Abstract

The fidelities of the Kondo and the Friedel-Anderson (FA) impurities are calculated numerically. The ground states of both systems are calculated with the FAIR (Friedel artificially inserted resonance) theory. The ground state in the interacting systems is compared with a nullstate in which the interaction is zero. The different multi-electron states are expressed in terms of Wilson states. The use of $N$ Wilson states simulates the use of a large effective number $N_{\text{eff}}$ of states. A plot of $\ln(F)$ versus $N \propto \ln(N_{\text{eff}})$ reveals whether one has an Anderson orthogonality catastrophe at zero energy. The results are at first glance surprising. The $\ln(F) - \ln(N_{\text{eff}})$ plot for the Kondo impurity diverges for large $N_{\text{eff}}$. On the other hand, the corresponding plot for the symmetric FA impurity saturates for large $N_{\text{eff}}$ when the level spacing at the Fermi level is of the order of the singlet-triplet excitation energy. The behavior of the fidelity allows one to determine the phase shift of the electron states in this regime.

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1 Introduction

In the process of modeling a complicated physical state by a simplified model it is of great interest how well the model agrees with the real state. To measure this agreement one compares the two states with each other. If the states are electronic wave functions then the comparison can be performed as a scalar product between the two wave functions. The result is called the fidelity, and it is defined as

\[ F = |\langle \Psi_{\text{model}} | \Psi_{\text{real}} \rangle| \]  

(1)

It turns out that this concept is also useful when the system (for example the Hamiltonian) depends on a parameter \( \lambda \). Then one can define the fidelity as

\[ F = |\langle \Psi_\lambda | \Psi_0 \rangle| \]

This definition is slightly different from the definition of the differential fidelity \( F(\lambda, d\lambda) \)

\[ F(\lambda, d\lambda) = |\langle \Psi_\lambda | \Psi_{\lambda+d\lambda} \rangle| = 1 - \frac{1}{2} G(\delta\lambda)^2 \]

(2)

where \( G \) is the fidelity susceptibility [1], [2], [3], [4], [5].

If for example a potential in the Hamiltonian is given by \( \lambda V \), then when the potential \( \lambda V \) acts in the whole volume (as for example in the periodic Hubbard model) the fidelity susceptibility is generally proportional to the number of band electrons. (For phase transitions such as quantum critical points it can increase faster than linearly with the number of band electrons). Therefore it is of interest how the fidelity of a system depends on the number of conduction electrons.

The definition of the fidelity is connected with the Anderson orthogonality catastrophe (AOC) as introduced by Anderson [6]. Anderson showed that the ground state of a system of \( N \) fermions is orthogonal to the ground state in the presence of a finite-range scattering potential, as \( N \) approaches infinity \( \ln(F) \propto -\ln(N) \). This AOC has been intensively studied in connection with the Kondo effect [7], [8], [9], [10], [11], [12], [13] where a magnetic d-impurity interacts with the conduction electrons through an exchange interaction \( J s \cdot S \), where \( s \) and \( S \) are the spins of the conduction electrons and the d-impurity.

In this paper we study the fidelity for the Kondo and the Friedel-Anderson (FA) impurities. Both systems are known to possess a singlet ground state. For sufficiently large Coulomb repulsion between the spin-up and down impurity state the FA impurity shows a behavior that is very similar to the Kondo impurity. Schrieffer and Wolff [14] showed that in the range of a local moment the FA Hamiltonian can be transformed into a Kondo Hamiltonian plus a number of additional terms \( \hat{H}_t \). Therefore it suggests that the fidelities of the two systems should behave similarly. That is the reason why we choose both systems for our investigation.

For the calculation of the fidelity we divide the Hamiltonian into two parts: there is a part \( \hat{H}^{\lambda=0} \) that is kept constant and a second part \( \hat{H}^{\lambda} \) that is varied during the calculation. In many cases the Hamiltonian \( \hat{H}^{\lambda} \) depends on several parameters. The FA impurity is an
example. In this case one can choose different paths in the parameter space. The paths are called a fidelity paths in which the parameters $\lambda$ describe the position on the paths.

For the numerical evaluation we use the ground state which we obtain with the FAIR (Friedel Artificially Inserted Resonance) theory [15], [16], [17], [18], [19], [20], [21], [22], [23].

2 Theoretical Background

2.1 Kondo impurity

The Kondo system consists of a band of free s-electrons and a d-impurity with spin $S = 1/2$. Its Hamiltonian is given by

$$\hat{H}^K = \hat{H}^0 + \hat{H}^{\text{ex}}$$

with

$$\hat{H}^\lambda=0 = \hat{H}^0 = \sum_{\nu=1}^{N} \varepsilon_{\nu} \hat{c}_{\nu,\sigma}^\dagger \hat{c}_{\nu,\sigma}$$

For the Kondo impurity we replace $\lambda$ by $J$.

$$\hat{H}^{\text{ex}} = \hat{H}' = v_a 2 J \left( \sum_{\alpha,\beta} \hat{\Psi}_\alpha^\dagger (0) \hat{s}_{\alpha,\beta} \hat{\Psi}_\beta (0) \right) \cdot \mathbf{S}$$

$$= v_a J \left[ \left( S_+ \hat{\Psi}_\uparrow^\dagger (0) \hat{\Psi}_\uparrow (0) + S_- \hat{\Psi}_\uparrow^\dagger (0) \hat{\Psi}_\downarrow (0) \right) \right.$$  

$\left. + S_z \left( \hat{\Psi}_\uparrow^\dagger (0) \hat{\Psi}_\downarrow (0) - \hat{\Psi}_\downarrow^\dagger (0) \hat{\Psi}_\uparrow (0) \right) \right]$ (3)

where $S_+, S_-, S_z$ are the spin operators of the impurity with spin $S = 1/2$, $\hat{\Psi}_\alpha (0)$ and $\hat{\Psi}_\beta (0)$ represent field operators of the conduction electrons and $\hat{s}_{\alpha,\beta}$ are the components of the Pauli operators $\sigma$ divided by two. The product $v_a J \hat{\Psi}_\sigma^\dagger (0) \hat{\Psi}_{\sigma'} (0)$ yields an energy since $\hat{\Psi}_\sigma^\dagger (0) \hat{\Psi}_{\sigma'} (0)$ has the dimension of a density. The operators $\hat{c}_{\nu,\sigma}^\dagger$ and $\hat{c}_{\nu,\sigma}$ are the creation and annihilation operators for the Wilson states of free electrons (see appendix).

The FAIR ground state for the Kondo Hamiltonian is

$$\Psi_K = \left[ B \hat{a}_{0,\uparrow}^\dagger \hat{d}_{\downarrow}^\dagger + C \hat{d}_{\uparrow}^\dagger \hat{b}_{0,\downarrow}^\dagger \right] \prod_{i=1}^{n} \hat{a}_{i,\uparrow}^\dagger \prod_{j=1}^{n} \hat{b}_{j,\downarrow}^\dagger \Phi_0$$

$$+ \left[ C' \hat{b}_{0,\uparrow}^\dagger \hat{d}_{\uparrow}^\dagger + B' \hat{d}_{\uparrow}^\dagger \hat{a}_{0,\downarrow}^\dagger \right] \prod_{i=1}^{n} \hat{b}_{i,\uparrow}^\dagger \prod_{j=1}^{n} \hat{a}_{j,\downarrow}^\dagger \Phi_0$$ (4)

Here the states $\hat{a}_{0,\downarrow}^\dagger$ and $\hat{b}_{0,\uparrow}^\dagger$ are two artificial resonance states. The second part of the state (lower line) is essentially the spin-reversed first part (after it is spin-ordered). In the ground state one has $B' = B$ and $C' = C$ and one of the coefficients, for example $B$, is much larger than the other so that the relative occupations differ by a factor of about 100. Therefore the FAIR state $\hat{a}_{0,\downarrow}^\dagger$ is roughly the always quoted s-electron state that forms a singlet state with the d-impurity. Details of the ground state energy and the spatial polarization and density is discussed in [19], [20], [21].
2.2 Friedel-Anderson impurity

For real d-electrons one has an on-site Coulomb repulsion of the d-electrons among each other. This is described for the Friedel-Anderson (FA) impurity by a simplified Hamiltonian

\[
\hat{H}_{FA} = \sum_{\sigma} \left\{ \sum_{\nu=0}^{N-1} \varepsilon_{\nu} \hat{c}^{\dagger}_{\nu,\sigma} \hat{c}_{\nu,\sigma} + \sum_{\nu=0}^{N-1} V_{\nu}^{sd}[\hat{d}^{\dagger}_{\sigma} \hat{c}_{\nu,\sigma} + \hat{c}^{\dagger}_{\nu,\sigma} \hat{d}_{\sigma}] + E_d \hat{d}^{\dagger}_{\sigma} \hat{d}_{\sigma} \right\} + U n_{d\uparrow} n_{d\downarrow} \tag{5}
\]

The fact that a d-impurity has five different orbital states is simplified into the non-degenerate case with only one d-state with spin up and another one with spin down. The \( \hat{c}^{\dagger}_{\nu,\sigma} \) are the creation operators for conduction electrons with spin \( \sigma \) and \( \hat{d}^{\dagger}_{\sigma} \) is the corresponding operator for the d-electron with spin \( \sigma \). Further \( V_{\nu}^{sd} \) is the matrix element for a transition between the conduction electron \( \hat{c}^{\dagger}_{\nu,\sigma} \) and the d-electron \( \hat{d}^{\dagger}_{\sigma} \). The most intensively studied case is the symmetric FA impurity where \( E_d = -U/2 \).

The FAIR ground state of the FA impurity is

\[
\Psi_{SS} = \left[ A \hat{a}^{\dagger}_{0,\uparrow} \hat{b}^{\dagger}_{0,\downarrow} + B \hat{a}^{\dagger}_{0,\downarrow} \hat{b}^{\dagger}_{0,\uparrow} + C \hat{d}^{\dagger}_{\uparrow} \hat{d}^{\dagger}_{\downarrow} + D \hat{d}^{\dagger}_{\downarrow} \hat{d}^{\dagger}_{\uparrow} \right] \prod_{i=1}^{n-1} \hat{a}^{\dagger}_{i,\uparrow} \prod_{i=1}^{n-1} \hat{b}^{\dagger}_{i,\downarrow} \Phi_0 \tag{6}
\]

In the ground state the coefficients \( X' = X \) where \( X \) stands for \( A, B, C, D \). Again the second line is essentially the first line with reversed spins.

3 Numerical Evaluation

Since any solution of the Kondo or FA impurity has to include states with very small energy (less than the Kondo energy with typical values of \( 10^{-5} \) or \( 10^{-6} \) in units of the bandwidth) we use Wilson states (see appendix) as the basis of our calculation. The smallest level separation at the Fermi level for \( N \) Wilson states is \( \delta E = 2 \times 2^{-N/2} \). This energy is essential in the fidelity calculation. A spectrum with equidistant levels would contain \( N_{\text{eff}} = 2/\delta E \) states. For \( N = 48 \) the effective number of states \( N_{\text{eff}} \) would be \( N_{\text{eff}} = 2/\delta E = 2^{N/2} \) which is \( 2^{24} \approx 1.7 \times 10^7 \). This shows that with a moderate number of Wilson states one simulates a large number of band electrons.

3.1 Kondo impurity

For the Kondo impurity the Hamiltonians \( \hat{H}^{\lambda=0} \) and \( \hat{H}^{\lambda} \) have the form

\[
\hat{H}^{\lambda=0} = \sum_{\nu=1}^{N} \varepsilon_{\nu} \hat{c}^{\dagger}_{\nu,\sigma} \hat{c}_{\nu,\sigma}
\]
\[ \hat{H}^\lambda = \lambda \hat{H}^{ex} \]

For comparison the state with \( \lambda = 0 \) is required. We call this state the nullstate. We choose for the nullstate

\[ \Psi^{\lambda=0} = \frac{1}{\sqrt{2}} \left( \hat{c}^{\dagger}_{n,\uparrow} \hat{d}^{\dagger}_{\downarrow} + \hat{d}^{\dagger}_{\uparrow} \hat{c}^{\dagger}_{n,\downarrow} \right) \prod_{\nu=1}^{n-1} \hat{c}^{\dagger}_{\nu,\uparrow} \prod_{\nu=1}^{n-1} \hat{c}^{\dagger}_{\nu,\downarrow} \Phi_0 \]

with \( n = (N/2 + 1) \). This represents a half-filled band for the spin-up and down conduction electrons plus a pseudo-singlet state between the d-electron \( \hat{d}^{\dagger} \) and the first electron state above the Fermi level. We call it a pseudo-singlet state because there is no coupling between \( \hat{c}^{\dagger} \) and \( \hat{d}^{\dagger} \) since \( \lambda J \) is zero. The two components are two degenerate ground states, and their combination represents the symmetry of the Kondo ground state.

In the next step the numerical FAIR ground states are calculated for a given value of \( \lambda J \) for a total number of Wilson states of \( N = 20, 24, 28, 32, 36, 40, 44 \) and \( 48 \). Then the scalar product (the fidelity \( F \)) between the nullstate and the FAIR ground state of the FA impurity is calculated. In Fig.1 the logarithm of the fidelity \( \ln (F) \) is plotted for different \( J \) as a function of the number of Wilson states \( N \). As we pointed out above the number of Wilson states \( N \) corresponds to an effective number of electrons \( N_{eff} \). With \( N = 2 \star \log_2 N_{eff} \) a plot of \( \ln (F) \) versus \( N \) corresponds to log-log-plot between \( F \) and \( N_{eff} \).

Fig.1: The logarithm of the fidelity \( \ln (F) \) for a Kondo impurity is plotted versus the number of Wilson states \( N \). The nullstate for \( J = 0 \) is described in the text. (The arrows are explained in the discussion).

One obtains a set of curves that show in principle a linear dependence of \( \ln (F(0, J)) \) on \( N \) at large values of \( N \). For the \( J = 0.15 \) and \( 0.12 \) curves the linear behavior is dominant for
most of the region shown. With decreasing values of $J$ the onset of the linear range moves to larger values of $N$. For $J = 0.05$ and 0.04 the linear part is outside of the calculated and drawn regime. In the linear regime all curves show the same slope of $m = 0.088$. So we observe that the fidelity depends on the effective number of states as

$$
\ln (F(0, J)) \propto -0.088N \approx -0.088 \times 2 \log_2(N_{eff}) \approx -0.25 \ln (N_{eff})
$$

or

$$
F(0, J) \propto \frac{1}{N_{eff}^{1/4}}
$$

If we consider the differential fidelity between $J = 0.09$ and 0.10 then one obtains an interesting result that is shown in Fig.2. For small numbers of Wilson states $F(0.09, 0.10)$ is close to one. Then it decreases for $N$ between 25 and 35 and assumes a constant value of about 0.95 for larger $N$. Fig.2 demonstrates very nicely that the slopes of the $\ln (F)$ versus $N$ curves are the same at sufficiently large $N$ (for $J = 0.09$ and 0.1). The additional states close to the Fermi energy have the same phase shift as we will discuss below. Fig.2 also shows that the internal structure of the Kondo impurity for these $J$-values experiences a relative change at $N \approx 30$. Below we discuss that this is in the range of the singlet-triplet excitation energy for the two $J$-values.

Fig.2: The relative fidelity $F$ between Kondo impurities with $J = 0.09$ and $J = 0.10$ is plotted as a function of $N$.

### 3.2 Friedel-Anderson impurity

The FA impurity is described by several independent parameters, the s-d-hopping matrix element $|V_{sd}|^2$, the energy of the d-state $E_d$ and the exchange energy $U$. Therefore one
can choose many different fidelity paths. In this investigation we consider essentially two
different paths; (i) the symmetric FA impurity case with $|V_{sd}|^2 = 0.05$, $U = \lambda U_0$ ($U_0 = 1$)
and $E_d = -\frac{1}{2}\lambda U_0$, (ii) the asymmetric FA impurity with constant $|V_{sd}|^2 = 0.05$ and $U = 1$
and varying $E_d$ in the range ($-1 < E_d < 0$).

**Symmetric case:** Here we use for the nullstate the parameters $E_d = 0$ and $U = 0$. This
represents the Friedel resonance with the d-energy at the Fermi level. Fig.3 shows a several
examples of the fidelity for $E_d = -0.5$ and $U = 1$ where $|V_{sd}|^2$ takes the values 0.05, 0.04, 0.03
and 0.025.

![Fig.3: The logarithm of the fidelity ln (F) for the symmetric
Friedel-Anderson impurity is plotted versus the number of Wilson
states $N$. The nullstate for $U = 0$ is the symmetric Friedel impurity
with the $|V_{sd}|^2$ and $E_d = 0$.]

Fig.3 shows that the fidelity is essentially constant for $|V_{sd}|^2 = 0.05$ but decreases for
$|V_{sd}|^2 = 0.025$ with increasing $N$. However, for large $N$ the fidelity approaches a constant
value. (The arrows in Fig.3 are explained in the discussion).

The values of the fidelity for $|V_{sd}|^2 = 0.05$, $U = 1$ and $E_d = -0.5$ vary over the whole
range of $20 \leq N \leq 48$ by less than 2%. This independence of the fidelity of the number
of Wilson states is observed in the whole range $0 < \lambda < 1$ with $U = \lambda U_0$ and $E_d = -\frac{1}{2}U_0$
($U_0 = 1$). In addition the fidelity shows a quadratic dependence on $\lambda$ as is shown in Fig.4
for $N = 32$. We observe the relationship

$$F(\lambda) = 1 - \frac{1}{2}G\lambda^2$$
where $G$ the fidelity susceptibility has the value of $G = 0.63$. There is no unusual or singular behavior of the fidelity in the symmetric case.

Asymmetric case: Next we study the fidelity of the FA impurity along the path with $|V_{sd}|^2 = 0.05$, $U = 1$ while $E_d$ is varied between $-1$ and $0$. As the nullstate we use the symmetric state with $|V_{sd}|^2 = 0.05$, $U = 1$ and $E_d = -0.5$. Fig. 5 shows a typical diagram of the fidelity $\ln (F)$. It shows a relatively small reduction of $\ln (F)$ with $N$. The small deviation at $N = 48$ is due to the fact that the calculation of the FA ground state requires a very large number of iterations to optimize the low energy states close to the Fermi energy. The ground-state energy has to be optimized up to an accuracy better than $10^{-12}$. This high
accuracy is normally not needed for any other physical properties.

Fig. 5: The logarithm of the fidelity $\ln(F)$ between two FA impurities as a function of $N$. The impurities possess the same $|V_{sd}|^2 = 0.05$ and $U = 1$ but possess different values of $E_d = -0.5$ and $E_d = -0.25$.

The slope $d(\ln F)/dN$ is shown in Fig. 6 as a function of $E_d$. This slope is, of course, zero at $E_d = -0.5$ because here the fidelity state and the null state are identical. These results show that in the asymmetric case one observes a reduction of the fidelity for large number
of states $N_{\text{eff}}$ but the effect is much smaller than in the Kondo impurity.

![Graph of Friedel-Anderson impurity](image)

**Fig. 6:** The slope as shown in Fig. 5 of $\ln(F)$ versus $N$ as a function of $E_d$ of the fidelity state for the asymmetric FA impurity.

### 3.3 Friedel impurity

The FA impurity is defined by three parameters. Its fidelity is independent of $N$ along the path $U = \lambda U_0, E_d = -\frac{1}{2}U_0$ and (slightly) singular along other paths, for example along the path where only $E_d$ is varied. This raises the question whether the singular behavior of $\ln(F)$ is a consequence of the Coulomb interaction and the resulting Kondo ground state or whether it is a trivial result of the single particle potentials $V_{sd}$ and $E_d$. Therefore it is an obvious necessity to check this question. Such a check is easy done by investigating the simple spinless Friedel impurity which is defined by the two parameters $|V_{sd}|^2$ and $E_d$.

In the first Friedel investigation we choose for the nullstate the parameters $|V_{sd}|^2 = 0.05$ and $E_{d,0} = 0$. Then a series of fidelity series are performed with the same value for $|V_{sd}|^2$ and values for $E_d$ between $-0.7$ and $+0.7$. The plots of $\ln(F)$ versus $N$ yield straight lines with a relatively small slope. These slopes are plotted in Fig. 7 as a function of $E_d$. At $E_d = 0$ the slope is, of course, zero because both states are identical. As a whole one obtains a bell-shaped curve for the slopes. This demonstrates that a simple change of $E_d$ yields a singular $\ln(F)$ for large $N$ without any electron-electron interaction.
Fig. 7: The slope of $\ln (F)$ versus $N$ for the asymmetric Friedel impurity as a function of $E_d$. The nullstate is a Friedel impurity with $E_d = 0$ and the same $|V_{sd}|^2 = 0.05$.

In a second series of simulations the same nullstate is chosen with $|V_{sd}|^2 = 0.05$ and $E_{d,0} = 0$. For the fidelity states the s-d-hopping matrix $|V_{sd}|^2$ is varied between $5 \times 10^{-5}$ and 0.05. For each value of $|V_{sd}|^2$ the fidelity approaches a constant value for a sufficiently large number of Wilson states. There is no singular behavior of $\ln (F)$ as a function of $N$. Of course, the constant value of the fidelity depends on $|V_{sd}|^2$. This dependence of $F$ is shown
in Fig.8 as a function of \( \ln \left( |V_{sd}|^2 \right) \).

![Graph showing fidelity as a function of \( \ln \left( |V_{sd}|^2 \right) \).](image)

Fig.8: Fidelity between a two Friedel states as a function of \( \ln \left( |V_{sd}|^2 \right) \) in the fidelity state while the nullstate has \( |V_{sd}|^2 = 0.05 \). Both states have identical values of \( E_d = 0, U = 0 \). The fidelity shows essentially no dependence on the number of Wilson states \( N \).

4 Discussion

In our fidelity calculation we use the Wilson basis for the conduction band in the (normalized) energy range \((-1 : +1)\). The density of Wilson states is very thin far away from the Fermi level and increases exponentially close to the Fermi level. There is no question that the Wilson basis does not describe well the density of states of a resonance far below or above the Fermi level where the level separation is much larger than the resonance width. Therefore it is a legitimate question whether this handicap of the Wilson basis disqualifies it for fidelity calculations.

To clarify this question let us compare two different wave functions: \( \Psi_1 \) describes the ground state of of a system with a resonance at \( \varepsilon_{d,1} = -0.8 \) and \( \Psi_2 \) has a resonance at \( \varepsilon_{d,2} = -0.4 \). Both resonances are sharp and have a width of \( \Delta = 0.05 \). To simplify the situation we assume that the s-d-matrix element vanishes for \( |\varepsilon - \varepsilon_{d,i}| > 0.1 \). In both systems the conduction band is half filled (all states in the energy range \((-1 \leq \varepsilon \leq 0)\) are occupied). Intuitively one might assume that the wave functions of \( \Psi_1 \) and \( \Psi_2 \) are quite different because their resonances don’t overlap. However, this is not the case. The scalar product (fidelity) \( \langle \Psi_1 | \Psi_2 \rangle \) is essentially one. The reason is that in both wave functions the d-state and the band states in the range \((-1 \leq \varepsilon \leq 0)\) are all occupied so that their wave
functions are given by

$$ \Psi_1 \approx \Psi_2 \approx \hat{d}^\dagger \prod_{\varepsilon < 0} \hat{c}_\varepsilon^\dagger \Phi_0 $$

where $\hat{c}_\varepsilon^\dagger$ describes the band states with the energy $\varepsilon$. The different density of states far below the Fermi level (as well as far above) is not important for the fidelity. What counts in the fidelity is the occupation of states close to the Fermi level. For this reason the Wilson basis is particularly well suited for fidelity calculations because it emphasizes the states close to the Fermi level where it counts and it does not waste states far away from the Fermi level. In the appendix we demonstrate that it is the (smallest) level separation at the Fermi level which determines the fidelity. Halving the level separation by introducing one additional state above and below the Fermi level has the same effect as doubling the number of states (which also halves the level spacing at the Fermi level).

An important question in this investigation is whether the fidelity identifies and helps to understand interacting electron systems. Both the Kondo and the FA impurities possess a singlet ground state. For sufficiently large Coulomb repulsion between the spin-up and down impurity states the FA impurity shows a behavior that is very similar to the Kondo impurity.

A comparison between Fig.1 for the Kondo impurity and Fig.3 for the FA impurity shows that the fidelities of the two systems behave very differently. For the following discussion it will be useful to calculate the singlet-triplet excitation energy for the two systems. In table I the relaxed singlet-triplet excitation energy $\Delta E_{st}$ is collected for the parameters of the Kondo impurity investigated in [19]. The relaxed singlet-triplet excitation energy $\Delta E_{st}$ is obtained by optimizing the two bases $\{\hat{a}_i^\dagger\}$ and $\{\hat{b}_i^\dagger\}$ independently in the singlet state and the triplet state.

For the development of the ground state it is important that the smallest level separation $\delta E$ at the Fermi level (which is $\delta E = 2 \times 2^{-N/2}$) is less than the excitation energy $\Delta E_{st}$. Therefore we collect in table I also the critical number of Wilson states $N_{st} \approx 2 \times \left[\log_2 \left(1/\Delta E_{st}\right)\right] + 1$ that yields a level separation of about $\Delta E_{st}$. In Fig.1 this critical value is marked with a small arrow. One recognizes that for $N < N_{st}$ the fidelity is essentially constant and for $N > N_{st}$ the logarithm of the fidelity changes linearly with $N$.

| J     | $\Delta E_{st}$ | $N_{st}$ |
|-------|-----------------|----------|
| 0.15  | $9.1 \times 10^{-4}$ | 22       |
| 0.12  | $1.65 \times 10^{-4}$ | 26       |
| 0.10  | $2.53 \times 10^{-5}$ | 32       |
| 0.09  | $7.02 \times 10^{-6}$ | 36       |
| 0.08  | $1.52 \times 10^{-6}$ | 40       |
| 0.07  | $2.41 \times 10^{-7}$ | 44       |
| $<0.07$ | $<10^{-7}$ | $>48$   |

Table I: The relaxed singlet-triplet excitation energy $\Delta E_{st}$ for the Kondo impurity as a function of $J$. The third column gives the (closest) number of Wilson states $N_{st}$ so that the
The smallest level separation is roughly equal to the excitation energy $\Delta E_{st}$.

In Table II the corresponding data $\Delta E_{st}$ and $N_{st}$ are collected for different values of $|V_{sd}|^2$ for the FA impurity. In Fig.3 the critical values of $N_{st}$ are also marked on the curves. However, now the behavior is almost reversed compared with the Kondo impurity. For the FA impurity we observe essentially a linear decrease of $\ln (F)$ with increasing $N$ for $N < N_{st}$ and a saturation of $\ln (F)$ for $N > N_{st}$. In particular there is no singular behavior of $\ln (F)$ for large $N$.

| $|V_{sd}|^2$ | $\Delta E_{st}$ | $N_{st}$ |
|-----------|----------------|----------|
| 0.05      | $8.33 \times 10^{-4}$ | 22       |
| 0.04      | $1.35 \times 10^{-4}$ | 26       |
| 0.03      | $3.23 \times 10^{-6}$ | 38       |
| 0.025     | $2.65 \times 10^{-7}$ | 44       |

Table II: The relaxed singlet-triplet excitation energy $\Delta E_{st}$ as a function of $|V_{sd}|^2$. The third column gives the (closest) number of Wilson states $N_{st}$ so that the smallest level separation is roughly equal to the excitation energy $\Delta E_{st}$.

This may be rather surprising since the symmetric FA impurity approaches the Kondo impurity asymptotically for small $|V_{sd}|^2 / U$, but this is not reflected by the fidelity behavior.

Recently Weichselbaum et al. [24] calculated the fidelity of the FA impurity using the numerical renormalization group (NRG) theory. They obtained in general a logarithmic decrease of the fidelity. However, they used very different fidelity paths. In one example they varied the energy of the d-level and kept the other parameters constant. Therefore we performed a similar calculation which is shown in Fig.5. We believe, however, that the linear decrease of $\ln (F)$ with $N$ is not a many-body effect. Therefore we have calculated the fidelity of the simple non-interacting Friedel impurity. Fig.7 shows that one obtains a singular behavior of $\ln (F)$ for large $N$. This is not surprising since it was derived earlier by Anderson and is known as the Anderson orthogonality catastrophe. We believe that the singular behavior as observed by Weichselbaum et al. is due to the change of the potential scattering in the underlying Friedel resonance. Weichselbaum et al. use rather small parameters of $U, E_d$ and $|V_{sd}|^2$ such as $U = 0.12$ and $\Gamma_{\mu} = \pi |V_{sd\mu}|^2 \rho_{\mu} = 0.01$ and several hybridization processes $\mu$ ($\rho_{\mu}$ is the density in the band $\mu$). We did not extend our software to several hybridization processes since we concluded that our two examples of the Kondo and the FA impurity already illuminate the physics.

We suggest the following mechanisms for the different behavior of the fidelity $\ln (F)$ as a function of $N$. In the Kondo impurity we compare the Kondo solution with the $J = 0$ state. The latter is a homogeneous electron gas with the same density at the impurity as anywhere else. For small $J$ the magnetic d-electron causes only a relatively small change for
small $N$ since the Kondo ground state has not yet developed. When $N$ becomes larger than $N_{st}$ the Kondo ground state has formed and causes a phase shift of $\pi/2$ for all electrons with smaller energy. This phase shift is the reason why the scalar product with the free electron case ($J = 0$) goes to zero, i.e. $\ln (F)$ diverges. It is analogous to the Anderson orthogonality catastrophe.

The difference between the Kondo and the symmetric FA impurity is that we don’t compare the latter with the free electron case but with a state that has the same s-d-potential $|V_{sd}|^2$. If one chooses for the nullstate the symmetric Friedel impurity then all electrons within the resonance width already have a phase shift of $\pi/2$ in the nullstate. On the other hand in the singlet ground state of the FA impurity all electrons with energy smaller the $\Delta E_{st}$ also have a phase shift of $\pi/2$. Since this is the same phase shift as in the nullstate it does not reduce the scalar product of the fidelity between the nullstate and the singlet ground state with increasing $N$. The fidelity becomes asymptotically constant.

Finally it is tempting to compare the ground-state wave function of a Kondo impurity with that of a FA impurity. From tables I and II one finds that the Kondo impurity with $J = 0.12$ and the FA impurity with $|V_{sd}|^2 = 0.04$, $U = 1$ and $E_d = -0.5$ have roughly the same singlet-triplet excitation energy ($1.65 \times 10^{-4}$ versus $1.35 \times 10^{-4}$). Therefore we calculate the scalar product which yields the similarity between the wave functions for different $N$. This similarity (which is defined in the literature as fidelity) is plotted in Fig.9. It shows that $F$ is close to 1.0 and approaches a constant value of 0.95 for large $N$. This confirms the similarity between the Kondo and the FA impurity (for large $U/|V_{sd}|^2$), and the phase shift
in both systems close to the Fermi level is essentially the same.

![Graph of Fig.9](image)

Fig.9: The similarity (fidelity) between the ground state of a Kondo and a FA impurity as a function of the number of Wilson states. The parameters of the impurities are shown in the figure.

The minimum of the curve is at about $N = 24$. This corresponds to a level separation at the Fermi energy of $2 \times 2^{-N/2} \approx 1.2 \times 10^{-4}$. This is of the order of the singlet-triplet excitation energy of the two systems.
5 Conclusion

In this paper the ground states of the Kondo impurity and the Friedel-Anderson impurity are calculated for many parameters and seven different numbers $N$ of Wilson states using the FAIR theory. The effective number of band electrons is $N_{\text{eff}} \approx 2 \times 2^{N/2}$. For each number of Wilson states the resulting ground states (which we denote as fidelity states) are compared with the corresponding ground states for zero interaction, the so-called nullstates. The fidelity is obtained by forming the scalar product between the fidelity state and the nullstate for each $N$. Then the logarithm of the fidelity $\ln(F)$ is plotted versus $N \approx 2 \log_2 (N_{\text{eff}}/2)$.

The fidelity shows very different behavior for the Kondo and the Friedel-Anderson impurities. In the symmetric FA impurity it saturates at large values of $N$ while for the Kondo impurity the logarithm $\ln(F)$ diverges. This result demonstrates that the behavior of the fidelity depends as much on the choice of the simple nullstate as on the interacting fidelity state.

For the symmetric FA impurity we choose a nullstate with $U = 0$ and $E_d = 0$ (to maintain the symmetry) but leave $|V_{sd}|^2$ constant. Here the s-electrons close to the Fermi energy already have a phase shift of $\pi/2$ in the nullstate. The interacting ground state introduces a phase shift of $\pi/2$ as well in a narrow energy range about the Fermi energy. Therefore if one increases the number of states closer and closer to the Fermi level the phase shift in the nullstate and the fidelity state are the same and the scalar product does not change. On the other hand, for the Kondo impurity we set $J = 0$ and obtain a nullstate whose conduction band is the free electron band that has no phase shift, and the fidelity decreases with increasing $N$. It is not sufficient to turn off the interaction in the nullstate. One also has to know or investigate the phase shift of its s-electrons close to the Fermi level.

In this respect the fidelity calculations yield comparative information about the s-electrons at the Fermi level. In addition a change in the slope of $\ln(F)$ versus $N$ indicates at which energy the inner structure changes, either of the nullstate or the fidelity state.

If we compare two multi-electron states then the behavior of the fidelity does not tell us whether none, one or both are interacting electron systems. The fidelity does not correlate with the many-body physics of the problems.

Finally, we observed that the fidelity of ground states of the Kondo and the FA Hamiltonians with similar Kondo temperatures does not show an Anderson orthogonality catastrophe, but on the contrary is relatively close to one and becomes constant with an increasing number of Wilson states $N$. 

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6 Appendix

A Wilson’s states

Wilson considered an s-band with a constant density of states and the Fermi energy in the center of the band. By measuring the energy from the Fermi level and dividing all energies by the Fermi energy Wilson obtained a band ranging from $-1$ to $+1$. To treat the electrons close to the Fermi level at $\zeta = 0$ as accurately as possible he divided the energy interval $(-1:0)$ geometrically at energies of $\zeta_\nu = \zeta_{\nu+1} - \zeta_\nu = 1/2^{\nu+1}$ and average energy $\varepsilon_\nu = (\zeta_{\nu+1} + \zeta_{\nu-1})/2$.

Wilson rearranged the quasi-continuous original electron states $\varphi_k(x)$ in such a way that only one state within each cell $C_\nu$ had a finite interaction with the impurity. Assuming that the interaction of the original electron states $\varphi_k(x)$ with the impurity is independent of $k$, this interacting state in $C_\nu$ had the form

$$\psi_\nu(x) = \sum \psi_\nu \varphi_k(x) / \sqrt{Z_\nu}$$

where $Z_\nu$ is the total number of states $\varphi_k(x)$ in the cell $C_\nu$ ($Z_\nu = Z(\zeta_{\nu+1} - \zeta_\nu)/2$, $Z$ is the total number of states in the band). There are $(Z_\nu-1)$ additional linear combinations of the states $\varphi_k$ in the cell $C_\nu$ but they have zero interaction with the impurity and were ignored by Wilson as they are within this paper.

The interaction strength of the original basis states $\varphi_k(x)$ with the d-impurity is assumed to be a constant, $v_{sd}$. Then the interaction between the d-state and the Wilson states $\psi_\nu(x)$ is given by

$$V_{sd}(\nu) = V_{sd}^0 \sqrt{(\zeta_{\nu+1} - \zeta_\nu)/2}$$

where $|V_{sd}^0|^2 = \sum_k |v_{sd}|^2 = \sum_\nu |V_{sd}(\nu)|^2$.

A.1 FAIR theory

Let us first consider the Friedel impurity without spin. Its Hamiltonian is

$$\hat{H}_F = \sum_{\nu=1}^{N} \varepsilon_\nu \hat{c}_\nu^{\dagger} \hat{c}_\nu + E_d \hat{d}_\sigma^{\dagger} \hat{d}_\sigma + \sum_\sigma V_{sd}^{\sigma} \left( \hat{c}_\nu^{\dagger} \hat{d}_\sigma + \hat{d}_\sigma^{\dagger} \hat{c}_\nu \right)$$

We call this Hamiltonian sub-diagonal because it is diagonal in the states $\hat{c}_\nu^{\dagger}$ but not between $\hat{d}_\sigma^{\dagger}$ and $\hat{d}_\sigma$. (We use here the creation operators to denote the corresponding states $\hat{c}_\nu^{\dagger} \Phi_0$ or $\hat{d}_\sigma^{\dagger} \Phi_0$, where $\Phi_0$ is the vacuum).

By diagonalization one finds the exact eigenstates

$$\hat{b}_j^{\dagger} = \sum_{\nu=1}^{N+1} \beta_j^{\nu} \hat{c}_\nu^{\dagger} + \beta_j \hat{d}_\sigma^{\dagger}$$

and a diagonal Hamiltonian. The ground state with $n$ electrons is given by

$$\Psi_F = \prod_{j=1}^{n} \hat{b}_j^{\dagger} \Phi_0$$
where \( \Phi_0 \) is the vacuum state.

Of course, one can reverse the process and starting from the diagonal Hamiltonian \( \hat{H} = \sum_j E_j \hat{b}_j \hat{b}_j^\dagger \) extract the resonance state \( \hat{d}^\dagger \) and build an arbitrary orthonormal basis out of the \( \hat{b}_j^\dagger \) which is orthogonal to \( \hat{d}^\dagger \). The Hamiltonian will not be diagonal in this basis. So in the final step one sub-diagonalizes the Hamiltonian excluding the state \( \hat{d}^\dagger \) in the process.

This reverse process can also be applied to the s-electron part of \( \hat{H}_F \). One can build an arbitrary state \( \hat{a}_0^\dagger = \sum_\nu \alpha_0^\nu \hat{c}_\nu^\dagger \). In the next step one builds a new orthonormal conduction band basis \( \{ \hat{a}_i^\dagger \} \) with \( (N-1) \) states which are also orthogonal to \( \hat{a}_0^\dagger \). Again the Hamiltonian \( \hat{H}^0 \) will not be diagonal and in the final step one sub-diagonalizes the Hamiltonian excluding the state \( \hat{a}_0^\dagger \) in the process. Now \( \hat{a}_0^\dagger \) is an artificial Friedel resonance, i.e. the FAIR state. The state \( \hat{a}_0^\dagger \) determines the composition of the whole basis \( \{ \hat{a}_i^\dagger \} \).

This FAIR concept is rather flexible because \( \hat{a}_0^\dagger \) can be any combination of the s-states \( \hat{c}_\nu^\dagger \). It turns out that there is one special state \( \hat{a}_0^\dagger \) with which one can construct the exact ground state of the Friedel resonance. With this special FAIR state the Friedel ground state takes the form

\[
\Psi_F = \left( A \hat{a}_0^\dagger + B \hat{d}^\dagger \right) \prod_{i=1}^{n-1} \hat{a}_i^\dagger \Phi_0
\]

This ground state of the Friedel resonance has the great advantage that \( \hat{d}^\dagger \) is only hybridized with one single s-electron \( \hat{a}_0^\dagger \). The FAIR state \( \hat{a}_0^\dagger \) is in a way representing all other s-electrons. \( \left( A \hat{a}_0^\dagger + B \hat{d}^\dagger \right) \) forms a composed state which shifts the energy of all the other electron states (introducing a phase shift). It is the building block for the compact ground state of the FA and the Kondo impurity.

### B Relation between Wilson state number \( N \) and effective number of electrons \( N_{eff} \)

The Wilson states are defined by the ratio \( \Lambda \). However, for some physical properties this sub-division of the energy band is too coarse. We observed an error in the amplitude of the Friedel oscillation of about 10% for \( \Lambda = 2 \) which became of the order of 1% for when the intervals where sub-divided twice (corresponding to \( \Lambda = \sqrt{2} \) [21]). Therefore we checked whether the coarse sub-division of the band caused any error for the fidelity calculation. For this purpose we calculated the fidelity between two Friedel resonances with two different d-energies, \( E_{d1} = 0 \) and \( E_{d2} = -1 \). In both cases the s-d-coupling is \( |V_{sd}|^2 = 0.05 \). In Fig.10 the squares give the plot of \( \ln(F) \) versus the number of Wilson states for \( \Lambda = 2 \), which is equivalent to all the plots in this paper. Then we subdivided each cell into two equal subcells (full circles) and again each subcell into two new subcells (full triangles).
number of states increased each time by a factor two but we plotted the newly calculated \( \ln(F) \) as a function of the original number \( N \) of Wilson states. First we observe that the resulting straight lines are perfectly parallel. Secondly the two sub-divisions into equal subcells reduced the smallest energy \( \delta E \) at the Fermi level by a factor of \( 4 = 2^2 \). This means that after two subdivisions the smallest \( \delta E \) for \( N \) Wilson states is equal to the original \( \delta E \) for \( (N+4) \) Wilson states. For example, the plot shows that the square at \( N = 36 \) has the same value as the triangle at \( N = 32 \). If one would plot \( \ln(F) \) versus \( 2 \log_2 (1/\delta E) \) all points would fall on one straight line (the one with the squares), although the number of states used in the calculation are varied by a factor four. This demonstrates that the fidelity depends essentially on the smallest energy \( \delta E \) at the Fermi energy and not on the total number of states.

Fig.10: The logarithm of the fidelity between two Friedel impurities with different d-level energies. The squares are for a regular Wilson spectrum. For the circles each Wilson energy cell is divided into two cells increasing the number of states to \( 2N \). For the triangles the original energy cells are divided into four cells yielding \( 4N \) states. Therefore the new states are essentially a factor 2 and 4 closer, and the smallest energy separation is smaller by a factor 2 and 4. The fidelity is plotted in all cases versus the original number of Wilson states. The straight lines are perfectly parallel. In addition a triangle at \( N = 36 \) has the same smallest energy as a square at \( N = 40 \), and indeed they have the same fidelity.
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