The Inner Life of the Kondo Ground State: An Answer to Kenneth Wilson’s Question

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Abstract

The Kondo ground state has been investigated by numerical and exact methods, but the physics behind these results remains veiled. Nobel prize winner Wilson, who engineered the break through in his numerical renormalization group theory, commented in his review article ”the author has no simple explanation ...for the crossover from weak to strong coupling”. In this article a graphical interpretation is given for the extraordinary properties of the Kondo ground state. At the crossover all electron states in the low energy range of $k_B T_K$ are synchronized. An internal orthogonality catastrophe is averted.

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1 Introduction

This year 2014 is the fiftieth anniversary of Kondo’s [1] seminal paper ”Resistance minimum in Dilute Magnetic Alloys” and the fortieth anniversary of Wilson’s [2] renormalization paper about the Kondo effect. For 50 years the Kondo effect has been investigated with the most sophisticated theoretical methods [3], [4], [5], [6], [7], [8], [9], [10], [11], [12], [13], [14], [15]. Kondo [1] solved the puzzle of the low-temperature resistance increase in dilute magnetic alloys [16] above the Kondo temperature $T_K$. Wilson calculated the Kondo ground-state properties with a numerical renormalization, known as NRG theory. He observed a crossover from weak to strong coupling with increasing $n$ (number of renormalization steps). In this article the FAIR solution of the Kondo ground-state [17] is applied to reproduce and interpret Wilson’s results (FAIR=Friedel artificially inserted resonance).
2 Wilson’s Numerical Renormalization Theory

The interaction between a magnetic impurity and the conduction electrons can be described by an exchange interaction with the potential $-2J(S \cdot s) \delta(r)$, $J < 0$ where $S$, $s$ are the spins of the impurity and the conduction electrons. Wilson invented and applied a number of tricks to tackle the Kondo ground-state. Using a band with a constant density of states and a band width of $2W$ he divided all energies by $W$, yielding a band range $(-1 : 1)$ with the Fermi level at 0. Then Wilson made the (almost) infinite number of $s$-electron states $\varphi_k \dagger$ manageable by dividing the band into energy cells. (I use the same symbol for a state, (for example $\varphi_k$), when addressing it by a creation operator $\varphi_k \dagger$, an annihilation operator $\hat{\varphi}_k$ or as a wave-function $\tilde{\varphi}_k(r)$).

In Fig.4 in the appendix Wilson’s sub-division is shown. The ranges $(-1 : 0)$ and $(0 : 1)$ are split at $\pm 1/2, \pm 1/4, \pm 1/8, ..., \pm 1/2 \nu, ..., \pm 1/2 \infty$. In the next step Wilson combined all states $\varphi_k$ within each cell $C_\nu$ into a single state $c_\nu \dagger$ (as the normalized sum of all states $\varphi_k$ within the cell). These states $c_\nu$ I will call Wilson states. They contain the full interaction of all electrons in the cell with the impurity.

From these states $c_\nu$, Wilson constructed a series of new states $f_{\mu} \dagger$. The state $f_0 \dagger$ is the normalized sum of all the original band states $\varphi_k \dagger$. It is concentrated at the impurity, being a Wannier state of the $s$-band. The next state $f_1 \dagger$ surrounds the inner state $f_0 \dagger$ and is itself surrounded by $f_2 \dagger$, etc. All the $f_\mu \dagger$ surround the magnetic impurity like onion shells. Their width in real space increases each time by a factor of two. Wilson chose the states $f_{\mu, \sigma} \dagger$ in such a way that their Hamiltonian is that of a linear chain with next nearest neighbor coupling. Only the states $f_0 \dagger, \sigma$ interact with the impurity. He solved this Hamiltonian by renormalization, i.e. by initially cutting off the chain at a small $n$ and solving the resulting Hamiltonian $H_n$ by diagonalization. With the eigenstates of $H_n$ and the states $f_{(n+1)\uparrow}, f_{(n+1)\downarrow}$ Wilson built the next Hamiltonian $H_{n+1}$. This NRG cycle is repeated. The number of basis states increases at each NRG step by a factor of four (yielding $4^n$) but is generally limited to the 1000 states with the lowest energies.

Wilson compared the resulting excitation spectrum for a finite exchange interaction, for example $J = -0.055$, with the spectrum for $J = 0$ and $J = -\infty$. For a small number $n$ of NRG steps the spectrum of $H_n$ resembled that of $J = 0$. But after a critical number $n_0$ the spectrum crossed over, resembling the strong coupling case $J = -\infty$. In addition, Wilson observed that the effective number of band electrons changed from odd to even at the transition.

With this work Wilson achieved a break through in the low-temperature properties of the Kondo effect. From the flow diagram and the fixed-point properties he obtained an effective Hamiltonian for low temperatures. Evaluation of his numerical results lead Nozieres [7] to the Fermi-liquid description of the Kondo ground-state.

Despite this great success, it appears that Wilson was not completely satisfied with his achievement. In his review article about the Kondo renormalization Wilson wrote ([2], page 810): "Why the crossover from weak to strong coupling takes place will not be explained. The author has no simple physical explanation for it. It is the result of a complicated..."
Numerical calculation”.

The reason that Wilson had no simple interpretation of his results, i.e., that the physics of the Kondo ground-state is so veiled, is due to the fact that the wave function of the ground-state is so intangible. In NRG only a tiny fraction of the ground-state Slater states can be maintained, which makes it very difficult to uncover the hidden physics. Unfortunately the exact solution using the Bethe-ansatz [12], [13], [14] does not help because it is very difficult to extract the wave function from this ansatz.

3 Magnetic and Kondo Ground-State in FAIR

The author has developed in the past years a very compact solution for the Kondo ground-state. It is known as the FAIR solution of the Kondo ground-state. A short review is given in the festschrift to Jaques Friedel’s 90’s birthday [17] with extended references therein. Although it is not an exact solution as the Bethe-ansatz, it describes the physics of the Kondo ground-state very well, and it is well equipped to answer Wilson’s implicit questions behind the physics of the NRG cross-over.

Kondo and Wilson used a rigid magnetic impurity in their initial calculations. However, the most common group of magnetic impurities are 3d-atoms dissolved in a host. These impurities possess d-resonances. Friedel [18] and Anderson [19] showed that a sufficiently large Coulomb exchange interaction between opposite d-spins creates a magnetic moment in the d-states. Anderson reduced the ten-fold degeneracy of the FA-impurity to a two-fold degeneracy, making it de facto an impurity with \( l = 0 \) and \( s = 1/2 \) (it is still called a d-impurity). This Anderson model is used in most theoretical calculations of the Kondo effect of d-impurities. Schrieffer and Wolff [20] showed that for sufficiently strong Coulomb interaction the Anderson model yields the Kondo effect. Krishna-murthy, Wilkins, and Wilson [5] performed NRG calculations for the FA-impurity and obtained an equivalent crossover. Here I will discuss the Kondo ground-state of the d-impurity because it demonstrates an interesting feedback of the singlet state on the electronic structure of its magnetic components.

In the FAIR approach we use the same trick as Wilson to reduce the large number of s-electron states. The positive and negative bands of s-electrons are repeatedly sub-divided. But we stop the sub-division when a given number \( N = 2n \) of energy cells \( \mathcal{E}_{\nu} \) is obtained, \( n \) cells below and \( n \) cells above the Fermi level at energy zero. For each energy cell a Wilson state is constructed. Then the smallest level spacing between the resulting Wilson states is (next to the Fermi level) equal to \( \delta = 2^{-n+1} \) (in units of \( \varepsilon_F \) or \( W \)). The corresponding size of the host is \( R \approx 2^n \lambda_F / 4 \) where \( \lambda_F \) is the Fermi wave length. As in NRG the sample size doubles when \( n \) is increased by one. Out of the Wilson states two fair states \( a_{0\uparrow}^\dagger \) and \( b_{0\downarrow}^\dagger \) of spin-up and down are composed.

The easiest way to explain the logic behind the FAIR approach is to compare it with a monarch whose subjects elect an ombudsman. This ombudsman does all the negotiation with the king relieving all the other subjects from this duty. In our case the \( d_{\uparrow}^\dagger \)-state is the king and the spin-up s-states \( c_{\nu\uparrow}^\dagger \) are the subjects. The latter elect the fair state \( a_{0\uparrow}^\dagger \) as
ombudsman who now exclusively negotiates with the $d^\uparrow$-state. This negotiation occurs in form of s-d-hopping between $d^\uparrow$ and $a^\dagger_{0\uparrow}$, from which the remaining subjects $a^\dagger_0$ are excluded. Their only function is to optimally elect and equip the ombudsman, i.e. fair state. (Of course, the remaining $(N-1)$ s-states $c^\dagger_{\nu \downarrow}$ have to be rebuilt so that they are orthogonal to $a^\dagger_{0\uparrow}$, orthonormal to each other and diagonal in the band Hamiltonian $H^0$. Because of the spin, there is a second royal copy, consisting of $d^\downarrow$ and $b^\dagger_{0\downarrow}$. In the appendix the FAIR method is summarized for a simple Friedel resonance.

This idea may appear too simple to work but actually it yields a much better magnetic state for the Anderson model than the mean field theory \cite{21}. Equation (1) shows the structure of the magnetic state. For sufficiently strong Coulomb interaction it assumes a magnetic moment, i.e. $|B|^2 \neq |C|^2$. For $|B|^2 >> |A|^2, |C|^2, |D|^2$ the net d-spin is down. The Coulomb repulsion affects only the term $Dd^\dagger_\downarrow d^\dagger_\uparrow$ and the s-d-hopping is, for example, observed between the terms $Ba^\dagger_{0\uparrow}d^\dagger_\downarrow, Aa^\dagger_{0\uparrow}b^\dagger_{0\downarrow}$. The two half-filled FAIR bands $|0_{a^\dagger_1}\rangle = a^\dagger_1...a^\dagger_{n_1}\Omega$ and $|0_{b^\dagger_1}\rangle = b^\dagger_1...b^\dagger_{n_1}\Omega$ don’t participate in any of the interactions ($\Omega =$ vacuum state).

$$\Psi_{MS\downarrow} = \left[ Aa^\dagger_{0\uparrow}b^\dagger_{0\downarrow} + Ba^\dagger_{0\uparrow}d^\dagger_\downarrow + Cd^\dagger_\uparrow b^\dagger_{0\downarrow} + Dd^\dagger_\uparrow d^\dagger_\downarrow \right]|0_{a^\dagger_1}\rangle |0_{b^\dagger_1}\rangle$$ (1)

Fig.1 shows the electron structure of a magnetic d-impurity in the FAIR description graphically. If one suppresses the spin-flip processes then one obtains an enforced magnetic ground-state $\Psi_{MS\downarrow}$ with net spin-down moment. The spin-up and -down FAIR bands are shown in the $\{a^\dagger_{i\uparrow}\}$- and $\{b^\dagger_{i\downarrow}\}$-bases. The d-states are drawn to the left and right of the FAIR bands. The circles within the FAIR bands represent the fair states $a^\dagger_{0\uparrow}$ and $b^\dagger_{0\downarrow}$, white is empty and black is occupied. The figure shows the Slater state with the largest amplitude. The double arrows indicate the transitions between the d- and the fair states via s-d-coupling. One obtains for the magnetic state a total of four Slater states with the four possible occupations of d- and fair states as shown in equ. (11). The explicit form of the magnetic solution is obtained by varying the composition of the two fair states $a^\dagger_{0\uparrow}$ and $b^\dagger_{0\downarrow}$ and minimizing the energy expectation value of the Anderson Hamiltonian. The fair states determine the remaining FAIR band states $a^\dagger_{i\uparrow}, b^\dagger_{i\downarrow}$ and the coefficients $A, .., D$ uniquely.

Although the total spin of $\Psi_{MS\downarrow}$ in equ. (11) is zero the d-impurity possesses a finite magnetic moment. The band electrons which appear to compensate the moment are pushed to the surface of the host.
If one reverses all spins in Fig.1 then one obtains an impurity $\Psi_{MS\uparrow}$ with net spin up. (A modified version of) Both states together will form the Kondo ground-state. But let us first consider the enforced magnetic state $\Psi_{MS\downarrow}$ with a net d-spin down. Its half-filled band states are $|0_a\uparrow\rangle|0_b\downarrow\rangle$. Since the orbital wave functions $a_i^\uparrow$ and $b_j^\downarrow$ of the fair states are different the corresponding bands $\{a_i^\uparrow\}$ and $\{b_j^\downarrow\}$ are different too (the net spin of the impurity breaks the up-down symmetry). Any transition between $\Psi_{MS\downarrow}$ and $\Psi_{MS\uparrow}$ contains the multi-electron scalar products (MESP)

$$\langle 0_b\downarrow|0_a\uparrow|0_b\downarrow\rangle = \langle 0_b\downarrow|0_a\uparrow\rangle \langle 0_a\uparrow|0_b\downarrow\rangle = |\langle 0_a|0_b\rangle|^2$$

(2)

The MESP $\langle 0_a|0_b\rangle$ is often called the fidelity $F$. It can be calculated from the $\Psi_{MS\downarrow}$ alone if one takes only the orbital parts of $|0_a\uparrow\rangle$ and $|0_b\downarrow\rangle$. The single electron states $a_i^\uparrow$ and $b_j^\downarrow$ in Fig.1 experience the opposite polarization potential. Therefore one expects that $\langle 0_a|0_b\rangle$ in equ. (2) decreases with increasing electron number or volume. It should show an orthogonality catastrophe.

### 4 Internal Orthogonality Catastrophe

We first check the fidelity $\langle 0_a|0_b\rangle$ for the (enforced) magnetic state $\Psi_{MS\downarrow}$ as a function of $n$ (where $n$ is half the number of Wilson states, $n = N/2$). The smallest level spacing is $2^{-n+1}$ and the effective size of the host is $2^n \lambda_F/4$. In Fig.2 the logarithm of the fidelity $\ln (F) = \ln \langle 0_a|0_b\rangle$ is plotted as a function of $n$ for the magnetic state of a d-impurity (stars). The parameters of the d-impurity are: d-state energy $E_d = -0.5$, Coulomb energy $U = 1$ and s-d-hopping matrix element $|V_{sd}|^2 = 0.03$. We find a linear dependence of $\ln (F)$ on $n$, i.e., the fidelity $\langle 0_a|0_b\rangle$ decreases exponentially with $n$. This causes an internal orthogonality catastrophe (IOC), in analogy to Anderson’s orthogonality catastrophe [22].
This IOC makes the transition matrix element between $\Psi_{MS\downarrow}$ and $\Psi_{MS\uparrow}$ arbitrarily small for large sample volume and would prevent any energy reduction in the singlet state. Therefore the IOC has to be averted in the Kondo ground-state.

When spin-flip processes are permitted between $\Psi_{\downarrow}$ and $\Psi_{\uparrow}$ then the system forms a singlet state. A new optimization yields new compositions of the *fair* states $a_0^\dagger$ and $b_0^\dagger$ which yields new FAIR bands. The ground-state is the (normalized) sum of the state in Fig.1 and its spin-inverted image. The composition of $\Psi_{MS\downarrow}$ and $\Psi_{MS\uparrow}$ changes to a very different form which I denote as $\Psi_{SS\downarrow}$ and $\Psi_{SS\uparrow}$ and the singlet ground-state is the normalized sum of $\Psi_{SS\downarrow}$ and $\Psi_{SS\uparrow}$. Now the fidelity shows a completely different behavior (full circles in Fig.2). At about $n = 15$, the fidelity becomes constant. The singlet state prevents the IOC. As we will see below this transition into a constant fidelity at about $n = 15$ is closely related to Wilson’s track change in the NRG ladder.

![Fig.2: The internal fidelity in the magnetic state (stars) and the singlet state (full circles) as a function of $n$. (2n is the number of Wilson states per spin. The radius of the host is $2^n \lambda_F / 4$).](image)

5 Energy Shifts due to the Magnetic Impurity

The formation of the singlet ground-state has a dramatic effect on the electronic band structure. This becomes even more obvious when one investigates the energy spectrum $E_{i}^{a}$ and $E_{i}^{b}$ of the two FAIR-bands. In the absence of the d-impurity the energy spectra for spin-up and down are, of course, equal. We denote these initial energies as $\varepsilon_{i}$. \{For the first $n - 1$ states this energy depends exponentially on $i$ and has the values $\varepsilon_{i} = -3/2 * 2^{-i}$, while $\varepsilon_{n} = -2^{-n}$. Above the Fermi level one has the mirror image of the negative energies. The total number of Wilson states for a given $n$ is $N = 2n$. (The FAIR bands have one state less).\}

Now we can plot the relative energy shift $r_{i} = (E_{i} - \varepsilon_{i}) / (\varepsilon_{i+1} - \varepsilon_{i})$ for the two FAIR
bands, the \( \{a_i^\dagger\} \) - and the \( \{b_i^\dagger\} \) -band as a function of \( i \). This is done in Fig.3. The abscissa gives the number \( i \) of the (energy ordered) Wilson states. The second abscissa below is the corresponding energy scale.

We first discuss the energy shift in the magnetic state \( \Psi_{MS\downarrow} \) (open triangles) (they are the same in \( \Psi_{MS\uparrow} \)). The increase of \( r_i \) from the left to the right of Fig.3 is due to the fact that the FAIR bands have one state less than the band of Wilson states. The value of \( r_i \) represents essentially the phase shift of the state \( a_i^\dagger \) or \( b_i^\dagger \) in units of \( \pi \). One recognizes that \( r_i \), i.e. the phase shifts are very different for the FAIR bands anti-parallel and parallel to the net spin of the impurity. Close to the Fermi level the difference in \( r_i \) is almost equal to one, i.e. one level spacing.

![Fig.3: The relative energy shifts \( r_i \) of the FAIR bands \( \{a_i^\dagger\} \) and \( \{b_i^\dagger\} \) as a function of \( i \) or energy (lower scale) for the magnetic state \( \Psi_{MS\downarrow} \) (open symbols) and the component \( \Psi_{SS\uparrow} \) of the singlet state (full symbols).](image)

In the singlet state the relative energy shift \( r_i \), shown as full triangles, presents a rather fascinating behavior. For \( |E| > 2^{-10} \) the values of \( r_i \) for the singlet and magnetic states are quite close. However, if one approaches the low energy region, \( |E| < 2^{-15} \), then the band energies \( E_a^i \) and \( E_b^i \) move towards each other and become essentially identical. The corresponding states \( a_i^\dagger \) and \( b_i^\dagger \) become synchronized. As a consequence the internal orthogonality catastrophe is averted in the Kondo ground-state.

The physical reason for the synchronization at low energy is the following. In the Kondo ground-state one has a competition between polarization energy and spin-flip energy. The spin-flip energy likes the two FAIR bands \( \{a_i^\dagger\} \) and \( \{b_i^\dagger\} \) to be synchronized because its (transition) matrix element is proportional to \( |\langle 0 |a|0_b \rangle|^2 \). The polarization energy wants to
shift the \( \{ a^\dagger \} \) and \( \{ b^\dagger \} \) bands in opposite directions. At large (absolute) energies \(|E|\) the polarization energy wins. Only for small energies of the order of \( k_B T_K \) (i.e. \( n > n_0 \)) does the spin-flip gain a minor victory by synchronizing the two bands in the very small energy range of the Kondo energy.

The synchronization of the two electron bases close to the Fermi level, i.e. the suppression of the internal orthogonality catastrophe, is therefore a characteristic property of the Kondo ground-state. In the process the two \textit{fair} states \( a^\dagger_0 \) and \( b^\dagger_0 \) dramatically change their composition. In the singlet state for \( n > n_0 \) they increase their weight at very small energies.

Wilson’s renormalization can be roughly visualized by means of the single Fig.3. The figure corresponds to roughly \( n = 30 \) NRG steps. If one wants to visualize the situation after 10 NRG steps one removes in Fig.3 the inner section for \( 11 \leq i \leq 50 \) and joins the remaining outer parts, then one obtains, at least qualitatively, the relative energy shifts \( r_i \) for \( n = 10 \). One easily recognizes that the crossover has not yet taken place. In our case it occurs in the range \( 13 < n < 17 \).

6 The Physics of the Bound Electron in the Singlet State

Wilson observed in his normalization sequence that the spectrum changed as if one electron was removed at the Fermi level when the system had crossed over from weak to strong coupling. The general interpretation is that the impurity has bound one conduction electron and formed a singlet state, removing this electron from the band.

In Fig.3 one recognizes that for the singlet state and \( n = 30 \) the energies \( E^a_i \) and \( E^b_i \) (for the same \( i \) close to the Fermi level, i.e. close to \( n = 30 \)) possess the same energy. An even number of band electrons fills the two FAIR bands up to the same energy.

If one removes the inner forty states (as discussed above) then one obtains roughly the energy shifts for \( n = 10 \). Now the energy shifts \( r_i \) for the two FAIR bands in the singlet state differ roughly by one, \( \Delta r_i = r^a_i - r^b_i \approx 1 \) or \( (E^a_i - E^b_i) \approx (\varepsilon_{i+1} - \varepsilon_i) \). Here the energies \( E^a_i \) lie about one level higher than \( E^b_i \) (for the same \( i \)). Now an odd number of electrons would fill the two FAIR bands up to the same energy. This is exactly what Wilson observed. It is due to the synchronization of the electron states within \( k_B T_K \) of the Fermi level. Of course, this is only possible when there are levels within \( k_B T_K \) of the Fermi level. For a spherical host this requires that the radius is larger than the Kondo length.

7 Summary

In summary the synchronization of the FAIR band states close to the Fermi level averts the internal orthogonality catastrophe between the states \( \Psi_{SS^\uparrow} \) and \( \Psi_{SS^\downarrow} \). It arises because it permits the system to lower its potential energy due to a tiny but finite spin-flip energy between these two states. It is also this synchronization that appears to remove an electron.
from the conduction band. At the same time the composition of the fair states $a_0^\dagger$ and $b_0^\dagger$ changes dramatically, which in turn changes the spectrum of the two FAIR bands. This changes the charge distribution around each $\Psi_{SS\sigma}$ within a radius of the Kondo length, that is known as the Kondo cloud. It is this low energy synchronization process which makes the Kondo effect such a extraordinary phenomenon.

This might be the physical interpretation Wilson was looking for.
A Definition of Wilson states

The ranges \((-1:0)\) and \((0:1)\) are split at \(\pm 1/2, \pm 1/4, \pm 1/8, \ldots \pm 1/2^\nu, \ldots \pm 1/2^\infty\). In the next step Wilson combined all states \(\varphi_k^\dagger\) within each cell \(\mathcal{E}_\nu\) into a single state \(c_\nu^\dagger\) (as the normalized sum of all states \(\varphi_k^\dagger\) within the cell). These states \(c_\nu^\dagger\) I will call Wilson states. They contain the full interaction of all electrons in the cell with the impurity.

![Diagram](image_url)

Fig.4: The energy cells \(\mathcal{E}_\nu\), the definition of the Wilson states \(c_\nu^\dagger\) and their energies \(\varepsilon_\nu\).

B Summary of the FAIR method

The FAIR ansatz can be best explained by the example of a spinless Friedel resonance. In this case one has a (conduction) band of \(N\) states \(\{c_\nu^\dagger\}\) and a single (non-magnetic) d-impurity, the so-called d-resonance. The d-state couples to every band state through the s-d-matrix element \(V_{sd}\). In the FAIR ansatz one constructs one fair state \(a_0^\dagger\) out of the band states, i.e. as a normalized superposition of band state wave functions. In the ground-state only this fair state interacts with the d-state. From the remaining \((N-1)\) band states a new FAIR band \(\{a_i^\dagger\}\) is constructed. (First the \(a_i^\dagger\) are made orthogonal to \(a_0^\dagger\) and orthonormalized. Then the band-Hamiltonian \(H_{0,ij} = \left< a_i^\dagger \Omega | H^0 | a_j^\dagger \Omega \right>\) for \(i, j > 0\) is diagonalized). The fair state \(a_0^\dagger\) is an artificial Friedel resonance; it is coupled to each of the new band states \(a_i^\dagger\) by a matrix element \(V_{fr}^i\). The original band Hamiltonian \(H^0 = \sum_\nu \varepsilon_\nu c_\nu^\dagger c_\nu\) is transformed
into a Hamiltonian with an (artificial) resonance state $a_0^\dagger$

$$H^0 = \sum_{i=1}^{N-1} E_i a_i^\dagger a_i + E^0 a_0^\dagger a_0 + \sum_{i=1}^{N-1} V_{fr}^i \left( a_i^\dagger a_0 + a_0^\dagger a_i \right)$$

In the ground-state the d-state couples only to the fair state by the matrix element $V_0^{sd}$ (which yields a $2 \times 2$ matrix) and the ground-state for a half-filled band becomes

$$\Psi_{FR} = \left( A a_0^\dagger + B d^\dagger \right) \prod_{i=1}^{n-1} a_i^\dagger \Omega \quad (3)$$

Remarkably equ. (3) represents the exact ground-state of the Friedel resonance, and it has the advantage that it separates the states with zero and one d-state.

For the Friedel resonance the composition of the fair state $a_0^\dagger$ is given by an exact formula. In other cases such as the Kondo impurity one obtains the fair states by variation (i.e. minimizing the ground-state energy).

C The Kondo ground-state for $J = -\infty$, an exact FAIR solution

Actually the wave function of the Kondo ground-state for $J = -\infty$, which Wilson and others used, is a very simple example of a FAIR solution. If for example the impurity spin points down ($S_\downarrow$) then the term $-2JS_\downarrow S_z \delta (r)$ attracts all anti-parallel spin-up states with a finite amplitude at $r = 0$ and builds out of all band states a new state $\tilde{a}_{0\uparrow} (r)$ with the maximum amplitude at $r = 0$. It is given by

$$\tilde{a}_{0\uparrow} (r) = \frac{1}{A} \sum_{\nu} \tilde{c}_{\nu\uparrow}^* (0) \tilde{c}_{\nu\uparrow} (r)$$

where $\tilde{c}_{\nu\uparrow}^* (0)$ is the conjugate complex amplitude of the Wilson state $\tilde{c}_{\nu\uparrow} (r)$ at $r = 0$ and $A$ is the renormalization factor.

If the band has $N$ states $\tilde{c}_{\nu\uparrow} (r)$ (or $c_{\nu\uparrow}$) then the remaining $(N - 1)$ states have to be rebuilt so that they are orthogonal to $\tilde{a}_{0\uparrow} (r)$, orthonormal to each other and diagonal in the band Hamiltonian $H^0$. We call this new band $\left\{ a_{i\uparrow}^\dagger \right\}$, $i > 0$ a FAIR band. Actually the impurity spin $S_\uparrow$ not only transforms the anti-parallel conduction band but also the parallel one. In the latter any state with a finite amplitude at $r = 0$ is forbidden. This means that all spin-down band states have to be orthogonal to $\tilde{a}_{0\downarrow} (r)$. Since the orbital parts of $a_{0\uparrow}$ and $a_{0\downarrow}$ are identical the corresponding band states $a_{i\uparrow}$ and $a_{i\downarrow}$ possess the same orbital wave functions.

If we ignore the spin-flip part of the exchange interaction for a moment then we obtain the magnetic ground-state

$$\Psi_{MS,\downarrow} = S_\downarrow a_{0\uparrow}^\dagger |0_{a\uparrow}\rangle |0_{a\downarrow}\rangle \quad (4)$$
where \( |0_{\uparrow}\rangle = \prod_{i=1}^{n} a_{i\uparrow}^{\dagger} \Omega \) represents the half-filled \( \{ a_{i\uparrow}^{\dagger} \} \)-bands for spin up (\( \Omega \) is the vacuum state). The states \( a_{0\uparrow}^{\dagger} \) and \( a_{0\downarrow}^{\dagger} \) are artificial Friedel resonance states, denoted as *fair* states. The band states \( \{ a_{i\uparrow}^{\dagger} \} \) and \( \{ a_{i\downarrow}^{\dagger} \} \), \( (i > 0) \) represent two new conduction bands, the FAIR bands.

If one includes the spin-flip terms in the Hamiltonian then equ. (5) represents the ground-state of the Kondo impurity. It is a simple version of a FAIR ground-state which is an exact solution for \( J = -\infty \).

\[
\Psi_0 = \frac{1}{\sqrt{2}} \left( S_{\downarrow} a_{0\uparrow}^{\dagger} - S_{\uparrow} a_{0\downarrow}^{\dagger} \right) |0_{\uparrow}\rangle |0_{\downarrow}\rangle \tag{5}
\]

For \( J = -\infty \) the anti-parallel and the parallel *fair* states have the same orbital wave function \( \tilde{a}_0 (r) \). This is no longer the case for a finite value of \( J \).

## D The magnetic mean field solution

It is worth noting that Anderson’s mean field solution for the magnetic state can be exactly expressed by a FAIR solution with the appropriate *fair* states. But it is not the optimal magnetic state. By optimizing the two *fair* states \( a_{0\uparrow}^{\dagger} \) and \( b_{0\uparrow}^{\dagger} \) one finds a different magnetic solution which has a considerably lower ground-state energy [21]. This FAIR solution requires twice the Coulomb exchange energy as in mean-field theory to form a magnetic moment. The FAIR approach should be included in spin-density functional theory calculations of the magnetic moment of single impurities because its solution is superior to the presently applied mean-field approximation.
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