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Towards verified numerical renormalization group calculations

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Abstract. Numerical approaches are an important tool to study strongly correlated quantum systems. However, their fragility with respect to rounding errors is not well studied and numerically verified enclosures of the results are not available. In this work, we apply interval arithmetic to the well established numerical renormalization group scheme. This extension enables us to provide a numerically verified NRG excitation spectrum.

1 Introduction

Wilson's numerical renormalization group scheme [1–5] is one of the most important numerical schemes in the field of strongly correlated quantum systems allowing to track the full crossover from weak to strong coupling within the Kondo problem.

The Kondo model and the associated Kondo resonance can be seen as the prime examples for correlated quantum systems. The Kondo problem itself can be traced back to the experiments by de Haas and van den Berg [6] in the early 1930s which displayed an increase in resistivity of noble metals like gold or silver. It took 30 years until Kondo [7,8] could relate the increase of resistivity to dynamical scattering at magnetic impurities. But it was only more than 30 years later that Wilson could provide a rigorous solution of the Kondo model based on his numerical renormalization group (NRG) technique. A few years later Andrei [9] and Vigman [10] could verify the numerical solution of Wilson by a Bethe ansatz solution. Besides its importance in describing magnetic impurities in metals it is also important in understanding the transport properties of quantum dots [11] and often appears as effective model in understanding correlated quantum systems, e.g. the dynamical mean field theory [12,13]. For an overview see [4].

Besides being used for decades it was realized only recently [14], that numerical rounding errors lead to the appearance of a new fixed point within the NRG. Most strikingly this fixed point obeys a scaling law with respect to the precision of the underlying arithmetic and behaves like a typical physical fixed point. In this work, we investigate, whether one can use interval arithmetic to signal the breakdown of the numerics and to provide a scaling regime where the correctness of the numerical result can be guarantied.

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2 Interval arithmetic

Interval arithmetic was already introduced by Ramon Moore [15] in the 1960s as an approach to bound rounding errors in mathematical computations. Within interval arithmetic [15–18] one represents a number not by a single discretized floating point value. Instead it is represented by two floating point values, a lower and an upper bound presenting an enclosure of the the desired values x,

$$x \in [\underline{x}, \overline{x}] \quad \underline{x} \leq \overline{x}. \tag{1}$$

In addition all operations $\star$ and functions $f(x)$ are extended on intervals in such a way

$$[\underline{z}, \overline{z}] = [\underline{x}, \overline{x}] \star \left[\underline{y}, \overline{y}\right] \ : \ \forall x \in [\underline{x}, \overline{x}] \wedge y \in \left[\underline{y}, \overline{y}\right] \ x \star y \in [\underline{z}, \overline{z}] \tag{2}$$

$$[\underline{z}, \overline{z}] = f\left([\underline{x}, \overline{x}]\right) \ : \ \forall x \in [\underline{x}, \overline{x}] \ f(x) \in [\underline{z}, \overline{z}] \tag{3}$$

that the function values of $f(x)$ are contained in the result for all $x \in [\underline{x}, \overline{x}]$, and similarly for all operations $\star$. For example the addition of two intervals is now given by

$$[\underline{x}, \overline{x}] + \left[\underline{y}, \overline{y}\right] = \left[\underline{\underline{x} + \underline{y}}, \overline{\overline{x} + \overline{y}}\right] \tag{4}$$

where $\underline{\underline{x} + \underline{y}}$ is the sum $\underline{x} + \underline{y}$ rounded downwards on the level of the numerical precision, while $\overline{\overline{x} + \overline{y}}$ is the sum $\overline{x} + \overline{y}$ rounded upwards. Provided all operations are implemented with the necessary rounding modes interval arithmetic allows for an enclosure of the actual result. However, in general it is not possible to obtain the smallest possible enclosure of equations (2) and (3). In general one should expect that interval arithmetic overestimates the actual numerical error in cases where one simply replaces the floating point values by interval arithmetic in a given code. A prime example is given by the square function evaluated on an interval containing zero, e.g. $[-1, 1]$

$$\left([-1, 1]\right)^2 = [0, 1] \tag{5}$$

$$[-1, 1] \cdot [-1, 1] = [-1, 1]\,. \tag{6}$$

Since the square function maps a real value on a non-negative number we obtain equation (5) from the definition equation (3). In contrast, according to equation (2) the evaluation of the product equation (6) has to include the negative part. One should note, that the result of equation (6) encloses the result of equation (5). In the following, we investigate the results of NRG simulations by simply replacing the floating point values in [14] by an interval arithmetic.

3 Kondo model

Here, we follow precisely [14] in the description as well as the code used. Note that the description in [14] is based on Sections `VII` and `VIII` of [1].

The Kondo model describes a local impurity coupled to a conduction band, where the conduction band is transformed into spherical harmonics around the impurity and only the s-wave contributions are kept. The remaining model of a spin impurity

coupled to a half infinite chain is then discretized on a logarithmic scale. The system is then tridiagonalized leading to the following form:

$$\mathcal{H}_M = J\vec{\hat{S}}\vec{\hat{s}}_1 + \sum_{n=2}^{M} t_{n-1} \sum_{\sigma} \hat{c}^{\dagger}_{n,\sigma}\hat{c}_{n-1,\sigma} + \text{h.c.} \tag{7}$$

Here, we follow the usual convention of $\vec{\hat{S}}$ being the $SU(2)$ spin operator of the impurity, $\vec{\hat{s}}_1$ is the spin operator of the first conduction band site, $\hat{c}_{n,\sigma}$ ($\hat{c}^{\dagger}_{n,\sigma}$) is the annihilation (creation) operator for a conduction band fermion with spin σ in energy shell n. J denotes the Heisenberg exchange coupling and

$$t_n = t\Lambda^{(n-1)/2} \tag{8}$$

is taken in its most simplistic form ignoring any corrections stemming from the original band structure as we are interested in the low energy physics only. For a justification for this Hamiltonian we refer to excellent articles by Wilson [1,2]. However, for this work it is sufficient to know that $\mathcal{H}$ (7) describes a single spin coupled to a 1D like tight binding chain where the nth site represents the physics at energy scale $t\,\Lambda^{-(n-1)/2}$. In the following we have set $t = 1$.

The most prominent property of the Kondo model is the flow from a weak coupling regime represented by a spin impurity coupled weakly to the conduction band consisting of M sites, to a strong coupling regime, where the spin impurity forms a singlet with the conduction band fermions leading to a singlet weakly coupled to an effective conduction band consisting of $M - 1$ sites. For a discussion of the parity effect with respect to M we refer to [14].

In order to obtain this flow the NRG starts with a system consisting of the impurity spin and the first conduction band site, that is with Hamiltonian (7) setting $M = 1$. One then iteratively increases the number of conduction band sites by one. Since the associated Hilbert space will increase by a factor of four in each step one has to introduce a truncation scheme. Within the NRG scheme one truncates the Hilbert space after each diagonalization to the m eigen states lowest in energy. In addition one performs a shift of the eigen values such that the lowest eigen value is zero, $E_0 = 0$.

Since the low energy scale of the Hamiltonian (7) decreases by $\Lambda^{-1/2}$ in each iteration step one rescales the Hamiltonian in order to keep the excitation energies of order one

$$\widetilde{\mathcal{H}}_M = \Lambda^{M/2}\mathcal{H}_M. \tag{9}$$

In this form one can now investigate the flow of the spectrum. Of course, in order to get the corresponding physical scale one has to undo the scaling. The striking feature of the Kondo model is the appearances of a scale T_{K}

$$T_{\text{K}} = D\sqrt{J/D}\,\mathrm{e}^{-D/J} \tag{10}$$

with $D = 4t$ the band width of the Hamiltonian (7) and t the band hopping element equation (8).

As an example we provide in Figure 1 the RG flow for a Kondo system with a spin coupling of $J = 0.6$. There we show the flow of the five lowest excitation energies vs. the energy scale $t_M = \Lambda^{-(M-1)/2}$ in units of T_{K}. In this computation the particle number and the S^z component of the total spin were explicitly conserved by working with a block matrix representation of the Hamiltonian and we truncated the

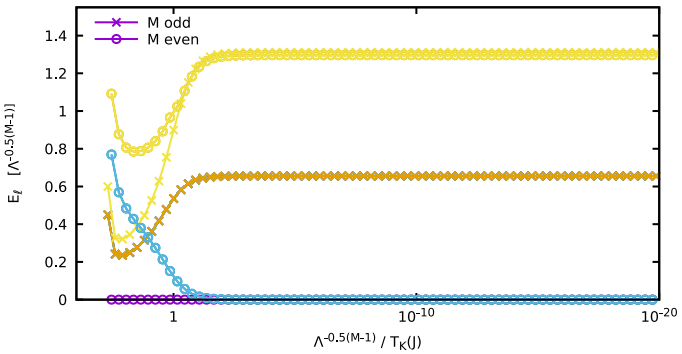

Fig. 1. The RG flow of the low energy spectrum for a Kondo model with $J = 0.6$, $\Lambda = 2.0$, and $m = 2000$, where the N and S^z conservation is explicitly enforced. The results are split into odd conduction band sites ($\circ$) and even conduction band sites ($\times$).

Hilbert space to at most $m = 2000$ states. One clearly observes the crossover regime at T_K and the flow towards the strong coupling regime at low energies. For a detailed description we refer to [1,2,14]. We would like to remark that m refers to taking the mth eigenvalues as a cutoff reference and the number of states kept is increased in the case we hit a degeneracy of the spectrum. In this way, we avoid a trivial breaking of the symmetries [19,20]. Here, we assumed that energy differences below 10^{-11} signal a degenerate energy subspace.

4 NRG with interval arithmetics

In order to track rounding issues we performed the following change to our code. We replaced the data type from `double` to `interval<double>` which is straightforward everywhere with the exception of the diagonalization of the Hamiltonian matrix. Here we took the simple approach of extracting a median matrix

$$\mathrm{median}\left([\underline{x}, \overline{x}]\right) = \left(\underline{x} + \overline{x}\right)/2 \tag{11}$$

$$h_{x,y} = \mathrm{median}(H_{x,y})\,. \tag{12}$$

We then diagonalize matrix h in a standard way, as its elements are of type `double`. We then take the resulting transformation matrix U as the transformation matrix and obtain the new energy eigenvalues as the diagonal elements obtained by a base transformation of H via U:

$$E = \mathrm{diag}\left(U^+ \cdot H \cdot U\right). \tag{13}$$

We would like to point out that these changes are rather simple and should be applicable to any NRG implementation.

In result, we now obtain an interval for each energy value where the width of the interval

$$\mathrm{width}\left([\underline{x}, \overline{x}]\right) = \overline{x} - \underline{x} \tag{14}$$

provides an error bar for the calculation.

In Figure 2, we provide the results for an interval version of the results presented in Figure 1. Figure 3 corresponds to the same system with $\Lambda = 3.0$ and $m = 500$. The

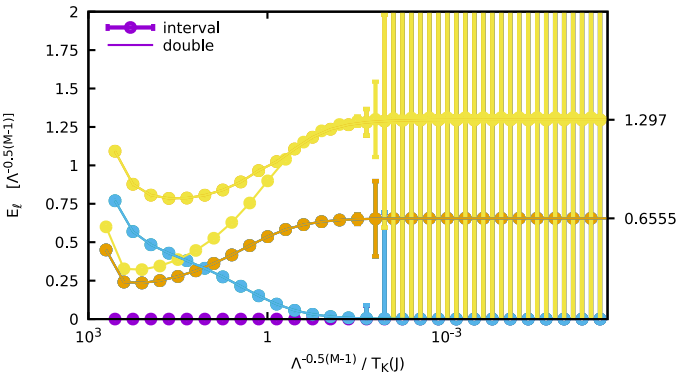

Fig. 2. The RG flow of the low energy spectrum for a Kondo model with $J = 0.6$, $\Lambda = 2.0$ and $m = 2000$, where the N and S^z conservation is explicitly enforced. The lines correspond to the results to a standard NRG using `double` arithmetics as presented in Figure 1. The ∘ correspond to the median of the obtained excitation energies. The error bars correspond to the width of the excitation energy intervals. In the left part of the figures, the error is smaller then the symbol size. The energy values provided on athe left y-axis are taken from Wilson's original work [1] for the lowest eigen values in the large M limit in the case of $\Lambda = 2$.

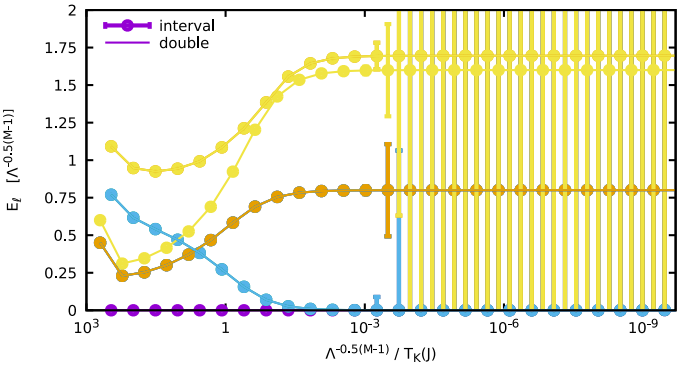

Fig. 3. The RG flow of the low energy spectrum for a Kondo with $J = 0.6$, $\Lambda = 3.0$ and $m = 500$, where the N and S^z conservation is explicitly enforced. The lines correspond to the results to a standard NRG using `double` arithmetics. The ∘ correspond to the median of the obtained excitation energies. The error bars correspond to the width of the excitation energy intervals.

first observation from these results is that one can actually perform an interval version of the NRG scheme and the median of the energy eigenvalue intervals corresponds to those of an NRG with standard `double` arithmetics during the complete crossover to the strong coupling regime and verified that this crossover is not due to rounding errors. As a benchmark for our implementation we added the energy values for the lowest excitation in the large M limit on the left y-axis in Figure 2 as provided in [1].

In Figure 4, we provide the width of the energy eigenvalue intervals corresponding to the results in Figure 3. Here, we witness a power law increase of the width of the energy eigenvalue intervals with respect to the low energy scale. Once the width of the energy intervals gets larger than the actual level splitting the interval arithmetic signals the end of a numerically verified spectrum of the NRG scheme. We would

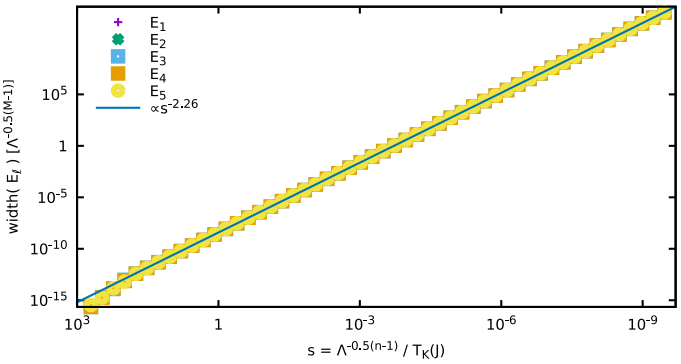

Fig. 4. The width of the energy eigenvalue intervals RG corresponding to the results of Figure 3. The line is a power law fit resulting in an exponent of $\alpha \approx -2.26$.

like to point out that this does not imply that a corresponding NRG calculation within `double` arithmetic breaks down. As pointed out in the introduction the interval scheme employed here will overestimate the corresponding numerical error and tighter bounds should be possible.

5 Summary and outlook

In this work, we extended Wilson's NRG scheme to interval arithmetics which allows us to provide a numerical guarantee on the obtained NRG spectrum, provided the width of the energy eigenvalue intervals do not signal a break down. We presented results keeping $m = 2000$ states after each NRG step. This is sufficiently large enough to demonstrate, that one is not restricted to toy calculations. The approach presented provides a measure to assure that the result is not dominated by the finite precision arithmetic as the parity breaking fixed point in [14].

The numerics presented here proofs numerically that the Kondo scale is not an artefact of the numerics. While this is not questioned within the Kondo model, the technique presented here could be useful in situations where the physics is not well understood.

One of the main advantages of the NRG scheme is its clear foundation and the stability of the NRG procedure and the stability and problems have been analyzed [1–5,20]. The numerics presented in this work can be seen as a worst case scenario where rounding of intermediated results is performed in a way to obtain the largest possible deviation due to rounding errors. The results should therefore be seen as a warning that even in the case of such a well defined and stable scheme as the NRG results can be spoiled by the underlying arithmetic and one should always accompany numerics with benchmark results.

Within the scheme employed here we observe a power law increase of the width of the energy eigenvalue intervals with respect to the inverse RG scale which currently limits the applicability of the verified NRG scheme to not too small energy scales. We therefore had to choose a rather large Kondo coupling, $J = 0.6$. For significantly smaller couplings the error would blow up before the strong coupling regime is reached.

It remains an open question whether this could be significantly improved by the application of an interval version of the diagonalization tailored to obtain smaller bounds on the eigen values and therefore leading to a verified NRG scheme applicable in the whole parameter regime. Alternatively one could apply a multi-precision

interval library in a similar way as in [14] to extend the range of applicability of the approach presented in this work.

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Author contribution statement

All authors contributed equally to the manuscript and the acquisition of the results.

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