



MICROSCOPIC THEORY FOR TRIPLET PAIRING IN AN ANDERSON LATTICE

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A microscopic mechanism for triplet pairing of conduction electrons is discussed. It is argued, that the effective f-f interaction on an uranium atom in a metallic lattice may be attractive. A unitary transformation of an Anderson (empty) lattice hamiltonian results in a Fröhlich like hamiltonian with the phonons replaced by doubly (de) occupied f states.

Recently the uranium compounds UBe_{13} and UPt_3 have attracted considerable attention, because in these solids superconductivity and "heavy fermion" properties co-exist^{1,2,3,4}. It has been suggested, that these systems are "triplet" superconductors for a number of reasons^{5,6}.

It is often assumed, that paramagnon exchange is the microscopic origin of the triplet pairing in these superconductors, like in 3He ^{7,8}. Nevertheless, this point is far from being settled, as paramagnon theory predicts a positive pressure induced change in T_c ⁹, contrary to experimental results¹⁰. Strong Coulomb repulsion between uranium 5f electrons is believed to prevent the formation of conventional s-wave Cooper pairs on the one hand⁶ and on the other hand the 5f states act as a reservoir of quasi localized quenched moments close to a magnetic transition, thus having strong spin fluctuations, which may bind conduction electrons into p-wave Cooper pairs⁹.

The aim of this paper is to point out that the Coulomb repulsion at the uranium sites may be very small due to screening and may even be exceeded by the local 5f Hund's Rule exchange interactions, resulting in a net local attraction between parallel spins in the uranium 5f shell. We show that hybridization between conduction states and 5f states then leads to a net attraction between parallel spins in the conduction bands near E_F . We will show, that there is indeed a close relation between an Anderson Lattice type hamiltonian and a triplet BCS hamiltonian.

Before turning to the actual model we will first briefly discuss the energetics of a single 5f atom. We will do this for the case of an atom having almost unoccupied f levels. Clearly this situation is quite different from what is expected to be found in uranium compounds, but we will argue later, that our findings can be applied to the more general f^n state under certain circumstances. Restricting our discussion to the lowest Hund's Rule states of each multiplet, we can express the energy of an atom having zero, one or two f electrons as¹¹:

$$\begin{aligned} E(f^0(1S)) &= 0 \\ E(f^1(2F)) &= \epsilon_f \\ E(f^2(3H)) &= 2\epsilon_f + U - J \end{aligned}$$

where U and J are shorthand for Coulomb monopole interactions and exchange plus multipole interactions, expressed in terms of Slater integrals as:

$$\begin{aligned} U &= F^0 \\ J &= \frac{1}{9} F^2 + \frac{17}{363} F^4 - \frac{25}{14157} F^6 \end{aligned}$$

If we put such an atom into a solid, the one electron potential ϵ_f changes and the Coulomb interactions are screened due to the response of the electron gas to a polarity change of the 5f shell. In Mn¹², Ni¹³ and Cu¹⁴ the reduction of F^0 due to screening is about 20 eV compared to the theoretical bare atomic values of Mann's tables¹⁵. In the rare earths this reduction is 23 eV on the average^{16,17}. The multipole integrals, on the other hand, are only slightly reduced in these cases, indicating that the electron gas does not respond to the details of the charge distribution in a given polarity state. This is the reason, why atomic like multiplets are observed in valence XPS, BIS and XAS of the rare earths^{18,19} and Mn impurities^{12,20}. It is also the principle origin of the large Hubbard gap in systems where the d or f shell is half occupied, such as Eu, Gd and Mn impurities, as these gaps have a lower bound of $21J$, even when F^0 is screened to zero.

We believe, that localized behavior and strong screening also exist in actinide compounds for a number of reasons:

- (1) Bandstructure calculations of uranium compounds show that the dispersional part of the 5f bands are extremely narrow, especially in view of the fact, that part of the width is due to spin orbit splitting^{21,22,23}.
- (2) BIS and XPS valence spectra of UO_2 and other actinide oxides can be explained quite well with atomic multiplet theory^{24,25}, indicating that in the solid the F^2 , F^4 and F^6 integrals are not strongly different from atomic values. Now the bare atomic theoretical value of F^0 is 19.3 eV for uranium¹⁵. Assuming that the same mechanisms exist in the iron row elements, the lanthanides and the actinides, we expect a reduction of about 20 eV, thus reducing F^0 to (almost) zero. In fact, comparison of the combined XPS and BIS valence spectra of UAl_2 , UPt_3 ²⁶ and UBe_{13} ²⁷ with those of Pr or Nd¹⁸ shows, that the Hubbard gap must be much smaller

in the former case, which we also expect from the smaller bare F^0 integral. Of course we must remember, that the interpretation of the (inverse) photoemission spectra of uranium intermetallic compounds is highly non-trivial, as initial and final states are presumably of mixed valent character, like in Ce ^{28,29}. We see, that, although the Coulomb interaction is strongly reduced, the exchange interactions are not, so that a simple band theory of uncorrelated particles is probably not applicable. In Ref.17 we use atomic values for F^2 , F^4 and F^6 and a strongly screened F^0 to show, that the atom fluctuates between f^2 , f^3 and f^0 , whereas f^1 is relatively high in energy. In our model we will reverse the picture in order to avoid cumbersome mathematics: The lowest state is $f^0(^1S)$, $f^1(^3P)$ is at the energy ϵ_f and the energy of $f^2(^3H)$ is ϵ_H . We will assume, that f^3 and higher polarity states as well as the other terms of the f^2 multiplet have high enough energies to be irrelevant to our discussion. We will also assume that there are only two f orbitals f_1 and f_2 that mix into the ground state, each one coupling to an orthogonal conduction band, also carrying the index $m = 1$ or 2 .

The model hamiltonian is:

$$H = H_0 + H_1 \tag{1}$$

$$H_0 = \sum_{Rm\sigma} (\epsilon_f f_{Rm\sigma}^+ f_{Rm\sigma}) + \sum_{R\sigma\sigma'} U(n_{f,\sigma,\sigma'}) \left\{ f_{R1\sigma}^+ f_{R1\sigma'} + f_{R2\sigma}^+ f_{R2\sigma'} \right\} + \sum_{km\sigma} (\eta_k c_{km\sigma}^+ c_{km\sigma}) \tag{2}$$

$$H_1 = \sum_{Rkm\sigma} \left(\frac{1}{\sqrt{N}} V_{km} e^{ik \cdot R} f_{Rm\sigma}^+ c_{km\sigma} + H.C. \right) \tag{3}$$

where $U(f^2(^3H)) = \epsilon_H - 2\epsilon_f$

and all other terms are assumed to be high in energy and are projected out with $U \rightarrow \infty$. In the case of a single impurity at site 0 we can apply the Schrieffer-Wolff transformation^{30,31} taking f^0 as the polarity of the atom and obtain a transformed hamiltonian

$$\tilde{H} = \sum_{km\sigma} (\eta_k c_{km\sigma}^+ c_{km\sigma}) + \sum_{kq\sigma} \left(\frac{1}{N} W_{kq} c_{km\sigma}^+ c_{qm\sigma} \right)$$

where

$$W_{kq} = -\frac{1}{2} V^2 \left(\frac{1}{\epsilon_f - \eta_k} + \frac{1}{\epsilon_f - \eta_q} \right) \tag{4}$$

Similarly, if the polarity is f^2 we obtain

$$\tilde{H} = \sum_{km\sigma} (\eta_k c_{km\sigma}^+ c_{km\sigma}) + \sum_{kq\sigma'} \left(\frac{1}{N} J_{kq} \langle f^2 | f_{m\sigma}^+ f_{m\sigma'} | f^2 \rangle c_{km\sigma}^+ c_{qm\sigma'} \right)$$

where

$$J_{kq} = -\frac{1}{2} V^2 \left(\frac{1}{\epsilon_f - \epsilon_H - \eta_k} + \frac{1}{\epsilon_f - \epsilon_H - \eta_q} \right) \tag{5}$$

which is the usual Kondo hamiltonian. The lowest order term in the Schrieffer-Wolff transformation also gives us terms corresponding to the annihilation and creation of two conduction electrons and a polarity change of two charges

in the f shell. In their original paper³⁰ Schrieffer and Wolff recognized the occurrence of such terms, but discarded them, because polarity

changes by two charges were high energy states irrelevant to the topic of the Kondo effect. In our case, however, these states become important as we want to consider the limit where their energies are low.

Let us turn to the lattice hamiltonian of Eqs. 1-3. We make a transformation $\tilde{H} = e^{-S} H e^S$, such that the terms linear in H_1 vanish. This leads to

$$\tilde{H} = H_0 + \tilde{H}_2 + \tilde{H}_3 + \tilde{H}_4 + \dots \tag{6}$$

$$\langle \alpha | S | \beta \rangle = \frac{\langle \alpha | H_1 | \beta \rangle}{E_\beta - E_\alpha} \tag{7a}$$

$$\langle \alpha | \tilde{H}_2 | \beta \rangle = \langle \alpha | \frac{1}{2} [H_1, S] | \beta \rangle = \frac{1}{2} \sum_\gamma \left(\frac{1}{E_\beta - E_\gamma} + \frac{1}{E_\alpha - E_\gamma} \right) \langle \alpha | H_1 | \gamma \rangle \langle \gamma | H_1 | \beta \rangle \tag{7b}$$

$$H_n = \frac{n-1}{n(n-2)} [\tilde{H}_{n-1}, S] \tag{7c}$$

The terms quadratic in H_1 are provided by \tilde{H}_2 and for our discussion there are three relevant types of matrix elements $\langle \alpha | \tilde{H}_2 | \beta \rangle$:
 (1) α and β correspond to f^0 at all lattice sites.
 (2) idem., except at site R , where α corresponds to f^0 and β to f^2 . Terms connecting f^0 to f^1 at two different sites have zero amplitude.
 (3) idem., except at site R , where α and β correspond to f^2 .

These terms are readily obtained and read:

$$\tilde{H}_{2,1} = \frac{1}{N} \sum_{kq\sigma} \left\{ e^{iR \cdot (k-q)} W_{kq} c_{km\sigma}^+ c_{qm\sigma} \right\} \tag{8a}$$

$$\tilde{H}_{2,2} = \frac{1}{N} \sum_{k'k''m_s} \left\{ T_{kk'} e^{i(k \cdot R + k' \cdot R')} \sum_{\sigma\sigma'} (c_{k1\sigma}^+ c_{k'2\sigma'} + f_{R1\sigma} f_{R'2\sigma'} + H.C.) \right\} \tag{8b}$$

$$\tilde{H}_{2,3} = \frac{1}{N} \sum_{kq\sigma\sigma'} \left\{ e^{iR \cdot (k-q)} J_{kq} \langle f^2 | f_{Rm\sigma}^+ f_{Rm\sigma'} | f^2 \rangle c_{km\sigma}^+ c_{qm\sigma'} \right\} \tag{8c}$$

where the summation over σ and σ' in Eq. 8b is subject to the conditions that the total spin is one and the z component is m_s and:

$$T_{kk'} = -\frac{1}{2} V_k V_{k'} \left\{ \frac{1}{\epsilon_f - \eta_k} + \frac{1}{\epsilon_f - \eta_{k'}} + \frac{1}{\epsilon_f - \epsilon_H + \eta_k} + \frac{1}{\epsilon_f - \epsilon_H + \eta_{k'}} \right\} \tag{9}$$

($R=R'$)
 = 0 ($R \neq R'$)
 and W_{kq} and J_{kq} are already defined in Eqs. 4 and 5. $\tilde{H}_{2,1}$ is a renormalization of the conduction electron energies due to hybridization with the f^1 states. This term can be included in H_0 without affecting the physics. $\tilde{H}_{2,3}$ describes the spin flip scattering of the conduction electrons from the $f^2(^3H)$ local moments. These terms are extremely important if f^2 is lower in energy than f^0 and may result in Kondo compensation of the magnetic moment at low temperatures. They also cause a renormalization of the $f^2(^3H)$ energies, which we symbolically indicate by replacing ϵ_H in H_0 with $\tilde{\epsilon}_H$. $\tilde{H}_{2,2}$ describes simultaneous hops of two conduction electrons to a $5f$ site. We can use formal exciton notation for the f^2 states, where the electrons are separated with a spatial vector Δ :

$$B_{q\uparrow\Delta}^+ = \frac{1}{\sqrt{N}} \sum_{R'} \left\{ e^{iq \cdot R'} f_{R+\frac{1}{2}\Delta}^+ f_{R-\frac{1}{2}\Delta}^+ \right\}$$

and similar expressions for the other two spin functions. These states have energies $2\epsilon_f$ for $\Delta \neq 0$ and ϵ_H for $\Delta = 0$. Now Eq.8 becomes:

$$\tilde{H}_2 = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}\mathbf{q}\mathbf{m}_s} \left(\sum_{\sigma\sigma'} \left\{ T_{\mathbf{k}\mathbf{q}} c_{\mathbf{k}1\sigma}^\dagger c_{\mathbf{q}2\sigma'} + P_{\mathbf{k}+\mathbf{q}\mathbf{m}_s} 0 + \text{H.C.} \right\} \right) \quad (10)$$

which is quite similar to a Fröhlich interaction,³² except that the role of phonons is taken over by f^2 states and that pairs of creation operators occur instead of pairs consisting of one creation and one annihilation operator.

Now there are two ways that two conduction electrons are coupled in fourth order of H_1 :

- (1) The simultaneous (de)occupation of f^2 states quadratic in \tilde{H}_2 .
- (2) Through the fourth order term in the Schrieffer-Wolff transformation \tilde{H}_4 of Eqs. 6 and 7.

The first possibility is easily accomplished by a second transformation, similar to the treatment of electron-phonon interactions. One simply looks for a generator S that removes all terms linear in \tilde{H}_2 , as in Eqs. 6 and 7. Such a transformation also modifies \tilde{H}_3 , \tilde{H}_4 etc. by adding fifth and sixth order terms in H_1 to them. As we won't consider terms of fifth and higher order, this is no point of concern. The lowest order term in our new hamiltonian \tilde{H} is quadratic in \tilde{H}_2 and we will indicate it with \tilde{H}_4 :

$$\tilde{H}_4 = \frac{1}{N} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}\mathbf{q}'\mathbf{m}_s} \sum_{\sigma\sigma'} \left(v(\mathbf{k},\mathbf{k}',\mathbf{q},\mathbf{q}') \delta(\mathbf{k}+\mathbf{k}'-\mathbf{q}-\mathbf{q}') c_{\mathbf{q}1\sigma}^\dagger c_{\mathbf{q}'1\sigma'}^\dagger c_{\mathbf{q}'2\sigma'} c_{\mathbf{k}'2\sigma'} c_{\mathbf{k}1\sigma} \right) \quad (11)$$

where

$$v(\mathbf{k},\mathbf{k}',\mathbf{q},\mathbf{q}') = -\frac{1}{2} T_{\mathbf{k}\mathbf{k}'} T_{\mathbf{q}\mathbf{q}'} \left(\frac{1}{\epsilon_H - \eta_{\mathbf{k}} - \eta_{\mathbf{k}'}} + \frac{1}{\epsilon_H - \eta_{\mathbf{q}} - \eta_{\mathbf{q}'}} \right)$$

$$\langle [B_{\mathbf{k}+\mathbf{k}'\mathbf{m}_s} 0, B_{\mathbf{q}+\mathbf{q}'\mathbf{m}_s} 0] \rangle \quad (12)$$

As the two particle states $B_{\mathbf{q}\mathbf{m}_s}^\dagger |\psi\rangle$ are no real bosons, we expect some difficulties with this expression as soon as the f^2 states become thermally occupied. As long as $|\psi\rangle$ contains no f^2 character, the commutator in Eq. 12 conserves momentum:

$$\langle f^0 | [B_{\mathbf{k}\mathbf{m}_s} 0, B_{\mathbf{q}\mathbf{m}_s}^\dagger] | f^0 \rangle = \delta_{\mathbf{k}\mathbf{q}} \quad (13)$$

The mixing in of f^2 states through thermal fluctuations will destroy momentum conservation and decrease the coherent part of the interaction. In Fig. 1 we see, that our interaction is attractive and increases as ϵ_H approaches zero. For $\epsilon_H = 2\epsilon_f$ we have $T_{\mathbf{k}\mathbf{k}'} = 0$ resulting in no coupling, as expected. However, if $\epsilon_H > 2\epsilon_f$ we get again an attractive interaction, which is rather unphysical, as the f electrons repel each other in this limit. Another unphysical behaviour is near $\epsilon_H = \epsilon_f$, where $T_{\mathbf{k}\mathbf{k}'}$ has a pole.

Both problems are solved, if we add \tilde{H}_4 to the interaction, so that we add up all quartic terms contributing to the electron-electron interaction. The expressions for \tilde{H}_3 and \tilde{H}_4 are:

$$\tilde{H}_3 = \frac{1}{3} [[H_1, S], S] \text{ and } \tilde{H}_4 = \frac{1}{8} [[H_1, S], S], S] \quad (14)$$

\tilde{H}_3 does not contribute to electron-electron coupling in fourth order, as it changes the f occupation by one or three. In \tilde{H}_4 there are two different channels that contribute: (1) $|\mathbf{k}\rangle$ scatters to $|\mathbf{R}_1\rangle$ and then to $|\mathbf{k}'\rangle$ followed by a similar

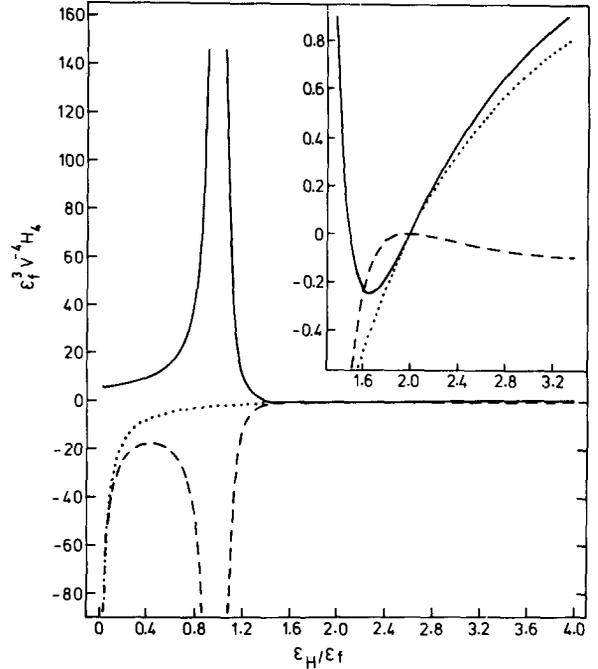


Fig. 1. Effective conduction electron interactions \tilde{H}_4 (solid curve), \tilde{H}_4 (broken) and H_{int} (dotted) as a function of ϵ_H/ϵ_f . The insert shows an expanded view of the region around $\epsilon_H/\epsilon_f = 2$.

process involving $|\mathbf{q}\rangle, |\mathbf{R}\rangle$ and $|\mathbf{q}'\rangle$. (2) A simultaneous hop of \mathbf{k} and \mathbf{q} to f^2 and back to \mathbf{k}' and \mathbf{q}' . Terms where \mathbf{k} and \mathbf{q} are scattered to different sites \mathbf{R} and \mathbf{R}' cancel in the summation over both channels. The matrix elements of \tilde{H}_4 are:

$$\langle \beta | \tilde{H}_4 | \alpha \rangle = \frac{1}{8} \sum_{\mu\gamma\rho} \left(\langle \beta | H_1 | \gamma \rangle \langle \gamma | H_1 | \mu \rangle \langle \mu | H_1 | \rho \rangle \langle \rho | H_1 | \alpha \rangle \right. \\ \left. \left[\frac{3}{(E_\beta - E_\gamma)(E_\alpha - E_\rho)} \left[\frac{1}{E_\rho - E_\mu} + \frac{1}{E_\gamma - E_\mu} \right] + \frac{1}{(E_\rho - E_\mu)(E_\mu - E_\gamma)} \right. \right. \\ \left. \left. \left[\frac{1}{E_\alpha - E_\rho} + \frac{1}{E_\beta - E_\gamma} \right] \right] \right) \quad (15)$$

In the case that $|\alpha\rangle$ and $|\beta\rangle$ refer to f^0 states, this expression can be worked out for conduction states near E_f :

$$\tilde{H}_4 = \frac{1}{N} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}\mathbf{q}'\mathbf{m}_s\sigma\sigma'} \left\{ \delta(\mathbf{k}+\mathbf{k}'-\mathbf{q}-\mathbf{q}') \left(\frac{2}{\epsilon_f^3} + \frac{1}{\epsilon_f(\epsilon_f - \epsilon_H)} \right) \right. \\ \left. \left[\frac{3}{\epsilon_f + \epsilon_f - \epsilon_H} \right] c_{\mathbf{q}1\sigma}^\dagger c_{\mathbf{q}'1\sigma'}^\dagger c_{\mathbf{q}'2\sigma'} c_{\mathbf{k}'2\sigma'} c_{\mathbf{k}1\sigma} \right\} \quad (16)$$

The sum of \tilde{H}_4 and \tilde{H}_4 in the region $\pm\epsilon_H$ around E_f is

$$H_{int} = \frac{V^4}{N\epsilon_f^3} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}\mathbf{q}'\mathbf{m}_s\sigma\sigma'} \left\{ \left(2 - \frac{4\epsilon_f}{\epsilon_H} \right) \delta(\mathbf{k}+\mathbf{k}'-\mathbf{q}-\mathbf{q}') \right. \\ \left. c_{\mathbf{q}1\sigma}^\dagger c_{\mathbf{q}'1\sigma'}^\dagger c_{\mathbf{q}'2\sigma'} c_{\mathbf{k}'2\sigma'} c_{\mathbf{k}1\sigma} \right\} \quad (17)$$

In Fig. 1 we show \tilde{H}_4 , \tilde{H}_4 and H_{int} as a function of ϵ_H/ϵ_f . Clearly H_{int} behaves regular for $\epsilon_H > 0$ and becomes repulsive for $\epsilon_H > 2\epsilon_f$. We see, that there are two important regions:

- (1) Small ϵ_H . The dominant channel is the Fröhlich type interaction of Eq. 10. This interaction must be worked out to sufficiently high order as ϵ_H approaches zero.

(2) $\epsilon_H \geq \epsilon_f$. The electron electron coupling becomes small and Eq. 17 is a fairly good lowest order approximation to the electron electron attraction. Eq. 17 can also be obtained from fourth order Rayleigh-Schrödinger perturbation theory, or by solving the two particle greens-function in the empty band limit.

At first glance Eq. 17 seems to give a repulsion for $\epsilon_H < 0$. However, in this case one has to do the theory starting from an f^2 ansatz, so that the commutator of Eq. 12 reverses sign. The net result is again an attractive interaction. There are a few problems in this case, related to the fact that $f^2(^3H)$ are three-fold spin degenerate. If, for example, all moments point in the same direction, triplet pairing will occur for one spin direction only. A similar problem exists if the moments are ordered anti-ferromagnetically. If, on the other hand, the local moments are compensated by the spin-flip terms of Eq. 8c to form a Kondo singlet, each of the three spin states is equally occupied and the commutator of Eq. 12 obtains the value $-1/3$. This seems to be reasonable in UB_{13} and UPT_3 which have Kondo resp. spin fluctuation

temperatures of ca $10 K^{1,2,3,4}$, which is much larger than the temperatures where superconductivity sets in.

We conclude that triplet pairing of conduction states may be mediated by simultaneous hops into the uranium atoms. This can result in an attraction between parallel spins if the Coulomb repulsion is sufficiently screened. It looks like a challenge to find out, whether the effective attraction can be enhanced by tuning the relative energy positions of the f^0 and f^2 states. Such tuning could in principle be possible by varying the partner element of uranium, or even by replacing uranium itself with atoms where we expect a small Coulomb repulsion, narrow f or d bands and an almost unscreened Hund's Rule exchange.

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