Numerical Renormalization Group Analysis of Interacting Quantum Dots

Walter Hofstetter
Theoretische Physik III, Elektronische Korrelationen und Magnetismus,
Universität Augsburg, 86135 Augsburg

Abstract. Wilson's Numerical Renormalization Group (NRG) is so far the only
nonperturbative technique that can reliably access low–energy properties of quan-
tum impurity systems. We present a recent extension of the method, the DM–NRG,
which yields highly accurate results for dynamical quantities at arbitrary frequen-
cies and temperatures. As an application, we determine the spectrum of a quantum
dot in an external magnetic field. Furthermore, we discuss magnetic impurities
with orbital degeneracy, which have been inferred in recent experiments on quantum
dots in an Aharonov-Bohm geometry. It is demonstrated that for spinless
electrons, interference between neighbouring levels sets the low–energy scale of the
system. Switching on an external field leads to a remarkable crossover into a regime
dominated by orbital Kondo screening. We predict that the broadening–induced
level splitting should be clearly visible in measurements of the optical absorption
power. A more general model including the electron spin is studied within an ex-
tended two-band NRG procedure. We observe competition between interference
and Kondo screening, similar to the situation in two-impurity models (RKKY).

1 Introduction

Quantum impurity models and their low-temperature properties are of cen-
tral importance in condensed matter physics. They show characteristic many-
body effects like the screening of a local moment by conduction electrons (the
Kondo effect) which was first observed in measurements on dilute magnetic
impurities in metals (see [1]). More recently, artificial nanostructures (quan-
tum dots [2] or surface atoms probed by STM [3]) with tunable parameters
provided new representations of the Anderson or Kondo model [4].
In theory, a very fruitful line of research was opened by the development of
dynamical mean-field theory (DMFT) [5] where correlated lattice systems
are mapped onto effective impurity models which are then accessible in a
controlled way [6].

In this article, we focus on semiconductor nanostructures, where – at the
moment – experiments with the highest level of control can be performed.
Electronic transport through ultra-small quantum dots, where the charging
energy is the largest energy scale, has been studied extensively over the last
few years [7]. Due to the quantization of charge the transport is dominated
by Coulomb blockade. More recently, experiments revealed that the Kondo
effect leads to an enhancement of the conductance – the zero bias anomaly – in the Coulomb blockade regime as predicted some time ago.

Theoretical modelling of these systems is usually based on the Kondo or Anderson Hamiltonians describing a localized spin (orbital) which is coupled to one or several conduction electron reservoirs. In the regime of interest, this coupling is the usually the smallest energy scale. It was realized very early that a treatment of these models based on perturbation theory fails due to logarithmic divergences below a characteristic temperature scale, the Kondo temperature $T_K$.

Solution of the Kondo problem at $T \ll T_K$ thus required a non-perturbative technique, which was provided by Wilson’s pathbreaking Numerical Renormalization Group (NRG). It proved to be very successful in clarifying the low-energy properties of various impurity problems, and it will be the method of choice for analyzing more complex quantum dot systems.

In this article we give a short introduction to the NRG technique, including in particular a recently developed density-matrix formalism (the DM-NRG) necessary for a reliable calculation of dynamical quantities. Using the new algorithm, impurity spectra are calculated for a quantum dot in an external magnetic field. Finally, we discuss the subtle interplay between interference and interaction which arises in a quantum dot with orbital degeneracy.

2 Generalized Numerical Renormalization Group

In the following, we consider the Anderson Hamiltonian

$$H_{\text{and}} = \sum_{\mathbf{k} \sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k} \sigma}^\dagger c_{\mathbf{k} \sigma} + \sum_{\mathbf{k}\sigma} V_{\mathbf{k}} \left( f_{\sigma}^\dagger c_{\mathbf{k} \sigma} + h.c. \right) + U n_f^+ n_f + \epsilon_f n_f - h S_f^z (1)$$

where the hybridization $\Gamma(\omega) = 2\pi \sum_k |V_k|^2 \delta(\omega - \epsilon_k)$ between the f impurity and the reservoir electrons $c_{\mathbf{k}\sigma}$ is balanced by a local Coulomb repulsion $U$ which suppresses double occupancy of the impurity. In addition, a local magnetic field $h$ is coupled to the impurity spin $S_f$. Units are chosen as $\hbar = k_B = \mu_B = g = 1$ and the half bandwidth is given by $D = 1$.

The key idea introduced by Wilson is the logarithmic discretization of the conduction band shown in Fig. 1, where each energy scale is represented by a single fermionic degree of freedom. After performing a Lanczos transformation (for details see [13,14,15]) the conduction band can be written as a linear chain shown in Fig. 2

$$H_{\text{and}} = \sum_{n=0}^{\infty} \epsilon_n \left( d_{n\sigma}^\dagger d_{(n+1)\sigma} + h.c. \right)$$

(2)

with hopping coefficients decaying exponentially as $\epsilon_n \sim \Lambda^{-n/2}$. In this representation, the impurity is only coupled to the maximally localized reservoir.
state \( d_0 = (1/\sqrt{N}) \sum_k c_k \). The transformed model – while still a nontriv-

\[ \begin{array}{c}
-\Lambda^{-1} & -\Lambda^{-2} & \cdots & \Lambda^{-2} & \Lambda^{-1} \\
-1 & 0 & 1 & \varepsilon/D
\end{array} \]

Fig. 1. Logarithmic discretization of the conduction band.

\[ \begin{array}{c}
-\Delta/2 & 0 & -1/2
\end{array} \]

Fig. 2. Linear chain representation of the Anderson impurity Hamiltonian.

\[ U,h \]

Fig. 3. Iterative diagonalization of the impurity problem.

In the iterative diagonalization scheme, the number of iterations corresponds to the temperature one is interested in according to \( T_N = c \Lambda^{-(N-1)/2} \),
where $c$ is a constant of order one. For calculating static thermodynamic expectation values, all necessary information is thus obtained because only excitations on the scale $T_N$ are relevant. As an example, consider the impurity magnetization

$$< S^z_f > = Z^{-1} \sum_m e^{-\beta E_m} < m | S^z_f | m >_N$$

where the $|n>$ are the many-particle eigenstates of $H$ and $Z$ is the partition function. Due to the Boltzmann factor, higher excitations – already lost in iteration $N$ – can be safely neglected at this point.

The situation changes completely when we consider a dynamical quantity like the spin–resolved spectral density

$$A_{\sigma}(\omega) = \sum_{nm} | < m | f_{\sigma}^\dagger | n >|^2 \delta (\omega - E_m + E_n) \frac{e^{-\beta E_m} + e^{-\beta E_n}}{Z}.$$  

Obviously, spectral information at frequencies $\omega \gg T_N$ requires matrix elements between low-lying states and excitations which in iteration $N$ are not available anymore (they have already been lost by truncation). In order to deal with this situation, the following two-stage procedure has to be employed:

1. NRG iterations are performed down to the temperature $T_N$ of interest, in particular we choose $T_N \ll T_K$ to calculate ground-state properties. In each iteration step, we keep the information on the transformation between one set of eigenstates and the next, i.e. we save the corresponding unitary matrix. After obtaining the relevant excitations at temperature $T_N$ one can define the density matrix

$$\hat{\rho} = Z^{-1} \sum_m e^{-E_m^N/T_N} |m >_N < m|$$

which completely describes the physical state of the system. The equilibrium Green’s function can be written as

$$G_\uparrow(t) = i \theta(t) \text{Tr} \left( \hat{\rho} \left\{ f_\uparrow(t), f_\uparrow^\dagger(0) \right\} \right)$$

2. Now we repeat the iterative diagonalization for the same parameters. Each iteration step $N'$ yields the single-particle excitations (and matrix elements of $f^\dagger$) relevant at a frequency $\omega \sim T_{N'}$. But instead of using (3), we now employ (5) and evaluate the spectral function with respect to the correct reduced density matrix (2): As depicted in Fig. 4, the complete chain is split into a smaller cluster of length $N'$ and an environment containing the remaining degrees of freedom. In the product basis of these two subsystems, the full density matrix has the form

$$\hat{\rho} = \sum_{m_1 m_2, n_1 n_2} \rho_{m_1 n_1, m_2 n_2} |m_1 >_{\text{env}} |n_1 >_{\text{sys}} < n_2 | < m_2|$$
which is in general not diagonal anymore. Performing a partial trace on the
environment then yields the density submatrix

$$\rho_{\text{red}}^{n_1 n_2} = \sum_{n_1 > n_2} \rho_{n_1 n_2}^{\text{sys}}, \quad \rho_{n_1 n_2}^{\text{red}} = \sum_m \rho_{mn m n_2}$$

(8)

This projection is easily done using the previously stored unitary transforma-
tion matrices. Note that $\rho_{\text{red}}$ – defined only on the shorter chain – contains
all the relevant information about the quantum mechanical state of the full
system.

The single–particle spectrum calculated in this way is shown in Fig. 4.

With increasing magnetic field, the Kondo resonance is suppressed and event-
ually merges with the lower atomic level. Regarding the total density of
states (DOS) $A(\omega) = \sum_\sigma A_\sigma(\omega)$, the Kondo peak is split by the field and
the DOS at the Fermi level strongly reduced. This effect has been observed
directly in measurements of the differential conductance through a quantum
dot [3].

**Fig. 5.** Spin–dependent (left) and total (right) impurity spectral density at zero
temperature for $\Gamma = 0.02$, $U = 5\Gamma$, and $\epsilon_f = -2.5\Gamma$. The Kondo temperature is
$T_K = 6.8 \times 10^{-4}$. 
3 Interference and Interaction in Multi–Level Dots

After the discussion of the spin–degenerate Anderson impurity model \[1\] in the last section, we now consider the effect of orbital degeneracy. We will first study a dot consisting of two levels without spin or, equivalently, two dots in an Aharonov-Bohm (AB) geometry with one level per dot in the presence of an interdot Coulomb repulsion \(U\). Such a system is of fundamental interest since the two possible paths through the dot (via level 1 or 2) can interfere with each other. The interference can be controlled by an AB flux and has attracted much interest due to the possibility of realizing AB interferometers \[22\] or using the coherent properties in connection with quantum computing \[23\]. Furthermore, there is enhanced experimental interest to study quantum dots in the strong tunneling regime where the level broadening is of the order of the level spacing. In this case, transport is inevitably controlled by multi-level physics.

Let us first discuss the case of spinless electrons, assuming e.g. a large Zeeman splitting \[24\]. The Hamiltonian is then written as

\[
H = \sum_{kr} \varepsilon_{kr} a_{kr}^\dagger a_{kr} + \sum_{rkj} (V_{rj} a_{kr}^\dagger c_j + \text{h.c.}) + \sum_j \varepsilon_j c_j^\dagger c_j + Un_1 n_2
\]

where \(j = 1, 2\) labels the two levels and the dot is connected to two reservoirs \(r = L, R\) via tunnel barriers. Note that the index labelling the dots is not present in the reservoirs – this model contains no conserved quantum number corresponding to spin, unlike previous studies \[25,26,27,28\]. The tunnel matrix elements are assumed to be real except for an AB-phase, i.e. we attach a phase factor \(e^{i\phi}\) to \(V_{2L}\). The level broadening is defined by \(\Gamma_j = 2\pi|V_{rj}|^2 \rho_0\), where \(\rho_0\) is the density of states in the leads, which we assume to be constant in the energy range of interest. The total broadening of each level is therefore given by \(\Gamma = \Gamma_j^L + \Gamma_j^R\).

Since both levels overlap with the reservoirs, they have an effective overlap matrix element \(\Delta\), which induces a level splitting \(\delta \tilde{\varepsilon} = \sqrt{\delta \varepsilon^2 + |\Delta|^2}\) where

![Fig. 6. Two quantum dots in an Aharonov–Bohm geometry.](image-url)
\( \delta \epsilon = \epsilon_2 - \epsilon_1 \) denotes the bare level spacing. Within second-order perturbation theory it is established that \( \Delta \) vanishes for the noninteracting dot, while

\[
\Delta \sim \frac{\sqrt{\Gamma_1 \Gamma_2}}{\pi} + \sqrt{\frac{\Gamma_1 \Gamma_2}{\Delta \epsilon}} \ln \left( \frac{U}{\omega_c} \right)
\]

(10)
in the case of strong on-site repulsion \( U \gg |\epsilon|, \Gamma \). For positive level energies, the tunnel splitting can be observed directly as a shift of the upper level position (see Fig. 7) in the total spectral density

\[
A(\omega) = -\frac{1}{\pi} \sum_{i,j=1,2} \text{Im} G_{ij}(\omega^+).
\]

(11)
For low lying levels \( \epsilon < -\Gamma \) and a large Coulomb repulsion, the dot is singly occupied at low temperatures. In this case, the effective level splitting shows up in a many-body resonance (“shoulder”) in the spectral density at a positive frequency \( \omega \sim \delta \epsilon \), see Fig. 7. This new many-body energy scale can be seen most clearly in a microwave absorption experiment, where transitions between the two dot levels are induced due to the dipole operator \( \hat{O} = c_1^\dagger c_2 + c_2^\dagger c_1 \). The corresponding spectral density

\[
\rho_{\text{abs}}(\omega) = Z^{-1} \sum_{mn} \langle n | \hat{O} | m \rangle^2 \delta (\omega + E_n - E_m) \left( e^{-\beta E_n} - e^{-\beta E_m} \right)
\]

(12)
displays a well-pronounced resonance at the frequency \( \delta \epsilon \) (see Fig. 7).

For \( \phi = \pi \) and \( \Gamma_j^R = \Gamma_j^L \), the tunnel splitting is zero, and the system is shown to be equivalent to an Anderson model with Zeeman splitting \( \delta \epsilon \). This can be seen most easily by introducing the new levels

\[c_{\text{even(odd)}} = (1/\sqrt{2}) (c_1 \pm c_2)\]

(13)
which are then coupled to the right and left reservoirs, respectively. In this way, an orbital Kondo effect can be realized in a quantum dot even in the absence of an a priori conserved quantum number like spin. The crossover between the interference– and Kondo–dominated regimes upon increase of the AB–phase $\phi$ is most clearly seen in the single particle spectrum (Fig. 8) where the Kondo resonance gradually develops as $\phi \to \pi$. Experimentally, the absorption power may be more easily accessible: With increasing $\phi$, the absorption maximum is shifted from $\delta \tilde{\epsilon}$ to $\min(T_K, \delta \epsilon)$, while at the same time the absorption intensity strongly increases (see Fig. 8).

![Graph showing the effect of the AB-phase on the single-particle spectrum.](image)

**Fig. 8.** Left: Effect of the AB–phase $\phi$ on the single–particle spectrum. The total spectral density is shown for $\epsilon_1 = -1.6 \Gamma$, $\delta \epsilon = 0$, $U = 8.1 \Gamma$, and $T = 0$. Insets: Partial spectral densities for levels $c_1$ (left) and $c_2$ (right). Same parameters as above, but with a finite level splitting $\delta \epsilon = 0.08 \Gamma$. Right: Absorption power for $U = 33 \Gamma$, $\epsilon_1 = -3.3 \Gamma$, $\delta \epsilon = 0.16 \Gamma$, $T = 0$ and different values of $\phi$.

So far, we have assumed that both levels are equally broadened by the reservoir, i.e. $\Gamma_1 = \Gamma_2$. In experiments, this need not be the case, although tuning within $\delta \Gamma = 20\%$ seems feasible. In order to clarify whether the orbital Kondo effect discussed previously is still visible under these conditions, we have therefore determined the influence of an asymmetric broadening on the single particle spectrum (Fig. 9). In the Kondo regime $\phi \approx \pi$ our model then corresponds to an effective Anderson Hamiltonian with spin–dependent hybridization, which is interesting in itself and has not been studied before. For the parameters used, we find a robust Kondo peak, which is split, but remains clearly visible even at an asymmetry of $\delta \Gamma = 100\%$. We therefore conclude that the orbital Kondo effect discussed here should be accessible under realistic experimental conditions.
Fig. 9. Effect of an asymmetric broadening of the two levels for \( U = 16.2 \Gamma_1, \epsilon_1 = -3.2 \Gamma_1, \Phi = \pi, T = 0 \) and different values of \( \Gamma_2 \). For comparison, the influence of a finite level splitting is also shown.

Finally, we would like to extend our model to include the electron spin, which should give rise also to a magnetic Kondo effect. In this case, the dot Hamiltonian has to be generalized as

\[
H_{\text{dot}} = \sum_j \varepsilon_j c_{j\sigma}^\dagger c_{j\sigma} + U n_1 n_2 + U_1 n_{1\uparrow} n_{1\downarrow} + U_2 n_{2\uparrow} n_{2\downarrow}
\]  

(14)

where \( n_i = \sum_{\sigma} n_{i\sigma} \). For the special case of \( U = U_1 = U_2 \) and \( \delta \varepsilon = 0 \), this model has been studied before \[27,28\]. In realistic double–dot systems, however, we expect \( U < U_{1,2} \). This is the parameter regime we will address here.

NRG calculations for the model including spin are very expensive from a computational point of view. This is due to the larger size of the conduction band Hilbert space, which now contains four instead of two additional fermionic degrees of freedom per iteration, as shown in Fig. 10. In our calculations, we kept about up to 1000 levels in each iteration step, which for 20 iterations required about 10 hours of CPU time on an IBM Power 3.

Fig. 10. Effective NRG Hamiltonian for the spin–degenerate dot \[14\].
Results are shown in Fig. 11. For vanishing AB–phase $\phi$, the two dot levels are coupled to the same reservoir. The resulting RKKY interaction \cite{29} leads to an effective ferromagnetic exchange coupling between the levels. For zero interdot correlation ($U = 0$), the resulting side peaks dominate the single–particle spectrum (left plot). In addition, the screening of the total dot spin leads to the Kondo resonance at the Fermi level, which is suppressed for increasing broadening $\Gamma$.

![Fig. 11. Partial spectral density for level $c_1$ of a spin–degenerate double quantum dot. Left: $U = 0$, $U_1 = U_2 = 2.0$, $\varepsilon_1 = \varepsilon_2 = -1.0$ and $\Phi = T = 0$ with varying $\Gamma$. Right: Same parameters, but now $\Gamma = 0.61$ is fixed and the interdot interaction $U$ is tuned to different values.](image)

Switching on the interdot $U$ as shown in the right plot of Fig. 11 enhances the lower side peak. At $U = 1$, a discontinuous change in the ground state occupation number occurs, while at even larger values of $U$, one again obtains the interference “shoulder” already discussed in the spinless case.

For a finite AB–phase $\phi$ we expect interplay of the orbital and magnetic Kondo effects, which will be the subject of a future publication \cite{30}.

4 Conclusion

In this paper we have discussed Wilson’s Numerical Renormalization Group, a powerful nonperturbative method designed specifically to calculate low–temperature properties of quantum impurity systems. It is the only method that yields reliable results for systems with very different energy scales (small Kondo temperature $T_K$, large bandwidth). Recent experimental progress in the fabrication of ultrasmall quantum dots has made the preparation of artificial Kondo “atoms” with well–controlled parameters possible. NRG is the method of choice for the theoretical interpretation of spectral and transport measurements in terms of single impurity models.

We have presented an extended NRG algorithm (DM–NRG) suitable for calculating low–temperature dynamics in the full frequency range. This
Numerical Renormalization Group has been applied to calculate the spectrum of a quantum dot in a magnetic field.

Furthermore, we have studied the interplay between interference and Kondo correlations in multi–level quantum dots. Orbital Kondo screening has been observed which can be tuned by an external Aharonov–Bohm phase and should be most easily visible in the optical absorption power. Additional spin degeneracy gives rise to the (Spin–) Kondo effect and causes an effective RKKY–interaction between the two dot levels. We expect competition between magnetic and orbital screening in the presence of a finite AB–phase. These results should be useful for the interpretation of recent experiments on vertically coupled dots (see e.g. [31]) or lateral multi–dot arrangements [32].

In future applications of the NRG method, more complex impurities will be considered – one may even try to model the lowest excitations of a complete molecule in order to describe recent transport experiments, see e.g. [33]. From the methodical point of view, the extension of NRG to non–equilibrium calculations remains a major challenge.

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