Oscillations of the magnetic polarization in a Kondo impurity at finite magnetic fields.

Gerd Bergmann
Department of Physics
University of Southern California
Los Angeles, California 90089-0484
e-mail: bergmann@usc.edu

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Abstract

The electronic properties of a Kondo impurity are investigated in a magnetic field using linear response theory. The distribution of electrical charge and magnetic polarization are calculated in real space. The (small) magnetic field does not change the charge distribution. However, it unmasks the Kondo cloud. The (equal) weight of the d-electron components with their magnetic moment up and down is shifted and the compensating s-electron clouds don't cancel any longer (a requirement for an experimental detection of the Kondo cloud). In addition to the net magnetic polarization of the conduction electrons an oscillating magnetic polarization with a period of half the Fermi wave length is observed. However, this oscillating magnetic polarization does not show the long range behavior of Rudermann-Kittel-Kasuya-Yosida oscillations because the oscillations don't extend beyond the Kondo radius. They represent an internal electronic structure of the Kondo impurity in a magnetic field.

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1 Introduction

The properties of magnetic impurities in a metal is one of the most intensively studied problems in solid state physics. The magnetic impurity combines two fascinating phenomena, (i) the formation of a magnetic moment (\( \mathbf{M} \)) in a host \([1], [2]\) due to the Coulomb interaction and (ii) the formation of a non-magnetic singlet state at low temperatures \([3], [4], [5], [6], [7], [8], [9], [10], [11], [12], [13]\). The electronic structure of this singlet or Kondo ground state has been investigated using a large number of sophisticated methods, for example: scaling \([14]\), renormalization \([15], [16], [17], [18]\) Fermi-liquid theory \([19], [20]\), slave-bosons (see for example \([21]\)), large-spin limit \([22], [23]\), local moment approach \([24], [25]\), Bethe ansatz \([26], [27], [28]\). The author has added in recent years a new approach, the FAIR method, (FAIR for Friedel Artificially Inserted Resonance) which yields a very compact approximate ground state of the Friedel-Anderson and the Kondo impurity \([29], [30], [31]\).

One of the most controversial aspects of the Kondo ground state is the so-called Kondo cloud within the radius \( r_K \) where \( r_K \) is called the Kondo length

\[
    r_K = \frac{\hbar v_F}{k_B T_K} \tag{1}
\]

\((k_B T_K = \varepsilon_K = \text{Kondo energy}, v_F = \text{Fermi velocity of the conduction electrons})\).

The idea is to divide the ground state \( \Psi_K \) of a Kondo impurity into two parts with opposite d-spins. The question is whether the conduction electrons compensate the magnetic moment of the d-electron forming of a Kondo cloud in each part. This question has been highly controversial over the last 30 years (for references see for example \([32]\)).

Recently the author \([33]\) calculated the internal electronic structure of a Kondo impurity in real space using the FAIR solution of the Kondo ground state. This solution consists of only four Slater states and is well suited to calculate spatial properties which are difficult to obtain with other methods. The calculation showed that indeed a Kondo cloud of s-electrons compensates perfectly the magnetic moment of the d-electrons in the Kondo ground state.

However, to study the polarization Kondo cloud experimentally one needs a finite magnetic field because in zero magnetic field the polarization clouds of the magnetic components cancel. The magnetic field should be small enough so that the Kondo state is neither destroyed nor dramatically changed by the field. Therefore, in this paper I will use linear response theory to calculate the electronic structure of a Kondo impurity in a small magnetic field.

The magnetic properties, such as susceptibility, of the Kondo ground state in a magnetic field have been studied theoretically in a number of papers \([34], [35], [36], [37]\). However, to the best of my knowledge this is the first investigation of the effect of a magnetic field on the electronic structure in real space. The number of real space calculations in the Kondo ground state is still rather limited. Recently Affleck, Borda and Saleur \([38]\) calculated the Friedel oscillations in the vicinity of a Kondo impurity by means of NRG calculations (Numerical Renormalization Group). The author repeated their calculation with the FAIR method and found good agreement with the NRG approach.
2 Theoretical Background

2.1 The FAIR approach

The basic idea of the FAIR method can be best explained for a Friedel resonance with the Hamiltonian

\[
H_F = \sum_{\nu=0}^{N-1} \varepsilon_\nu c_\nu^\dagger c_\nu + E_d d^\dagger d + \sum_{\nu=0}^{N-1} V_{sd}(\nu)[d^\dagger c_\nu + c_\nu^\dagger d]
\]

It has been shown by the author \[39\], \[40\] that the exact \( n \)-particle ground state of a Friedel Hamiltonian can be expressed as by the sum of two Slater states.

\[
\Psi_F = \left( Aa_0^\dagger + Bd^\dagger \right) \prod_{i=1}^{n-1} a_i^\dagger \Phi_0
\]  

The state \( a_0^\dagger = \sum \alpha_\nu c_\nu^\dagger \) is a localized state which is composed of the states \( c_\nu^\dagger \). The states \( \{a_i^\dagger\} \) represent an \( N \)-dimensional orthonormal basis representing the same Hilbert space as the basis \( \{c_\nu^\dagger\} \). The state \( a_0^\dagger \) determines uniquely the full basis \( \{a_i^\dagger\} \).

In this basis the conduction electron Hamiltonian \( H_0 = \sum_{\nu=1}^{N} \varepsilon_\nu c_\nu^\dagger c_\nu \) takes the form

\[
H_0 = \sum_{i=1}^{N-1} E_i a_i^\dagger a_i + E_0 a_0^\dagger a_0 + \sum_i V_{fr} (i) [a_0^\dagger a_i + a_i^\dagger a_0]
\]

As one can see the structure of \( H_0 \) is identical to the structure of the Friedel Hamiltonian. The state \( a_0^\dagger \) represents an artificially inserted Friedel resonance state. Therefore I call \( a_0^\dagger \) a "Friedel Artificially Inserted Resonance" state or FAIR-state. The use of the FAIR-states is at the heart of my approach to the FA- and Kondo impurity problem. Therefore I call this approach the FAIR method.

In the ground state \( \Psi_F \) the \((n-1)\) lowest states \( a_i^\dagger \) are occupied (starting at \( i = 1 \)). The states \( a_0^\dagger \) and \( d^\dagger \) are mixed. Further details are reviewed in the appendix.

2.2 The Kondo impurity in a magnetic field

The Kondo Hamiltonian in zero magnetic field has the form

\[
H = \sum_{\nu=0}^{N-1} \sum_{\alpha} \varepsilon_\nu c_{\nu,\alpha}^\dagger c_{\nu,\alpha} + \sum_{\nu,\nu'=0}^{N-1} 2J_{\nu,\nu'} \sum_{\alpha,\alpha'} c_{\nu,\alpha}^\dagger s_{\alpha,\alpha'} c_{\nu',\alpha'} \cdot S
\]  

where \( s = \sigma/2 \) is half the Pauli matrix vector, \( S \) is the impurity spin 1/2. The conduction electron band is expressed by discrete Wilson states \( c_\nu^\dagger \) which have a logarithmic energy scale (see appendix). \( J_{\nu,\nu'} \) is the matrix element of the exchange interaction between the Wilson states \( c_\nu^\dagger \) and \( c_{\nu'}^\dagger \) via the impurity.

In previous papers the author introduced a very compact (approximate) solution for the Kondo Hamiltonian which consists of four Slater states. (The path to this solution is briefly sketched in the appendix).
\[
\psi_K = B a_{01}^\dagger d_1^\dagger |0_{a1}0_{b1}\rangle + B d_{11}^\dagger a_{01}^\dagger |0_{b1}0_{a1}\rangle + C d_{11}^\dagger b_{01}^\dagger |0_{a1}0_{b1}\rangle + C b_{01}^\dagger d_1^\dagger |0_{b1}0_{a1}\rangle
\] (4)

Because of the spin degeneracy of the electrons two FAIR states \(a_{01}^\dagger\) and \(b_{01}^\dagger\) and the corresponding bases \(\{a_{01}^\dagger\}\) and \(\{b_{01}^\dagger\}\) are needed. The many-electron state \(|0_{a1}0_{b1}\rangle\) is defined as

\[
|0_{a1}0_{b1}\rangle = \prod_{j=1}^{n-1} a_{j1}^\dagger \prod_{k=1}^{n-1} a^\dagger_k |\Phi_0\rangle
\]

The FAIR states \(a_{0\sigma}^\dagger\) \((b_{0\sigma}^\dagger)\) and the d states \(d_{\pm\sigma}\) form a bound two-electron state with negative energy.

The four Slater states are abbreviated as

\[
\Psi_K = B\Psi_{ad} + B\Psi_{da} + C\Psi_{db} + C\Psi_{bd}
\] (5)

(The interpretation of \(\Psi_{ad}\) is that the MM-up electrons use the basis \(\{a_{01}^\dagger\}\) and the state \(a_{01}^\dagger\) is occupied \((d_1\) empty\) while the MM-down electrons use the other basis \(\{b_{01}^\dagger\}\) and the state \(d_{01}^\dagger\) is occupied \((b_{01}^\dagger\) empty\). Since the ansatz for the Kondo ground state consists of four Slater states its secular matrix has the dimension four. One may consider the four Slater states as four basis states of an effective Hamiltonian, the \(4 \times 4\) secular matrix. The components of this effective Hamiltonian are the expectation values of the original Hamiltonian between the Slater states.

The two FAIR states \(a_{01}^\dagger = \sum_\nu \alpha_0^\nu c_\nu^\dagger\) and \(b_{01}^\dagger = \sum_\nu \beta_0^\nu c_\nu^\dagger\) determine uniquely the full basis \(\{a_1^\dagger\}\) and \(\{b_1^\dagger\}\). The two FAIR states \(a_{01}^\dagger\) and \(b_{01}^\dagger\) are numerically optimized and determine the secular matrix and the ground state \(\Psi_K\).

Spin-flip processes are only included in the matrix elements between the FAIR states \(a_{0\sigma}^\dagger\), \(b_{0\sigma}^\dagger\) and the \(d_{\pm\sigma}\) states. In the following I will refer to this effective Hamiltonian - secular matrix as the "\textit{secular Hamiltonian}".

If one applies a magnetic field \(B\) in z-direction then the energy of electrons with their moment pointing upwards is reduced by \(E_B = \mu_B B\) while those with their moment pointing down is increased by \(E_B\). Since within this paper the orientation of the magnetic moment of the electrons is of primary interest I use the symbol \(\uparrow\) for magnetic moment up or in short MM-up and \(\downarrow\) for MM-down.

Applying a magnetic field corresponds to an external Hamiltonian

\[
H^{ex} = -E_B \sum_\nu \left( (\hat{n}_{\nu\uparrow} - \hat{n}_{\nu\downarrow}) + (\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow}) \right)
\]

where \(\hat{n}_{\nu\sigma}\) is the number operator for the conduction electron (Wilson) states. The interaction of the magnetic field with the conduction electrons yields essentially the Pauli susceptibility in which we are not interested at this point. Since the magnetic field is introduced in linear response its effect on the conduction electrons can be ignored. However, for finite magnetic fields this is not correct as will be discussed in the appendix together with a sketch of the four Slater states in a magnetic field.
Since the effect of the magnetic field on the conduction electrons can be discarded the effective perturbation Hamiltonian of the magnetic field has the form

\[ H^{ex} = -E_B (\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow}) = E_B (\hat{n}_{d\downarrow} - \hat{n}_{d\uparrow}) \]

3 Linear Response to a Magnetic Field

The FAIR ground state (5) of the Kondo Hamiltonian is an exact eigenstate of the (approximate) secular Hamiltonian (which is given in the appendix for \( J = 0.1 \)). The ground state has the coefficients \((B, B, C, C)\) (with \( B = 0.70313, C = 0.0626 \) for \( J = 0.1 \)).

If we apply a magnetic field \( B \) which corresponds to a magnetic energy \( E_B \) then we obtain a polarization in our system. The perturbation Hamiltonian in the Heisenberg picture is

\[ H^{ex}_H (t') = E_B e^{iHt'/\hbar} (\hat{n}_{d\downarrow} - \hat{n}_{d\uparrow}) e^{-iHt'/\hbar} \]

If one switches on the field at the time \( t_0 \) then this alters the wave function by adding a perturbation state

\[ |\delta \Psi_K\rangle = -\frac{i}{\hbar} e^{-iHt'/\hbar} E_B \int_{t_0}^{t} dt' e^{iHt'/\hbar} \left[ (\hat{n}_{d\downarrow} - \hat{n}_{d\uparrow}) e^{-iHt'/\hbar} \left( \begin{pmatrix} Ba_{0\uparrow}^\dagger d_{\downarrow}^\dagger + C d_{\uparrow}^\dagger b_{0\downarrow}^\dagger \rangle |0_{a\uparrow}0_{b\downarrow}\rangle \\
+ (Cb_{0\uparrow}^\dagger d_{\downarrow}^\dagger + Bd_{\uparrow}^\dagger a_{0\downarrow}^\dagger) \rangle |0_{b\uparrow}0_{a\downarrow}\rangle \end{pmatrix} \right] \]

The term in the square brackets yields

\[ \left[ \left( Ba_{0\uparrow}^\dagger d_{\downarrow}^\dagger - C d_{\uparrow}^\dagger b_{0\downarrow}^\dagger \right) |0_{a\uparrow}0_{b\downarrow}\rangle + \left( Cb_{0\uparrow}^\dagger d_{\downarrow}^\dagger + Bd_{\uparrow}^\dagger a_{0\downarrow}^\dagger \right) |0_{b\uparrow}0_{a\downarrow}\rangle \right] e^{-iE_0t'/\hbar} \]

This state is perpendicular to \( |\Psi_K\rangle \) and can be expanded in terms of the other three solutions of the \( 4 \times 4 \) secular matrix

\[ = \sum_{\lambda} \alpha_{\lambda} |\psi_{\lambda}\rangle e^{-iE_\lambda t'/\hbar} \]

where \( |\psi_{\lambda}\rangle \) oscillates with the frequency \( E_\lambda/\hbar \). This yields for

\[ \int_{t_0}^{t} dt' e^{iHt'/\hbar} \left[ \ldots \right] e^{-iE_0t'/\hbar} = \sum_{\lambda=1}^{3} \frac{i\hbar}{(E_0 - E_\lambda + i\eta\hbar)} \alpha_{\lambda} |\psi_{\lambda}\rangle e^{-i(E_0 - E_\lambda)t'/\hbar} \]

Here a factor \( e^{\eta t'} \) with \( \eta \to 0^+ \) is inserted for convergence reasons. Then the lower integration limit yields zero for \( t_0 - \to -\infty \). (Afterwards \( \eta \) is discarded).

Then one obtains for the linear response wave function

\[ |\delta \Psi_K (t)\rangle = -E_B \sum_{\lambda=1}^{3} \frac{1}{E_{\lambda,0}} \alpha_{\lambda} |\psi_{\lambda}\rangle e^{-iE_\lambda t'/\hbar} \]

where \( E_{\lambda,0} = -(E_0 - E_\lambda) > 0 \)
3.1 Magnetic moment

Next we calculate the magnetic moment (in units of $\mu_B$). The operator in the Schroedinger picture is $(\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow})$. The expectation value of the moment $\langle \mu \rangle$ is

$$\langle \mu \rangle = 2 \text{Re} \langle \delta \Psi_K(t) \rangle \langle (\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow}) \rangle \Psi_K(t)$$

We calculate

$$\langle \delta \Psi_K(t) \rangle \langle (\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow}) \rangle \Psi_K(t) = \left\langle \sum_{\lambda=1}^{3} \frac{-E_{\lambda}}{E_{\lambda,0}} \alpha_{\lambda} \psi_{\lambda} e^{-iE_{0} t/\hbar} \langle (\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow}) \rangle \Psi_K(0) e^{-iE_{0} t/\hbar} \right\rangle$$

$$= \left\langle \sum_{\lambda=1}^{3} \frac{E_{\lambda}}{E_{\lambda,0}} \alpha_{\lambda} \psi_{\lambda} \left[ \sum_{\lambda=1}^{3} \alpha_{\lambda} \psi_{\lambda} \right] \right\rangle$$

While the four Slater states in equ. (4) are not orthogonal with respect to each other, the eigenstates $|\psi_{\lambda}\rangle$ of the secular Hamiltonian are. Therefore one obtains for the magnetic moment

$$\langle \mu \rangle = 2E_B \sum_{\lambda=1}^{3} \frac{1}{E_{\lambda,0}} |\alpha_{\lambda}|^2$$

(6)

For the example with the exchange interaction strength $J = 0.1$ I have collected the secular Hamiltonian, its eigenvectors and its eigenvalues in the appendix. One obtains for the linear response wave function $|\delta \Psi_K(0)\rangle = 0.984 |\psi_1\rangle + 0.158 |\psi_3\rangle$. Because of the energy denominators ($E_1 - E_0 = 2.38 \times 10^{-4}$, $E_3 - E_0 = 0.522$) the contribution of $|\psi_3\rangle$ to the magnetic moment is almost $10^{-5}$ smaller and one obtains for $\langle \mu \rangle$ in good approximation

$$\langle \mu \rangle = 2E_B \frac{1}{E_{1,0}} |\alpha_{1}|^2 = \frac{(0.984)^2}{2.38 \times 10^{-4}} 2E_B = 8140 \times E_B$$

3.2 Kondo temperature

In numerical normalization group (NRG) calculations one uses the susceptibility to define the Kondo temperature as $k_B T_K = 1/(4\chi)$. The susceptibility is, in linear response, $\chi = \langle \mu \rangle / (E_B)$. If one applies this method to the example with $J = 0.1$ one obtains

$$k_B T_K = \frac{E_B}{4 \langle \mu \rangle} = 3.07 \times 10^{-5}$$

In the past we have used the energy difference between the singlet ground state and the relaxed triplet state for the definition of the Kondo energy. For $J = 0.1$ this yields $k_B T_K^* = 2.36 \times 10^{-5}$. These two values are surprisingly close together if one considers that there is some arbitrariness in the definition of the Kondo temperature and that almost every theoretical approach to the Kondo problem has a different definition.
4 Net Spin Polarization

The ground state of the Kondo impurity does not possess any spin- or magnetic moment polarization because of its symmetry between MM-up and down states. Therefore one has to separate the ground state mathematically into its two magnetic components to answer the question about the existence of a Kondo cloud. The author showed that there is a Kondo cloud in the magnetic components of the Kondo ground state. But this polarization cloud can not be observed in the ground state. To measure the Kondo cloud one has to disturb the ground state sufficiently so that the symmetry between MM-up and down is removed but not too much so that the Kondo state is not destroyed. A magnetic field of the right strength might do the job.

In linear response the interference between the ground state $\Psi_K$ and the linear response state $\delta \Psi_{LS}$ gives the change of the electron density and electron polarization due to a small magnetic field. The calculation of this interference is quite similar to the author’s calculation of the Kondo cloud in the previous paper [33].

When one uses the Slater state basis $(\Psi_{ad}, \Psi_{da}, \Psi_{db}, \Psi_{bd})$ the ground state $\Psi_K = \psi_0$ has the components $(B, B, C, C)$ and the linear response state $\delta \Psi = \alpha_1 (2E_B/\Delta E_0) \psi_1$ has the components

$$\alpha_1 \frac{2E_B}{\Delta E_0} (B', -B', -C', C')$$

where $(B', -B', -C', C')$ is the eigenvector of the first excited state $|\psi_1\rangle$ and for $J = 0.1$ the components have the values $B = 0.70313$, $C = 0.0626$ and $B' = 0.7055$, $C' = 0.0635$ (see appendix).

If we denote the electron density between two Slater states $|\Psi_\alpha\rangle$ and $|\Psi_\beta\rangle$ as $\langle \Psi_\alpha | \hat{\rho} (r) | \Psi_\beta \rangle = \rho_{\alpha,\beta} (r)$ then the total change of density due to the magnetic field is

$$\delta \rho (r) = \alpha_1 \frac{4E_B}{\Delta E_0} \left( BB' (\rho_{ad,ad} - \rho_{da,da}) + CC' (\rho_{db,db} - \rho_{bd,db}) + (BC' + CB') (\rho_{ad,db} + \rho_{da,db} + \rho_{db,da} + \rho_{bd,da}) \right) = 0 \quad (7)$$

Since the state $|\Psi_{da}\rangle$ is just the state $|\Psi_{a,d}\rangle$ with reversed spins the two states have the same charge density and the opposite spin density or polarization. The same applies for the pairs $(\rho_{db,db}; \rho_{bd,db})$, $(\rho_{ad,db}; \rho_{da,db})$ and $(\rho_{da,db}; \rho_{ad,db})$. Therefore one realizes that there is no change of the charge density. On the other hand the polarization which is defined as $p_{\alpha,\beta} = \rho_1|_{\alpha,\beta} - \rho_1|_{\alpha,\beta}$ reverses sign when the spins are reversed. Therefore one has for example $p_{\alpha,\beta} = -p_{\beta,\alpha}$. This yields a total polarization of

$$p (r) = \alpha_1 \frac{8E_B}{\Delta E_0} (BB' p_{ad,ad} + CC' p_{db,db} + (BC' + CB') (p_{ad,db} + p_{da,db})) \quad (8)$$

If one divides by $\langle \mu \rangle = \alpha_1^2 2E_B/\Delta E_{10}$ this yields for our example ($J = 0.1$)

$$\frac{p (r)}{4 \langle \mu \rangle} = \left[ 0.504 \, p_{ad,ad} + 4.1 \times 10^{-3} \, p_{db,db} + 9.2 \times 10^{-2} \, (p_{ad,db} + p_{da,db}) \right] \quad (9)$$

where $BB'/\alpha_1 = 0.504$. 


The calculation of the charge density of the Slater states is described in detail in ref. ?? A summary is given in the appendix. The calculation can be performed for the one, two or three dimensional case. Since the Kondo impurity couples only to a single angular momentum of the conduction electrons (for example \( l = 0 \)) it represents essentially a one-dimensional problem. If one defines the charge density as a one-dimensional density \( \delta q/\delta r \) (for example in three dimension the charge \( \delta q \) between two spheres of radii \( r \) and \( r + \delta r \)) then the calculation and the results are essentially identical in all dimensions. (The main difference is that the oscillatory part of the charge shows a dimensional phase shift of \( D \pi/2 \), see equ. (10)).

The four Slater states of the ground state and the linear response state are composed of Wilson states \( \psi_\nu(\xi) \). Here \( \xi \) is the the distance from the impurity in units of half the Fermi length \( \lambda_F/2 \) so that \( \xi = r/ (\lambda_F/2) \). The explicit form of \( \psi_\nu(\xi) \) (using the logarithmic energy scale with \( \Lambda = 2 \), see appendix) for \( \nu < (N/2 - 1) \) is

\[
\psi_\nu(\xi) = 2\sqrt{2^{\nu+2}} \sin \left( \frac{\pi \xi}{2^{\nu+2}} \right) \cos \left( \pi \xi \left( 1 - \frac{3}{2^{\nu+2}} \right) \right)
\]

This state has a fast-oscillating component \( \cos \left( \pi \xi \left( 1 - \frac{3}{2^{\nu+2}} \right) \right) \) (in space) and a slowly varying component \( \sin \left( \pi \xi \left( 1 - \frac{3}{2^{\nu+2}} \right) \right) \). The first component yields the Friedel and RKKY oscillations while the second part yields the background electron density which is given by

\[
\rho_\nu^0(\xi) = |\psi_\nu(\xi)|^2 = 2^{\nu+3} \sin^2 \left( \frac{\pi \xi}{2^{\nu+2}} \right) / (\pi \xi)^2
\]

The appendix gives a more detailed discussion of the calculation of density and polarization.

I will divide the calculation into two parts, (i) averaging over the fast-oscillating contribution to calculate the overall spin polarization and (ii) focus on the fast-oscillating part which will yield oscillations of the spin polarization.

### 4.1 Background polarization

Since \( B \) and \( B' \) are much larger than \( C \) and \( C' \) the dominant contribution comes from the first term in equ. ?? The prefactor of the second term is smaller by a factor 100. The prefactors of \( p_{db} \) and \( p_{ad} \) are smaller by a factor 10. However, their contribution is in addition reduced because the bases for MM-up (and MM-down) are different in the two states and therefore the interference terms are essentially reduced by the square of the multi-scalar product

\[
\left\langle \prod_{j=1}^{n-1} a_i^\dagger \Phi_0 \prod_{j=1}^{n-1} b_i^\dagger \Phi_0 \right\rangle
\]

This multi-scalar product is about 0.14, which reduces the contribution of \( p_{db} \) and \( p_{ad} \) by an additional factor of about 1/50. Therefore these terms will be neglected in the calculation. For the discussed example (\( J = 0.1 \)) the polarization is given to good accuracy by

\[
p(\xi) \approx 2 \left\langle \mu \right\rangle p_{ad,ad} = - \left\langle \mu \right\rangle (p_{da,da} - p_{ad,ad})
\]
In Fig.1 the integrated polarization is plotted in units $2\langle \mu \rangle$ as a function of the log $\xi$ where $\xi = 2r/\lambda_F$ is the distance from the impurity in units of half the Fermi wave length.

![Graph of integrated polarization](image)

**Fig.1:** The integrated polarization of the ground state in a magnetic field in units of $2\langle \mu \rangle$ where $\mu$ is the magnetization in units $\mu_B$.

### 4.2 Polarization oscillations

In the vicinity of a Kondo impurity one obtains Friedel oscillations which have the magnitude (in reduced units)

$$\rho_{Fr}(\xi) - \rho_0 = -\frac{C_D}{\xi K} A_p \left( \frac{\xi}{\xi K} \right) \cos \left( 2\pi \xi - D\pi \right)$$

(10)

where $D$ is the dimension of the system, the coefficients $C_D$ have the values $C_1 = 1/(2\pi)$, $C_2 = 1/(2\pi^2)$ and $C_3 = 1/(4\pi^2)$ in one, two and three dimensions [38]. $r_K = \hbar v_F/k_B T_K$ is the Kondo length. The period in $\xi$ is equal to 1. The function $A_p(\xi/\xi_K)$ is a universal function which approaches the values 0 for $\xi/\xi_K << 1$ and 2 for $\xi/\xi_K >> 1$. (I skipped the phase shift $\delta_P$ due to potential scattering). I will use the magnitude of the Friedel oscillations as a scale for the polarization oscillations in a magnetic field. Therefore I define an amplitude $A_p(\xi/\xi_K)$ so that the calculated polarization in one dimension is given by

$$p(\xi) = -\frac{1}{2\pi \xi} A_p \left( \frac{\xi}{\xi K} \right) \cos \left( \pi \xi - \frac{\pi}{2} - \delta_p \right)$$

(11)

The calculated polarization oscillations are proportional to $-\cos (2\pi \xi)$. They are shown in Fig.4a-e for different distances from the impurity. Each time two periods are plotted. The
average distances in Fig.2a-e vary between $\xi = 7$ and $\xi = 32767$. The minima lie at integer values of $\xi$ and the maxima at half integer ($\xi = 2r/\lambda_F$).
Fig. 2: Oscillations of $2\pi p(\xi)$ ($p(\xi)$ is the magnetic polarization) as a function of $\xi = 2r/\lambda_F$. Two two periods of the oscillations are shown for different distances from the impurity. The average distances are from (a) to (e): 7, 63, 511, 4047 and 32767.
In Fig. 3 the envelope of the oscillations of $2\pi\xi \ast p(\xi)$, i.e. the maxima and minima are plotted as triangles. The full points give the average of $2\pi\xi \ast p(\xi)$ as a function $l = \log_2(\xi)$. The amplitude is given by half the difference between the maximum and minimum curve. The amplitude does not show the expected long-range behavior of $p(\xi) \simeq 1/(2\pi\xi)$ (which should be a constant in Fig. 2). For small distances the average is close to zero and for distances of the order of the Kondo length the amplitude is roughly equal to the average. For distances larger than the Kondo length the oscillations fade away. As discussed below they don’t extend far beyond the Kondo length.

5 Discussion and Conclusion

A magnetic field alters the ground state of the Kondo impurity and yields in linear response

$$\Psi_K = B (1 - \varepsilon) \Psi_{a,d} + B (1 + \varepsilon) \Psi_{da} + C (1 + \varepsilon') \Psi_{db} + C (1 - \varepsilon') \Psi_{bd}$$

with

$$\varepsilon = \alpha_1 \frac{2E_B}{\Delta E_{01}} B' = 1.013 \langle \mu \rangle \quad \varepsilon' = \alpha_1 \frac{2E_B}{\Delta E_{01}} C' = 1.031 \langle \mu \rangle$$
Therefore one has \( \varepsilon \approx \varepsilon' \approx \langle \mu \rangle \) and the components with the d magnetic moment parallel to the magnetic field are relatively increased in their amplitude by the value of the magnetization \( \langle \mu \rangle \). Therefore the part of the Kondo cloud which is due to \( \Psi_{da} \) is now only partially compensated by \( \Psi_{a,d} \). The same applies to \( \Psi_{db} \) and \( \Psi_{bd} \). Therefore it is not surprising that the net polarization has the same shape as the hidden Kondo cloud which the author calculated recently. One even expects the scaling factor of about 2 \( \langle \mu \rangle \). The polarization cloud extends to a distance of 2\(^{14.9} \) which corresponds to \( 1.5 \times 10^4 \lambda_F \) being of the order of the Kondo length. Using the Kondo energy \( k_B T_K \approx 3.1 \times 10^{-5} \) one obtains for the Kondo length \( r_K = \hbar v_F / k_B T_K = \lambda_F / (2 \pi k_B T_K) \approx 5.1 \times 10^3 \lambda_F \) where Wilson’s linear dispersion relation between energy and wave vector is used.

On the other hand the position dependence of the polarization oscillation is at first rather surprising. The amplitude of \( (C_D / \xi^D) \cos (\pi \xi) \) has a maximum at roughly the position \( \xi \approx 2^{10.5} = 1.45 \times 10^3 \) which is smaller than the Kondo length but corresponds roughly to the distance at which the Friedel oscillation began to develop. Since the Friedel oscillations are suppressed at short distances it is not surprising that the polarization oscillations are suppressed within this range. But why do they disappear at larger distances. Here one can consider two physical scenarios:

- The magnetic field polarizes the Kondo impurity and generates a magnetic moment at the impurity. This magnetic moment scatters MM-up and down electrons differently and as a result one obtains RKKY oscillations which should depend as \( \xi^{-D} \) on the distance from the impurity.

- The Kondo impurity modifies the electronic structure of the host within the distance of the Kondo impurity. The polarization oscillations are restricted to the region into which the Kondo cloud of the impurity extends.

It appears that the polarization oscillations (for small magnetic fields) are not due to the scattering of conduction electrons by the impurity. Instead they show the structure of the Kondo cloud and therefore they are restricted to distances of the order of the Kondo radius.

6 Appendix

6.1 The FAIR Method

The ansatz for the ground state of the Kondo Hamiltonian (equ.4) has been derived from the ground state of the Friedel-Anderson impurity. The Hamiltonian of the Friedel-Anderson impurity is given

\[
H_{FA} = \sum_{N-1} \left\{ \sum_{\nu=0}^{N-1} \varepsilon_{\nu} c_{\nu \sigma}^\dagger c_{\nu \sigma} + E_d d_{\sigma}^\dagger d_{\sigma} + \sum_{\nu=0}^{N-1} V_{sd}(\nu) \left[ d_{\sigma}^\dagger c_{\nu \sigma} + c_{\nu \sigma}^\dagger d_{\sigma} \right] \right\} + U n_{d \uparrow} n_{d \downarrow}
\]

In mean-field approximation the Hamiltonian one replaces \( n_{d+} n_{d-} \rightarrow n_{d+} \langle n_{d-} \rangle + \langle n_{d+} \rangle n_{d-} - \langle n_{d+} \rangle \langle n_{d-} \rangle \). After adjusting \( \langle n_{d+} \rangle \) and \( \langle n_{d-} \rangle \) self-consistently one obtains two Friedel...
resonance Hamiltonians with a spin-dependent energy of the $d_\sigma$-state: $E_{d,\sigma} = E_d + U \langle n_{d,-\sigma} \rangle$. The mean-field wave function is a product of two Friedel ground states for spin up and down
\[ \Psi_{mf} = \Psi_F^\uparrow \Psi_F^\downarrow . \]

As discussed in section II the ground state of the Friedel Hamiltonian can be expressed as a function of two Slater states, one consisting of only conduction electrons and the other containing one d-electron.
\[ \Psi_F = \left( A a_0^\dagger + B d^\dagger \right) \prod_{i=1}^{n-1} a_i^\dagger \Phi_0 \]
The state $a_0^\dagger$ is called the FAIR state.

The product of the two Friedel ground states in the mean field approximation can be expanded and yields a "magnetic state"
\[ \Psi_{MS} = \left[ Aa_{01}^\dagger b_{01}^\dagger + Ba_{01}^\dagger d_{01}^\dagger + Cd_{01}^\dagger b_{01}^\dagger + Dd_{01}^\dagger d_{01}^\dagger \right] |0_{a1}0_{b1}\rangle \]
where $\{a_i^\dagger\}$ and $\{b_i^\dagger\}$ are two (different) bases of the $N$-dimensional Hilbert space and $a_0^\dagger, b_0^\dagger$ are two different FAIR states.

\[ |0_{a1}0_{b1}\rangle = \prod_{j=1}^{n-1} a_{j1}^\dagger \prod_{j=1}^{n-1} b_{j1}^\dagger |\Phi_0\rangle \]
The state (12) opens a wide playing field for optimization: (i) The FAIR states $a_0^\dagger$ and $b_0^\dagger$ can be individually optimized to minimize the energy expectation value (ground-state energy). Each FAIR state defines uniquely a whole basis $\{a_i^\dagger\}, \{b_i^\dagger\}$. The coefficients $A, B, C, D$ can be optimized. This yields a much better treatment of the correlation effects. The resulting state is denoted as the (potentially) magnetic state $\Psi_{MS}$.

The magnetic state $\Psi_{MS}$ is used as the building block for the singlet state. $\Psi_{MS}$ together with its counterpart where all spins are reversed yield two states $\Psi_{MS}(\uparrow\downarrow)$ and $\Psi_{MS}(\downarrow\uparrow)$. The singlet ground state is then given by
\[ \Psi_{SS} = \Psi_{MS}(\uparrow\downarrow) + \Psi_{MS}(\downarrow\uparrow) \]
A new optimization of the FAIR states and the coefficients changes $a_0^\dagger$ and $b_0^\dagger$ drastically increases the weight at low energies.

The Kondo Hamiltonian represents a limit of the Friedel-Anderson Hamiltonian by suppressing zero and double occupancy of the d-states. This leads to the approximate ground state in chapter II.

### 6.2 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 $(-1 : 0)$ at energies of $-1/\Lambda, -1/\Lambda^2, -1/\Lambda^3, \ldots$ i.e. $\zeta_\nu = -1/\Lambda^\nu$. This yields energy cells $C_\nu$ with the range $\{ -1/\Lambda^\nu : -1/\Lambda^{\nu+1} \}$ and the width $\Delta_\nu = \zeta_{\nu+1} - \zeta_\nu = 1/\Lambda^{\nu+1}$. During this paper generally the value $\Lambda = 2$ is chosen. (In this paper I count the energy cells and the Wilson states from $\nu = 1$ to $N$.)

Wilson rearranged the quasi-continuous original electron states $\varphi_k(r)$ 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 $\varphi_k(r)$ with the impurity is $k$-independent this interacting state in $C_\nu$ had the form

$$\psi_\nu(r) = \sum_{\xi} c_{\xi} \varphi_k(r) / \sqrt{Z_\nu}$$

where $Z_\nu$ is the total number of states $\varphi_k(r)$ 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 $\varphi_k(r)$ with the d-impurity is assumed to be a constant. Then the exchange interaction between two Wilson states $\psi_\nu(r)$ and $\psi_\mu(r)$ is given

$$J_{\nu,\mu} = \sqrt{Z_\nu / Z} \sqrt{Z_\mu / Z} J = \sqrt{(\zeta_{\nu+1} - \zeta_\nu) / 2 \sqrt{(\zeta_{\mu+1} - \zeta_\mu) / 2}} J.$$

### 6.3 The Slater states in a finite magnetic field

In Fig.4 the energy bands of the conduction electrons $a_{i,\sigma}^\dagger$ and $b_{j,\sigma}^\dagger$ are drawn together with the FAIR states $a_{0,\sigma}^\dagger$ and $b_{0,\sigma}^\dagger$ and the d states $d_\sigma^\dagger$. We have four Slater states. The first Slater state is occupied with $(n - 1)$ electrons of the basis $\{ a_{i,\uparrow}^\dagger \}$ and $(n - 1)$ electrons of the basis $\{ b_{i,\downarrow}^\dagger \}$, the FAIR state $a_{0,\uparrow}^\dagger$ and the d-state $d_{\uparrow}$. In the absence of a magnetic field the second Slater state is obtained by reversing all moments. So in the second Slater state the MM-up electrons would be filled into the $\{ b_{i,\uparrow}^\dagger \}$ basis and the MM-down electrons into the $\{ a_{i,\downarrow}^\dagger \}$ basis. However, since the magnetic field shifts MM-up and MM-down electrons in different directions, the basis are slightly altered to $\{ b_{i,\uparrow}^\dagger \}$ and $\{ a_{i,\downarrow}^\dagger \}$.

The energies of $a_{0,\uparrow}^\dagger$ and $b_{0,\downarrow}^\dagger$ are non-zero and opposite equal. In the first two Slater states the $a_{0,\uparrow}^\dagger$ state with negative energy is occupied while in the last two Slater states the $b_{0,\downarrow}^\dagger$ state with positive energy is occupied. The occupation probability of the last two is smaller by roughly a factor 100 than for the first two.
Fig. 4: A drawing of the four Slater states in the Kondo ground state. In each Slater state a FAIR state \((a_0^\dagger \text{ or } b_0^\dagger)\) and a d-state with opposite spins (magnetic moment) are occupied. The energies of the FAIR states are non-zero and opposite equal. The brackets below the bands show which basis the Wilson states occupy. A magnetic field has shifted the moment up and down bands in different directions.

The magnetic field moves the MM-up and the MM-down bands in opposite direction by \(\pm E_B\). The Fermi levels of MM-up and MM-down electrons readjust by electron spin flips to the same height. As a consequence the Fermi momenta are slightly different for MM-up and the MM-down electrons.
In the present calculation the slight shift of the bands is neglected because the shift is very small compared to the band energy. The Wilson states in the shifted bands measure their energies from the new Fermi level. Then the energy of the Wilson states is not changed except for the first and last Wilson state. The small change for \( \nu = 1 \) which extends from \(-1 \pm E_B\) to \(-\frac{1}{2}\) and for \( \nu = N \) which extends from \(+\frac{1}{2}\) to \(1 \pm E_B\) is neglected. Since the FAIR bases are constructed from the Wilson states their energies are, in first approximation not affected by the magnetic field.

A finite magnetic field has, however, an important effect on the matrix elements. If one considers two Wilson states \( c_{\nu \uparrow}^\dagger \) and \( c_{\nu \downarrow}^\dagger \) with the same energy but different MM then their orbital wave functions are not identical. As a consequence the scalar product between the orbital parts of \( c_{\nu \uparrow}^\dagger \) and \( c_{\nu \downarrow}^\dagger \) is no longer equal to one but reduced to \( 1 - \frac{2E_B}{\zeta_{\nu+1} - \zeta_{\nu}} \) (for \( 2E_B < (\zeta_{\nu+1} - \zeta_{\nu}) \)). In the FAIR method such matrix elements occur only between the FAIR states. Since the present calculation is performed in linear response this problem does not arise. But for finite fields it will be important.

### 6.4 The Secular Hamiltonian and its Eigenstates

The FAIR solution for the Kondo ground state is given by the ansatz (4) which consists of four Slater states. With this state \( \Psi_K \) one can calculate the expectation value of the Hamiltonian \( H_K \) (equ. (3)). The minimization of this expectation value with respect to the four coefficients (which at this stage are considered as independent) yields a \( 4 \times 4 \) secular matrix. In parallel the variation and optimization of the FAIR states \( a_0^\dagger \) and \( b_0^\dagger \) yields the optimal bases \( \{ a_i^\dagger \} \) and \( \{ b_i^\dagger \} \) with the lowest ground-state energy. (The calculation and optimization of the energy expectation value has been described in ref. [31]).

The secular matrix possesses four eigenvectors with four energy eigenvalues. The coefficients of the eigenvector with the lowest energy are the coefficients of the ground state \( |\psi_0\rangle = |\Psi_K\rangle \). The other eigenvectors represent excited states \( |\psi_1\rangle, |\psi_2\rangle, |\psi_3\rangle \) which are needed in the linear response calculation. With respect to these eigenvectors and their energy the secular matrix plays the role of a Hamiltonian, which I baptized the **secular Hamiltonian**. For \( J = 0.1 \) and a Wilson basis with \( \Lambda = 2 \) and \( N = 50 \) this secular Hamiltonian is given below by equ. (13).

\[
H_{\text{sec}} = \begin{pmatrix}
-3.0013 & -0.0019237 & -0.46265 & -0.057213 \\
-0.0019237 & -3.0013 & -0.057213 & -0.46265 \\
-0.46265 & -0.057213 & -2.4887 & -0.029434 \\
-0.057213 & -0.46265 & -0.029434 & -2.4887
\end{pmatrix}
\] (13)

The four eigenvectors of (13) are given by the four columns of the \( 4 \times 4 \)-matrix (14) below.

\[
\begin{pmatrix}
0.70313 & 0.70547 & -0.076084 & 0.49993 \\
0.70313 & -0.70547 & -0.076084 & -0.49993 \\
0.06256 & 0.063539 & 0.70447 & -0.70438 \\
0.06256 & -0.063539 & 0.70447 & 0.70438
\end{pmatrix}
\] (14)
The eigenvalues are \((E_0, E_1, E_2, E_3) = (-3.0056, -3.0053, -2.4856, -2.4831)\). The energy difference \((E_1 - E_0)\) is \(E_{1,0} = 2.38 \times 10^{-4}\). The band energies for the occupied states in basis \(\{a_{i}\}\) is \(E_{bd} (a) = -1.4988\) and for the basis \(\{b_{i}\}\) is \(E_{bd} (b) = -1.22305\).

6.5 The wave function of Wilson’s states in real space

For the discussion of the wave functions in real space we assume a linear dispersion relation between energy and momentum, a constant density of states and a constant amplitude at \(r = 0\). Then the interaction between the original basis states \(\varphi_k (r)\) and the d-impurity will be constant for all k-states. These assumptions are the same as in Wilson’s treatment of the Kondo impurity. We define the wave functions \(\varphi_k (r)\) in such a way that the results apply for the impurity problem in one, two and three dimensions.

6.5.1 One-dimensional case

Let us start with the one-dimensional problem. Here we have the impurity at the position zero and the conduction electrons are located in the range between 0 and \(L\). The wave functions \(\varphi_k (r)\) have the form \(\varphi_k (r) = \sqrt{2/L} \cos (kr)\). There is another set of eigenstates \(\bar{\varphi}_k (r) = \sqrt{2/L} \sin (kr)\). These states don’t interact with the impurity at the origin. Therefore they don’t have any bearing on the impurity problem.

6.5.2 Three-dimensional case

In three dimensions the free electron states can be expressed as \(\varphi_k (r) \propto Y_{l}^{m} (\theta, \phi) j_l (kr)\) where \(Y_{l}^{m}\) is a spherical harmonics and \(l, m\) are the angular momentum and magnetic quantum numbers. \(j_l (kr)\) is a spherical Bessel function. Its long range behavior is given by \((1/kr) \sin (kr - l\pi/2)\). Only the states with the same \(l\) as the impurity couple to the impurity. All the other states for different \(l\) belong to the group of inert states \(\bar{\varphi}_k (r)\).

If one calculates the density of the wave function, integrating in the three-dimensional case over the spherical surface \(4\pi r^2\) and averaging over short range (Friedel) oscillations then one obtains in the

\[-\begin{align*}
\bullet\ & \text{one-dimensional case}: \langle 2/L \rangle \cos^2 (kr) = 1/L \\
\bullet\ & \text{three-dimensional case}: \rho_k (r) = \langle 2/L \rangle \sin^2 (kr - l\pi/2) = 1/L
\end{align*}\]

In both cases one obtains essentially the same density. Therefore it is sufficient to use the one-dimensional approach for calculating the density of a Kondo cloud. It is equivalent to the 3-dimensional case integrated over the spherical surface.
6.5.3 The wave functions in one dimension

While the energy is measured in units of the Fermi energy the momentum will be measured in units of the Fermi wave number. We assume a linear dispersion relation for $0 \leq \kappa \leq 2$ with

$$
\zeta = (\kappa - 1)
$$

Here $\kappa = k/k_F$ is dimensionless. It is useful to measure distances also in dimensionless units. We define $\xi = \frac{1}{\pi k_F} r = \frac{r}{\lambda_F/2}$. Then $\xi$ gives the distance from the impurity in units of $\lambda_F/2$.

The (almost) continuous states $\varphi_\kappa$ are given as

$$
\varphi_\kappa (\xi) = \sqrt{\frac{2}{L}} \cos (\pi \kappa \xi)
$$

where $L$ is the length of the one-dimensional box. The boundary condition $\cos (\pi \kappa L) = 0$ yields $\kappa = (\lambda + 1/2) / L$ (where $\lambda$ is an integer. The maximum value of $\lambda$ is the integer of $(2L)$, since $\kappa$ is dimensionless then $L$ is also dimensionless). Therefore we have $Z = 2L$ states in the full band of width 2.

To obtain the Wilson state we have to sum the states $\varphi_\kappa (\xi)$ over all states within an energy cell. If the cell ranges from $\left(\zeta_\nu : \zeta_{\nu+1}\right)$ corresponding to a $\kappa$-range $(1 + \zeta_\nu) < \kappa < (1 + \zeta_{\nu+1})$ then we represent all the states in this energy interval by

$$
\psi_\nu (\xi) = \frac{1}{\sqrt{(\zeta_{\nu+1} - \zeta_\nu) L}} \sum_{1 + \zeta_\nu < \kappa < 1 + \zeta_{\nu+1}} \sqrt{\frac{2}{L}} \cos (\pi \kappa \xi)
$$

From $Z_\nu = L (\zeta_{\nu+1} - \zeta_\nu)$ states we have (according to Wilson) constructed one state $\psi_\nu (\xi)$ which couples to the impurity. Similarly one can construct $(Z_\nu - 1)$ additional linear combinations of $\varphi_\kappa (\xi)$ which are orthonormal and do not couple to the impurity at the origin. We denote these states as $\varphi_{\kappa,l} (\xi)$. They are as inert to the impurity as the states $\varphi_\kappa (\xi)$ and will be included in the quasi-vacuum.

After integration the wave function of the state $c_\nu^\dagger$ has the form for $\nu < N/2$

$$
\psi_\nu (\xi) = \frac{2 \sqrt{2}}{\sqrt{(\zeta_{\nu+1} - \zeta_\nu) \lambda}} \sin \left( \frac{\pi \xi (\zeta_{\nu+1} - \zeta_\nu)}{2} \right) \cos \left( \frac{\pi \xi (2 + \zeta_\nu + \zeta_{\nu+1})}{2} \right)
$$

For the logarithmic energy scale ($\Lambda = 2$) this yields for $\nu < N/2 - 1$ using $\zeta_\nu = -1/2^\nu$

$$
\psi_\nu (\xi) = 2 \sqrt{2^{\nu+2}} \sin \left( \frac{\pi \xi}{2^{\nu+2}} \right) \cos \left( \pi \xi \left( 1 - \frac{3}{2^{\nu+2}} \right) \right)
$$

Similarly one obtains for in the positive energy range

$$
\psi_{N-1-\nu} (\xi) = 2 \sqrt{2^{\nu+2}} \sin \left( \frac{\pi \xi}{2^{\nu+2}} \right) \cos \left( \pi \xi \left( 1 + \frac{3}{2^{\nu+2}} \right) \right)
$$

The two wave functions $\psi_{N/2-1}$ and $\psi_{N/2}$ are special because their $\kappa$-range is the same as their neighbors $\psi_{N/2-2}$ and $\psi_{N/2+1}$ All four states close to the Fermi level have the same $\kappa$-range of $2^{-N/2-1}$. One has to pay special attention to this complication.
6.6 Density of the Wilson states in real space

The density of a single state $\psi_\nu (\xi)$ is given by the square of the function $\psi_\nu (\xi)$ in equ. (15).

$$|\psi_\nu (\xi)|^2 = \frac{8}{(\zeta_{\nu+1} - \zeta_\nu)} \sin^2 \left( \frac{\pi (\zeta_{\nu+1} - \zeta_\nu)}{2} \right) \cos^2 \left( \frac{\pi \xi (2 + \zeta_\nu + \zeta_{\nu+1})}{2} \right)$$

This density has a fast oscillating contribution which yields the Friedel oscillations. We first average over the fast oscillation (which has a period of the order of 1 in units of $\lambda_F/2$). Then we obtain for the Wilson states for $\nu < N/2$ where $(\zeta_{\nu+1} - \zeta_\nu) = \frac{1}{2^{\nu+1}}$

$$\rho_\nu^0 (\xi) = |\psi_\nu (\xi)|^2 = 2^{\nu+3} \frac{\sin^2 \left( \frac{\pi \xi}{2^{\nu+2}} \right)}{(\pi \xi)^2}$$

(16)

In the numerical calculation we will use (most of the time) $N = 50$ Wilson states. The different wave functions $\psi_\nu (\xi)$ have very different spatial ranges and therefore very different densities, the lowest being of the order of $2^{-25} < 3 \times 10^{-8}$. This means that it is not useful to calculate the density as a function of $\xi$ because this density varies over a range of $2^{25}$. Instead, we use the integrated density, integrated from 0 to $\xi$.

$$q_\nu^0 (\xi) = \int_0^\xi |\psi_\nu (\xi')|^2 d\xi' = 2^{\nu+3} \int_0^\xi \frac{\sin^2 \left( \frac{\pi \xi'}{2^{\nu+2}} \right)}{(\pi \xi')^2} d\xi'$$

$$= 2 \int_0^{\pi u/2} \frac{\sin^2 \left( \frac{\pi u}{(\pi u)^2} \right)}{(\pi u)^2} du$$

One realizes that a single integral yields the integrated density for (almost) all wave function $\psi_\nu (\xi)$. The state $\psi_0 (\pi \xi)$ lies roughly in the range $\xi < 2^2$, i.e. the integrated density $q_\nu (\xi) = \int_0^\xi |\psi_0 (\pi \xi)|^2 d\xi'$ increases in this range to 90%. Therefore the states $\psi_\nu (\xi)$ and $\psi_{N-1-\nu} (\pi \xi)$ essentially lie in the range $\xi < 2^{\nu+2}$ (in units of $\lambda_F/2$). For a total of $N = 50$ Wilson states the maximum range of the wave functions is roughly $2^{N/2-1} = 2^{26}$.

We may define as a ruler a linear array $I (s)$ where $s$ is an integer, $(-N/2 \leq s < N)$ as

$$I (s) = 2 \int_0^{2^s} \frac{\sin^2 \left( \frac{\pi u}{(\pi u)^2} \right)}{(\pi u)^2} du$$

Then the integrated density of the state $\psi_\nu$ in the range from 0 to $2^l$ is given by

$$q_\nu^0 (2^l) = \int_0^{2^l} |\psi_\nu (\xi')|^2 d\xi' = 2 \int_0^{2^{l-1}} \frac{\sin^2 \left( \frac{\pi u}{(\pi u)^2} \right)}{(\pi u)^2} du = I (l - \nu - 2)$$

$I (l - \nu - 2)$ gives the integrated density of the wave function $\psi_\nu$ within the radius $2^l$. 

20
6.6.1 Interference terms in the density

The Wilson states \( \psi_\nu (\xi) \) or \( c^\dagger_\nu \) represent the free electron states in the impurity problem. With the impurity we express the ground state in terms of new states \( a^\dagger_i = \sum_{\nu=0}^{N-1} \alpha^\nu_i c^\dagger_\nu \). Their integrated density is given by

\[
\mathcal{\rho}_i (2^l) = \int_0^{2^l} \left| \sum_{\nu=0}^{N-1} \alpha^\nu_i \psi_\nu (\xi) \right|^2 d\xi
\]

The quadratic terms can be evaluated with the same ruler \( I(s) \) as before. But this time one has in addition interference terms \( \psi_\nu (\xi) \psi_\nu (\xi) + \lambda (\xi) \). These terms depend on two parameters, \( \nu \) and \( \lambda \). So one needs for each \( \lambda \) a different ruler. Furthermore the interference terms depend on the sub-bands of \( \psi_\nu (\xi) \) and \( \psi_{\nu+\lambda} (\xi) \). If both states lie either in the negative energy sub-band \( (\nu, \nu + \lambda < N/2) \) or in the positive sub-band \( (\nu, \nu - \lambda \geq N/2) \) then one obtains one set of rulers \( I_0 (\nu, \lambda) \) and if they lie in opposite sub-bands then one obtains another set of rulers \( I_1 (\nu, \lambda) \). As an example one obtains

\[
I_0 (s, \lambda) = 2\sqrt{2} \int_0^{2^l} \frac{\sin (\pi u) \sin (\pi \frac{\lambda u}{2})}{(\pi u)^2} \cos \left( 3\pi u \left( 1 - \frac{1}{2\lambda} \right) \right) du
\]

For \( I_1 (\nu, \lambda) \) one has to replace the minus sign in the cosine function by a plus sign. Furthermore one has to treat the terms where \( \nu + \lambda = N/2 - 1 \) separately because one state lies at the Fermi level and has a different cell width.

6.6.2 The net integrated density

If we occupy all Wilson states below the Fermi level then we obtain \( \prod_{\nu=0}^{n-1} c^\dagger_\nu \Phi_0 \) with \( n = N/2 \) and \( \Phi_0 \) the vacuum state. This state is not really the free electron ground state. To obtain the latter we have also to occupy the states \( \varphi_\kappa (\xi) \) and \( \varphi_\kappa (\xi) \). They don’t interact with the impurity but they are occupied. Therefore we define as quasi-vacuum \( \Phi'_0 \) the state in which all states \( \varphi_\kappa (\xi) \) and \( \varphi_\kappa (\xi) \) with \( \kappa < 1 \) are occupied. Then the ground state is \( \Psi_0 = \prod_{\nu=0}^{n-1} c^\dagger_\nu \Phi'_0 \). This state has a constant electron density in real space.

In the presence of the impurity the new ground state \( \Psi_{\text{new}} = \prod_{i=0}^{n-1} a^\dagger_i \Phi'_0 \) must also contain this quasi vacuum, i.e., the non-interacting states must be occupied up to the Fermi level. Since the inert states are occupied in \( \Psi_0 \) and \( \Psi_{\text{new}} \) they cancel out when one calculates the change in the electron density. The net density of the new state \( \Psi_{\text{new}} \) is the difference between \( \rho (\Psi_{\text{new}}) \) and \( \rho (\Psi_0) \). Since the inert states cancel out one can ignore their existence during this calculation.
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