# Numerical RG and quantum impurity problems

**CMT** Journal Club, given by Phil Derry *May 29th*, *2015* 

Thomas Veness

# References

- Ken Wilson's original NRG for the Kondo Model (lots of interesting background, but quite expansive!): Rev. Mod. Phys. 47, 773 (1975)
- A significantly clearer, detailed "instruction manual" for NRG for the Anderson Impurity Model: Phys. Rev. B **21**, 1003 (1980)
- Ralf Bulla's 2008 NRG review now the standard NRG reference, with good discussion of applications: Rev. Mod. Phys. **80**, 395 (2008)
- NRG formulated in terms of tensor networks/MPS: Phys. Rev. B 86, 245124 (2012)

# 1 Overview

- Introduction and history
- "Wilson's NRG"
- Modern NRG
- Applications

# 2 Quantum impurity problems

What are they and why do they have this name? We generally mean a small quantum mechanical system coupled to a large quantum mechanical system i.e. some small, finite set of states coupled to some continuum system. Traditionally this comes about because we have a physical situation like an iron (magnetic) impurity in gold. We can also find examples of this in atoms adsorbed onto a surface. They are applicable to nano-scale

physics, as well as being at the heart of techniques like DMFT. These models are applicable to these kinds of physical situations.

#### 2.1 Why are they interesting and hard?

In the 1930s, it was noticed that some samples of gold didn't have the resistance profile as a function of temperature that was expected. Instead of going to zero, as would be expected from a simple phonon model, but instead had a minimum. This wasn't understood, but it was shown that the minimum scaled in the impurity density as  $T_{\rm min} \propto c_{\rm imp}^{1/5}$ , so the impurities were definitely important.



Figure 1: Resistance minimum as a function of temperature i.e. the Kondo effect

Kondo modelled this by a Hamiltonian of the form

$$H_{Sd} = \sum_{k} \varepsilon_{k} c_{k,\sigma}^{\dagger} c_{k,\sigma} + J \mathbf{S} \cdot \mathbf{S_0}$$
(1)

This is a very common kind of Hamiltonian for quantum impurity models. Kondo performed perturbation theory to third order in J and found that

$$R = c_{\text{Phonon}}T^5 + R_{\text{imp}} + c_{\text{imp}}(J^2 + \rho J^3 \ln D/T)$$
(2)

This has a minimum that occurs as observed, but we have a resistance that diverges at low T. In the best-case scenario we find that

$$J^2 = \rho J^3 \log D/T \tag{3}$$

i.e.

$$T_K = De^{-1/\rho J} \tag{4}$$

Anderson proposed the idea that can be understood now as perturbative one-loop RG. What he did was to take the conduction band that runs between energies [-D, D]. He then integrated out the energies about the edge of the band on a scale  $\delta D$ . These give rise to one-loop Feynman diagrams. Doing this gives an effective model with a new J and a smaller D. Iterating this gives rise to a scaling equation

$$\frac{\mathrm{d}\rho J}{\mathrm{d}\ln D} = -2(\rho J)^2 \tag{5}$$

And therefore

$$\tilde{D}e^{-1/\rho J} = De^{-1/\rho J} = T_K \tag{6}$$

For a very weakly coupled impurity i.e. a small but non-zero J, the coupling will eventually, at some very low energy, scale to infinity. This is a partial solution that gives us some idea of what's going on, but it's not fantastic as it's perturbative in J, which still eventually blows up.

### 3 Wilson's NRG

The perturbative approach is doomed to fail, as we can't consistently take a small parameter in which to perform the calculation. What we really want is a fully non-perturbative technique that uses RG. The cost is that we have to do it numerically. There are four key steps to this RG procedure

- 1. Logarithmic discretisation
- 2. Mapping to a one-dimensional chain (Wilson chain)
- 3. Iterative diagonalisation procedure
- 4. Successive Hilbert space truncation

In many ways this is a bespoke technique and is set up specifically for quantum impurity problems. This is an essentially exact solution (i.e. can reach arbitrary degree of accuracy). This will give us a complete crossover from a free spin at high temperature to the strongcoupling fixed point. We will consider not the Kondo model, but instead the Anderson impurity model. We have a charge degree of freedom which is coupled by some hopping.

Traditionally, one would calculate with flat bands, but we can handle a band with a generic density of states  $\rho(\omega)$ . The Hamiltonian is given by

$$H = \sum_{k} \varepsilon_{k} c_{k,\sigma}^{\dagger} c_{k,\sigma} + \sum_{\sigma} \varepsilon_{d} d_{\sigma}^{\dagger} d_{\sigma} + U n_{\uparrow} n_{\downarrow} + \sum_{\sigma,k} V_{k} d_{\sigma}^{\dagger} c_{k,\sigma} + \text{h.c.}$$
(7)

The effect of the bath on the impurity is all contained in the function

$$\Delta(\omega) := \pi \sum_{k} V_k \delta(\omega - \varepsilon_k) \tag{8}$$

Which is essentially the imaginary part of the local density of states i.e.

$$\Delta(\omega) = -V^2 \text{Im}G_{\text{loc}}(\omega) = V^2 \rho(\omega)$$
(9)

The form of  $\rho(\omega)$  can have a profound effect on what happens. In a flat band, we find a normal Anderson model, but we can get very different physics in general. We consider here the flat band i.e. a constant density of states at the Fermi level.



Figure 2: Flat density of states

					+	-	_		+	<i>,</i>
-	$1 - \Lambda$	$-1 - \Lambda$	-2		Λ	-2	$\Lambda^{-}$	- 1	1	

Figure 3: Logarithmic discretisation

#### 3.1 Logarithmic discretisation

This is the key step and therefore requires some motivation. We want to look at exponentially small excitations which effect the physics. If we wrote down a physical model, it would have to be exponentially long. We therefore discretise logarithmically so that we can reach exponentially small excitations in a linear chain length. If, for simplicity, we scale everything by the bandwidth D s.t. we work in a band running from [-1, 1], we partition this by some parameter  $\lambda$  into logarithmic intervals, we can then assign a pole at each  $\Lambda^{-n}$ such that

$$\int \mathrm{d}\omega\rho(\omega) = \gamma_n^{\pm 2} \tag{10}$$

$$\frac{\int \mathrm{d}\omega\rho(\omega)\omega}{\int \mathrm{d}\omega\rho(\omega)} = \xi_n^{\pm} \tag{11}$$

We can now sample exponentially finely around the Fermi point. We can now write



Figure 4: Logarithmic discretisation example weights



Figure 5: One-dimensional chain

$$H = H_{\rm imp} + \sum_{n,\sigma} \xi_n^+ a_{n,\sigma}^\dagger a_{n,\sigma} + \xi_n^- b_{n\sigma}^\dagger b_{n,\sigma} + V \sum_{n,\sigma} d_\sigma^\dagger \left( \sqrt{\frac{\gamma_n^+}{\pi}} a_{n,\sigma} + \sqrt{\frac{\gamma_n^-}{\pi}} b_{n,\sigma} \right) + \text{h.c.} \quad (12)$$

We can consider these as Fourier modes. We have thrown away some states, but we have discarded them in a controlled fashion. We have discarded the states which couple indirectly, but as we take  $\Lambda \to 1$  we recover the model exactly again. We now have an infinite but discretised version on the model.

#### 3.2 Mapping to a one-dimensional chain

This is a Lanczos-type algorithm: we start with a seed orbital. This gives us an infinite chain with the impurity at one end. For the flat-band case, we can show that

$$t_n \stackrel{n \gg 1}{\longrightarrow} \frac{1}{2} (1 + \Lambda^{-1}) \Lambda^{-n/2} \tag{13}$$

We can now really see the RG structure. If we added an extra orbital, then each successive orbital tells us about finer energy scales in the problem. These orbitals can be thought of physically as being energy shells around the impurity, but this is not necessarily the best way to think about it.

We now have a one-dimensional chain with nice properties. We still have an infinite chain, and we wish to do numerics. So, where does this leave us?

#### 3.3 Iterative diagonalisation

The crux of the calculation is that these couplings fall off exponentially fast. We can therefore think about diagonalising some finite chain and then adding more onto it, diagonalising at every step. We can now define the whole Hamiltonian as

$$H = \lim_{N \to \infty} \left[ \Lambda^{-(N-1)/2} H_N \right] \tag{14}$$

$$H_n = \Lambda^{(n-1)/2} \left[ H_{\rm imp} + V \sum_{\sigma} \left( d^{\dagger}_{\sigma} f_{0,\sigma} + \text{h.c.} \right) + \sum_{\sigma,m=0}^n \varepsilon_m f^{\dagger}_{n,\sigma} f_{m,\sigma} + \sum_{\sigma,m=0}^n t_m f^{\dagger}_{m,\sigma} f_{m,\sigma} + \text{h.c.} \right]$$
(15)

We can now define a transformation between the two

$$R(H_N) = H_{N+1} \tag{16}$$

Going to a larger Hilbert space and looking at lower energy scales means that R can be understood as some sort of RG step. We will end up looking at the flow of the energy levels as we iterate. This gives us a way to step between chain sizes. We still have the problem of diagonalising longer and longer chains.

#### 3.4 Successive Hilbert space truncation

In DMRG we have to work hard to decide what states to throw away. Here, the story is very different, as we know we can throw away the high energy states. This is because if we have a high-energy state, we know that adding on more states only changes the energy levels on a smaller scale, so the high energy states will *never* change the low-energy physics. We take our energy levels, rescale them by  $\Lambda^{1/2}$ , couple the new states of the chain and then truncate the high-energy states. We therefore expect to see comparable energy scales between steps and observe the flow of the energy levels.

This is difficult to understand physically. It would be easier if we could calculate thermodynamic quantities to have a grip on this. If we consider a Wilson chain of length N, there is a temperature at which all states we keep are full anyway and everything we throw away is always empty. There is therefore a temperature at which the chain is very well described by the model. Note that the energy levels are many-particle energy levels and are therefore *not* local quantities.

$$T_N = \frac{\Lambda^{-(N-1)/2}}{\bar{\beta}} \tag{17}$$

We normally calculate impurity contributions i.e. the differences of quantities between those of the free model and that with the impurity.

We then find that the impurity has a certain behaviour as a function of temperature. Plotting as a function of this temperature, we can find the full crossover as a function of temperature.

## 4 Applications

The original formulation of the NRG and of DMRG look very different. It is only fairly recently that all of the concepts have been linked and this is under the conceptual framework of MPS. Every time we couple another orbital, we are performing a matrix product. In order to calculate dynamical quantities, we want to reconceptualise DMRG. Instead of starting with a chain of length 1 and build up, we actually start with a chain of length N and turn on *couplings* successively. We then have that the states of each iteration are given by



Figure 6: Overall procedure



Figure 7: Anderson impurity model results

$$|se\rangle_n = |s\rangle_n \otimes |e\rangle_n \tag{18}$$

Each action of the NRG procedure plucks a state from the environment and couples it to the system. This is just a matrix product, the matrices are those which diagonalise each set of state successively. The bond order in the DMRG language is the number of states we keep at each iteration.

If we consider all of the discarded states that were thrown away, if we were to keep all of them we would have a complete basis. We can then write down a density matrix and then calculate, for example, impurity Greens functions

$$G_{\rm imp} = \langle \langle d_{\sigma}, d_{\sigma}^{\dagger} \rangle \rangle_{\omega} \tag{19}$$

and indeed calculate essentially anything we want. In addition, the link to DMRG gives us a way to sense check the NRG procedure, as we can see how much weight we are throwing away at each state.

## 5 Closing remarks

*DMFT*: Map a lattice (correlated) onto a single impurity with a dynamic band which changes and self-consistently work out structure of conduction band. This is a local self-energy for each site instead of have non-local correlations.

*Multiple-impurity*: can get critical physics with two-channel Kondo or quantum dots *Spin-boson models* can be examined via these techniques.

Despite being originally reasonably niche, there are many more applications being developed.