Spin wave excitations in the antiferromagnetic Heisenberg-Kondo model for heavy fermions.

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Abstract.
Recent inelastic neutron scattering experiments in CeIn$_3$ and CePd$_2$Si$_2$ single crystals measured spin wave excitations at low temperatures. These two heavy fermion compounds exhibit antiferromagnetic long-range order, but a strong competition between the Ruderman-Kittel-Kasuya-Yosida(RKKY) interaction and Kondo effect is evidenced by their nearly equal Neél and Kondo temperatures. Our aim is to show how magnons such as measured in the antiferromagnetic phase of these Ce compounds, can be described with a microscopic Heisenberg-Kondo model introduced by J.R.Iglesias, C.Lacroix and B.Coqblin, used before for studies of the non-magnetic phase. The model includes the correlated Ce-4f electrons hybridized with the conduction band, where we also allow for correlations, and we consider competing RKKY (Heisenberg-like $J_H$) and Kondo ($J_K$) antiferromagnetic couplings. Carrying on a series of unitary transformations, we perturbatively derive a second-order effective Hamiltonian which, projected onto the antiferromagnetic electron ground state, describes the spin wave excitations, renormalized by their interaction with correlated itinerant electrons. We numerically study how the different parameters of the model influence the renormalization of the magnons, yielding useful information for the analysis of inelastic neutron scattering experiments in antiferromagnetic heavy fermion compounds. We also compare our results with the available experimental data, finding good agreement with the spin wave measurements in cubic CeIn$_3$.

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1. Introduction

The description of heavy fermion compounds is challenging due to the rich variety of phase diagrams they present, and the anomalous physical properties which may be found. Among them, appear the Ce and U compounds which exhibit long-range antiferromagnetism (AF) at low temperatures (for example, among antiferromagnetic Ce compounds, CeRh$_2$Si$_2$ exhibits the highest ordering temperature $T_N = 36K$, with local magnetic ordered moments of $1.34 - 1.42\mu_B$ per Ce, i.e. relatively large, compared to the full Ce$^{3+}$ free-ion value: $2.54\mu_B$).[1] Depending on the particular compound,[2] the antiferromagnetism takes different forms (magnitude of the local moments varies widely: e.g. $0.001\mu_B$ as in CeRu$_2$Si$_2$ or $0.02\mu_B$ in UPt$_3$, to $1.55\mu_B$ as in UCu$_5$; as does the spin configuration: with three-, two- or one-dimensional AF structures observed). Antiferromagnetism may also appear competing or coexisting with superconductivity,[3, 4] for which spin fluctuation-mediated pairing mechanisms are explored.[5] Non-Fermi liquid behaviour may appear,[6] and quantum criticality has become a subject of intensive study in these compounds, both experimentally and theoretically.[4, 7, 8, 9, 10, 11] The crossover from the antiferromagnetic state to the non-magnetic heavy fermion state, which can be tuned by pressure, doping or magnetic field, is one of the most interesting problems in strongly correlated $f-$compounds.

The physical properties of these compounds are determined by the strongly correlated $f-$electrons present ($4f$ in Ce; $5f$ in U) and their hybridization with the conduction band. The RKKY indirect exchange interaction between $f-$ local magnetic moments, favouring the establishment of long-range magnetic order, competes with the screening of these moments by the conduction electrons, described by the Kondo effect.[12] This competition is the subject of the Doniach diagram,[13] which compares the variation of the Néel and Kondo-impurity temperatures with increasing antiferromagnetic intrasite exchange coupling $J_K$, between local $f$-moments and conduction electron spins. Compounds with similar magnetic ordering temperature $T_N$ and Kondo temperature $T_K$, the temperature below which magnetic susceptibility saturates indicating coherent Kondo-singlet formation, are ideally suited to the study of this RKKY-Kondo competition. In this regard, experiments on CeM$_2$Sn$_2$ ($M=$Ni, Ir, Cu, Rh, Pd, and Pt: $4d$ or $5d$ transition metals)[14] and CeX$_2$Si$_2$ ($X=$Au, Pd, Rh, Ru) [15] were undertaken, indicating that departures between theory and experiments resulted from the use of Kondo impurity relations. The Kondo-lattice model, instead, consisting of a lattice of local magnetic moments coexisting with a conduction band, has proved appropriate for the description of many $4f$ and $5f$ materials, in particular most Ce (or Yb) compounds, respectively corresponding to a configuration close to $4f^1$ (or $4f^{13}$), where one $4f$ electron (or hole) interacts with the conduction electrons.[10, 16] In 1997 a revisited Doniach diagram was introduced, including short-range antiferromagnetic correlations in the Kondo lattice, in order to improve the
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description and, in particular, to account for the observed pressure dependence of $T_K$ in CeRh$_2$Si$_2$.\[16\] The situation is more complex in Uranium compounds, where U has a $5f^n$ configuration with $n=2$ or 3, since the $5f$ electrons are much less localized than the $4f$ electrons of rare earths. Regarding spin dynamics, it is not clear that Ce and U compounds are intrinsically similar.\[2\] In the following we will focus on Ce-compounds, except otherwise specifically stated.

Experimentally, while the magnetic response due to Kondo spin fluctuations in the paramagnetic state of heavy fermions is well studied, relatively little is known about the nature of the magnetic excitations in the ordered phase of Kondo lattices,\[2\] on which our present study will focus. Being still an unsolved problem how to describe on equal terms both the Kondo effect and antiferromagnetism,\[19\] here we will focus on systems with relatively large local magnetic moments and study them deep inside the antiferromagnetic phase: far from the antiferromagnetic quantum critical point, where spin fluctuations would become more relevant.

A few years ago CePd$_2$Si$_2$\[20\] single crystals were studied with inelastic neutron scattering: below the antiferromagnetic ordering temperature strongly dispersive spin wave excitations were found, with an anisotropic damping, which coexisted with the Kondo-type spin fluctuations also present above $T_N$. At $T = 1.5K$ these spin waves were measured along various BZ paths: they were found to present an energy gap of 0.83 meV and to extend up to almost 3.5 meV. CePd$_2$Si$_2$ has a bcc tetragonal structure, and its antiferromagnetic ground state is characterized by propagation vector: $\vec{q} = (1/2, 1/2, 0)$, with ordered moments: $S = 0.66\mu_B$, $T_N = 8.5K$ and $T_K = 10K$, and linear electronic specific heat coefficient $\gamma = 250 \text{ mJ/mol K}^2$. Under pressure application, at 28.6 kbar the system undergoes a transition into a superconducting phase with critical temperature of 430 mK.\[21, 22\] More recently, inelastic neutron studies of CeIn$_3$ single crystals were performed, with similar results.\[21\] Well defined spin wave excitations with a bandwidth of 2 meV and a gap of 1.28 meV were found in the antiferromagnetic phase,\[21\] coexisting with Kondo-type spin fluctuations and crystal-field excitations which also appeared above $T_N = 10K = T_K$. CeIn$_3$ crystallizes in a cubic (fcc) structure, with an antiferromagnetic structure characterized by magnetic propagation vector $\vec{q} = (1/2, 1/2, 1/2)$, with ordered moments: $S = 0.5\mu_B$ and $\gamma = 130 \text{ mJ/mol K}^2$. Under application of pressure, at 26.5 kbar the system undergoes a transition into a superconducting phase with critical temperature of 200 mK.\[21\] Recently, similar antiferromagnetic magnon excitations were measured by inelastic neutron scattering in CeCu$_2$.\[23\] an anisotropic antiferromagnetic heavy fermion compound with $T_N = 3.5K$ and $T_K = 4K$.

In next section, we will briefly introduce the microscopic Heisenberg-Kondo model proposed by J.R.Iglesias, C.Lacroix and B.Coqblin,\[16\] to study the non-magnetic phase of heavy fermion AF compounds, to which we shall add conduction electron correlations. We will then present our calculation for the renormalization of spin wave excitations due to their interaction with the correlated conduction electrons (the Appendix complements this section). In Section\[5\] we will discuss the results of our study, show how the different
Spin wave excitations in the antiferromagnetic Heisenberg-Kondo model for heavy fermions. Parameters of the model influence the renormalization of the magnons, and compare our results with the available experimental data.\cite{20, 21} In Section 5 we summarize and point out that the present work should yield useful information for the analysis and prediction of inelastic neutron scattering experiments in heavy fermion AF compounds, as CeRh$_2$Si$_2$.

2. Microscopic model, and perturbative approach.

In order to describe the Ce-heavy-fermion systems exhibiting antiferromagnetic long-range order we have used the microscopic model which has been proposed by Coqblin et al.\cite{16} to describe the competition between the Kondo effect and the RKKY interaction, in compounds where departures from the original Doniach picture\cite{13} appear. In principle, both the RKKY magnetic coupling and the Kondo effect can be obtained from the Kondo intrasite-exchange term, but when dealing with approximations it is difficult to assure that both effects are taken into account if an explicit intersite exchange (as the effective RKKY interaction or, depending on the system, also the direct exchange) is not included in the Hamiltonian.\cite{10} The model\cite{16} consists of a Kondo lattice, featuring local magnetic moments coupled both to conduction electrons, by a Kondo-type interaction $J_K$, and, among themselves, by an antiferromagnetic RKKY-type exchange $J_H > 0$. The moments are assumed to order below the Néel temperature $T_N$, but we will concentrate on the zero-temperature limit. The Hubbard-correlated conduction electrons occupy a non-degenerate band. Therefore, the model may be represented in standard notation by the following Heisenberg-Kondo Hamiltonian:

\begin{equation}
H = H_{\text{Heis}} + H_{\text{band}} + H_{\text{Kondo}}
\end{equation}

\begin{equation}
H_{\text{Heis}} = J_H \sum_{i \langle m \rangle} \mathbf{S}_i \cdot \mathbf{S}_m - B_a \left( \sum_{l \in A} S_l^z - \sum_{j \in B} S_j^z \right)
\end{equation}

\begin{equation}
H_{\text{band}} = \sum_{i \sigma} \epsilon_i n_{i \sigma} + \sum_{i \langle m \rangle \sigma} t_{i \sigma m \sigma} c_{i \sigma}^\dagger c_{m \sigma} + U \sum_i n_{i \uparrow} n_{i \downarrow}
\end{equation}

\begin{equation}
H_{\text{Kondo}} = J_K \left( \sum_{l \in A} \mathbf{s}_l \cdot \mathbf{S}_l + \sum_{j \in B} \mathbf{s}_j \cdot \mathbf{S}_j \right)
\end{equation}

where we have included in $H_{\text{Heis}}$ an anisotropy field $B_a > 0$, which is physically realized by the crystal field in the heavy fermion systems. It will be shown to play a crucial role with respect to the stability of the AF spin waves.

Here $i \langle m \rangle$ indicates that the lattice site index $m$ runs over the $z$ nearest neighbours of site $i$ which, in turn, runs over the $N$ sites of the full lattice. The itinerant electron spin is $s_{i \langle j \rangle}$, while $A, B$ label the two interpenetrating sublattices with $N/2$ sites each, where local moments, $S_{l \in A}$ and $S_{j \in B}$, with opposite moment direction, sit. The Kondo exchange $J_K$ could in principle have either sign (though for heavy fermion compounds, it would be antiferromagnetic: $J_K \geq 0$).
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2.1. Diagonalization of $H_{Heis}$.

We diagonalize the Heisenberg term, by representing the local moments operators in the Holstein-Primakoff approximation, which is appropriate at temperatures much lower than $T_N$. Namely, we take

$$\vec{S}_l = (S^+_l, S^-_l, S^z_l) \sim (\sqrt{2}Sb^+_l, \sqrt{2}Sb^-_l, S - b^+_lb_l)$$

$$\vec{S}_j \sim (\sqrt{2}Sb^+_j, \sqrt{2}Sb^-_j, -(S - b^+_jb_j))$$

(5)

where $b^+_l(\dagger)$ and $b^+_j(\dagger)$ are the bosonic spin-deviation operators in sublattices $\mathcal{A}$ and $\mathcal{B}$, respectively. Going to reciprocal space in the reduced Brillouin zone (RBZ) one gets an anharmonic Hamiltonian in the spin-deviation $\{b^+_l,b^-_l\}$ operators. It’s convenient for what follows to recall that a generic anharmonic Hamiltonian of the form:

$$H_{anh} = \sum_q F_q (b^+_q b^-_q + b^+_q b^-_q) + \sum_q G_q (b^+_q b^-_q + b^+_q b^-_q)$$

(6)

where $F_q, G_q$ are $c$-numbers, is diagonalized by a Bogolyubov transformation, which introduces the AF spin wave operators $\{a^+_q, a^-_q\}$ according to:

$$b^+_q = a^+_q \text{Ch} (\vartheta_q) + a^-_q \text{Sh} (\vartheta_q)$$

$$b^-_q = a^+_q \text{Ch} (\vartheta_q) + a^-_q \text{Sh} (\vartheta_q)$$

(7)

The diagonalization condition is $\text{Th} (2\vartheta_q) = -G_q/F_q$. The diagonalized Hamiltonian (defining $\text{sgn} (x) = x/|x|$) reads:

$$e^S H_{anh} e^{-S} = H_{diag} = \sum_q \text{sgn} (F_q) \sqrt{F^2_q - G^2_q} (a^+_q a^-_q + a^+_q a^-_q)$$

(8)

Stability of the system requires the renormalized frequency to be real and positive. Reality imposes the condition $F^2_q > G^2_q$, i.e. the anharmonic part must have an amplitude smaller than the harmonic part. If the renormalized frequencies are real, their positiveness is assured by the additional constraint $F_q > 0$.

In our case the diagonalization condition for $H_{Heis}$ reads:

$$\text{Th} (2\vartheta_q) = -G_q/F_q = - \left( \frac{J_H S}{zJ_H S + B_a} \right) \sum_{\Delta_{ij}} \cos (q\Delta_{ij})$$

(9)

In the absence of the interaction with the fermions, i.e. in the limit of vanishing $J_K$, the frequency of the bare AF spin waves would be ($z$ is the number of nearest neighbors and $\Delta_{ij}$ is the vector joining two n.n.sites)

$$H_{Heis} = \sum_q \hbar\Omega_q \left(a^+_qa^-_q + \frac{1}{2}\right)$$

(10)

$$\hbar\Omega_q = (zJ_H S + B_a) \sqrt{1 - \left[ \frac{J_H S \sum_\Delta \cos (q\Delta_{ij})}{zJ_H S + B_a} \right]^2}$$

(11)
2.2. Diagonalization of $H_{\text{band}}$.

The band electrons described by $H_{\text{band}}$ can be in either the paramagnetic (PM) or AF state, according to the values of the bandwidth $W = 2zt$ and of the Hubbard correlation $U$. To diagonalize $H_{\text{band}}$ we will use a reformulation of Gutzwiller’s variational approach for the description of antiferromagnetism in narrow bands due to Spalek et al.\cite{Spalek2021} This approach allows to connect smoothly the PM state for $U \ll W$ to standard (mean-field) Slater band-insulator for $U \approx W$ and to the localized Mott antiferromagnetic insulator for $U \gg W$. One expresses the correlation-induced bandwidth reduction in the paramagnetic (PM) state by a Gutzwiller-type factor $\Phi(n, \rho)$ depending on the band filling $n$ and on the probability of double occupancy $\rho = N^{-1} \sum_{\ell} \langle n_{\ell \uparrow} n_{\ell \downarrow} \rangle$. The correlated band energies $\varepsilon^U_k$ are given by:

$$\varepsilon^U_k = \Phi(n, \rho) \varepsilon^0_k$$

(12)

$$\Phi(n, \rho) = 1 - \left(\frac{n}{2 - n}\right) \left(1 - \frac{4\rho}{n^2}\right)$$

where $\varepsilon^0_k$ are the uncorrelated band energies. The $U$-depending optimal value of $\rho$ is found at zero temperature by minimizing the PM energy

$$E^{PM} = \Phi(n, \rho) \sum_{k\sigma} \varepsilon^0_k \langle n_{k\sigma}\rangle + NU\rho$$

(13)

at given $n$ and $U$.

Assuming that the electrons have an AF ground state of Néel-type, one adopts the standard Slater formalism only with the PM energies renormalized according to Eq.\cite{Gutzwiller1963} We therefore introduce the fermion operators for this AF Slater-type state $\{\alpha^{(\uparrow)}_{k\sigma}, \beta^{(\uparrow)}_{k\sigma}\}$ by the transformation

$$c_{k\sigma}^\dagger = \alpha_{k\sigma}^\dagger \cos \zeta_{k\sigma} - \beta_{k\sigma}^\dagger \sin \zeta_{k\sigma}$$

$$c_{k+Q,\sigma}^\dagger = \alpha_{k\sigma}^\dagger \sin \zeta_{k\sigma} + \beta_{k\sigma}^\dagger \cos \zeta_{k\sigma}$$

(14)

where $Q = (1/2, 1/2, 1/2)$ in units of $2\pi/a$ is the wavevector characterizing the AF magnetic state and $k$ is a wavevector belonging to the reduced Brillouin zone (RBZ) defined by $|k| \leq |Q|$. The diagonalization condition for $H_{\text{band}}$ in a lattice with an inversion center yields:

$$\tan (2\zeta_{k\sigma}) = -\sigma \frac{U \langle s \rangle_{\alpha\beta}}{\Phi \varepsilon_k} \equiv \sigma \tan (2\zeta_k),$$

(15)

where the amplitude of the AF order parameter $\langle s \rangle_{\alpha\beta}$ of the itinerant electrons (staggered magnetization, or band electron polarization), is given by:

$$\langle s \rangle_{\alpha\beta} = \frac{1}{2N} \sum_{k \in \text{RBZ}, \sigma} \left( \langle n^\alpha_{k\sigma} \rangle - \langle n^\beta_{k\sigma} \rangle \right) \sin 2\zeta_k$$

(16)

Let’s stress that Eq.\cite{Gutzwiller1963} does not set the sign of $\langle s \rangle_{\alpha\beta}$. When introducing the interaction with the ordered local moments, its sign will be set according to

$$\langle s \rangle_{\alpha\beta} = -\text{sgn} (J_K) \langle s \rangle_{\alpha\beta}$$

(17)
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so that a positive $J_K$ means an antiparallel orientation with respect to the local moment staggered magnetization, assumed positive by definition, and vice versa.

The resulting diagonal bare electron Hamiltonian is:

$$H_{AF}^{band} = \sum_{k \in RBZ, \sigma} \left[ E^{\alpha}_{k\sigma} n^{\alpha}_{k\sigma} + E^{\beta}_{k\sigma} n^{\beta}_{k\sigma} \right] - U N \left( \frac{n^2}{4} - \langle s \rangle^2_{\alpha\beta} \right),$$

where the bare electron eigenenergies (actually spin-independent) read ($x = \alpha, \beta$):

$$E^{x}_{k\sigma} = \frac{1}{2} \langle n \rangle_{\alpha} + (1 - 2\delta_{x\alpha}) \sqrt{\Phi^2 \epsilon^2_{k} + U^2 \langle s \rangle^2_{\alpha\beta}},$$

where $\delta_{x\alpha}$ denotes the Kronecker delta. Notice that $\alpha$ is the lower subband. The subband filling factors $\langle n^{x}_{k\sigma} \rangle = \langle n^{x}_{k, -\sigma} \rangle = \left[ \exp \left( E^{x}_{k\sigma} - \mu \right) / k_B T + 1 \right]^{-1}$ also depend on $\langle s \rangle_{\alpha\beta}$ through $E^{x}_{k\sigma}$ so that Eq.16 has to be solved self-consistently.

3. The Kondo coupling.

Taking into account the orientation of the local-moment magnetization, we shall distinguish in the Kondo term the longitudinal $H^z_K$ from the transverse $H^\perp_K$ contributions. By taking as positive $z$ direction the direction of $S_l \in A$, they are defined as:

$$H^z_K = J_K \left( \sum_{l \in A} s_l^z S_l^z + \sum_{j \in B} s_j^z S_j^z \right)$$

$$H^\perp_K = \frac{J_K}{2} \left[ \sum_{l \in A} (s_l^+ S_l^- + H.c.) + \sum_{j \in B} (s_j^+ S_j^- + H.c.) \right]$$

3.1. The longitudinal part $H^z_K$ of the Kondo coupling term.

It is convenient to rewrite the longitudinal Kondo term by decomposing it into the two sublattices contributions. For a given sublattice $\mathcal{X} = A, B$ we have from Eq.[20]:

$$\sum_{l \in \mathcal{X}} \left( S - b_l^\dagger b_l \right) s_l^z$$

$$= (2\delta_{\mathcal{X}A} - 1) \left[ \frac{1}{2} \sum_{\sigma, l \in \mathcal{X}} \sigma n_{l\sigma} - \frac{1}{2} \sum_{\sigma, l \in \mathcal{X}} b_l^\dagger b_l \sigma n_{l\sigma} \right]$$

$$= H^z_{\mathcal{X}1} + H^z_{\mathcal{X}2} \quad (\mathcal{X} = A, B)$$

This expression, rewritten in terms of the operators $\left\{ \alpha^{(1)}_p \right\}$ and $\left\{ \alpha^{(1)}_p, \beta^{(1)}_p \right\}$ which diagonalize, respectively, $H_{Heis}$ and $H_{band}$, yields several contributions. The first one, not containing Bose operators, is:

$$H^z_{A1} + H^z_{B1} = \frac{J_K}{2} S \sum_{p, \sigma} \left[ (n^{\alpha}_{\sigma p} - n^{\beta}_{\sigma p}) \sin (2\zeta_p) \right]$$

$$+ \frac{J_K}{2} S \sum_{p, \sigma} \sigma \cos (2\zeta_p) \left( \beta^\dagger_{\sigma p} \alpha_p^\dagger + \alpha^\dagger_{\sigma p} \beta_p^\dagger \right)$$

where $n^{\alpha}_{\sigma p} = \langle n^{\alpha}_{k_p \sigma} \rangle$ and $n^{\beta}_{\sigma p} = \langle n^{\beta}_{k_p \sigma} \rangle$ are the subband occupation numbers.
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Notice that the second term in Eq. 23 describes a Kondo-induced hybridization between the bare electrons.

The second contribution $H_{X}^{z}(X = A, B)$ describes scattering terms between the spin waves and itinerant electrons. It reads:

$$H_{X}^{z} = -\frac{J_{K}}{2N} \sum_{pqrs,\sigma} \alpha_{r\sigma}^{\dagger} \alpha_{p+q-r,s} \left[ (2\delta_{XA} - 1) \sin \zeta_{r} + \sigma \cos \zeta_{r} \right] \times$$

$$\times \left[ \cos \zeta_{p+q-r} + (2\delta_{XA} - 1) \sigma \sin \zeta_{p+q-r} \right] V_{pq}$$

$$- \frac{J_{K}}{2N} \sum_{pqrs,\sigma} \alpha_{r\sigma}^{\dagger} \beta_{p+q-r,s} \left[ (2\delta_{XA} - 1) \sin \zeta_{r} + \sigma \cos \zeta_{r} \right] \times$$

$$\times \left[ -\sigma \sin \zeta_{p+q-r} + (2\delta_{XA} - 1) \cos \zeta_{p+q-r} \right] V_{pq}$$

$$- \frac{J_{K}}{2N} \sum_{pqrs,\sigma} \beta_{r\sigma}^{\dagger} \alpha_{p+q-r,s} \left[ -\sin \zeta_{r} + (2\delta_{XA} - 1) \sigma \cos \zeta_{r} \right] \times$$

$$\times \left[ \cos \zeta_{p+q-r} + (2\delta_{XA} - 1) \sin \zeta_{p+q-r} \right] V_{pq}$$

$$- \frac{J_{K}}{2N} \sum_{pqrs,\sigma} \beta_{r\sigma}^{\dagger} \beta_{p+q-r,s} \left[ -\sin \zeta_{r} + (2\delta_{XA} - 1) \sigma \cos \zeta_{r} \right] \times$$

$$\times \left[ -\sigma \sin \zeta_{p+q-r} + (2\delta_{XA} - 1) \cos \zeta_{p+q-r} \right] V_{pq} \tag{24}$$

where $V_{pq}$ is a bosonic operator:

$$V_{pq} = a_{p}^{\dagger} a_{q} \text{Ch}(\vartheta_{q}) \text{Ch}(\vartheta_{p}) + a_{-p}^{\dagger} a_{q} \text{Ch}(\vartheta_{q}) \text{Sh}(\vartheta_{p})$$

$$+ a_{p}^{\dagger} a_{-q} \text{Sh}(\vartheta_{q}) \text{Ch}(\vartheta_{p}) + \left( a_{-p}^{\dagger} a_{q}^{\dagger} + \delta_{pq} \right) \text{Sh}(\vartheta_{q}) \text{Sh}(\vartheta_{p}) \tag{25}$$

By inserting the identity $1 = \delta_{pq} + (1 - \delta_{pq})$ in Eq. 24 we can distinguish between the contributions containing the diagonal and non-diagonal parts of $V_{pq}$. The term in $H_{X}^{z}$ containing the diagonal part $V_{pp}\delta_{pq}$, after symmetrizing with respect to $\pm q$, can be further decomposed as $H_{ABS2, diag}^{z0} + H_{ABS2, diag}^{z}$ where the boson-independent term

$$H_{ABS2, diag}^{z0} = -\frac{J_{K}}{2} \sum_{p,\sigma} \left[ \sin(2\zeta_{p}) \right] \left[ n_{p\sigma}^{\alpha} - n_{p\sigma}^{\beta} \right] \left( \frac{2}{N} \right) \sum_{q} \text{Sh}^{2}(\vartheta_{q})$$

$$- \frac{J_{K}}{2} \sum_{p,\sigma} \sigma \left[ \cos(2\zeta_{p}) \right] \left[ \beta_{p\sigma}^{\dagger} \alpha_{p\sigma} + \alpha_{p\sigma}^{\dagger} \beta_{p\sigma} \right] \left( \frac{2}{N} \right) \sum_{q} \text{Sh}^{2}(\vartheta_{q}) \tag{26}$$

contributes, together with $H_{A1}^{z} + H_{B1}^{z}$ (Eq. 23), to the electronic Hamiltonian, yielding modified band energies and an additional inter-subband Kondo-induced hybridization.
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of the bare AF electrons. The remaining term $H^z_{AB2,\text{diag}}$ contains bosons and reads:

$$H^z_{AB2,\text{diag}} = -\frac{J_K}{4} \sum_{p,q} \sin (2\zeta_p) \left( n^\alpha_{p,\sigma} - n^\beta_{p,\sigma} \right) \left( \frac{2}{N} \right) \sum_q \text{Ch} \left( 2\vartheta_q \right) \left( a^\dagger_q a_q + a^\dagger_{-q} a_{-q} \right)$$

$$+ \frac{J_K}{4} \sum_{p,q} \left[ -\sigma \cos (2\zeta_p) \right] \left( \beta^\dagger_{p,\sigma} \alpha_{p,\sigma} + \alpha^\dagger_{p,\sigma} \beta_{p,\sigma} \right) \left( \frac{2}{N} \right) \sum_q \text{Ch} \left( 2\vartheta_q \right) \left( a^\dagger_q a_q + a^\dagger_{-q} a_{-q} \right)$$

$$+ \frac{J_K}{4} \sum_{p,q} \left[ -\sin (2\zeta_p) \right] \left( n^\alpha_{p,\sigma} - n^\beta_{p,\sigma} \right) \left( \frac{2}{N} \right) \sum_q \text{Sh} \left( 2\vartheta_q \right) \left( a^\dagger_q a^\dagger_{-q} + a_q a_{-q} \right)$$

Finally, the non-diagonal part of $H^z_{A2} + H^z_{B2}$ is:

$$H^z_{AB2,\text{nondiag}} = \frac{J_K}{2} \left( \frac{2}{N} \right) \sum_{p,q,\sigma} \left[ \sin (\zeta_r + \zeta_{p+r-q}) \left( \beta^\dagger_{r,\sigma} \beta_{p+r-q,\sigma} - \alpha^\dagger_{r,\sigma} \alpha_{p+r-q,\sigma} \right) \right. - \left. \sigma \cos (\zeta_r + \zeta_{p+r-q}) \left( \beta^\dagger_{r,\sigma} \alpha_{p+r-q,\sigma} + \alpha^\dagger_{r,\sigma} \beta_{p+r-q,\sigma} \right) \right] V_{pq} \left( 1 - \delta_{pq} \right)$$

3.2. Effect of $H^z_K$ on the electronic Hamiltonian.

The appearance of the above-mentioned Kondo-induced hybridization terms between the itinerant electrons (Eqs. 23 and 26) suggests to perform a joint diagonalization of $H_{band}$ and such terms. It is convenient to define the number of AF spin waves at zero temperature for the Heisenberg Hamiltonian $N_{SW}^{\text{AF}}$, expressing the zero-point deviation for the local moments when $J_K = 0$, and the measurable amplitude of the local moment polarization $\langle S^z_0 \rangle$ as:

$$N_{SW}^{\text{AF}} = \left( \frac{2}{N} \right) \sum_q \text{Sh}^2 \left( \vartheta_q \right) \quad \langle S^z_0 \rangle = S - N_{SW}^{\text{AF}}$$

where $\vartheta_q$ was defined in Eq. 9.

Thus, the hybrid Hamiltonian to be diagonalized may be written:

$$H^{\text{hyd}}_0 = \sum_{p,\sigma} \left( E^\alpha_{p,\sigma} n^\alpha_{p,\sigma} + E^\beta_{p,\sigma} n^\beta_{p,\sigma} \right) + \frac{J_K}{2} \sum_{p,\sigma} \left[ \sin (2\zeta_p) \right] \left( n^\alpha_{p,\sigma} - n^\beta_{p,\sigma} \right)$$

$$+ \frac{J_K}{2} \sum_{p,\sigma} \sigma \left[ \cos (2\zeta_p) \right] \left( \beta^\dagger_{p,\sigma} \alpha_{p,\sigma} + \alpha^\dagger_{p,\sigma} \beta_{p,\sigma} \right)$$

The diagonalization is realized by introducing the hybridized Fermi operators $A^\dagger_{p,\sigma}, B^\dagger_{p,\sigma}$ through the unitary transformation:

$$\alpha^\dagger_{p,\sigma} = A^\dagger_{p,\sigma} \cos \xi_{p,\sigma} + B^\dagger_{p,\sigma} \sin \xi_{p,\sigma}$$

$$\beta^\dagger_{p,\sigma} = -A^\dagger_{p,\sigma} \sin \xi_{p,\sigma} + B^\dagger_{p,\sigma} \cos \xi_{p,\sigma}$$

(31)
Spin wave excitations in the antiferromagnetic Heisenberg-Kondo model for heavy fermions.

The diagonalization condition requires:

\[
\tan (2\xi_p) = \frac{J_K \langle S_0^z \rangle \cos (2\zeta_p)}{E_p^3 - E_p^0 + J_K \langle S_0^z \rangle \sin (2\zeta_p)}
\]

(32)

\[
= \sigma \frac{J_K \langle S_0^z \rangle |\varepsilon_p|}{(E_p^3 - E_p^0) \sqrt{\Phi^2 \varepsilon_p^2 + U^2 (\langle s^z \rangle_{\alpha\beta})^2 + U |J_K \langle S_0^z \rangle|}}
\]

where in the second line we have explicitated \(\sin (2\zeta_p)\) and \(\cos (2\zeta_p)\).

Therefore the electronic Hamiltonian in diagonal form reads:

\[
H_{el}^0 = \sum_{\rho,\sigma} (E^{A\rho}_{\sigma \rho} n^{A\rho}_{\sigma \rho} + E^{B\rho}_{\sigma \rho} n^{B\rho}_{\sigma \rho})
\]

(33)

with hybridized energies given by \((X = A, B)\):

\[
E^X_{\rho \sigma} = \frac{1}{2} [E_p^3 + E_p^0]
\]

\[
- \left( \delta_{X\alpha} - \frac{1}{2} \right) \sqrt{[E_p^3 - E_p^0 + J_K \langle S_0^z \rangle \sin (2\zeta_p)]^2 + [J_K \langle S_0^z \rangle \cos (2\zeta_p)]^2}
\]

(34)

The evaluation of the band AF order parameters in the hybridized basis, as detailed in the Appendix, yields:

\[
\langle s^z \rangle_{AB} = -\text{sgn} (J_K) \frac{1}{2N} \sum_{\rho,\sigma} \{ \sin [2 (\zeta_p + \xi_p)] \langle n^A_{\rho \sigma} \rangle - \sin [2 (\zeta_p - \xi_p)] \langle n^B_{\rho \sigma} \rangle \}
\]

Notice that in the limit \(J_K \to 0\), i.e. \(\xi_p \to 0\) we recover the result of Eq.16 for the isolated band

\[
\lim_{J_K \to 0} \langle s^z \rangle_{AB} = -\text{sgn} (J_K) \frac{1}{2N} \sum_{\rho,\sigma} \sin (2\zeta_p) \left[ \langle n^A_{\rho \sigma} \rangle - \langle n^B_{\rho \sigma} \rangle \right]
\]

(36)

Conversely, for the case of a band, too weakly correlated to order antiferromagnetically by itself, i.e. for \(U \to 0\), \(\zeta_p \to 0\), we get the Kondo-induced band staggered moment

\[
\lim_{U \to 0} \langle s^z \rangle_{AB} = -\text{sgn} (J_K) \frac{1}{2N} \sum_{\rho,\sigma} \sin (2\xi_p) \left[ \langle n^A_{\rho \sigma} \rangle + \langle n^B_{\rho \sigma} \rangle \right]
\]

(37)

Therefore, due to Eq. 32 in this case the band polarization is explicitly proportional to the effective field \((- |J_K| \langle S_0^z \rangle)\) provided by the local moments, though oppositely oriented.

3.3. The longitudinal Kondo term \(H^z_K\) in the hybrid \(\{A^{(i)}_{\rho \sigma}, B^{(i)}_{\rho \sigma}\}\) basis.

The longitudinal Kondo term obtained above consists of two contributions, namely \(H_{AB2,diag}^z\) (Eq.27) and \(H_{AB2,nondiag}^z\) (Eq.28) which have to be explicitated in the electronic hybrid basis\(\{A^{(i)}_{\rho \sigma}, B^{(i)}_{\rho \sigma}\}\). Defining \(Z_p = \zeta_p - \xi_p\), we get:
Spin wave excitations in the antiferromagnetic Heisenberg-Kondo model for heavy fermions.

The transverse Kondo term reads:

\[ I_d = H_{\text{ABS2,diag}}^{\perp} (\alpha_{p\sigma}^{(t)}, \beta_{p\sigma}^{(t)} \rightarrow A_{p\sigma}^{(t)}, B_{p\sigma}^{(t)}) \]

\[ = \frac{J_K}{2N} \sum_{p,\sigma} \left[ -\sin(2Z_p) \left( n_{p\sigma}^A - n_{p\sigma}^B \right) - \sigma \cos(2Z_p) \left( A_{p\sigma}^\dagger B_{p\sigma} + B_{p\sigma}^\dagger A_{p\sigma} \right) \right] \times \]

\[ \times \sum_q \text{Ch} (2\vartheta_q) \left( a_q^\dagger a_q + a_{-q}^\dagger a_{-q} \right) \]

\[ + \frac{J_K}{2N} \sum_{p,\sigma} \left[ \sin(2Z_p) \left( n_{p\sigma}^A - n_{p\sigma}^B \right) - \sigma \cos(2Z_p) \left( A_{p\sigma}^\dagger B_{p\sigma} + B_{p\sigma}^\dagger A_{p\sigma} \right) \right] \times \]

\[ \times \sum_q \text{Sh} (2\vartheta_q) \left( a_q^\dagger a_q + a_{-q}^\dagger a_{-q} \right) \]

(38)

and

\[ I_{nd} = H_{\text{ABS2,nondiag}}^{\perp} (\alpha_{p\sigma}^{(t)}, \beta_{p\sigma}^{(t)} \rightarrow A_{p\sigma}^{(t)}, B_{p\sigma}^{(t)}) \]

\[ = \frac{J_K}{N} \sum_{pq,\sigma} \left[ -\sin [(Z_r + Z_{p+r-q})] \left( A_{r\sigma}^\dagger A_{p+r-q,\sigma}^\dagger - B_{r\sigma}^\dagger B_{p+r-q,\sigma}^\dagger \right) \right. \]

\[ - \sigma \cos [(Z_r + Z_{p+r-q})] \left( A_{r\sigma} B_{p+r-q,\sigma}^\dagger + B_{r\sigma}^\dagger A_{p+r-q,\sigma} \right) \]

\[ \times V_{pq} (1 - \delta_{pq}) \]

(39)

3.4. The transverse Kondo term \( H_K^{\perp} \) in the hybrid \( \{ A_{p\sigma}^{(t)}, B_{p\sigma}^{(t)} \} \) basis.

The transverse Kondo term reads:

\[ H_K^{\perp} = \frac{1}{2} J_K \left( \sum_{l \in A, \sigma = \pm} s_l^\sigma S_l^{-\sigma} + \sum_{j \in B, \sigma = \pm} s_j^\sigma S_j^{-\sigma} \right) \]

(40)

By expressing the local moments in terms of the spin wave operators \( a_q^{(t)} \), and the electronic part in terms of the hybrid operators \( \{ A_{p\sigma}^{(t)}, B_{p\sigma}^{(t)} \} \), we get:

\[ I^{\perp} = H_K^{\perp} (\alpha_{p\sigma}^{(t)}, \beta_{p\sigma}^{(t)} \rightarrow A_{p\sigma}^{(t)}, B_{p\sigma}^{(t)}) = \]

\[ = \frac{J_K}{2} \sqrt{\frac{S}{N}} \sum_{pq,\sigma} A_{p\sigma}^\dagger A_{p+q,-\sigma}^\dagger a_q^\dagger \left[ \text{Ch} (\vartheta_q) C_{AA}^{+\perp} (p, q) + \text{Sh} (\vartheta_q) C_{BB}^{+\perp} (p, q) \right] \]

(41)

\[ + \frac{J_K}{2} \sqrt{\frac{S}{N}} \sum_{pq,\sigma} A_{p\sigma}^\dagger B_{p+q,-\sigma} a_{-q} \left[ \text{Sh} (\vartheta_q) C_{AA}^{\perp\perp} (p, q) + \text{Ch} (\vartheta_q) C_{BB}^{\perp\perp} (p, q) \right] \]

\[ + \frac{J_K}{2} \sqrt{\frac{S}{N}} \sum_{pq,\sigma} \sigma A_{p\sigma}^\dagger B_{p+q,-\sigma} a_{-q} \left[ \text{Ch} (\vartheta_q) C_{AB}^{\perp\perp} (p, q) - \text{Sh} (\vartheta_q) C_{BA}^{\perp\perp} (p, q) \right] \]

\[ + \frac{J_K}{2} \sqrt{\frac{S}{N}} \sum_{pq,\sigma} \sigma A_{p\sigma}^\dagger B_{p+q,-\sigma} a_{-q} \left[ \text{Sh} (\vartheta_q) C_{AB}^{\perp\perp} (p, q) - \text{Ch} (\vartheta_q) C_{BA}^{\perp\perp} (p, q) \right] \]

\[ + (A \rightleftharpoons B) \]

(42)

where the numerical coefficients \( C_{XY}^{\pm\pm} (p, q) \) \( (X, Y = A, B) \), depending on the angles \( \zeta_p \)

and \( \xi_p \) (Eqs. [15] and [32]) are explicitated in the Appendix.
Spin wave excitations in the antiferromagnetic Heisenberg-Kondo model for heavy fermions.

4. Perturbative derivation of the effective magnon Hamiltonian.

We will now describe the perturbative treatment performed to derive the effective second-order Hamiltonian for magnons. We begin by rearranging the total Hamiltonian, separating it into a basic part \( H_0 \), and a perturbation \( I \). The basic part consists of the bare magnon part \( H_{\text{Heis}} \) (Eq. 10) plus the diagonalized electron Hamiltonian \( H_{0}^{\text{el}} \) (Eq.33). The perturbation includes the full transverse Kondo coupling term \( I^\perp \) and the boson-dependent part of the longitudinal Kondo Hamiltonian \( I^z \), i.e. the terms not included in \( H_{0}^{\text{el}} \). Explicitly we have:

\[
H = H_0 + I = H_0 + (I^z + I^\perp) \\
H_0 = H_{\text{Heis}} + H_{0}^{\text{el}} \\
I^z = I_d^z + I_{nd}^z \\
I^\perp = I^\perp
\]  

where \( I_d^z, I_{nd}^z \) and \( I^\perp \) are respectively given by Eqs.38, 39 and 42.

In the following, the effect of the total perturbation \( I = I_d^z + I_{nd}^z + I^\perp \) will be taken into account through a Fröhlich-type of truncated unitary transformation [25]. We determine the generator \( R \) of the appropriate canonical transformation by eliminating from the transformed Hamiltonian the first order term in the perturbation \( I \). To this aim, we impose

\[
I + i[ R, H_0 ] = 0.
\]

Introducing the notation \( R \equiv R_d^z + R_{nd}^z + R^\perp \), we decompose this constraint into three separate equations, which can be solved [26] yielding:

\[
R^{(z,\perp)} = \lim_{t \to 0} \frac{i}{\hbar} \int_{-\infty}^{t} I^{(z,\perp)}(x) dx.
\]

Each term in the perturbation produces a corresponding term in the generator, namely, from \( I_d^z \) and \( I_{nd}^z \) we obtain the "longitudinal" generators \( R_d^z \) and \( R_{nd}^z \) while from \( I^\perp \) we obtain the "transverse" generator \( R^\perp \). The terms \( R_d^z, R_{nd}^z \) and \( R^\perp \) are detailed in the Appendix. By this procedure, we obtain the second-order effective Hamiltonian for the magnon-conduction electron system as:

\[
H_{\text{eff}} = H_0^0 + \frac{1}{2} \left[ R_d^z + R_{nd}^z + R^\perp, I_d^z + I_{nd}^z + I^\perp \right] + O \left( I_d^z, I_{nd}^z, I^\perp \right)^3
\]  

(44)

Let us anticipate here that one finds that the perturbative parameter which actually controls this expansion, is the ratio \(|J_K/J_H|\) weighted by coefficients depending on the electronic band structure and filling, whose expressions are detailed in the Appendix. These electronic coefficients effectively reduce the magnitude of the perturbative control parameter from the raw value \(|J_K/J_H|\), leading to a smooth convergence of the perturbative expansion even when \(|J_K/J_H|\) is near or exceeds one. This will become clear when we present our numerical results for the renormalized magnons in the next section.

Finally, we make a projection onto the AF fermion wavefunction to obtain a second-order effective Hamiltonian for the magnons \( H_{\text{SW}}^{\text{eff}} \). Let us remark that, when taking the average \( \langle H_{\text{eff}} \rangle_{\text{Fermi}} \) over the AF Fermi wavefunction, we find

\[
\langle [ R_d^z, I_d^z ] \rangle_{\text{Fermi}} = \langle [ R_d^z, I_{nd}^z ] \rangle_{\text{Fermi}} = \langle [ R_d^z, I_{d}^z ] \rangle_{\text{Fermi}} = \langle [ R_{nd}^z, I_d^z ] \rangle_{\text{Fermi}} = 0
\]  

(45)
so that the effective spin wave Hamiltonian has the simpler form

\[ H_{SW}^{eff} \equiv \langle H_{eff} \rangle_{Fermi} = \]

\[ = \sum_{k\sigma} (\mathcal{E}_{k\sigma}^{A} \langle n_{k\sigma}^{A} \rangle + \mathcal{E}_{k\sigma}^{B} \langle n_{k\sigma}^{B} \rangle) + \sum_{q} \frac{\hbar \Omega_{q}}{2} (a_{q}^{\dagger}a_{q} + a_{-q}^{\dagger}a_{-q}) \]

\[ + \frac{1}{2} \langle [R_{d}^{z}, I_{d}^{z}] + [R_{nd}^{z}, I_{nd}^{z}] + [R_{\perp}^{z}, I_{\perp}^{z}] \rangle_{Fermi} \]  

(46)

where

\[ \langle n_{k\sigma}^{X} \rangle = \left[ \exp (\mathcal{E}_{k\sigma}^{X} - \mu) / k_{B}T + 1 \right]^{-1} \]  

(47)

Each one of the perturbative contributions above can be decomposed as a sum of harmonic and anharmonic terms: thus

\[ \frac{1}{2} \langle [R_{d}^{z}, I_{d}^{z}] \rangle_{Fermi} = \sum_{q} \mathcal{G}_{q}^{har} (a_{q}^{\dagger}a_{q} + a_{-q}^{\dagger}a_{-q}) \]

\[ + \sum_{q} \mathcal{G}_{q}^{anhar} (a_{q}^{\dagger}a_{-q}^{\dagger} + a_{q}a_{-q}) \]  

(48)

\[ \frac{1}{2} \langle [R_{nd}^{z}, I_{nd}^{z}] \rangle_{Fermi} = \frac{1}{4} \sum_{q} \hbar (D_{q}^{z+} + D_{q}^{z-}) (a_{q}^{\dagger}a_{q} + a_{-q}^{\dagger}a_{-q}) \]

\[ + \frac{1}{4} \sum_{q} \hbar (\varpi_{q}^{z+} + \varpi_{q}^{z-}) (a_{q}^{\dagger}a_{-q} + a_{q}a_{-q}) \]  

(49)

and

\[ \frac{1}{2} \langle [R_{\perp}^{z}, I_{\perp}^{z}] \rangle_{Fermi} = \frac{1}{4} \sum_{q} \sum_{X,Y=A,B} \mathcal{T}_{q}^{XY} (a_{q}^{\dagger}a_{q} + a_{-q}^{\dagger}a_{-q}) \]

\[ + \frac{1}{4} \sum_{q} \sum_{X,Y=A,B} (S_{q}^{XY1} + S_{q}^{XY2}) (a_{q}^{\dagger}a_{-q} + a_{q}a_{-q}) \]  

(50)

The numerical coefficients entering Eqs. 48 - 50 are given by long and complicated expressions, which we detail in the Appendix. Here we just point out that both the harmonic and the anharmonic parts in \( H_{SW}^{eff} \) have contributions from both longitudinal and transverse Kondo terms.

By further defining

\[ \hbar \Phi_{q} = \hbar \Phi_{-q} = \mathcal{G}_{q}^{har} + \frac{1}{4} \left( \mathcal{T}_{q}^{AA} + \mathcal{T}_{q}^{BB} + \mathcal{T}_{q}^{AB} + \mathcal{T}_{q}^{BA} \right) + \frac{1}{4} (\hbar D_{q}^{z+} + \hbar D_{q}^{z-}) \]

and

\[ \hbar \Psi_{q} = \hbar \Psi_{-q} = \mathcal{G}_{q}^{anhar} + \frac{1}{4} \sum_{X,Y=A,B} (S_{q}^{XY1} + S_{q}^{XY2}) + \frac{1}{4} \hbar (\varpi_{q}^{z+} + \varpi_{q}^{z-}) \]  

(52)

we arrive at the overall effective Hamiltonian:

\[ \langle H \rangle_{Fermi} = \sum_{q} \hbar \left( \frac{\Omega_{q}}{2} + \Phi_{q} \right) (a_{q}^{\dagger}a_{q} + a_{-q}^{\dagger}a_{-q}) + \sum_{q} \hbar \Psi_{q} (a_{q}^{\dagger}a_{q} + a_{-q}^{\dagger}a_{-q}) + \text{const}. \]  

(53)
Spin wave excitations in the antiferromagnetic Heisenberg-Kondo model for heavy fermions.

With one last Bogolyubov transformation

\[ d_q^\dagger = a_q^\dagger \text{Ch} (\eta_q) + a_{-q} \text{Sh} (\eta_q) \]
\[ d_q = a_{-q}^\dagger \text{Sh} (\eta_q) + a_q \text{Ch} (\eta_q) \]  

where

\[ \text{Th} (2\eta_q) = -\frac{\hbar \Psi_q}{\Omega_q/2 + \Phi_q} \]  

we diagonalize the effective Hamiltonian for the spin excitations (Eq. 53), yielding:

\[ H_{SW}^{eff} = \sum_q \hbar \left[ \left( \frac{\Omega_q}{2} + \Phi_q \right) \sqrt{1 - \frac{\Psi_q^2}{(\Omega_q/2 + \Phi_q)^2}} \right] (d_q^\dagger d_q + d_{-q}^\dagger d_{-q}) \]

\[ \equiv \sum_q \hbar \tilde{\Omega}_q d_q^\dagger d_q \]  

where:

\[ \tilde{\Omega}_q \equiv \text{sgn} (\Omega_q + 2\Phi_q) \sqrt{\Omega_q + 2\Phi_q}^2 - 4\Psi_q^2 \]  

is the renormalized frequency of the antiferromagnetic spin waves. In almost all the cases investigated numerically we have found that \( \Phi_q \leq 0 \) so that the overall effect of the interaction of the local moments with the AF band is, in general, a softening of the spin waves with respect to the non-interacting case. Hardening for some wave vectors was obtained only for extremely large values of \( |J_K| \approx t \), outside the range of Kondo coupling values estimated for the heavy fermion compounds addressed here. Notice that, in the absence of the effective anisotropy field \( B_a \) produced by the crystal field, at \( q = 0 \), due to \( \lim_{q \to 0} \Omega_q = 0 \), one would get \( \tilde{\Omega}_q < 0 \). A non-vanishing crystal field thus appears necessary for the stability of the renormalized spin waves. Also, our result of Eq. 57 suggests that the gap measured at \( q = 0 \) should not be taken for a direct estimation of \( B_a \), because it also depends on the value of \( |J_K/J_H| \).

It is interesting to mention that the observed number of Kondo-renormalized spin waves in the interacting system \( N_{SW}^{\text{K}} \) is:

\[ \left( \frac{2}{N} \right) \sum_q \langle d_q^\dagger d_q \rangle = \left( \frac{2}{N} \right) \sum_q \langle a_q^\dagger a_q \rangle \text{Ch} (2\eta_q) + \left( \frac{2}{N} \right) \sum_q \text{Sh}^2 (\eta_q) \]
\[ = \left( \frac{2}{N} \right) \sum_q \langle b_q^\dagger b_q \rangle \text{Ch} (2\vartheta_q) \text{Ch} (2\eta_q) \]
\[ + \frac{1}{2} \left( \frac{2}{N} \right) \sum_q \left[ \text{Ch} (2\vartheta_q) \text{Ch} (2\eta_q) - 1 \right] \]  

thus being always larger than the bare magnon value \( N_{SW}^{\text{H}} \) (Eq. 29). At zero temperature
we find that the observed Kondo-renormalized local-moment polarization $\langle S^z_K \rangle$ is:

$$\lim_{T \to 0} \langle S^z_K \rangle = S - \frac{1}{2} \left( \frac{2}{N} \right) \sum_q \left[ \text{Ch} \left( 2\vartheta_q \right) \text{Ch} \left( 2\eta_q \right) - 1 \right]$$

$$= S - \frac{1}{2} \left( \frac{2}{N} \right) \sum_q \left[ \frac{1}{\sqrt{1 - \gamma_q^2}} \sqrt{\frac{\Omega_q/2 + \Phi_q}{(\Omega_q/2 + \Phi_q)^2 - \Psi_q^2} - 1} \right]$$  (59)

indicating that the screening of the local moments due to their Kondo interaction
with the electrons enhances the zero-point-motion quantum fluctuations of the local
moments, already present in the bare AF Heisenberg case. This allows for a physical
interpretation of the softening effect which, as anticipated above, we obtain for these
renormalized magnons (detailed results in next section). The AF arrangement of local
moments produces an effective magnon Hamiltonian in the form of a harmonic plus
an anharmonic term, which we reduced above to a simple harmonic oscillator form by
the final Bogolyubov transformation. That type of transformation entails the increase
of the zero-point motion of the effective local moments, thus reducing the effective
local magnetic moments with respect to their value in the absence of Kondo coupling.
The relevant scale for the bare Heisenberg energies is determined by $zJ_H S(+B_a)$. In
the interacting case, by diagonalization we arrived to an expression of the effective
spin-wave Hamiltonian (Eq. [56]) representing it as a new Heisenberg-like harmonic
Hamiltonian in terms of an effective local moment $< S^z_K >$, reduced with respect to
the full local moment $S$. So now the relevant energy scale for the renormalized spin
waves is $z < S^z_K > J_H (+B_a)$, a value lower than in the non-interacting case due to
the Kondo screening of the local moments. In other words, the dynamical screening of
the local moments is naturally reflected in a Kondo-induced softening of the magnon
energies.

5. Results and discussion.

In previous section, we obtained a formally simple final expression for the renormalized
antiferromagnetic magnons given by Eq. [57], but one which depends on a series
of coefficients which are detailed in the Appendix. The quite complicated explicit
expressions for these perturbative coefficients, depend on the combined effect or interplay
of the different model parameters, and most coefficients involve multiple summations
over the reduced Brillouin zone. Therefore, our renormalized magnon results can only be
evaluated numerically, exploring wide ranges of the different model parameters, in order
to assess and compare the main effect of each of them. We will show that our model can
reasonably explain experimental magnon results [20, 21, 23] employing parameters in the
range which has been independently shown [27] to be appropriate for a phenomenological
fit of specific heat measurements in this family of antiferromagnetic heavy fermions. Our
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Figure 1. Simple cubic lattice: 1st Brillouin zone and special symmetry points.

The exploration of wide parameter ranges has also allowed us to verify that the convergence radius of the perturbative series which determines the magnon renormalization is much wider than one might naively have expected. As mentioned below Eq. (44), the results presented in this section evidence that the actual “small parameter” controlling this perturbative expansion is not just the bare \( \frac{|J_K|}{|J_H|} \) ratio. Indeed, in the renormalized magnon frequency this quantity appears always weighed by electronic structure- and filling-dependent coefficients which, when combined with suitable values of the other model parameters, effectively reduce the control parameter value from this ratio, leading to convergent results also for \( \frac{|J_K|}{|J_H|} > 1 \), as will be shown in this section.

The numerical study of our model has been done assuming two simple cubic interpenetrating magnetic sublattices, for simplicity and without much loss of generality (rigorously, under this assumption our results would correspond to a cubic (bcc) chemical lattice). Notice that CeIn\(_3\),\([21]\) one of the compounds where inelastic neutron scattering (INS) on single crystals has measured the magnons we aim to describe, is cubic (though fcc) and has a three-dimensional Néel-type antiferromagnetic structure. We evaluated the magnons at zero temperature, assuming an underlying 3D Néel-type antiferromagnetic ground state of the system. Our study focuses on parameter sets far away from the quantum critical region of these systems, i.e. deep inside the antiferromagnetic phase. In fact, our parameters lie well inside the AF stable region recently determined by a DMFT + NRG study\([28]\) of the magnetic phase diagram of the correlated Kondo-lattice (corresponding to the \( J_H = 0 \) case of our model: the addition of non-negligible AF-like RKKY coupling \( J_H \), as done here, will only increase the stability of the AF phase). As experimentally observed,\([21]\) in this range one might expect Kondo-type spin fluctuations to be less relevant, and the dispersive spin waves, object of our study, to appear in the AF phase. For simplicity, but also in accordance with experimental indications\([21]\), we have further assumed that there is one isolated crystal field level of Ce\(^{3+}\) which is relevant, hosting a spin \( S = 1/2 \) (in fact, \( S = 0.5\mu_B \) is the experimental magnitude of the local moments in CeIn\(_3\),\([21]\) ). The hopping parameter \( t \) was taken as unit of energy, being \( W = 12t \) the total bare electron bandwidth.

We shall start by discussing the general trends we have found in our numerical study
Spin wave excitations in the antiferromagnetic Heisenberg-Kondo model for heavy fermions. of the renormalized magnons given by Eq. 57 to subsequently focus on the description of the measured magnons in antiferromagnetic heavy fermion compounds. Once one takes into account the relative orientation of the band and local moment staggered polarizations according to Eq. 17, the results of our second-order perturbative treatment turn out to be independent of the sign of $J_K$.

Fig. 1 depicts the first Brillouin Zone (BZ) of the simple cubic lattice, and we include the notation for the special symmetry points and BZ paths on which the spin waves were numerically evaluated ($\Gamma \equiv O$ denotes the zone center, $\Delta \equiv X = 0.5\pi/a \,(1,0,0)$, $Y = 0.5\pi/a \,(0,1,0), Z = 0.5\pi/a \,(0,0,1)$). Let us mention here that for the BZ summations we have used the special-points BZ sampling method by Chadi-Cohen (CC), at 4th order, for the simple cubic lattice.[29] To obtain dressed magnons with the correct symmetry of the lattice, and to take into account that the multiple summations involve linear combinations of wavevectors, we have noticed [26] that it was not sufficient to include the basic CC set of wavevectors of the (reduced) first BZ octant, but one needs to extend it to the full first Reduced BZ (RBZ). Therefore one has to consider all the vectors obtained by applying the 48 symmetry operations of the $O_h$ group to the basic CC set. Thus, at 4th-order of the CC method, we have included 5760 special symmetry points for each RBZ summation. To achieve higher accuracy for our determination of

![Figure 2](image_url)  
**Figure 2.** Hybridized (A,B) electron bands ($\uparrow$) along selected BZ paths. Parameters: $S = 1/2; T = 0; t = 1 eV; J_H/t = 0.001; J_K/J_H = 20; n = 0.999$. $U/t$ values as detailed in inset.
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In Fig. 2 we show the typical conduction electron bandstructure near half-filling, given by Eq. (34). Notice that for each value of U only the lower band (denoted A) is filled. Chemical potential values obtained for the cases shown, are: \( \mu/t = -0.63, 0.84, 2.30, 2.33, 1.13 \) (the Fermi level is slightly below the top of the lower subband), respectively for \( U/W = 0.008, 0.25, 0.48, 0.49, 0.67 \) (i.e. the \( U/t \) values of Fig. 2). Near the two values: \( U/t = 5.8, 5.8652 \), the conduction electrons start to develop an AF spin polarization (see polarization values reported in Table I), which at \( U/t = 8 \) has increased to 0.35. The AF solution has a direct band gap, determined by the AF hybridized subband energies at the BZ point \( R \) on the cube diagonal (see Fig. 1). The size of the gap, as well as the energy of its centroid, increases with the magnitude of the electron correlation \( U \), while also a correlation-driven band-narrowing effect is seen to appear. For small \( J_K \) , the AF band gap value essentially depends on \( U \langle s \rangle_{\alpha\beta} \), with \( \langle s \rangle_{\alpha\beta} \approx \langle s \rangle_{\alpha\beta} \) growing with both the band filling \( n \) and the correlation \( U \). In Table 1 these trends of the band polarization with the different parameters are evidenced.

It is also interesting to compare our band polarization values (tabulated in Table I) with those reported in Fig. 2 of Ref. [28], for corresponding parameters. Notwithstanding the different respective treatments for the band electron correlations, we find quite reasonable agreement where we could check it. In the present work, focused on applications to the AF heavy fermion compounds where magnons were measured, we have used antiferromagnetic Kondo coupling values in a relatively narrow region around \( J_K/W \sim 10^{-5} - 10^{-3} \). In agreement with Peters and Pruschke,[28] in this parameter range we find spin polarizations characteristic of the RKKY regime: the local moments are almost fully polarized, while the corresponding band polarization obtained for \( U \sim 0 \) (i.e. unpolarized “PM” bare conduction band, corresponding e.g. to our data of the first two columns of Table I) is proportional to the “effective field” provided by the local spins, as mentioned in the last paragraph of Section 3.2. Our \( U/W = 0 \) results thus agree quite well with the corresponding ones of Ref. [28]. Since their results are given only for \( U/W = 0, 1 \) we could not make the comparison for intermediate \( U/W \) values.

We have also explored wider ranges of values for \( J_K \), to verify the consequences of Eq. (59). We have found that, if the renormalized spin waves are real and positive everywhere in the RBZ, then the local moment value is scarcely affected (reduced). Conversely, the larger are the regions of the RBZ where the Eq. (57) yields either negative or imaginary results, the stronger is the reduction of \( \langle S^z_K \rangle \), in qualitative agreement with the results of Ref. [28] for AF Kondo coupling.

In Fig. 3 we show the dependence of the renormalization of the antiferromagnetic magnons on the bare \( J_K/J_H \) ratio at half-filling (the most relevant filling for AF heavy fermion compounds) when the correlation \( U = 3t \) is not strong enough to appreciably AF-polarize the bare band \( U \langle s^z \rangle_{\alpha\beta} \approx 0 \): we labelled this case as PM, corresponding to a paramagnetic bare conduction band (at \( J_K = 0 \)). The top curve represents the bare magnons \( \Omega_q \) (independent of the conduction electrons). We have included a small
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Figure 3. (PM) $J_K/J_H$ dependence of renormalized AF magnons: magnon energy along selected BZ paths. Parameters: $S = 1/2; T = 0; t = 1eV; J_H/t = 0.001; n = 0.999; U/t = 6; B_a/t = 0.0005$. $J_K/J_H$ values as detailed in inset; $w_0$ denotes the bare magnons $\Omega_q$.

anisotropy field $B_a$, as inelastic neutron scattering experiments reporting a magnon gap indicate. [20] [21] As a general trend, anticipated in the last paragraph of previous section, we find that the renormalization reduces the spin wave frequency $\tilde{\Omega}_q$ with respect to bare $\Omega_q$, the effect growing with the ratio $|J_K/J_H|$. The softening is present throughout the whole RBZ, and is strongly dependent on the wavevector, being maximal around the $\Gamma$ point. In Fig. 4 we show the same quantities when the correlation $U = 6t$ is strong enough to start polarizing antiferromagnetically the bare conduction band, see Table I (therefore we have labelled this: AF). For higher $U/t$ one finds that the convergence of our perturbative series for the renormalized magnons (leading to physical non-negative energies) is limited to a more restricted range of values of the ratio $|J_K/J_H|$, with respect to the low correlation case. The reason for this behaviour is that the fermions which effectively interact with the local moments are those in a neighbourhood of the Fermi energy of width $\approx \hbar\Omega_{qp}$, as can be seen by looking at the explicit expressions of the renormalization coefficients in the Appendix. We use a Fröhlich-type of transformation as in the BCS theory of superconductivity, so that the same type of considerations about the effective interactions apply. Though not too visible in the cases shown of Fig. 2 which lead to well-defined renormalized magnons (except $U/t = 8$), we have checked
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Figure 4. (AF) $J_K/J_H$ dependence of renormalized AF magnons: magnon energy along selected BZ paths. Parameters: $S = 1/2; T = 0; t = 1eV; J_H/t = 0.001; n = 0.999; U/t = 6; B_a/t = 0.0005$. $J_K/J_H$ values as detailed in inset; $w_0$ denotes the bare magnons $\Omega_q$.

which are the main band-structure changes at larger $U/t$ values. Near half-filling, with the Fermi wavector at $R$, for $U \langle s^2 \rangle_{\alpha\beta} \approx 0$ ($U/t = 0.1, 3.0$) the AF subbands disperse strongly around $E_F$ resulting in a weak interaction with the local moments. But as the correlation increases, and $U \langle s^2 \rangle_{\alpha\beta}$ too, the lower AF subband, which contains the Fermi level around $R$, progressively flattens so that now more electrons effectively interact with the local moments. For the cases $U/t = 6, 8$ one also finds that another Fermi surface pocket appears around $M$.

Fig. 5 depicts the dependence of the renormalized magnons on the correlations in the conduction band ($U$), at half-filling: the trend is a larger softening of the magnons when $U$ is increased, and we show cases where $U/W$ ranges between 0.008 (for $U/t = 0.1$) and 0.49 ($U/t = 5.8652$). Notice that the increase of $U$ increases the $q$-dependence of the magnon renormalization. This results from the indirect effect which $U$ has on magnons (while $J_K$ has also a direct effect, since it appears also as explicit multiplicative factor of the perturbatively obtained magnon corrections). $U$ affects magnons through the modifications it induces in electron bandstructure, as discussed above in connection with Figs. 3 and 4, and through the $U$-dependence of the energy denominators in the perturbative coefficients which determine the $q$-dependent renormalization of
Spin wave excitations in the antiferromagnetic Heisenberg-Kondo model for heavy fermions. The recent more refined DMFT+NRG treatment of correlations in an extended Kondo lattice model\cite{28} unfortunately does not allow us comparison, here, as their finite U results are presented for antiferromagnetic $J_K$ outside the region of interest in our problem: their correlated AF Kondo coupling system is studied at much too large Kondo coupling (namely, $J_K = 0.5W = U$) for the antiferromagnetic state to remain stable, the stable phase near half filling in that case being the Kondo insulator with all moments locally quenched.

We exhibit the effects of doping on the magnon renormalization in Fig. 6. Here the deviation of the renormalized magnon energies from the bare magnon values increases with the filling: at half-filling the renormalization is largest, due to more conduction electrons contributing to the renormalization of magnons by coupling through Kondo interaction to the local moments. Doping away from half-filling we obtain a smooth reduction of such renormalization effects, as one would expect. Thus, both filling and electron correlation do increase the renormalization effects, and we have already mentioned that both lead to similar increases of the spin polarization of the conduction band (see Table I and Figs. 5-6). When entering the filling range of values at which the bare electron band ($J_K = 0$) develops an itinerant AF polarization, the renormalization effects become much stronger, as shown by the very different behaviour of the cases

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure5.png}
\caption{\textit{U} dependence of renormalized AF magnons: magnon energy along selected BZ paths. Parameters: $U/t$ as detailed in inset; $B_a/t = 0.0005$; others as in Fig. 2.}
\end{figure}
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Let us briefly refer again to the $q$-dependence of the AF magnon renormalization we find. Some anisotropy is present: a larger $q$-dependence is noticeable along BZ diagonal paths such as $O - M$ or $O - R$ (see e.g. Fig. 6) or paths along the symmetry axes. The renormalization effects are more pronounced at long wavelengths: in particular, they are maximal at the BZ center where we find a spin stiffness decreasing with doping, and increasing with $U$ or $J_K/J_H$. Making allowance for the quite different systems involved, let us mention that the renormalized AF magnon behavior we obtain contrasts with the one recently disclosed by INS measurements in ferromagnetic metallic manganites [31] where at low-$q$ the spin wave stiffness appears insensitive to doping, while magnons exhibit a doping-dependent renormalization at the BZ boundaries (recently suggested to be related to electronic correlations [32]).

At this point, let us compare our results with the few INS magnon measurements available for single crystals of antiferromagnetic heavy fermions. Comparison in more detail may be made only with CeIn$_3$, which is cubic (though f.c.c.) and presents a three-dimensional AF order as we have assumed for our calculation. The sets of parameters we find as allowing us a reasonable description of the INS magnon results which were described in the Introduction [21] as evidenced by inspection of the cases presented in our

Figure 6. Filling ($n$) dependence of renormalized AF magnons: magnon energy along selected BZ paths. Parameters: $n$ values as detailed in inset; $U/t = 5.865$; $B_n/t = 0.0005$; others as in Fig. 2.

$n = 0.9$ (PM band for $J_K = 0$) and $n = 0.999$ (AF band for $J_K = 0$).
figures, are similar to the parameter ranges independently suggested by other authors for this family of compounds. A concrete example is the fit of experimental specific heat curves for CeIn₃, made by Lobos et al.,[27] using a model related though not exactly identical to ours, within a phenomenological approach, who find: $J_H/t = 0.0014$, $t = 0.5eV$, $n = 1$ and $J_K/J_H = 980$. For CeRh₂Si₂ they instead estimate: $J_H/t = 0.0034$ and $J_K/J_H = 430$; and their data extrapolation for CePd₂Si₂ was: $J_H/t = 0.0034$ with a negligible $J_K/J_H$. [27]

6. Summary

In the present work, we have studied spin wave excitations in heavy fermion compounds with antiferromagnetic long-range order, where a strong competition of RKKY and Kondo screening is present, as evidenced by nearly equal magnetic ordering and Kondo temperatures. We have described these systems using a microscopic model including a lattice of correlated $f$-electron orbitals (as in $Ce$-, $U$- compounds of this family) hybridized with a correlated conduction band, in the presence of competing RKKY-Heisenberg and Kondo magnetic couplings. Through a series of unitary transformations we perturbatively derived a second-order effective Hamiltonian describing the antiferromagnetic spin wave excitations, renormalized by their interaction with the conduction electrons. We have numerically studied the effect of the different parameters of this effective model on the magnon energy renormalization. Apart from the expected increase of renormalization effects for larger Kondo coupling, we identify another relevant ingredient. Magnon renormalization is also amplified by spin polarization of the conduction electrons: either if it originates from large correlations between the carriers or by an increase of the electron filling. We have been able to find appropriate sets of model parameters to describe the few existing measurements of magnons by inelastic neutron scattering in single crystal samples of antiferromagnetic heavy fermion $Ce$ compounds (such as CeIn₃, CePd₂Si₂, CeCu₂). Our parameter sets agree with the ranges independently proposed for these materials, by phenomenological fits of other experiments like specific heat. Our results may provide information of interest for the prediction of inelastic neutron scattering experiments in other systems of this family, like CeRh₂Si₂, where there have been suggestions that the RKKY coupling should be stronger than the Kondo effect,[15] and the only existing NIS measurements are of poor quality: they were made on polycrystals[15] many years ago, with lower resolution.

As outlook towards related future work, we might mention the description of the experimentally reported magnon damping effects, and the study of the coexistence of antiferromagnetism and superconductivity in the context of the present model.
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7. Appendix.

7.1. Evaluation of the AF order parameter in the hybrid $\{A_{p\sigma}^{(t)}, B_{p\sigma}^{(t)}\}$ basis.

Using the real-space representation we have to evaluate

$$s_{Q}^{z} = \frac{1}{2N} \sum_{l \in A, \sigma} \sigma c_{l\sigma}^{\dagger} c_{l\sigma} - \frac{1}{2N} \sum_{j \in B, \sigma} \sigma c_{j\sigma}^{\dagger} c_{j\sigma}$$

(60)

Notice that Eq.(60) implicitly assumes that $\langle s_{Q}^{z} \rangle$ is positive on the $A$ sublattice, which is correct only for a FM Kondo coupling. To keep track of the correct sign for arbitrary sign of $J_K$ we have to use Eq.(17) yielding $\langle s_{Q}^{z} \rangle = -\text{sgn}(J_K) |\langle s_{Q}^{z} \rangle|$.

For a generic site $m \in A \cup B$ one has the standard decomposition:

$$c_{m\sigma}^{\dagger} = \frac{1}{\sqrt{N}} \sum_{p \in RBZ} c_{p\sigma}^{\dagger} e^{-ipR_m} + \frac{1}{\sqrt{N}} \sum_{p \in RBZ} c_{p+Q\sigma}^{\dagger} e^{-i(p+Q)R_m}$$

(61)

Substituting for $c_{p\sigma}^{\dagger}$, $c_{p+Q\sigma}^{\dagger}$ the $\{\alpha_{p\sigma}^{(t)}, \beta_{p\sigma}^{(t)}\}$ operators and recalling that on the $A$ sites $R_m = 2ma$ while on $B$ sites $R_m = (2m+1)a$ one has:

$$R_t \in A \quad c_{l\sigma}^{\dagger} = \frac{1}{\sqrt{N}} \sum_{p \in RBZ} [(\alpha_{p\sigma}^{\dagger} + \beta_{p\sigma}^{\dagger}) \cos \zeta_p + \sigma (\alpha_{p\sigma}^{\dagger} - \beta_{p\sigma}^{\dagger}) \sin \zeta_p] e^{-ipR_t}$$

$$R_j \in B \quad c_{j\sigma}^{\dagger} = \frac{1}{\sqrt{N}} \sum_{p \in RBZ} [(\alpha_{p\sigma}^{\dagger} - \beta_{p\sigma}^{\dagger}) \cos \zeta_p - \sigma (\alpha_{p\sigma}^{\dagger} + \beta_{p\sigma}^{\dagger}) \sin \zeta_p] e^{-ipR_j}$$

(62)

Expressing the $\{\alpha_{p\sigma}^{(t)}, \beta_{p\sigma}^{(t)}\}$ operators in terms of the $\{A_{p\sigma}^{(t)}, B_{p\sigma}^{(t)}\}$ basis the real space Fermi operators in the hybrid basis for $R_t \in A$ are given by:

$$c_{l\sigma}^{\dagger} = \frac{1}{\sqrt{N}} \sum_{p} [(A_{p\sigma}^{\dagger} + B_{p\sigma}^{\dagger}) \cos (\zeta_p - \xi_p) + \sigma (A_{p\sigma}^{\dagger} - B_{p\sigma}^{\dagger}) \sin (\zeta_p - \xi_p)] e^{-ipR_t}$$

and, for $R_j \in B$, by:

$$c_{j\sigma}^{\dagger} = \frac{1}{\sqrt{N}} \sum_{p} [(A_{p\sigma}^{\dagger} - B_{p\sigma}^{\dagger}) \cos (\zeta_p + \xi_p) - \sigma (A_{p\sigma}^{\dagger} + B_{p\sigma}^{\dagger}) \sin (\zeta_p + \xi_p)] e^{-ipR_j}$$

(63)

It follows:

$$\frac{1}{2N} \sum_{l \in A, \sigma} \sigma n_{l\sigma} = \frac{1}{4N} \sum_{p, \sigma} A_{p\sigma}^{\dagger} A_{p\sigma} \{\sigma + \sin [2(\zeta_p - \xi_p)]\} + \frac{1}{4N} \sum_{p, \sigma} B_{p\sigma}^{\dagger} B_{p\sigma} \{\sigma - \sin [2(\zeta_p - \xi_p)]\}$$

$$+ \frac{1}{4N} \sum_{p, \sigma} (A_{p\sigma}^{\dagger} B_{p\sigma} + B_{p\sigma}^{\dagger} A_{p\sigma}) \sigma \cos [2(\zeta_p - \xi_p)]$$

(64)

and

$$-\frac{1}{2N} \sum_{j \in B, \sigma} \sigma n_{j\sigma} = -\frac{1}{4N} \sum_{p} A_{p\sigma}^{\dagger} A_{p\sigma} \{\sigma - \sin [2(\zeta_p + \xi_p)]\} - \frac{1}{4N} \sum_{p} B_{p\sigma}^{\dagger} B_{p\sigma} \{\sigma + \sin [2(\zeta_p + \xi_p)]\}$$

$$+ \frac{1}{4N} \sum_{p} \sigma \cos [2(\zeta_p + \xi_p)] (A_{p\sigma}^{\dagger} B_{p\sigma} + B_{p\sigma}^{\dagger} A_{p\sigma})$$

(65)
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The Eqs. 64 and 65, when substituted into Eq. 60, yield:

\[
s_{AB}^z = \frac{1}{2N} \sum_{p,\sigma} \left\{ \sin \left[ 2 \left( \zeta_p + \xi_p \right) \right] A_{p\sigma}^\dagger A_{p\sigma} - \sin \left[ 2 \left( \zeta_p - \xi_p \right) \right] B_{p\sigma}^\dagger B_{p\sigma} \right\} \\
+ \frac{1}{4N} \sum_{p,\sigma} \sigma \left( A_{p\sigma}^\dagger B_{p\sigma} + B_{p\sigma}^\dagger A_{p\sigma} \right) \left\{ \cos \left[ 2 \left( \zeta_p - \xi_p \right) \right] + \cos \left[ 2 \left( \zeta_p + \xi_p \right) \right] \right\}
\]

When taking the Fermi average of Eq. 66, the terms \( A_{p\sigma}^\dagger B_{p\sigma} + B_{p\sigma}^\dagger A_{p\sigma} \) do not contribute and we obtain Eq. 35.

7.2. The coefficients \( C_{XY}^{\pm} (k, q) \) in Eq. 42.

It is convenient to define for short

\[
L_{k,p}^\lambda = \cos \left( Z_k + \lambda Z_p \right) \quad M_{k,p}^\lambda = \sin \left( Z_k + \lambda Z_p \right)
\]

\[
\lambda = \pm \quad Z_p = \zeta_p - \xi_p
\]

notice that \( L_{k,k}^+ = \cos (2Z_k) \) and \( M_{k,k}^+ = \sin (2Z_k) \). In Eq. 42 the coefficients \( C_{XY}^{+} (k, q) \) and \( C_{XY}^{-} (k, q) \) with \( X, Y = A, B \) then read:

\[
C_{XY}^{+} (k, q) = \delta_{XY} \left[ L_{k,k+q}^+ + (2\delta_{XA} - 1) M_{k,k+q}^- \right] \\
+ \left( 1 - \delta_{XY} \right) \left[ L_{k,k+q}^- + (1 - 2\delta_{XB}) M_{k,k+q}^+ \right]
\]

\[
C_{XY}^{-} (k, q) = \delta_{XY} C_{XX}^{+} (k, q) - (1 - \delta_{XY}) C_{YY}^{+} (k, q)
\]

7.3. The generators \( R_{d}^z \) and \( R_{nd}^z \).

In the perturbation we have several types of contributions. In \( I_{d}^z \) and \( I_{nd}^z \) we find terms with two types of products of Bose operators. The generator corresponding to the perturbation term of first type (number-conserving) like \( \sum_{pq,\sigma} C_{pq,\sigma} X_{r,\sigma}^\dagger Y_{p-q+r,\sigma} a_p^\dagger a_q \), where \( X = A, B \) while \( C_{pq,\sigma} \) is a numerical coefficient, is given by:

\[
\sum_{pq,\sigma} \frac{C_{pq,\sigma}}{\mathcal{E}_{X_{r,\sigma}} - \mathcal{E}_{Y_{p-q+r,\sigma}} + \hbar (\Omega_p - \Omega_q)} X_{r,\sigma}^\dagger Y_{p-q+r,\sigma} a_p^\dagger a_q
\]

The generator corresponding to the perturbation term of the second type like \( \sum_{pq,\sigma} C_{pq,\sigma} X_{p,\sigma}^\dagger Y_{p,\sigma} a_q^{(+) \dagger} a_{-q} \) reads

\[
\sum_{pq,\sigma} \frac{C_{pq,\sigma}}{\mathcal{E}_{X_{r,\sigma}} - \mathcal{E}_{Y_{p,\sigma}} \pm 2\hbar \Omega_q} X_{p,\sigma}^\dagger Y_{p,\sigma} a_q^{(+) \dagger} a_{-q}
\]

where the (+) sign applies for bosonic creation operators, and (−) for destruction operators.
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7.4. The generator $R^\perp$.

The generator $R^\perp$ resulting from the transverse Kondo term $I^\perp$, Eq.42, can be written as the sum of four contributions: $R^\perp = \sum_{X,Y=A,B} R^\perp_{XY}$, where:

$$R^\perp_{XY} = \sum_{\tau} X_{\tau} Y_{k+q,-\sigma} (W^\perp_{kq} a^\dagger_q + Z^\perp_{kq} a_{-q})$$

and the coefficients $W^\perp_{kq}$ and $Z^\perp_{kq}$ are given by:

$$W^\perp_{kq} = \frac{1}{2} \left[ \text{Ch} (\vartheta_q) - \text{Sh} (\vartheta_q) \right]$$

and

$$Z^\perp_{kq} = \frac{1}{2} \left[ \text{Ch} (\vartheta_q) - \text{Sh} (\vartheta_q) \right]$$

7.5. The coefficients of $(1/2) \langle [R, I] \rangle_{\text{Fermi}}$.

We have obtained the effective Hamiltonian in Eq.56. Taking advantage of the electron-hole symmetry, the coefficients will be now explicated assuming the paramagnetic band filling per site $n \leq 1$ so that $\langle n^B_{k,\sigma} \rangle = 0$ in the ground state.

7.5.1. The coefficients of $(1/2) \langle [R^z, I^z] \rangle_{\text{Fermi}}$. In Eq.48 the coefficients read:

$$G^\text{har}_{q} = -\frac{J^2}{16} \left( \frac{2}{N} \right) \sum_{\rho,\sigma} M^+_{\rho,\rho} M^+_{\sigma,\rho} \left[ \delta_{\rho,\sigma} + (1 - \delta_{\rho,\sigma}) \langle n^A_{\rho,\sigma} \rangle \right] \langle n^A_{\rho,\sigma} \rangle \frac{\text{Sh}^2 (2\vartheta_q)}{\hbar \Omega_q}$$

and

$$G^\text{anhar}_{q} = -\frac{J^2}{16} \left( \frac{2}{N} \right) \sum_{\rho,\sigma} M^+_{\rho,\rho} M^+_{\sigma,\rho} \left[ \delta_{\rho,\sigma} + (1 - \delta_{\rho,\sigma}) \langle n^A_{\rho,\sigma} \rangle \right] \langle n^A_{\rho,\sigma} \rangle \frac{\text{Sh} (4\vartheta_q)}{2\hbar \Omega_q}$$

7.5.2. The coefficients of $(1/2) \langle [R^z, I^z] \rangle_{\text{Fermi}}$. To write down the coefficients $a^\pm_{q}$ and $\varpi^\pm_{q}$ of Eq.49 it is convenient to introduce:

$$\text{Ch} (\vartheta_q + \vartheta_p) = G_{qp} \quad \text{Sh} (\vartheta_q + \vartheta_p) = \mathcal{S}_{qp}$$
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By defining

$$\mathcal{L}_{ppr}^+ = -M_{p,r-q+r}^+ \left( \mathcal{X}_{p,q-r,p}^{AA1} + \mathcal{X}_{p,q-r,r,q}^{AA2} \right) \mathcal{E}_{qq} \langle n_{q-r,q}^A \rangle$$

$$- L_{p,r-q+r}^+ \left( \mathcal{X}_{r,p-q+r,p}^{BA1} + \mathcal{X}_{r,p-q+r,q}^{BA2} \right) \mathcal{E}_{qp} \langle n_{q-r,q}^A \rangle$$

$$+ M_{r,p-q+r}^+ \left( \mathcal{X}_{q,p-r,p}^{AA3} + \mathcal{X}_{q,p-r,q}^{BA} \right) \mathcal{S}_{qp} \langle n_{q-r,q}^A \rangle$$

$$+ L_{r,p-q+r}^+ \left( \mathcal{X}_{q,p-r,q}^{BA3} + \mathcal{X}_{p,q-r,q}^{BA4} \right) \mathcal{S}_{qp} \langle n_{q-r,q}^A \rangle$$

(77)

and

$$\mathcal{L}_{pqr}^- = + M_{p,r-q+r}^+ \left( \mathcal{X}_{p,q-r,q}^{AA1} + \mathcal{X}_{p,q-r,q}^{AA2} \right) \mathcal{E}_{qp} \langle n_{r,q}^A \rangle$$

$$+ L_{p,r-q+r}^+ \left( \mathcal{X}_{r,p-q+r,r,q}^{BA1} + \mathcal{X}_{r,p-q+r,p}^{BA2} \right) \mathcal{E}_{qp} \langle n_{r,q}^A \rangle$$

$$- M_{r,p-q+r}^+ \left( \mathcal{X}_{q,p-r,q,p}^{AA3} + \mathcal{X}_{q,p-r,q}^{BA} \right) \mathcal{S}_{qp} \langle n_{r,q}^A \rangle$$

$$- L_{r,p-q+r}^+ \left( \mathcal{X}_{q,p-r,q,p}^{BA3} + \mathcal{X}_{p,q-r,q,p}^{BA4} \right) \mathcal{S}_{qp} \langle n_{r,q}^A \rangle$$

(78)

where \((X = A, B)\)

$$\mathcal{X}_{rxyw}^{XX1} = - \frac{2\delta XA - 1}{E_y - E_{x+y-w} + \hbar (\Omega_w - \Omega_x)} \text{Ch} (\vartheta_w) \text{Ch} (\vartheta_x)$$

(79)

$$\mathcal{X}_{rxyw}^{XX2} = - \frac{2\delta XA - 1}{E_y - E_{x+y-w} + \hbar (\Omega_w - \Omega_x)} \text{Sh} (\vartheta_w) \text{Sh} (\vartheta_x)$$

(80)

$$\mathcal{X}_{rxyw}^{XX3} = - \frac{2\delta XA - 1}{E_y - E_{x+y-w} + \hbar (\Omega_w + \Omega_x)} \text{Sh} (\vartheta_w) \text{Ch} (\vartheta_x)$$

(81)

$$\mathcal{X}_{rxyw}^{XX4} = - \frac{2\delta XA - 1}{E_y - E_{x+y-w} + \hbar (\Omega_w + \Omega_x)} \text{Sh} (\vartheta_w) \text{Ch} (\vartheta_x)$$

(82)

$$\mathcal{X}_{rxyw}^{XY1} = - \frac{\cos (Z_y + Z_{x-w+y})}{E_y - E_{x+y-w} + \hbar (\Omega_w - \Omega_x)} \text{Ch} (\vartheta_w) \text{Ch} (\vartheta_x)$$

(83)

$$\mathcal{X}_{rxyw}^{XY2} = - \frac{\cos (Z_y + Z_{x-w+y})}{E_y - E_{x+y-w} + \hbar (\Omega_w - \Omega_x)} \text{Sh} (\vartheta_w) \text{Sh} (\vartheta_x)$$

(84)

$$\mathcal{X}_{rxyw}^{XY3} = - \frac{\cos (Z_y + Z_{x-w+y})}{E_y - E_{x+y-w} + \hbar (\Omega_w + \Omega_x)} \text{Sh} (\vartheta_w) \text{Ch} (\vartheta_x)$$

(85)

$$\mathcal{X}_{rxyw}^{XY4} = - \frac{\cos (Z_y + Z_{x-w+y})}{E_y - E_{x+y-w} + \hbar (\Omega_w + \Omega_x)} \text{Sh} (\vartheta_w) \text{Ch} (\vartheta_x)$$

(86)

we can write

$$\hbar l^2 q = \frac{J_K}{2} \left( \frac{2}{N} \right)^2 \sum_{pq} (1 - \delta_{pq}) \mathcal{L}_{pq}^+$$

(87)
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Next, by defining

\[ M_{pqr}^+ = -M_{r,p-q+r}^+ \left( \mathcal{X}_{q,p-q+r,p}^{AA1} + \mathcal{X}_{q,p-q+r,-q}^{AA2} \right) \mathcal{S}_{qp} \left\langle n_{r,q,r}^A \right\rangle \\
- L_{r,p-q+r}^+ \left( \mathcal{X}_{q,p-q+r,p}^{AB1} + \mathcal{X}_{q,p-q+r,-q}^{AB2} \right) \mathcal{S}_{qp} \left\langle n_{r,q,r}^A \right\rangle \\
+ M_{r,p-q+r}^+ \left( \mathcal{X}_{q,p-q+r,p}^{AA3} + \mathcal{X}_{q,p-q+r,-q}^{AA3} \right) \mathcal{C}_{qp} \left\langle n_{r,q}^A \right\rangle \\
+ L_{r,p-q+r}^+ \left( \mathcal{X}_{q,p-q+r,p}^{BA3} + \mathcal{X}_{q,p-q+r,-q}^{BA3} \right) \mathcal{C}_{qp} \left\langle n_{r,q}^A \right\rangle \]  

(88)

and

\[ M_{pqr}^- = +M_{r,p-q+r}^+ \left( \mathcal{X}_{q,p-q+r,-q}^{AA1} + \mathcal{X}_{q,p-q+r,-q}^{AA2} \right) \mathcal{S}_{qp} \left\langle n_{r,q,r}^A \right\rangle \\
+ L_{r,p-q+r}^+ \left( \mathcal{X}_{q,p-q+r,p}^{AA4} + \mathcal{X}_{q,p-q+r,-q}^{AA4} \right) \mathcal{S}_{qp} \left\langle n_{r,q,r}^A \right\rangle \\
- M_{r,p-q+r}^+ \left( \mathcal{X}_{q,p-q+r,p}^{BA4} + \mathcal{X}_{q,p-q+r,-q}^{BA4} \right) \mathcal{C}_{qp} \left\langle n_{r,q,r}^A \right\rangle \\
- L_{r,p-q+r}^+ \left( \mathcal{X}_{q,p-q+r,p}^{BA4} + \mathcal{X}_{q,p-q+r,-q}^{BA4} \right) \mathcal{C}_{qp} \left\langle n_{r,q,r}^A \right\rangle \]  

(89)

we can write

\[ h\omega_q^{\pm} = \frac{J_K^2}{2} \left( \frac{2}{N} \right)^2 \sum_{p,q} (1 - \delta_{pq}) M_{pqr}^\pm \]  

(90)

7.5.3. The coefficients of \((1/2) \left\langle \left[ R^\dagger, I^\dagger \right] \right\rangle_{\text{Fermi}} \). In Eq.50, if \( n \leq 1 \), so that \( \left\langle n_{k,q}^B \right\rangle = 0 \) in the ground state, one finds \( T_{q}^{BB} = \mathcal{S}_{q}^{BB} = 0 \). The other \( T_{q}^{XY} \) coefficients, by defining \( \left\langle f_{k,k \pm q}^A \right\rangle = \left\langle n_{k,-q}^A \right\rangle - \left\langle n_{k,q}^A \right\rangle \), read:

\[ T_{q}^{AA} = \frac{J_K^2 S}{4N} \sum_{k,q} \mathcal{W}_{k,q} \mathcal{X}_{AA} \left( \nu_{k,q} \right) C_{AA}^\dagger (k + q, -q) \left\langle f_{k,k + q}^A \right\rangle \]

\[ + \frac{J_K^2 S}{4N} \sum_{k,q} \mathcal{W}_{k,q} \mathcal{X}_{BB} \left( \nu_{k,q} \right) C_{BB}^\dagger (k + q, -q) \left\langle f_{k,k + q}^A \right\rangle \]

\[ + \frac{J_K^2 S}{4N} \sum_{k,q} \mathcal{W}_{k,q} \mathcal{X}_{AA} \left( \nu_{k,q} \right) C_{AA}^\dagger (k - q, q) \left\langle f_{k,k - q}^A \right\rangle \]

\[ + \frac{J_K^2 S}{4N} \sum_{k,q} \mathcal{W}_{k,q} \mathcal{X}_{BB} \left( \nu_{k,q} \right) C_{BB}^\dagger (k - q, q) \left\langle f_{k,k - q}^A \right\rangle \]  

(91)

\[ T_{q}^{AB} = \frac{J_K^2 S}{2N} \sum_{k,q} \mathcal{W}_{k,q} \mathcal{X}_{AB} \left( \nu_{k,q} \right) C_{BA}^\dagger (k + q, -q) \left\langle n_{k,-q}^A \right\rangle \]

\[ + \frac{J_K^2 S}{2N} \sum_{k,q} \mathcal{W}_{k,q} \mathcal{X}_{AB} \left( \nu_{k,q} \right) C_{BA}^\dagger (k + q, -q) \left\langle n_{k,-q}^A \right\rangle \]

\[ - \frac{J_K^2 S}{2N} \sum_{k,q} \mathcal{W}_{k,q} \mathcal{X}_{AB} \left( \nu_{k,q} \right) C_{BA}^\dagger (k - q, q) \left\langle n_{k,-q}^A \right\rangle \]

\[ + \frac{J_K^2 S}{2N} \sum_{k,q} \mathcal{W}_{k,q} \mathcal{X}_{AB} \left( \nu_{k,q} \right) C_{BA}^\dagger (k - q, q) \left\langle n_{k,-q}^A \right\rangle \]  

(92)
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and

\[ T_{q}^{BA} = \frac{J_{K}^{2} S}{2N} \sum_{k} W_{k,q}^{BA} \text{Sh} (\vartheta_{q}) C_{AB}^{+-} (k + q, -q) \langle n_{k+q,\sigma}^{A} \rangle - \frac{J_{K}^{2} S}{2N} \sum_{k} W_{k,q}^{BA} \text{Ch} (\vartheta_{q}) C_{BA}^{+-} (k + q, -q) \langle n_{k+q,\sigma}^{A} \rangle + \frac{J_{K}^{2} S}{2N} \sum_{k} Z_{k,q}^{BA} \text{Ch} (\vartheta_{q}) C_{AB}^{+-} (k - q, q) \langle n_{k-q,\sigma}^{A} \rangle - \frac{J_{K}^{2} S}{2N} \sum_{k} Z_{k,q}^{BA} \text{Sh} (\vartheta_{q}) C_{BA}^{+-} (k - q, q) \langle n_{k-q,\sigma}^{A} \rangle \]

(93)

The \( S_{q}^{XY1} \) coefficients read:

\[ S_{q}^{AA1} = \frac{J_{K}^{2} S}{2N} \sum_{k} W_{k,-q}^{AA} \text{Ch} (\vartheta_{q}) C_{AA}^{+-} (k - q, q) \langle \tilde{N}_{k,-q,\sigma} \rangle + \frac{J_{K}^{2} S}{2N} \sum_{k} W_{k,-q}^{AA} \text{Sh} (\vartheta_{q}) C_{BB}^{+-} (k - q, q) \langle \tilde{N}_{k,-q,\sigma} \rangle \]

(94)

\[ S_{q}^{AB1} = -\frac{J_{K}^{2} S}{2N} \sum_{k} W_{k,-q}^{AB} \text{Ch} (\vartheta_{q}) C_{BA}^{+-} (k - q, q) \langle n_{k,-\sigma}^{A} \rangle + \frac{J_{K}^{2} S}{2N} \sum_{k} W_{k,-q}^{AB} \text{Sh} (\vartheta_{q}) C_{AB}^{+-} (k - q, q) \langle n_{k,-\sigma}^{A} \rangle \]

(95)

\[ S_{q}^{BA1} = \frac{J_{K}^{2} S}{2N} \sum_{k} W_{k,-q}^{BA} \text{Ch} (\vartheta_{q}) C_{AB}^{+-} (k - q, q) \langle n_{k,-\sigma}^{A} \rangle - \frac{J_{K}^{2} S}{2N} \sum_{k} W_{k,-q}^{BA} \text{Sh} (\vartheta_{q}) C_{BA}^{+-} (k - q, q) \langle n_{k,-\sigma}^{A} \rangle \]

(96)

The coefficients \( S_{q}^{XY2} \) can be obtained from \( S_{q}^{XY1} \) by interchanging \( W_{k,-q}^{XY} \) and \( \text{Ch} (\vartheta_{q}) \) respectively with \( Z_{k,-q}^{XY} \) and \( \text{Sh} (\vartheta_{q}) \).

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Table 1. Conduction band AF spin polarization, $< s^z >_{AB}$, dependence on other model parameters, for the cases depicted in respective Figs. 3 to 6. In first column we enter the relative Kondo coupling magnitude (cases of Fig. 3: notice that $J_K/W \sim J_K/J_H \times 10^{-4}$, here), while in second column we state the corresponding band polarization $< s^z >_{AB}$ obtained; similarly, for Fig.4 and the related 3rd and 4th columns of this table. In 5th column we enter the electron correlation $U/t$ cases from Fig. 5, and next column states the corresponding $< s^z >_{AB}$. In 7th column we enter filling $n$ values of Fig. 6, and in last column the corresponding $< s^z >_{AB}$ values.

| $J_K/J_H$ (PM) | $< s^z >_{AB}$ | $J_K/J_H$ (AF) | $< s^z >_{AB}$ | $U/t$ | $< s^z >_{AB}$ | $n$ | $< s^z >_{AB}$ |
|----------------|----------------|----------------|----------------|-------|----------------|----|----------------|
| 0.1            | -6.10E-7       | 1.0            | -7.20E-2       | 0.100 | -1.14E-4       | 0.100 | -3.81E-6       |
| 1.0            | -6.10E-6       | 4.0            | -7.20E-2       | 1.000 | -1.15E-4       | 0.500 | -2.96E-5       |
| 5.0            | -3.0E-5        | 5.5            | -7.20E-2       | 3.000 | -1.22E-4       | 0.600 | -3.97E-5       |
| 10.0           | -6.10E-5       | 7.0            | -7.20E-2       | 5.000 | -1.42E-4       | 0.700 | -5.24E-5       |
| 15.0           | -9.15E-5       | 5.5            | -7.20E-2       | 5.500 | -1.51E-4       | 0.800 | -6.92E-5       |
| 20.0           | -1.22E-4       | 5.800          | -3.52E-3       | 5.800 | -3.52E-3       | 0.850 | -8.00E-5       |
| 25.0           | -1.50E-4       | 5.8650         | -8.69E-3       | 5.8650 | -8.69E-3       | 0.900 | -9.94E-5       |
| 30.0           | -1.80E-4       | 5.8652         | -8.71E-3       | 5.8652 | -8.71E-3       | 0.999 | -8.69E-3       |