Research Article

Factorization of the $N$-Electron Wave Function in the Kondo Ground State

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The multielectron wave function of an interacting electron system depends on the size of the system, that is, the number of electrons. Here the question investigated is how the wave function changes for a symmetric Friedel-Anderson impurity when the volume is doubled. It turns out that for sufficiently large volume (when the level spacing is smaller than the resonance width) the change in the wave function can be expressed in terms of a universal single-electron state $|q\rangle$ centered at the Fermi level. This electron state is independent of the number of electrons and independent of the parameters of the Friedel-Anderson impurity. It is even the same universal state for a Kondo impurity and a symmetric Friedel impurity independent of any parameter. The only requirement is that the impurity has a resonance exactly at the Fermi level and that the level spacing is smaller than the resonance width. This result clarifies recent fidelity calculations.

1. Introduction

In the late 1960s Anderson [1] showed that the potential of a weak impurity in a metal host changes the total $n$-electron wave function of the conduction electrons dramatically. Actually with increasing number $N_c$ of electron states (which is achieved by increasing the volume) the scalar product between the wave functions of the $n$-electron host without and with the impurity approaches zero. This phenomenon is generally called the Anderson orthogonality catastrophe (AOC). In recent years this phenomenon has been somewhat generalized and decorated with the romantic name fidelity. The generalization is that one applies the AOC to an arbitrary system, which depends on one or several parameters $\lambda$. If the system consists of electrons then it is described by its Hamiltonian. The Hamiltonian may contain a term, which is proportional to a parameter $\lambda$. Suppose that one can calculate the ground state of the system for $\lambda = 0$ and for finite $\lambda$. Then the scalar product of the two wave functions is defined as the fidelity $F_N(0, \lambda)$ of the system. Here $N_c$ is the number of conduction electrons states, which is proportional to the volume. The fidelity depends on the size of the system and of particular interest is the limit for $N_c$ increasing towards infinity. If $F_N(0, \lambda)$ approaches zero in this limit (the thermodynamic limit), then one faces an AOC.

Our group studied recently the fidelity of the Friedel-Anderson impurity. This is an electron system with a $d$-atom as impurity. The energy of the $d$-electron lies at $E_d$ below the Fermi level. If one removes a $d$-electron, that is, creates a $d$-hole, then the conduction electrons can hop into the empty $d$-state with a hopping matrix element $V_{sd}$. The $d$-hole possesses a finite life time $\tau_d$ before it is refilled. Due to Heisenberg's uncertainty principle this life time broadens the energy level of the $d$-electron and transforms it into a $d$-resonance with a resonance width, which is of the order of $h/\tau_d$. In general the properties of a dissolved $d$-atom are more complicated because the different $d$-electrons repel each other due to the Coulomb interaction. In the theoretical investigation of such an impurity one studies (most of the time) a simplified model of a $d$-impurity with only two $d$-states, a spin-up and a spin-down $d$-state. Such an impurity was first studied by Friedel [2–5] and Anderson [6] and I call it the Friedel-Anderson (FA) impurity. The strength of the Coulomb interaction $U$ represents a parameter $\lambda$ as introduced in the fidelity. For $U = 0$ the impurity properties are much simpler. The impurity has a Friedel resonance at
the $d$-energy $E_d$ in each spin subband and is called a Friedel impurity.

While the wave function of the FA impurity is quite complex the density of states is simpler and qualitatively sketched in Figure 1 together with the density of states of a Friedel impurity. For both impurities the symmetric case is shown. In the Friedel impurity the resonance is positioned at the Fermi level ($E_d = 0$). In the FA impurity the $d$-state energy is positioned at $E_d = -U/2$ so that $E_d$ and $(E_d + U)$ lie symmetrically to the Fermi level. As a consequence there is an electron-hole symmetry. One obtains two $d$-resonances at roughly the energies $E_d = -U/2$ and $E_d + U = +U/2$ for spin-up and spin-down. These are known as the Hubbard resonances, and their width is twice the width of a Friedel resonance with the same $s$-$d$-hopping [7–9]. In addition one obtains a narrow resonance at the Fermi level, which is generally called the Kondo resonance (see for example [10]).

Two studies of the fidelity of the FA impurity have been published recently, one by Weichselbaum et al. [11] and one by our group [12]. In our investigation we calculated the fidelity between a symmetric Friedel impurity ($E_d = 0$, $U = 0$) and a symmetric FA impurity with finite Coulomb repulsion $U$ and $E_d = -U/2$. When level spacing $\delta E$ is smaller than the width of the Kondo resonance in Figure 1(b) then the fidelity did not change any more with increasing $N$.

In the fidelity calculations one has on one hand to increase the number of electron states dramatically. On the other hand one needs to keep the number of states relatively small because otherwise the numerics requires an unacceptable computer time. These opposing requirements are optimally fulfilled by an ingenious trick applied by Wilson. One considers a system with $2^{N/2}$ electron states. The conduction band is half filled and symmetric to the Fermi level. For simplicity one assumes a constant density of states and divides all energies by the Fermi energy. Then the conduction band extends from $(-1 : +1)$ as shown in Figure 2. In the next step one divides the lower (and upper) half of the band geometrically into cells with decreasing width so that one obtains an energy frame. In Figure 2 this energy frame has the values $-1$, $-1/2$, $-1/4$, $-1/8$, $-1/16$, $-1/32$, $0$, $1/32$, $1/16$, $1/8$, $1/4$, $1/2$, $1$ and defines $N$ energy cells $\mathcal{C}_e$ (in Figure 2 we have $N = 12$). The number $N$ is always even because there are as many negative as positive Wilson states. Each subdivision adds two states so that the number of subdivisions or iterations is equal to $N/2$.

The four energy cells close to the Fermi level (in Figure 2 $\mathcal{C}_5, \mathcal{C}_6, \mathcal{C}_7, \mathcal{C}_8$) may be considered to possess just one electron state each. The number of states per cell doubles with each step away from the Fermi level. (In Figure 2 $\mathcal{C}_1$ and $\mathcal{C}_2$ have 16 electron states and the whole band has 64.) Wilson reshifted these electron states in each cell in such a way that one of them, the state $c_{\nu}^\dagger$ in the cell $\mathcal{C}_e$, carried the full interaction with the $d$-impurity. The remaining states in the cell have zero interaction and are neglected. The width of the four smallest energy cells in the vicinity of the Fermi level determines the effective energy spacing $\delta E = 2^{-(N/2-1)}$ (in units of the Fermi energy). The effective number of electron states $N_{\text{eff}}$ is determined by the energy spacing at the Fermi level and is given by $N_{\text{eff}} = 2/\delta E = 2^{N/2}$ (for details see the discussion in [12]). According to the construction the number $N$ of Wilson states in FAIR is always even.

The Wilson states have two great advantages: (i) one can represent a band of $2^{N/2}$ electrons by just $N$ Wilson states and (ii) one can double the number of electrons by subdividing the cell directly below and the cell directly above the Fermi level into two equal halves. So the Wilson spectrum achieves the trick at doubling the effective number of states by adding just two states.

**Figure 1:** (a) The electron band of a symmetric Friedel impurity with the $d$-resonance at the Fermi level. (b) The effective band (density of states) after turning on the Coulomb repulsion $U$ and setting $E_d = -U/2$. The Friedel resonances are transformed into broad Hubbard resonances, roughly positioned at $E_d = -U/2$ and $E_d + U = +U/2$, far away from the Fermi level and an extremely narrow Kondo resonance at the Fermi level.
2. Theoretical Background

For the actual calculation I use the FAIR ground state for the different impurities [17–19]. The FAIR technique has been developed during the past few years by the author. FAIR stands for Friedel artificially inserted resonance. The FAIR ground state represents a very good approximation for the Friedel-Anderson and the Kondo impurities. It has reproduced a number of numerical results with good accuracy and produced a number of new results, such as the polarization of the Kondo cloud [20], oscillations in the Kondo cloud [21], Friedel oscillations of the FA impurity [22], and, in the magnetic pseudo-ground state, the magnetic moment [23], which roughly corresponds to the mean field result with half the Coulomb energy $U$ because of the reduced density of states in the $d$-resonances [9]. A review of the FAIR theory is given in [24].

The singlet ground state of the FA impurity, which consists of eight Slater states, was used to calculate the fidelity between the symmetric Friedel and the symmetric FA impurity [12]. Its wave function is essentially the superposition of two magnetic states $\Psi_{MS}$ with opposite magnetic moment. The magnetic state (with net spin-up) has the form

$$\Psi_{MS} = \left[ A a^\dagger_{0i} b^\dagger_{0i} + B a^\dagger_{0i} d^\dagger_i + C d^\dagger_i b^\dagger_{0i} + D d^\dagger_i d^\dagger_i \right] |0_i 0_i\rangle,$$

where $a^\dagger_{0i}$ and $b^\dagger_{0i}$ are two artificial resonance states or fair states in the spin-up and spin-down bands. It is defined and investigated in [9, 23] within FAIR formalism. Its magnetic moment is $|B^2 - C^2|$ in units of $\mu_B$.

The question in this paper is the following: what is the relation between $\Psi_{N-2}$ and $\Psi_N$ in the range of $N$ where the fidelity is constant? I arrive at the following result: for sufficiently large $N$ there is a single-electron state $q_i^\dagger$ such that $\Psi_N \approx q_i^\dagger q_i^\dagger \Psi_{N-2}$ with remarkable accuracy. This conclusion will be derived in detail below. (In this paper I denote single-electron states such as $\{q\}$ by their creation operator $q_i^\dagger$.)

The Kondo and the FA impurity problem have been exactly solved with the Bethe ansatz [13, 14]. I am told that it is very hard to extract the wave function from the Bethe-ansatz. The presently most frequently used numerical method for the investigation of the FA impurity is the numerical renormalization group (NRG) theory, which was developed by Wilson [15] 35 years ago and first applied to the FA impurity by Krishna-murthy et al. [16] in 1980. It derives the ground state through a large number of renormalization steps (of the order of 50 to 100 steps). In each step the number of Slater states is increased by a factor of 16. (A Slater state is defined as the product of $n$ single-electron states.) This yields a huge number of Slater states for the ground state and only a small number of the order of a few thousand Slater states are finally included in the calculation performed.

Suppose that for a half-filled band with $(N-2)$ Wilson states we calculate the ground state $\Psi_{N-2}$ of a given impurity and then repeat the calculation for a system with $N$ Wilson states for the same physical parameters, again half filled. The occupation of each spin band is either $(N-2)/2$ or $N/2$ which I define as $n = N/2$. The ground state with $N$ Wilson states has one additional spin-up electron and one additional spin-down electron. The ground state $\Psi_{N-2}$ can be easily expressed in the new basis. If we denote for a moment the two energy cells next to the Fermi level in the $(N-2)$-basis by $C^-$ and $C^+$ then these cells are each split into half in the $N$-basis. Consequently, the amplitude in each of the new states is just $1/\sqrt{2}$ of the amplitude in the original basis state. So the state $\Psi_{N-2}$ is exactly transferred into the $N$-state Wilson basis.

The composition, for example, of $a^\dagger_{0i}$ in terms of the $N$ Wilson states $c^\dagger_i$ is

$$a^\dagger_{0i} = \sum_{v=1}^{N} a^\dagger_{v} c^\dagger_i.$$

(2)

The fair states assume the effective interaction with the impurity. Since the electron system has two spin subbands one needs two fair states, the state $a^\dagger_{0i}$ for the spin-up subband and the state $b^\dagger_{0i}$ for the spin-down subband. The remaining states $a^\dagger_{i}$ in the spin-up subband are made orthogonal to each other and to $a^\dagger_{0i}$. In addition their free electron Hamiltonian matrix $(a^\dagger_{i} \Omega |H| a^\dagger_{i} \Omega)$ is subdiagonalized (excluding the row and column with $a^\dagger_{0i}$ matrix elements). As a result the state $a^\dagger_{0i}$ becomes an artificial Friedel resonance. The fair state $a^\dagger_{0i}$ determines uniquely the remaining band states $a^\dagger_{i}$ and $b^\dagger_{i}$ for $i \geq 1$ which form a new conduction band with one less electron (for each spin). The half-occupied bands are represented by

$$\langle 0_i | 0_i \rangle = \prod_{i=1}^{N-1} |a^\dagger_{i} b^\dagger_{i} \Phi_{0i}|,$$

where $N = N/2$.

The FA ground state is the normalized superposition of the magnetic states with net spin-up and net spin-down:

$$\Psi_{SS} = \Psi_{MS1} + \Psi_{MS1}.$$

(4)
The state Ψ_{SS} is obtained by reversing all spins in (1) (the spins are ordered in the same fashion as in (1)). The main numerical task is to find the optimal fair states \( a_q^0 \) and \( b_q^0 \) (which occur now in both spin directions). When this is achieved by variation the full wave function can be easily constructed.

The FAIR technique has a number of advantages. (i) Two single-electron states, the fair states \( a_q^0 \) and \( b_q^0 \), determine the full bases of the electron bands parallel and antiparallel to the impurity spin. Each fair state requires only a small number (of the order of 40) of coefficients \( a_q^0 \) of Wilson states. (ii) The ground states for the FA and the Kondo impurity consist of a small number of Slater states. (iii) The single-electron occupations in the different Slater states are well separated insofar as each Slater state possesses either zero, one, or two d-electrons.

So far the error margins of the FAIR technique have not been quantified. However, the quality of reproducing previous results justifies the use of this rather transparent method to predict new phenomena and uncover relationships and coherences, which were not transparent before.

3. Calculation and Results

In this paper I denote the singlet ground state \( \Psi_{SS} \) in the basis of \( N \) Wilson states by \( \Psi_N \). For the FA-impurity \( \Psi_N \) can be written as a sum of (eight) Slater states with \( N/2 \) spin-up and \( N/2 \) spin-down states. Each Slater state \( S^\pm_2 \) is the product of \( N/2 \) spin-up and \( N/2 \) spin-down electron states (creation operators applied to the vacuum state \( \Omega \)) and has a coefficient \( a_{S^\pm_2} \). I denote the sum of all these Slater states including their coefficients by \( A_{S^\pm_2}^\dagger \Omega = \Psi_N \). Similarly one can express the ground state for the \((N-2)\) Wilson basis as \( \Psi_{N-2} = B_{N-2}^\dagger \Omega \). Then one can multiply the state \( \Psi_N \) with the adjoint operator of \( B_{N-2}^\dagger \) that is, the corresponding annihilation operators and form the state

\[
\left( B_{N-2}^\dagger \right)^\dagger A_{S^\pm_2}^\dagger \Omega = B_{N-2}^\dagger A_{S^\pm_2}^\dagger \Omega = a_Q Q_2^\dagger \Omega. \tag{5}
\]

This procedure yields a two-electron state \( a_Q Q_2^\dagger \Omega \) with one electron in each spin. (\( a_Q \) is the amplitude and \( Q_2 \) is normalized.) In the final step I try to express the two-electron state \( Q_2^\dagger \) as the product of a spin-up and a spin-down single-electron state \( q^\uparrow_1 \) and \( q^\downarrow_1 \) with identical orbits:

\[
a_Q Q_2^\dagger \Omega \longrightarrow a_Q^2 q^\uparrow_1 q^\downarrow_1 \Omega. \tag{6}
\]

The value \( a_q \) is the amplitude of the (normalized) state \( q^\dagger \). The absolute value \( |a_q| \) is less than or equal to one. This can be seen in the following way: we form the \( N \)-particle state \( B_{N-2}^\dagger Q_2^\dagger \Omega \) and take the scalar product between \( B_{N-2}^\dagger \Omega \) and \( A_{S^\pm_2}^\dagger \Omega = \Psi_N \):

\[
\langle B_{N-2}^\dagger Q_2^\dagger \Omega | A_{S^\pm_2}^\dagger \Omega \rangle = \langle Q_2^\dagger \Omega | B_{N-2}^\dagger A_{S^\pm_2}^\dagger \Omega \rangle
\]

\[= \langle Q_2^\dagger \Omega | a_Q Q_2^\dagger \Omega \rangle = a_Q, \tag{7}
\]

where (5) is used. The scalar product is equal to \( a_Q \). The absolute value of the scalar product between two normalized \( N \)-electron states is less than or equal to one. Therefore one has \(|a_Q| \leq 1 \). Under optimal conditions the two-electron state \( Q_2^\dagger \) can be factored into two single-electron states, that is, \( a_Q Q_2^\dagger = (a_q q^\dagger_1)(a_q q^\dagger_2) \Omega \). One expects that the coefficient \( |a_q| \) is also less than or equal to one.

After the two ground states \( \Psi_N \) and \( \Psi_{N-2} \) are constructed in form of eight Slater states the calculation of \( B_{N-2}^\dagger A_{S^\pm_2}^\dagger \Omega \) consists mainly of scalar products between different \((n-1)\)-electron states \((n = N)/2\). The latter are determinants of single-electron scalar products. The resulting coefficients of \( a_Q Q_2^\dagger \Omega \) form a quadratic \((N+1) \times (N+1)\)-matrix in terms of \( N \) Wilson states plus one \( d \)-state for each spin. In the last step the two-electron state \( a_Q Q_2^\dagger \Omega \) is split into the product \((a_q q^\dagger_1)(a_q q^\dagger_2) \Omega \). This procedure is remarkably easy. Already the square root of the diagonal elements in \( a_Q Q_2^\dagger \Omega \) yields the absolute value of the coefficients of \((a_q q^\dagger_1)\Omega \), and the sign follows from the nondiagonal elements.

Table 1 shows the value \(|a_q| \) for a number of systems. The first column gives the impurity, the second the \( s-d \)-hopping strength, and the third column the number \( N \) of Wilson states. There are three different values of \( N \) used, \( N = 42, 32 \), and \( 22 \). The corresponding values of the smallest energy spacing are \( 2^{-20} \approx 10^{-6}, 2^{-15} \approx 3 \times 10^{-5} \), and \( 2^{-10} \approx 10^{-3} \).

For the FA impurities I used \( U = 1 \) and \( E_d = -0.5 \). In all these cases the split of the two-particle state \( a_Q Q_2^\dagger \Omega \) into two identical single-particle states with opposite spin worked very well. The coefficient \( a_q \) in column four is very close to one. The fifth column gives the Gaussian deviation \( E_d \) between \( a_Q Q_2^\dagger \Omega \) and \((a_q q^\dagger_1)(a_q q^\dagger_2) \Omega \). Obviously as soon as the smallest energy in the Wilson spectrum \( \delta E \) is sufficiently small compared to the resonance width of the impurity at the Fermi level then the state \( q^\dagger_1 \) is well defined and almost perfectly normalized. This means that the state \( \Psi_N \) can be constructed from the state \( \Psi_{N-2} \) by the relation

\[\Psi_N \equiv q^\dagger_1 q^\dagger_2 \Psi_{N-2}. \tag{8}\]

In all cases the extracted state \( q^\dagger_1 \) is mainly composed of basis states close to the Fermi level. In Table 1 the two last columns give the amplitudes of the state \( q^\dagger_1 \) below and at the new Fermi level in terms of Wilson states. These amplitudes agree almost perfectly.

Figure 3 shows the coefficients of \( q^\dagger_1 \) with respect to the Fermi level for pure Friedel impurities with \( N = 42 \) and very different \( s-d \)-hopping strengths \(|V_{sd}|^2\). It also shows the corresponding coefficients of \( q^\dagger_1 \) for FA impurities with \( N = 42 \) and different \(|V_{sd}|^2\) (which yield many orders of magnitude of different Kondo energies). In addition Figure 3 shows the effect of different \( N \) for a FA impurity with \(|V_{sd}|^2 = 0.05, U = 1 \), and \( E_d = -0.5 \). The Kondo energy is about \( 3.9 \times 10^{-3} \). For \( N = 22 \) the smallest energy spacing is about \( 10^{-3} \). Still the \( N = 22 \) curve is relatively close to the universal curve although Table 1 shows that its \(|a_q| \) is 0.979 is less close to one than for larger \( N \). For values of \( N \) where the smallest level spacing is of the order of the Kondo energy or larger the value of \( a_q \) decreases. Then the state \( \Psi_N \) can no longer be expressed as \( q^\dagger_1 q^\dagger_2 \Psi_{N-2} \) and the splitting of \( Q_2^\dagger \) into
The interpretation of the above results is that the complexity of the solutions of the FA and the Kondo impurity is not felt at energies sufficiently below the Kondo energy. We know from Wilson’s renormalization calculation that the structure of the ground state changes dramatically when the smallest level spacing $\delta E$ is of the order of the Kondo energy. After this metamorphosis the renormalization approaches a fixed point. From this behavior Nozieres [25] developed the Fermi liquid theory of the Kondo impurity (which applies also to the FA impurity). The present calculation provides quantitatively a universal state $q^1$, which has to be incorporated into the ground state for both spins when the Wilson basis is increased by 2 states. The fact that this is the same state for any impurity with a resonance at the Fermi level demonstrates that the Kondo and FA impurities have a resonance at the Fermi level. The result suggests an induction rule for the ground state with increasing number of Wilson states.

The accuracy of relation (8) is given by the scalar product between the left and right side. This is for the FA impurity and $N = 42$ already 0.996 (i.e., equal to $|\alpha_q|^2$) and approaches the value one with increasing $N$.

The fact that $q^1$ is the same state for any impurity with a resonance at the Fermi level is at the heart of our earlier discussed fidelity calculations. The fidelity is the scalar product between the ground states of the symmetric Friedel and FA impurities, $\langle \Psi_F^{\uparrow} | \Psi_{FA}^{\uparrow} \rangle$, which is compared with the corresponding scalar product in the ($N - 2$)-basis $\langle \Psi_{N-2}^{\uparrow} | \Psi_{N-2}^{FA \uparrow} \rangle$. (In both cases the bands are half-filled.) According to our present result we can express the latter as

$$\langle \Psi_N^{\uparrow} | \Psi_{N-2}^{FA \uparrow} \rangle \equiv \langle q^1_1 q^\dagger_{N-2} | q^1_1 q^\dagger_{N-2} \Psi_{N-2}^{FA \uparrow} \rangle = \langle \Psi_{N-2}^{\uparrow} | \Psi_{N-2}^{FA \uparrow} \rangle.$$

This relation confirms that the fidelity between the symmetric FA and the symmetric Friedel impurity approaches a finite value with increasing $N$ and does not experience an Anderson orthogonality catastrophe. Equation (8) yields an asymptotic recursion formula to construct $\Psi_N$ from a given $\Psi_{N_0}$, where $N_0$ is sufficiently large so that the smallest level spacing in the $N_0$-Wilson basis is smaller than the Kondo energy.

### 4. Conclusion

In the Wilson basis one can easily introduce two new states by splitting each of the states directly below and above the center of the band into two states of equal weight, creating
out of two old states four new ones. This reduces the smallest energy spacing by a factor of two and increases the effective number of states $N_{eff}$ by a factor of two. The relation between the ground states $\Psi_{N_{\text{sym}}}^N$ and $\Psi_{N_{\text{asym}}}^N$ of the two half-filled bands is investigated for several symmetric impurities, the Friedel, the Friedel-Anderson, and the Kondo impurity. The ground states are calculated with the FAIR technique. We observe that for sufficiently large $N$ the ground state $\Psi_{N_{\text{sym}}}^N$ can be obtained from $\Psi_{N_{\text{sym}}}^{N-2}$ by multiplying $\Psi_{N_{\text{sym}}}^{N-2}$ by two single-particle states $q^1_\uparrow$ and $q^1_\downarrow$. The composition of these states $q^1_\uparrow$ with respect to the Fermi level is independent of $N$ (for sufficient large $N$) and is independent of the resonance width of the impurity. This qualifies the state $q^1_\uparrow$ to be called universal. The state $q^1_\uparrow$ is not just universal for a given kind of impurity. It is superuniversal because it is even independent of the kind of impurity as long as the impurity has a resonance directly at the Fermi level. In particular it is independent of the complexity of the ground state of the FA or the Kondo impurity. All the complexity happens further away from the Fermi level. This result gives a simple confirmation and explanation of our previous fidelity calculations [12]. A similar investigation for the asymmetric FA impurity is in progress.

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