymmetric Anderson model at $U/\Delta_0 = 12$ and increasing values of $\varepsilon_d/\Delta_0 = -5, -3, -1, 0, +1, +3, +5$. FDM (solid lines), conventional approach (symbols). $\Lambda = 10$ with z -averaging [$n_z = 4, z = 1/8, 1/2, 3/8, 3/4$] [35].

where orthonormality $\langle lem | l' e' m' \rangle = \delta_{ll'} \delta_{ee'} \delta_{mm'}$, and the trace over the $N - m$ environment degrees of freedom $\sum_{lem} \dots = \sum_{lm} 4^{N-m} \dots$ has been used and $O_{ll}^m = \langle lm | \hat{O} | lm \rangle$. For other observables, such as the specific heat, or susceptibility, one requires a similar calculation for the conduction band contribution $\langle \hat{O} \rangle_{\rho_0}$, with ρ_0 the FDM of the non-interacting band. The impurity contribution is then obtained as $O_{\text{imp}} = \langle \hat{O} \rangle_{\rho} - \langle \hat{O} \rangle_{\rho_0}$.

For each temperature T and shell m , we require $w_m(T)$ and the factor $B_l^m(T) = e^{-\beta E_l^m} / Z_m$ where $Z_m = \sum_l e^{-\beta E_l^m}$. Numerical problems due to large exponentials are avoided by calculating $B_l^m(T) = e^{-\beta(E_l^m - E_0^m)} / Z'_m$ where $Z'_m = e^{\beta E_0^m} Z_m$ and E_0^m is the lowest discarded energy for shell m . Figure 12 shows results for the double occupancy of the Anderson model obtained within the FDM approach and comparisons with the conventional approach of Sec. 4.

Application to Dynamics

We consider a general fermionic/bosonic ($s = \pm 1$) retarded Green function

$$\begin{aligned} G_{AB}(t) &= -i\theta(t) \langle [A(t), B]_s \rangle \equiv -i\theta(t) \text{Tr} [\rho(A(t)B + sBA(t))] \\ &= -i\theta(t) [C_{A(t)B} + sC_{BA(t)}], \end{aligned} \quad (66)$$

where A, B are fermionic/bosonic operators, e.g. for the d-level Green function of our quantum dot $A = d_\sigma$ and $B = d_\sigma^\dagger$. The trace is evaluated using the complete basis set. We outline the derivation of $C_{A(t)B}$, with the expression for $C_{BA(t)}$ obtained in a similar manner. We have

$$\begin{aligned} C_{A(t)B} &= \text{Tr} [\rho A(t)B] = \sum_{lem} \langle lem | e^{iHt} A e^{-iHt} B \rho | lem \rangle \\ &= \sum_{lem} \sum_{l'e'm'} \langle lem | e^{iHt} A e^{-iHt} | l'e'm' \rangle \langle l'e'm' | B \rho | lem \rangle, \end{aligned} \quad (67)$$

which consists of three contributions with $m' = m, m' > m$ and $m' < m$. Consider the first contribution ($m' = m$), denoted by $C_{A(t)B}^{(i)}$. Using the NRG approximation $e^{-iHt} | l'e'm \rangle \approx e^{-iE_m t} | l'e'm \rangle$ and $\langle lem | A | l'e'm \rangle = \delta_{ee'} \langle lm | A | l'e'm \rangle = \delta_{ee'} A_{ll'}^m$, we have

$$C_{A(t)B}^{(i)} = \sum_{lm} \sum_{l'} e^{-i(E_l^m - E_l^m)t} A_{ll'}^m \sum_e \underbrace{\langle l'e'm | B \rho | lem \rangle}_{(B\rho)_{l'e,le}^m}$$

Inserting the FDM expression $\rho = \sum_m w_m \tilde{\rho}_m$ into $(B\rho)_{l'e,le}^m$ yields

$$\sum_e (B\rho)_{l'e,le}^m = B_{l'l}^m w_m e^{-\beta E_l^m} / Z_m,$$

hence we have,

$$C_{A(t)B}^{(i)} = \sum_m \frac{w_m}{Z_m} \sum_l \sum_{l'} e^{-i(E_{l'}^m - E_l^m)t} A_{ll'}^m B_{l'l}^m e^{-\beta E_l^m}. \quad (68)$$

The off-diagonal contributions with $m' > m$ and $m' < m$ in Eq. (67), which we label by $C_{A(t)B}^{(ii)}$ and $C_{A(t)B}^{(iii)}$, may be put into diagonal form by using $1_m^+ = \sum_{m'=m+1}^N \sum_{l'e'} |l'e'm'\rangle \langle l'e'm'| = \sum_{ke} |kem\rangle \langle kem|$ [Eq. (58)], thereby introducing kept states at iteration m (or m') in place of discarded states at iterations $m' > m$ (or $m > m'$),

$$\begin{aligned} C_{A(t)B}^{(ii)} &= \sum_{l'e'm' > m} \sum_{lem} \langle lem | e^{iHt} A e^{-iHt} | l'e'm' \rangle \langle l'e'm' | B \rho | lem \rangle \\ &= \sum_{lem} \sum_{ke'} \langle lem | e^{iHt} A e^{-iHt} | ke'm \rangle \langle ke'm | B \rho | lem \rangle \\ &\approx \sum_{lm} \sum_k e^{-i(E_k^m - E_l^m)t} A_{lk}^m \sum_e (B\rho)_{ke,le}^m \\ &= \sum_{lm} \sum_k e^{-i(E_k^m - E_l^m)t} A_{lk}^m B_{kl}^m e^{-\beta E_l^m} \frac{w_m}{Z_m} \end{aligned} \quad (69)$$

$$\begin{aligned} C_{A(t)B}^{(iii)} &= \sum_{lem > m'} \sum_{l'e'm'} \langle lem | e^{iHt} A e^{-iHt} | l'e'm' \rangle \langle l'e'm' | B \rho | lem \rangle \\ &= \sum_{l'e'm'} \sum_{ke'} \langle l'e'm' | B \rho | ke'm \rangle \langle ke'm | e^{iHt} A e^{-iHt} | l'e'm' \rangle \\ &\approx \sum_{l'm'} (B\rho)_{l'e',ke'} e^{-i(E_{l'}^{m'} - E_k^{m'})t} A_{kl'}^{m'} \end{aligned} \quad (70)$$

where the NRG approximation has been used together with $\sum_e (B\rho)_{ke,le}^m = B_{kl}^m e^{-\beta E_l^m} \frac{w_m}{Z_m}$. It is also easy to show that [51],

$$\text{Tr}_e [(B\rho)_{le,ke}^m] \equiv \sum_e [(B\rho)_{le,ke}^m] = \sum_{k'} B_{lk'}^m \underbrace{\sum_e \langle k'em | \rho | kem \rangle}_{R_{\text{red}}^m(k',k)} \quad (71)$$

where $R_{\text{red}}^m(k', k)$ is the reduced density matrix obtained from the FDM ρ by tracing out the degrees of freedom $e = (\alpha_{m+1}, \dots, \alpha_N)$ [10, 51], hence the contribution $C_{A(t)B}^{(iii)}$ may be written as

$$C_{A(t)B}^{(iii)} = \sum_{lm} (B\rho)_{le,ke} e^{-i(E_l^m - E_k^m)t} A_{kl}^m = \sum_{lkk'm} e^{-i(E_l^m - E_k^m)t} A_{kl}^m B_{lk'}^m R_{\text{red}}^m(k', k), \quad (72)$$

and

$$\begin{aligned} C_{A(t)B} &= C_{A(t)B}^{(i)} + C_{A(t)B}^{(ii)} + C_{A(t)B}^{(iii)} \\ &= \sum_m \frac{w_m}{Z_m} \sum_{ll'} e^{-i(E_{l'}^m - E_l^m)t} A_{ll'}^m B_{l'l}^m e^{-\beta E_l^m} + \sum_m \frac{w_m}{Z_m} \sum_{lk} e^{-i(E_k^m - E_l^m)t} A_{lk}^m B_{kl}^m e^{-\beta E_l^m} \\ &\quad + \sum_m \sum_{lkk'} e^{-i(E_l^m - E_k^m)t} A_{kl}^m B_{lk'}^m R_{\text{red}}^m(k', k) \end{aligned} \quad (73)$$

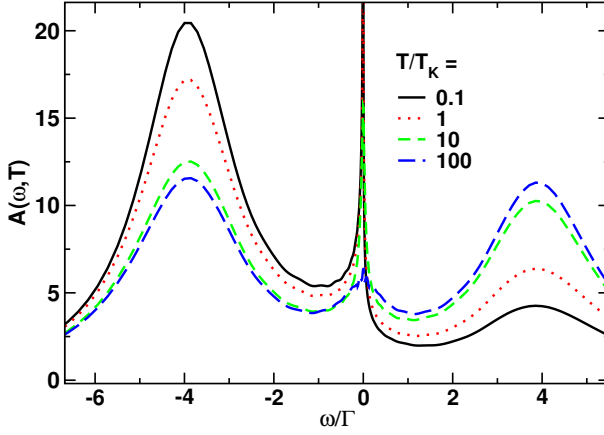


Fig. 13: Spectral function of a negative- U quantum dot modeled by the Anderson model with $U/\Gamma = -8$ at finite gate voltage $V_g = T_K$ and several temperatures, calculated within the FDM approach (adapted from [50]). The spectral function, polarized at low temperatures, becomes unpolarized at $T \gg T_K$.

Similar arguments lead to an expression for $C_{BA(t)}$ (exercise),

$$\begin{aligned}
C_{BA(t)} &= C_{BA(t)}^{(i)} + C_{BA(t)}^{(ii)} + C_{BA(t)}^{(iii)} \\
&= \sum_m \frac{w_m}{Z_m} \sum_{l'l} e^{-i(E_{l'}^m - E_l^m)t} A_{l'l}^m B_{l'l}^m e^{-\beta E_{l'}^m} + \sum_m \frac{w_m}{Z_m} \sum_{lk} e^{-i(E_l^m - E_k^m)t} A_{kl}^m B_{lk}^m e^{-\beta E_l^m} \\
&+ \sum_m \sum_{lkk'} e^{-i(E_k^m - E_l^m)t} A_{lk}^m B_{k'l}^m R_{\text{red}}^m(k, k'). \tag{74}
\end{aligned}$$

Fourier transforming $-i\theta(t)(C_{A(t)B} + sC_{BA(t)})$ using

$$\int_{-\infty}^{+\infty} -i\theta(t) e^{-i(E_{q'} - E_q)t} e^{i(\omega + i\delta)t} = 1/(\omega + i\delta - (E_{q'} - E_q)), \tag{75}$$

finally yields the Green function as

$$\begin{aligned}
G_{AB}(\omega + i\delta) &= \sum_{m=m_0}^N \frac{w_m}{Z_m} \sum_{l'l} A_{l'l}^m B_{l'l}^m \frac{e^{-\beta E_l^m} + s e^{-\beta E_{l'}^m}}{\omega + i\delta - (E_{l'}^m - E_l^m)} \\
&+ \sum_{m=m_0}^{N-1} \frac{w_m}{Z_m} \sum_{lk} A_{lk}^m B_{kl}^m \frac{e^{-\beta E_l^m}}{\omega + i\delta - (E_k^m - E_l^m)} + s \sum_{m=m_0}^{N-1} \frac{w_m}{Z_m} \sum_{lk} A_{kl}^m B_{lk}^m \frac{e^{-\beta E_l^m}}{\omega + i\delta - (E_l^m - E_k^m)} \\
&+ \sum_{m=m_0}^{N-1} \sum_{lkk'} A_{kl}^m B_{lk'}^m \frac{R_{\text{red}}^m(k', k)}{\omega + i\delta - (E_l^m - E_k^m)} + s \sum_{m=m_0}^{N-1} \sum_{lkk'} A_{lk}^m B_{k'l}^m \frac{R_{\text{red}}^m(k, k')}{\omega + i\delta - (E_k^m - E_l^m)} \tag{76}
\end{aligned}$$

The reduced density matrices appearing in Eq. (76) can be evaluated efficiently at all temperatures in a recursive manner [10]. The use of the complete basis set to calculate finite temperature Green functions ensures that the spectral sum rule $\int d\omega A_\sigma(\omega, T) = 1$ holds as an identity [10]. Furthermore, calculations at $\omega < T$ may be carried out without the need to restrict to a smaller cluster $M < N$, as was the case with the approach described in Sec. 4. Fig. 13 shows the spectral function of the negative- U Anderson model calculated from Eq. (76) at several temperatures.

For an application of this approach to thermoelectric properties of quantum dots see Ref. [51] and for a recent application to the magnetoresistivity and dephasing rate of multi-channel Kondo models see Ref. [31].

6 Recent Developments

The NRG has proved to be a reliable method for dealing with equilibrium properties of strongly correlated quantum impurity systems. Nevertheless, the method is still under development. In this section, we describe two areas where significant progress has been made, but where further work is needed. The first is in the transient response of a quantum impurity following either a quantum quench, a pulse of finite duration or a periodic train of pulses [53, 33, 55, 57, 58]. This is relevant, for example, in many pump-probe experiments [59, 60]. The second area is in developing ways to deal with real quantum impurities in metals or on surfaces, such as impurities with partially filled d- or f-levels, in which multiple channels (or bands) of the host may couple to the impurity.

Time-dependent NRG (TDNRG)

We are interested in the dynamics of a local observable \hat{O} following a quantum quench in which one or more system parameters of H change suddenly at $t = 0$. Thus, the time-dependence of H is described by $H(t) = \theta(-t)H^i + \theta(t)H^f$, with H^i and H^f being time-independent initial ($t < 0$) and final state ($t > 0$) Hamiltonians, respectively [53]. The time evolution of \hat{O} at $t > 0$ is then given by $O(t) = \text{Tr} [\rho(t)\hat{O}]$ where $\rho(t) = e^{-iH^f t} \rho e^{iH^f t}$ is the time-evolved density matrix and $\rho = e^{-\beta H^i} / \text{Tr}[\rho]$ is the density matrix of the initial state at inverse temperature β . In terms of the complete basis set, we have

$$\begin{aligned} O(t) &= \text{Tr} \left[e^{-iH^f t} \rho e^{iH^f t} \hat{O} \right] = \sum_{m=m_0}^N \sum_{le} \sum_f \langle lem | e^{-iH^f t} \rho e^{iH^f t} \hat{O} | lem \rangle_f \\ &= \sum_{mm'=m_0}^N \sum_{le'l'e'} \sum_f \langle lem | e^{-iH^f t} \rho e^{iH^f t} | l'e'm' \rangle_{ff} \langle l'e'm' | \hat{O} | lem \rangle_f. \end{aligned} \quad (77)$$

Making use of $1_m^+ = \sum_{m'=m+1}^N \sum_{l'e'} |l'e'm'\rangle \langle l'e'm'| = \sum_{ke} |kem\rangle \langle kem|$ [Eq. (58)], allows us to write[33]

$$\begin{aligned} O(t) &= \sum_{m=m_0}^N \sum_{rs \notin KK'} \sum_e \sum_f \langle sem | e^{-iH^f t} \rho e^{iH^f t} | rem \rangle_{ff} \langle rem | \hat{O} | sem \rangle_f \\ &\approx \sum_{m=m_0}^N \sum_{rs \notin KK'} \sum_e \sum_f \langle sem | e^{-iH_m^f t} \rho e^{iH_m^f t} | rem \rangle_{ff} \langle rem | \hat{O} | sem \rangle_f \\ &= \sum_{m=m_0}^N \sum_{rs \notin KK'} \left(\sum_e \sum_f \langle sem | \rho | rem \rangle_f \right) e^{-i(E_s^m - E_r^m)t} O_{rs}^m \\ &= \sum_{m=m_0}^N \sum_{rs \notin KK'} \rho_{sr}^{i \rightarrow f}(m) e^{-i(E_s^m - E_r^m)t} O_{rs}^m, \end{aligned} \quad (78)$$

in which r and s may not both be kept states, $O_{rs}^m = \sum_f \langle lem | \hat{O} | rem \rangle_f$ are the final state matrix elements of \hat{O} , which are independent of e , the NRG approximation

$$H^f |rem\rangle \approx H_m^f |rem\rangle = E_r^m |rem\rangle, \quad (79)$$

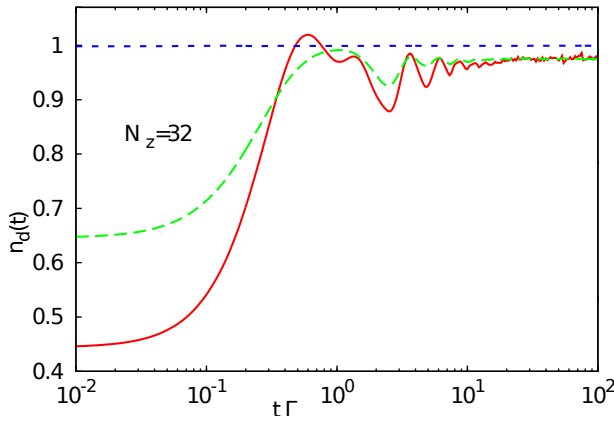


Fig. 14: Time dependence of the occupation number $n_d(t)$ of the Anderson model for $U/\Gamma = 12$ upon switching from the mixed valence regime ($\varepsilon_d = 0$) at $t < 0$ to the symmetric Kondo regime ($\varepsilon_d = -U/2$) at $t \geq 0$ at $T = T_K/10$ (red solid line), $T = 100T_K$ (green dashed line) and $T = 10^5T_K$ (blue dashed line). $\Lambda = 2$ with z -averaging ($N_z = 32$). Adapted from Ref. [57].

is adopted [in the second line of Eq. (78)], and $\rho_{sr}^{i \rightarrow f}(m) = \sum_e \langle sem | \rho | rem \rangle_f$ represents the reduced density matrix of the initial state projected onto the basis of final states (henceforth called the *projected density matrix*). The latter has been evaluated for the special choice of a density matrix defined on the longest Wilson chain

$$\rho = \sum_l |lN\rangle_i \frac{e^{-\beta E_l^N}}{Z_N} \langle lN|, \quad (80)$$

with $Z_N = \sum_l e^{-\beta E_l^N}$, in which only the discarded states of the last NRG iteration enter [33, 55]. More recently, the projected density matrix has been evaluated for a general initial density matrix, given by the full density matrix of the initial state [57]. This allows calculations to be carried out at arbitrary finite temperature, as shown in Fig. 14. While the short-time limit $O(t \rightarrow 0^+)$ in the TDNRG recovers the exact thermodynamic value $O^i = \text{Tr}[\rho O]$ in the initial state, the long-time limit suffers from an error of a few %. In addition, significant noise is observed at intermediate $t\Gamma \gtrsim 1$ to long times $t\Gamma \gg 1$. Attempts to further improve the method may be found in Ref. [57] and references therein. A generalization of the single-quench TDNRG formalism to multiple quenches, allowing applications to systems subject to general pulses or periodic driving fields, may be found in Ref. [58].

Multi-orbital and Multi-channel Models for Realistic Modeling

The Anderson impurity model is a starting point for describing many different systems, from the classic examples of transition metal magnetic impurities such as Fe or Mn in non-magnetic metals such as Au, rare-earth magnetic impurities in non-magnetic metals, such as Ce in LaAl_2 [24], or, magnetic ions such as Co, Fe and Ti adsorbed on surfaces of non-magnetic metals such as Cu or $\text{Cu}_2\text{N}/\text{Cu}$ (where the Cu_2N monolayer reduces the hybridization V to the substrate [61]). Of course, the relevant correlated orbitals in these systems are not the non-degenerate “s-levels” as in (3), but would be the 5-fold or 7-fold degenerate partially filled d- or f-orbitals in the case of transition metal or rare earth metal impurities, respectively. Furthermore, electrons in these partially filled shells would be subject to Coulomb, Hund’s exchange, spin-orbit and crystal-field interactions, often leading to non-degenerate low energy multiplets. In addition, these low energy multiplets, would hybridize with conduction channels of appropriate symmetry, and in general with many channels, not just one as in (3). Such a non-degenerate multi-channel Anderson model capable of describing a real-transition metal impurity would then look more

complicated than Eq. (3), e.g., the following model (but still neglecting spin-orbit and crystal field interactions),

$$\begin{aligned}
H = & \sum_{m\sigma} \varepsilon_{dm} n_{m\sigma} + \frac{1}{2} U \sum_{m\sigma} n_{m\sigma} n_{m-\sigma} + \frac{1}{2} U' \sum_{m \neq m'\sigma} n_{m\sigma} n_{m'-\sigma} + \frac{1}{2} (U' - J) \sum_{m \neq m'\sigma} n_{m\sigma} n_{m'\sigma} \\
& - \frac{J}{2} \sum_{m \neq m'\sigma} d_{m\sigma}^\dagger d_{m-\sigma} d_{m'-\sigma}^\dagger d_{m'\sigma} - \frac{J'}{2} \sum_{m \neq m'\sigma} d_{m\sigma}^\dagger d_{m-\sigma}^\dagger d_{m'-\sigma} d_{m'\sigma} \\
& + \sum_{km\sigma} \epsilon_{km\sigma} c_{km\sigma}^\dagger c_{km\sigma} + \sum_{km\sigma} V_{km\sigma} (c_{km\sigma}^\dagger d_{m\sigma} + h.c.)
\end{aligned}$$

would be closer describing a real transition metal impurity such as Mn in Cu. Despite its apparent complexity, this model, just like its simpler counterpart in Eq. (3), has the same general structure as Eq. (2) describing a general quantum impurity model, namely all many-body interactions (U, U', J, J') are contained in a local part H_{imp} , while the multi-channel bath H_{bath} represents non-interacting electrons coupling via a one-body hybridization to H_{imp} . While the NRG can be applied to such multi-channel models, for N_c -channels the Hilbert space grows as 4^{N_c} instead of 4 as for a single channel. The fraction of states that can be retained at each iteration is correspondingly smaller ($1/4^{N_c}$) than for a single channel ($1/4$), making accurate calculations difficult, particularly for dynamical quantities. While implementing all available symmetries ($U(1), SU(2), SU(3)$, parity etc), in order to increase the fraction of states that can be retained at each iteration, will help, such symmetries are not always present. At present, reliable NRG calculations for dynamics can be carried out for 3 channel models [31]. Increasing this to 5-channels would be a significant development, allowing many interesting realistic systems to be investigated with NRG in combination with ab-initio methods to extract the relevant model parameters [52, 62, 63]. We mention here one recent proposal for achieving this, which, however, has so far only been benchmarked on a 3-channel model [64]. As in the single-band case, we rewrite the above model in linear chain form with $H_{\text{bath}} = \sum_{m=1}^{N_c} \sum_{k\sigma} \epsilon_{km\sigma} c_{km\sigma}^\dagger c_{km\sigma} \rightarrow \sum_{m=1}^{N_c} \sum_{n=0}^{\infty} \sum_{\sigma} t_{mn} (f_{mn\sigma}^\dagger f_{m+1\sigma} + h.c.)$, where $t_{mn} \sim D_m \Lambda^{-n/2}$, $m = 1, \dots, N_c$ for N_c channels with half-bandwidths D_m . If all channels have the same band-width $D_m = D$, $m = 1, \dots, N_c$, the hoppings within a shell t_{mn} , $m = 1, \dots, N_c$ are constant one has to add all orbitals $f_{m+1\sigma}$, $m = 1, \dots, N_c$ of the next shell $n + 1$ in going from H_n to H_{n+1} in the NRG procedure of Sec. 3, before truncating the spectrum of H_{n+1} , hence leading to the above growth of the Hilbert space at each iteration. Choosing band-widths D_m with $D_1 > D_2 > \dots > D_{N_c}$, as suggested in Ref. [64], leads to an energy scale separation of the orbitals within each shell, i.e., $t_{mn} \sim D_m \Lambda^{-n/2}$ for fixed n decrease with $m = 1, \dots, N_c$. This allows adding the orbitals $f_{m+1\sigma}$, $m = 1, \dots, N_c$ of a given shell sequentially while simultaneously truncating the spectrum after each orbital is added. The calculation then resembles a single-channel calculation. The above energy scale separation is guaranteed provided $D_m/D_{m+1} = 1/g = \Lambda^{-1/2N_c}$ implying $t_{m+1n}/t_{mn} = g < 1$. Since the hoppings in this approach decrease by a factor $\Lambda^{-1/2N_c}$, a larger Λ will be required to obtain the same accuracy as a single channel calculation. In this way, the authors obtained accurate results for 3-channel and 3-impurity models.

7 Summary

Wilson's non-perturbative NRG transformation for the Kondo model has become a powerful tool for the study of quantum impurity models in general. It gives information on the many-

body eigenvalues and eigenstates of such models on all energy scales and thereby allows the direct calculation of their thermodynamic, dynamic, and transport properties. Recently, it has been further developed to yield the transient response of these systems to a sudden perturbation (a quantum quench) [33], the time-dependent NRG (TDNRG). Extensions of the TDNRG to general pulses using multiple quenches have also been made [57, 58]. The NRG also has potential to give information on the non-equilibrium steady-state transport through correlated impurity systems such as quantum dots. Recent work tries to construct a non-equilibrium density matrix for such systems by using the TDNRG to time-evolve from a known initial density matrix [65].

The method has been extended in new directions, such as to models with bosonic baths to study spin-boson models [28] and the interplay of correlations and phonon effects in Anderson-Holstein models [66]. It has also been used successfully to make progress on understanding the Mott transition, heavy fermion behaviour and other phenomena in correlated lattice systems [39, 67, 68, 69]. There is room for further improvement and extensions of the method both technically and in the investigation of more complex systems such as multi-channel models [70, 31, 64].

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Appendices

A Logarithmic discretization approximation

The approximation

$$H_c = \int_{-1}^{+1} d\varepsilon \varepsilon c_{\varepsilon\sigma}^+ c_{\varepsilon\sigma} \approx \sum_{n=0}^{\infty} (\varepsilon_{-n} c_{-n\sigma}^+ c_{-n\sigma} + \varepsilon_{+n} c_{+n\sigma}^+ c_{+n\sigma}) \quad (81)$$

used to replace the continuum band by the discrete one can be analyzed by introducing a complete orthonormal basis set of states for the conduction electrons in each interval $\pm[\Lambda^{-(n+1)}, \Lambda^{-n}]$ using the following wavefunctions

$$\psi_{np}^{\pm}(\varepsilon) = \begin{cases} \frac{\Lambda^{n/2}}{(1-\Lambda^{-1})^{1/2}} e^{\pm i\omega_n p \varepsilon} & \text{for } \Lambda^{-(n+1)} < \pm\varepsilon < \Lambda^{-n} \\ 0 & \text{otherwise} \end{cases} \quad (82)$$

Here p is a Fourier harmonic index and $\omega_n = 2\pi\Lambda^n/(1-\Lambda^{-1})$. The operators $c_{\varepsilon\sigma}$ can be expanded in terms of a complete set of new operators $a_{np\sigma}, b_{np\sigma}$ labeled by the interval n and the harmonic index p

$$c_{\varepsilon\sigma} = \sum_{np} [a_{np\sigma} \psi_{np}^+(\varepsilon) + b_{np\sigma} \psi_{np}^-(\varepsilon)]. \quad (83)$$

In terms of these operators, the Kondo Hamiltonian becomes,

$$\begin{aligned}
H_{KM} &= \frac{1}{2}(1 + \Lambda^{-1}) \sum_{np} \Lambda^{-n} (a_{np\sigma}^\dagger a_{np\sigma} - b_{np\sigma}^\dagger b_{np\sigma}) \\
&+ \frac{(1 - \Lambda^{-1})}{2\pi i} \sum_n \sum_{p \neq p'} \Lambda^{-n} (a_{np\sigma}^\dagger a_{np'\sigma} - b_{np\sigma}^\dagger b_{np'\sigma}) e^{\frac{2\pi i(p-p')}{1-\Lambda^{-1}}} \\
&+ J \sum_{\sigma\sigma'} f_{0\sigma}^+ \vec{\sigma}_{\sigma\sigma'} f_{0\sigma'} \cdot \vec{S}
\end{aligned} \tag{84}$$

where in terms of the new operators, $f_{0\sigma} = \frac{1}{\sqrt{2}} \int_{-1}^{+1} d\varepsilon c_{\varepsilon\sigma}$ contains only $p = 0$ states:

$$f_{0\sigma} = \frac{1}{\sqrt{2}} \int_{-1}^{+1} d\varepsilon c_{\varepsilon\sigma} = \left[\frac{1}{2}(1 - \Lambda^{-1}) \right]^{1/2} \sum_{n=0}^{\infty} \Lambda^{-n/2} (a_{n0\sigma} + b_{n0\sigma}) \tag{85}$$

We notice that only the $p = 0$ harmonic appears in the local Wannier state. This is a consequence of the assumption that the Kondo exchange is independent of k . Hence the conduction electron orbitals a_{np}, b_{np} for $p \neq 0$ only couple to the impurity spin indirectly via their coupling to the a_{n0}, b_{n0} in the second term of Eq. (84). This coupling is weak, being proportional to $(1 - \Lambda^{-1})$, and vanishes in the continuum limit $\Lambda \rightarrow 1$, so these states may be expected to contribute little to the impurity properties compared to the $p = 0$ states. This is indeed the case as shown by explicit calculations in [1, 2]. The logarithmic discretization approximation consists of neglecting conduction electron states with $p \neq 0$, resulting in H_c given by Eq. (81) with $c_{+n\sigma} \equiv a_{n,0\sigma}$ and $c_{-n\sigma} \equiv b_{n,0\sigma}$ and a discrete Kondo Hamiltonian given by Eq. (10).

B Lanczos procedure

Neglecting spin indices, the conduction electron operator is

$$H_c = \sum_k \varepsilon_k c_k^\dagger c_k$$

The Lanczos algorithm for tridiagonalizing this operator by repeated action on the normalized conduction electron Wannier state $|0\rangle = \frac{1}{\sqrt{N}} \sum_k c_k^\dagger |vac\rangle$, with $|vac\rangle$ the vacuum state and N the number of sites in the crystal, is

$$|1\rangle = \frac{1}{t_0} [H_c|0\rangle - |0\rangle\langle 0|H_c|0\rangle] \tag{86}$$

$$|n+1\rangle = \frac{1}{t_n} [H_c|n\rangle - |n\rangle\langle n|H_c|n\rangle - |n-1\rangle\langle n-1|H_c|n\rangle] \tag{87}$$

yielding

$$H_c = \sum_{n=0}^{\infty} \epsilon_n f_n^+ f_n + t_n (f_n^+ f_{n+1} + H.c.) \tag{88}$$

where the site energies are given by $\epsilon_n = \langle n|H_c|n\rangle$ and the hoppings t_n are obtained as normalizations from Eqs. (86)-(87).

C Comparison with Real Space RG

Real space RG methods have been used very successfully to investigate second order phase transitions [71]. In these methods, the form of the effective Hamiltonians, H_m , is such that only a small number of couplings (e.g. nearest-neighbour and next-nearest-neighbour couplings in the case of the 2D Ising model) is retained during the RG procedure. Despite this, highly accurate results can be obtained for critical properties. The reason for this is that second order critical points are governed by just a few relevant couplings, so an effective Hamiltonian retaining just these couplings is sufficient to describe the critical behaviour. In contrast, for the Kondo model, and, for quantum impurity models in general, the interest is in obtaining information about the many-body eigenstates and eigenvalues on all energy scales and not just close to a particular fixed point where simplifying assumptions about the effective Hamiltonian might hold. Consequently, a general form of the effective Hamiltonians, including relevant and irrelevant couplings, is required in order to follow the behaviour of the system as it flows via various unstable fixed points to the stable fixed point describing the interacting quantum mechanical groundstate. Such a general form is possible in the Kondo calculation as a result of the numerical representation of the H_m .

D Comparison with DMRG

The DMRG method [22, 23], differs from the NRG approach used in the Kondo calculation in several ways. The most important, and the reason for its success as applied to one-dimensional lattice models, is the criterion for choosing the basis states of the subsystems (the “block”, H_m in the Kondo calculation) used to extend the size of the system (the “superblock”, H_{m+1} in the Kondo calculation). These are chosen according to their weight in a reduced density matrix built from a few eigenstates of the larger system (in the Kondo calculation this reduced density matrix would be $\rho_m^{\text{red}} = \sum_{\alpha_{m+1}} \langle \alpha_{m+1} | \rho_{m+1} | \alpha_{m+1} \rangle$ where $|\alpha_{m+1}\rangle$ are the states of the $m + 1$ 'th site and ρ_{m+1} is the density matrix of H_{m+1}). That is, the states retained in the subsystems (similar to the lowest states retained in \bar{H}_m in the Kondo calculation) are in this case not necessarily the lowest energy states, but they are the states which couple most strongly, in the sense of having large eigenvalues in the reduced density matrix describing the subsystem, to the ones of interest, the target states of the larger system (in the Kondo calculation these might be taken to be the lowest few eigenstates of \bar{H}_{m+1}). The procedure gives highly accurate results for these target states, and therefore improves on real space NRG methods.

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