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Mixed Wave Function for Heavy Fermion Compounds

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Abstract

We propose a variational wave function for the ground state of the magnetic heavy fermion (HF) systems, in which both the Kondo and the RKKY interactions are variationally incorporated and the local f-orbital state exists as a linear combination of a full local moment state and a fully compensated state (mixed wave state). We describe the mechanism for the mixed wave ground state based on the large-N treatment of the Kondo lattice Hamiltonian added with RKKY interaction. With the mixed wave ground state we can explain several puzzling experiments in magnetic HF compounds such as a small value of local moment, coexistence of the antiferromagnetic (AFM) and the paramagnetic (PM) phases, local quantum criticality, etc.

Keywords : heavy fermion, Kondo, RKKY

I. Introduction

As a conventional wisdom, one often employs the Kondo mechanism to understand the HF behavior, in which the conduction electrons make bound states with the local f-orbital moments in a coherent fashion to result in fermionic quasiparticles integrating the local f-orbital moments with it. While it is still unclear how the single site Kondo mechanism can be generalized to the periodic lattice system, at least the above line of thinking seems to provide the correct energy scale, i.e. the coherent energy scale of forming heavy renormalized fermionic quasiparticles [1]. However, this phenomenological picture doesn't explain many experimental observations of HF systems, such as, strong temperature dependence of specific heat C(T) and bulk susceptibility χ(T) below the coherent temperature T_{coh} , the coexistence of the magnetism (often antiferromagnetism (AFM)) and the heavy quasiparticle in some compounds, and superconductivity in some other compounds [2].

Those compounds which display both HF properties as well as the magnetism (either magnetic fluctuations or the magnetic long range order (LRO)) are conveniently called "magnetic HF" by experimentalists. Then again the common wisdom for this class of HF systems is the competition between the Kondo coupling between the local f-orbitals and the conduction electrons and the RKKY interaction among the local f-orbitals themselves [3]. And at qualitative level the result of this competition is that the ground state should be either pure HF state (all local moment is completely compensated by conduction electrons) or pure magnetic state (no compensation of the local moment) depending on which energy scale is larger. Therefore, it is clear that a minimum requirement to understand experimental observations is that the true ground state wave function for the magnetic HF compounds should simultaneously possess both the heavy quasiparticle and local moment characters.

In this paper, we propose a variational wave function for the ground state of the magnetic HF

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systems, in which the local f-orbital wave function exists in the mixed states (a linear combination of the full local moment state and the fully compensated state), and we call it "mixed wave state" after the "mixed valence state" [4]. In the following sections, we show how this mixed wave state can be realized in the Kondo lattice model using the large-N scheme. This part is rather qualitative based on account of the energetics of the competition between different couplings. Once this mixed wave state is phenomenologically accepted, then this ground state properties can immediately provide explanations for the most puzzling questions of magnetic HF compounds: small uncompensated local moment, the coexistence of the AFM and PM domains (the PM domain can be even a superconducting phase), and as the most interesting possibility, the local quantum criticality coinciding with the magnetic criticality and its relation with the Fermi surface (FS) fluctuations, etc.

II. Mixed wave state (Duality wave function)

We start with the Kondo lattice Hamiltonian (KLH).

$$H = \sum_{k,m} \epsilon_{k,m} c\dagger_{k,m} c_{k,m} + \epsilon_f^0 \sum_{i,m} f\dagger_{i,m} f_{i,m} + \frac{J_{Kondo}}{N} \sum_i \vec{S}_i \cdot \vec{\sigma}_i + \frac{I_{RKKY}}{N^2} \sum_{<ij>} \vec{S}_i \cdot \vec{S}_j \quad (1)$$

where $c\dagger_{k,m}, c_{k,m}$ is the conduction electron creation and annihilation operators and $f\dagger_{i,m}$, $f_{i,m}$ are the local f-orbital operators, and the spin operators are the large N generalization of SU(2) spin $\vec{S}_i = f\dagger_{i,m} \vec{\tau} f_{i,m'}$ and $\vec{\sigma}_i = c\dagger_{i,m} \vec{\tau} c_{i,m'}$ for the f-orbital and conduction electron spins, respectively. The above Hamiltonian is the usual Kondo lattice Hamiltonian extended with the large N spin degeneracy $(m = 1, ..., N)$ and the f-orbital occupancy is constrained with $n_i^f = \sum_m f\dagger_{i,m} f_{i,m} = N q_0$ [5] representing the large on-site Coulomb interaction between the localized f-orbitals at the same site. Finally the RKKY interaction term between the f-orbitals is added [6]. The above Hamiltonian has been studied by numerous authors using various techniques [7]. Without the RKKY term, the various approximation (mainly the approximation treating the constraint $n_i^f = N q_0$ provides a solution of heavy renormalized coherent band(s) to explain the HF phenomena. When the RKKY term is added as in Eq.(1) not only any approximate solution becomes more complicated but more importantly the question of the correctness of treating the constraint becomes crucial because the fate of the competition/interplay between the Kondo and the RKKY interactions is largely unknown to determine the true ground state.

There are a few studies of the two impurity version of this model [8]. All these studies indicate that there is a critical ratio of interactions (J_{Kondo}/I_{RKKY}) from which the ground state flows away toward either a magnetically correlated state or the Kondo singlet state. While we learn from these studies that there is an interesting competition between the Kondo and RKKY interactions, a naive extension of this picture to the lattice system is not warranted.

As discussed in the introduction, motivated by experimental observations, we construct a new variational wave function for the ground state of the above Hamiltonian. We start with the f-orbital wave function as follows.

$$|f_{i,m}> = \sqrt{1-\alpha}|f_{i,m}>_{iti} + \sqrt{\alpha}|f_{i,m}>_{loc} \quad (2)$$

The above expression is designed to indicate that the f-orbital state in the ground state can be a superposition of two qualitatively different states; one is the itinerant state ($|f_{i,m}>_{iti}$) which makes a coherent singlet state with the conduction electrons via renormalized hybridization through Kondo coupling [7] and the other is the full local moment state ($|f_{i,m}>_{loc}$) which remains intact from forming Kondo singlet or heavy quasiparticle but couples only as a local magnetic moment with other electrons. With the above Ansatz for the f-orbital state, we diagonalize the Hamiltonian Eq.(1) in large N approximation. The ground state should determine the value of α to minimize the total energy of the Hamiltonian. This wave function, if it is realized as a true ground state, displays the mixed wave state in a same manner as the mixed valence state [4], and the origin of these mixed states is the strong onsite Coulomb interaction.

Assuming the variational Ansatz of Eq.(2), the Kondo coupling term in Eq.(1) is decomposed into two parts depending on which component of f-orbital states is involved.

$$\frac{J_{Kondo}}{N}\sum_i \vec{S}_i\cdot\vec{\sigma}_i = (1-\alpha)\frac{J_{Kondo}}{N} \cdot \sum_{i,m,m'} f\dagger_{i,m}c_{i,m}c\dagger_{i,m'}f_{i,m'} + \alpha\frac{J_{Kondo}}{N}\sum_i \vec{S}_i\cdot\vec{\sigma}_i \quad (3)$$

In the above equation, we rewrite the Kondo term coupled with the itinerant component of the f-orbital by the four fermionic expression often employed in the large-N treatment of Kondo coupling [7]. The second term represents the local moment part of the f-orbital state, which remains as a local moment and does not participate in forming the heavy quasiparticles. Now the Hamiltonian can be written as,

$$H = H_{Kondo} + H_{mag}, \quad (4)$$

$$H_{Kondo} = \sum_{k,m}\epsilon_{k,m}c\dagger_{k,m}c_{k,m} + \epsilon_f^0\sum_{i,m} f\dagger_{i,m}f_{i,m} + (1-\alpha)\frac{J_{Kondo}}{N}\sum_{i,m,m'} f\dagger_{i,m}c_{i,m}c\dagger_{i,m'}f_{i,m'}, \quad (5)$$

$$H_{mag} = \alpha\frac{J_{Kondo}}{N}\sum_i \vec{S}_i\cdot\vec{\sigma}_i + \alpha^2\frac{I_{RKKY}}{N^2}\sum_{<ij>}\vec{S}_i\cdot\vec{S}_j \quad (6)$$

H_{Kondo} part is well studied by many authors and in particular the large N technique is convenient to produce the heavy renormalized quasiparticle band(s). Switching on the Kondo coupling (J_{Kondo}), the ground state of H_{Kondo} lowers its energy compared to J_{Kondo}=0 state (ΔE_{Kondo}). H_{mag} part also should gain energy by developing a magnetic correlation, but the first term of H_{mag}, by coupling with the conduction electrons (***c*** electrons), also increases the kinetic energy of the H_{Kondo}.

Let us, first, consider H_{Kondo}. The only difference from the previous studies is that the Kondo coupling J_{Kondo} is replaced by (1-α) J_{Kondo} and also the f-orbital occupancy constraint is modified as $\boldsymbol{n}_i^f$= (1-α)Nq_0 (accordingly the Fermi surface volume changes with α). Introducing the Stratonovich-Hubbard decoupling field $\phi_0 = (1-\alpha)\frac{J_{Kondo}}{N}\sum_m < f\dagger_{i,m}c_{i,m} >$, H_{Kondo} is diagonalized and the renormalized ϵ_f is fixed to satisfy the constraint $\boldsymbol{n}_i^f$=(1-α)Nq_0. Following Read et al. (Ref. [3]), the Kondo energy gain ΔE_{Kondo} is written as,

$$\Delta E_{Kondo} = N\rho_0\phi_0^2\ln[\epsilon_f/D] - \epsilon_f(1-\alpha) + \frac{N}{J_K(1-\alpha)}\phi_0^2 \quad (7)$$

where D is the typical conduction band width and ρ_0 is the density of states (DOS) of it. The self-consistent equations are as follows.

$$N\rho_0\phi_0^2\frac{1}{\epsilon_f} = (1-\alpha) \quad (8)$$

$$\epsilon_f = D\exp[\frac{-1}{\rho_0 J_K(1-\alpha)}]. \quad (9)$$

Using the above equations, we find the Kondo energy gain per site is the following.

$$\Delta E_{Kondo} = -(1-\alpha)D\exp[\frac{-1}{\rho_0 J_K(1-\alpha)}]. \quad (10)$$

The system gains the above energy by compensating a fraction (1-α) of the local moments via Kondo screening and the conduction band becomes a renormalized heavy band(s). Now let us consider H_{mag}. The RKKY term would gain the following energy per site with the maximum polarization $< \vec{S}_i >= S_z = \frac{N-1}{2}$.

$$\Delta E_{RKKY} = -\alpha^2\frac{I_{RKKY}}{N^2}S_z^2 \sim O(N^0). \quad (11)$$

The first term of H_{mag} (Eq.(6)) now forces the AFM coupling of the conduction electrons (***c*** electrons) with a staggered field $\boldsymbol{h}^z_i$ or a staggered energy level $\Delta_i = \alpha \frac{J_K}{N} S_z$. With this staggered energy level for ***c*** -electrons, the renormalized heavy band(s) should further develop spin density wave (SDW) ordering and it will cost the kinetic energy increase as follows.

$$\Delta E_{kin} = \frac{1}{2}\rho_{HF}\ u_{k_F}^2 \Delta_i^2 + \frac{\rho_{HF}}{v_F^2(2k_F - Q)^2}\Delta_i^4 \dots \quad (12)$$

where ρ_{HF} is the DOS of the renormalized band at chemical potential and u_k is the Bogoliubov coefficient of c_k component of the renormalized band operators which diagonalize Eq.(5). v_F is the Fermi velocity and Q is the SDW ordering vector [9]. Finally, the total energy gain of H_{mag} with both the local magnetic and SDW orderings is as follows.

$$\Delta E_{mag} = -\rho_{HF}\ u_{k_F}^2 \Delta_i^2 - \alpha^2 \frac{I_{RKKY}}{N^2} S_z^2 \quad (13)$$

Now collecting all the energy gain and loss, the total energy difference by the Kondo and RKKY couplings is written as

$$\Delta E_{total} = \Delta E_{Kondo} + \Delta E_{kin} + \Delta E_{mag} \quad (14)$$

$$= -(1-\alpha) D \exp[\frac{-1}{\rho_0 J_{Kondo}(1-\alpha)}]$$

$$+ A^{(2)}\alpha^2 + A^{(4)}\alpha^4 + \dots \quad (15)$$

where $A^{(2)} = -\frac{1}{2}\rho_{HF}\ u_{k_F}^2 (\frac{J_{Kondo}}{N})^2 S_z^2 - \frac{I_{RKKY}}{N^2} S_z^2$, and $A^{(4)} = \frac{\rho_{HF}}{v_F^2 (k_F - Q)^2} (\frac{J_{Kondo}}{N})^4 S_z^4$. Note that $A^{(2)} < 0$, $A^{(4)} > 0$ and since $S_z \sim O(N)$ they are all $O(N^0)$. Ellipsis indicates the higher order terms ($O(\alpha^6)$ etc.)

Treating $A^{(2)}$ and $A^{(4)}$ as phenomenological parameters, in Fig.(1) we show the schematic total energy gain $\Delta E_{tot}(\alpha)$ of Eq.(15) for the three representative cases. There is always a local minimum with a finite value of α (due to $A^{(2)} < 0$, $A^{(4)} > 0$). However, when this local minimum is not a global minimum as in Fig.1.a, the ground state is a pure HF state (α=0, no magnetic HF) with fully screened local f-moments. In contrast, when this local minimum with a finite α becomes a global minimum as depicted in Fig. 1. b., then the ground state is a "mixed wave" state. If a fine tuning occurs such as using pressure, magnetic fields, chemical substitution, etc., then two minima can be degenerate with α≠0 and α=0 as in Fig.1.c. In this case, as the tuning parameter changes, the ground state goes through a first order transition accompanying with a jump of magnetization and FS volume.

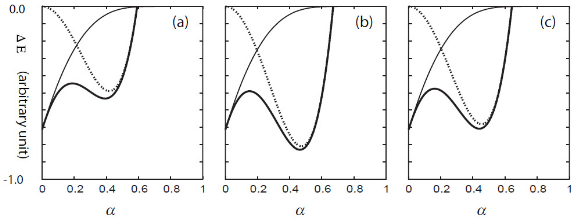

Fig. 1. Energy gains as a function of α for the representative cases of different ratios of Kondo and RKKY couplings: $\Delta E_{tot}(\alpha)$ (solid line), $\Delta E_{Kondo}(\alpha)$ (thin solid line), $\Delta E_{mag}(\alpha)+\Delta E_{kin}(\alpha)$ (dotted line).

III. Neutron diffraction(ND) and NMR experiments in URu_2Si_2

In our mixed wave state, the ground state is a superposition of the unscreened full local moments and the Kondo renormalized itinerant band(s). We first consider the consequence of this ground state for the measurement of the local moment by neutron diffraction (ND) experiment. At any given time, a fraction (α) of U sites have a full local moment and a fraction (1-α) of U sites are completely quenched by the conduction electrons. Now the unquenched local moment is partially screened by the opposite SDW moment developed by the renormalized itinerant band. This is the effective local moment. Now the ND should see the ensemble averaged size of the local moment, i.e. $\mu_{eff} = g\mu_B S_z^{eff} \times \alpha$. This value can be tiny ($\mu_{eff} \sim 0.03\mu_B$ for URu_2Si_2) while S_z^{eff} and m_z are not so tiny.

A recent NMR experiment by K. Matsuda et al.

[10] reports another puzzling data on magnetic moment. In this experiment, ^{29}Si NMR spectra clearly shows that ^{29}Si sites see both AFM ordered phase and the PM phase below the magnetic transition temperature T_0 and these authors interpret the data with a spatial inhomogeneous mixture of AFM and PM domains. From the estimated volume fraction of AFM domain, it is concluded that the actual size of local moment is at least 0.3 μ_B/U, an order of magnitude larger than the estimation from the neutron Bragg peak intensity [11]. In our picture, the coexistence of AFM and PM is not of a static inhomogeneous domain structure, but at any given time the ^{29}Si nuclei should see a fraction (α) of S_z^{eff} and a fraction (1-α) of zero moment from U sites. From this experiment we can read the size of SDW moment by $S_z^{eff}=S_z-m_z=0.3/g$ and $S_z=\mu_{para}/\ \mu_B=1.2/g$. Combining ND and NMR data, $\mu_{eff} \sim 0.03\ \mu_B = (0.3\ \mu_B \times \alpha)$, $\alpha \sim 0.1$ is estimated for URu_2Si_2 for ambient pressure. Also the observation of a distribution of local effective fields at ^{29}Si sites from ^{29}Si NMR by O.O. Bernal et al. [12] is a natural consequence of the local moment fluctuations of nearby U sites between zero and a finite value.

A strong pressure dependence of the local moment size from ND by H. Amitsuka et al. [12] (from 0.017 μ_B to 0.25 μ_B) and much slower increase of the magnetic ordering temperature (T_m) is not inconsistent with our model: the measured local moment size is (U full local moment – SDW moment) × α and in zeroth approximation T_m is $\sim\alpha^2$ (Eq.(6)) assuming the RKKY coupling I_{RKKY} constant [13]. Applying pressure should change α (increasing in URu_2Si_2) and T_m increases, but the increase of the effective local moment size should be a more complicate function of α.

IV. Local(momentum independent) quantum criticality and magnetic criticality

Many magnetic HF compounds exhibit non-Fermi liquid (NFL) behaviors in resistivity, specific heat, neutron scattering, susceptibility etc [14]. Often these behaviors coincide with the magnetic quantum transition (mostly AFM transition). However, theoretically any quantum critical fluctuations, which is spatially correlated, is not sufficient to explain the NFL behaviors. Therefore, what is naturally required is a "local quantum criticality" not only for NFL HF compounds but perhaps also for the high temperature superconducting materials.

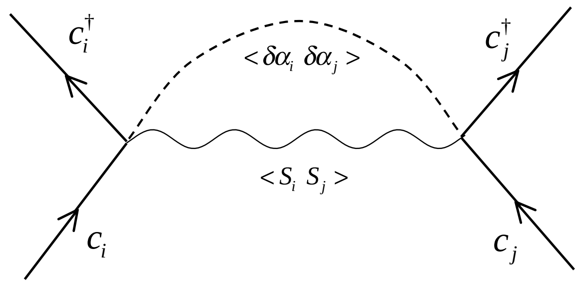

Fig. 2. Feynman diagram for the vertex of electron electron interaction mediated by magnetic fluctuations.

There are a few theoretical proposals [15, 16] of local quantum criticality in the strongly correlated electron system with different ideas. Our "mixed wave" ground state can provide a natural mechanism for the local quantum criticality, in particular, for NFL HF compounds. The first term of Eq.(6) provides a coupling between the conduction electrons (σ_i) and local spins (S_i), and the local spins develop its own dynamics through the RKKY interaction, which can go through the magnetic quantum criticality by tuning external parameters. This is a two component spin-fermion model recently proposed to study the superconductivity of $CeMIn_5$ [16]. Now in addition to the spatially correlated magnetic fluctuations, if the moment weight fluctuations $< \delta\alpha_i \delta\alpha_j >$ is allowed in higher order corrections, this fluctuations absorbs any value of momentum exchange just like impurities as far as the typical energy of this fluctuations is much higher than the typical low energy scale of the spin fluctuations $< S_i S_j >$. Then all conduction electrons around FS can be scattered off each other by a critical magnetic fluctuations with a help of the local moment weight fluctuations. This process is depicted diagramatically in Fig. 2. Therefore, in this picture the spatially correlated magnetic quantum criticality becomes a local quantum criticality with a help of the local moment weight fluctuations.

V. Conclusion

To summarize, we propose a new variational wave function for the magnetic HF which represents a mixed wave ground state. We use a mean field analysis in large N limit of the KLH added with RKKY interaction and show that this is indeed a generic ground state for a certain ratio of the couplings of Kondo and RKKY. Then we show that this mixed wave ground state can immediately provide natural explanations for the most puzzling observations in magnetic HF compounds (URu_2Si_2, UPt_3, $CeMIn_5$, $CeCu_{6-x}Au_x$, etc.) such as a tiny ordered magnetic moment, large specific heat jump, a coexistence of AFM and PM phases, a distribution of internal fields, and most interestingly the local quantum criticality coinciding with the spatial magnetic criticality.

Acknowledgments

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