Spin-Wave Excitations of Half-Filled Kondo Lattice Model

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The spin excitations in the antiferromagnetic phase of half-filled Kondo lattice model are studied by means of the decoupling approximation for spin Green’s function. The spin-wave spectrum is calculated as a function of Kondo coupling, and this is used to calculate the thermodynamic quantities at low temperatures. The Néel temperature of the form \( T_N = 0.087J^2 \ln(1/J) \) is obtained for the 3-dimensional case in the weak-coupling limit. It is pointed out that the ratio of the spin-wave velocity to the Néel temperature \( v_s/T_N \) is enhanced as the Kondo coupling becomes small, reflecting the long-range nature of effective interactions between localized spins.

The electronic states of heavy-fermion compounds have been extensively studied to understand a number of their anomalous properties due to strong correlations. The Kondo lattice model (KLM) and the periodic Anderson model (PAM) have been considered to give a microscopic basis to describe the characteristic features of these systems. It has been expected that KLM and PAM exhibit various types of magnetic long-range order due to effective RKKY interaction between localized spins. In particular, the properties of antiferromagnetically ordered (AFO) phase realized in the half-filled system have been studied by the Gutzwiller variational method [1][2] and the slave-boson mean-field approximation [3][4] in connection with the magnetic instability of heavy-fermion semiconductors [5]. However, the spin excitations and the resulting thermodynamic properties in AFO phase have not been fully understood, because the low-lying excitations are closely related to the non-local fluctuations neglected in these approximations. In the present paper, we are going to investigate these spin excitations in the AFO phase of KLM, making use of the spin Green’s functions in the decoupling approximation similar to the Tyabrikov method for the Heisenberg model [6]. The spin-wave excitation spectrum and the Néel temperature are determined from these Green’s functions.

The KLM with the nearest-neighbor hopping is described by the Hamiltonian

\[
H = -t \sum_{\langle ij \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + J \sum_i \vec{\sigma}_i \cdot \vec{S}_i,
\]

where \( c_{i\sigma}^\dagger \) and \( c_{i\sigma} \) represent the creation and annihilation operators of a conduction electron in Wannier state at the i-th site with spin \( \sigma \), respectively. The spin operator of conduction electron \( \vec{\sigma}_i \) is expressed in the form \( \vec{\sigma}_i = 1/2 \sum_{\sigma\sigma'} c_{i\sigma}^\dagger \tau_{\sigma\sigma'} c_{i\sigma'} \), where \( \tau \) is the Pauli matrix. In the following, we set \( t = 1 \), measuring all energies in the unit of \( t \).

In order to describe AFO phase in this model, we introduce the staggered magnetizations of localized spin and conduction electron, respectively:

\[
\langle S_i^z \rangle = \begin{cases} 
  m_s & \text{for A sublattice} \\
  -m_s & \text{for B sublattice}
\end{cases}
\]

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\[ \langle \sigma_i^z \rangle = \begin{cases} -m_c & \text{for A sublattice} \\ m_c & \text{for B sublattice}. \end{cases} \]

Then the Hamiltonian (1) is derived by the mean-field part \( H_0 \) and the residual-interaction part \( H_1 = H - H_0 \). The \( H_0 \) describes the conduction band in the staggered field, and can be regarded as the quasi-particle bands with spin-density-wave (SDW) modulation by means of the canonical transformation

\[ \alpha_k^{(\pm)} = u_k^A c_{k\sigma} + u_k^B c_{k\sigma}^\dagger, \]

with

\[ u_k^\pm = \sqrt{\frac{1}{2} \left( 1 \pm \frac{Jm_s}{2E_k} \right)}, \]

where \( c_{k\sigma}^{A(B)} \) is the Bloch transform of \( c_{i\sigma}^{A(B)} \) and \( E_k = \sqrt{\epsilon_k^2 + (Jm_s/2)^2} \) stands for the quasi-particle energy, and the wave vector \( k \) runs over reduced Brillouin zone. Making use of such a transformation, the Hamiltonian (1) is rewritten in the form:

\[ H = H_0 + H_1, \]

where

\[ H_0 = \sum_{k\sigma} (E_k \alpha_k^{(\pm)})^\dagger \alpha_k^{(\pm)} - E_k \alpha_k^{(-)}\alpha_k^{(-\dagger)} - Jm_c \sum_i (S_i^A - S_i^B) \]

and

\[ H_1 = J \sum_q \{(m_s - S_i^A)(m_c - \sigma_i^A) + (m_s - S_i^B)(m_c - \sigma_i^B)\} + J \sum_q \{\sigma_q^A S_{q-}^A + \sigma_q^A - S_{q+}^A + \sigma_q^B S_{q-}^B + \sigma_q^B - S_{q+}^B\}, \]

where \( \sigma_q \) and \( S_q \) are the Bloch representations of spin operators of conduction and localized spins, respectively. The simple mean-field treatment, which neglects \( H_1 \), produces the correct ground state of the large-S limit, providing the appropriate basis for further analysis. In order to study the effects brought about by the fluctuation \( H_1 \), we introduce the Green’s function of localized spins, \( \langle S_q^{A(B)}; S_{-q}^{A(-)} \rangle \), which satisfies the following equations of motion:

\[ z\langle S_q^{A+}; S_{-q}^- \rangle = 2\langle S_0^{A-} \rangle - J \sum_{q'}\{[\sigma_{q'}^A S_{q'}^{A+}; S_{-q}^A] + \langle S_{q'}^{A-}; S_{-q}^{A+} \rangle\}, \]

\[ z\langle S_q^{B+}; S_{-q}^- \rangle = -J \sum_{q'}\{[\sigma_{q'}^B S_{q'}^{B+}; S_{-q}^A] + \langle S_{q'}^{B-}; S_{-q}^{B+} \rangle\}. \]

Then the decoupling approximations such as

\[ \langle \sigma^z S^+; S^- \rangle \rightarrow \langle \sigma^z \rangle \langle S^+; S^- \rangle, \]

\[ \langle S^z \sigma^+; S^- \rangle \rightarrow \langle S^z \rangle \langle \sigma^+; S^- \rangle, \]

are employed for the higher-order Green’s functions, assuming the SDW state for carriers and Néel state for localized spins, respectively. This procedure is similar to the conventional Tyablikov method for the Heisenberg model. Thus we obtain

\[ (z - Jm_c)\langle S_q^{A+}; S_{-q}^- \rangle = 2m_s + Jm_s \sum_k [u_k^+ u_{k+q}^+ \langle \alpha_k^{(\pm)}\alpha_{k+q}^{(-)} \rangle S_{-q}^-]. \]
where use has been made of the relation

\[ (z + Jm_e)\langle S^B_+; S^-_q \rangle = Jm_s \sum_k [u^+_{k, q} \langle \alpha^{(+)}_k \alpha^{(-)}_{k+q}; S^-_q \rangle \]

Replacing \( z \) in eq.(7-a,b)

\[ (z \pm E_k \pm E_{k+q})\langle \alpha^{(+)}_k \alpha^{(+)}_{k+q}; S^-_q \rangle = \]

\[ \frac{J}{2N} \{1 - f(E_k) - f(E_{k+q})\} [u^+_{k, q} \langle S^A_+; S^-_q \rangle + u^+_{k, q} \langle S^B_+; S^-_q \rangle], \]

where \( f(E_k) \) is the Fermi distribution function. From this closed set of equations, we obtain the explicit expression for the spin Green’s function

\[ \langle S^A_+; S^-_q \rangle = \]

\[ \frac{2m_s \{1 - \frac{J^2}{2N} \phi_q(z)\} - \frac{J^2}{2N} \{ \chi^{AA}_0(0) + \chi^{AB}_0(0) - \chi^{AA}_q(z) \}} {\{1 - \frac{J^2}{2N} \phi_q(z)\}^2 z^2 - \{ \chi^{AA}_0(0) + \chi^{AB}_0(0) - \chi^{AA}_q(z) \}^2 - \{ \chi^{AB}_q(z) \}^2} \]

with

\[ \phi_q(z) = \frac{2}{N} \sum_k \frac{u^2_{k, q} - u^2_{k+q}}{z^2 - (E_{k+q} + E_k)^2} \]

\[ \chi^{AA}_q(z) = \frac{2}{N} \sum_k \frac{u^2_{k, q} - u^2_{k+q}}{z^2 - (E_{k+q} + E_k)^2} (E_{k+q} + E_k) \]

\[ \chi^{AB}_q(z) = \frac{2}{N} \sum_k \frac{2u^+_{k, q} u^+_{k+q}}{z^2 - (E_{k+q} + E_k)^2} (E_{k+q} + E_k), \]

where use has been made of the relation

\[ m_c = -\frac{Jm_s}{2} \{ \chi^{AA}_0(0) + \chi^{AB}_0(0) \}. \]

Replacing \( z \) in eq.(9) by \( \omega + i\delta \), the selfconsistent equation for the staggered magnetization \( m_s \) is given by

\[ \frac{1}{2} - m_s = -\frac{1}{\pi N} \sum_q \int_{-\infty}^{\infty} d\omega n(\omega) \text{Im} \langle S^A_+; S^-_q \rangle, \]

where \( n(\omega) \) is the Bose distribution function \( (e^{\beta\omega} - 1)^{-1} \) and \( \beta = T^{-1} \).

This Green’s function (9) has two types of poles corresponding to the Stoner and spin-wave excitations, respectively. Since the energy band of spin-wave excitations characterized by the energy scale \( 2Jm_e \) always lies lower than the continuum of the Stoner excitations \( E_{k+q} + E_k \) which have a gap \( 2Jm_s \) in the whole momentum space, in the weak coupling regime the spin-wave dispersion is well approximated in the form

\[ \Delta(q) = \frac{J^2}{2} \sqrt{\chi^{AA}_0 + \chi^{AB} - \chi^{AA}_q} - \chi^{AB}_q, \]
by replacing \( \chi(z) \) and \( \phi(z) \) by their values at \( z = 0 \). Our result (13) clearly shows the presence of the infinitesimal spin excitation at \( q = 0 \) which is expected from the Goldstone theorem. We note that in the single-site approximation such as Gutzwiller and slave-boson methods, there remains a finite spin excitation gap even in AFO phase. Since the spectral intensities of Stoner excitations are sufficiently small compared to those of spin-wave excitations in the weak coupling regime, in the following analysis we neglect the contributions from the Stoner excitations.

Let us first consider the asymptotic form of this dispersion at zero-temperature in the weak-coupling limit \( J \to 0 \). In this limit, we can show that \( \chi^{AA}_0 \) and \( \chi^{AB}_0 \) diverge as \( \ln J \), while \( \chi^{AA}_q \) and \( \chi^{AB}_q (q \neq 0) \) tend to a constant value. Therefore the equation (13) becomes independent of \( q \) in the limit \( J \to 0 \) with a jump at \( q = 0 \). This means that the results of the present theory at zero-temperature reduce to those of the mean-field theory in the weak-coupling limit, even although the effects of quantum fluctuation are included in the present decoupling scheme. This asymptotic behavior is independent of the dimensionality of the system and consistent with our previous work of 1D PAM [7].

For general couplings, equation (13) has been solved numerically, and the results are shown in Fig.1: Here, considering the weak coupling case, we use \( m_s = 1/2 \) and neglect deviation from it. The spin-wave dispersion strongly depends on the strength of Kondo coupling. It is found that the rapid increase in small-\( q \) region is gradually relaxed as \( J \) becomes large.

The linear expansion in \( q \) for eq.(13) yields the spin-wave velocity

\[
v_s = 0.088 J \sqrt{\ln \left( \frac{1}{J} \right)},
\]

for 3D KLM in the weak-coupling region. Similar results are also obtained for the lower dimensional systems: \( v_s/J \sqrt{\ln (1/J)} = 0.135 \) for 2D and 0.138 for 1D. Once the spin-wave velocity is determined, we can analytically calculate the specific heat and parallel suscepti-
bility in the low-temperature limit as follows:

\[ C_v = \frac{4\sqrt{3}\pi}{5} \left( \frac{T}{v_s} \right)^3, \tag{15} \]

\[ \chi_{//} = \frac{(\mu_B g)^2 T^2}{3 v_s^2}. \tag{16} \]

We can obtain the Néel temperature \( T_N \) by linearizing eq.(12) with respect to \( m_s \). Thus the equation for \( T_N \) is given by

\[ \frac{T_N}{J^2} = \frac{\chi_{N(0)}}{4} \left[ \frac{2}{N} \sum_q \frac{2\chi_N(0) + \chi_N(q)}{\chi_N(0) - \chi_N(q)} \right]^{-1} \tag{17} \]

where

\[ \chi_N(q) = \frac{2}{N} \sum_k \frac{1 - f_N(\epsilon_k) - f_N(\epsilon_{k+q})}{\epsilon_k + \epsilon_{k+q}} \tag{18} \]

and \( f_N(\epsilon_k) \) is the Fermi distribution function \( (e^{\beta \epsilon_k} + 1)^{-1} \) at \( T = T_N \). Equation (17) has been solved numerically with respect to \( T_N \) for various Kondo couplings \( J \), and the results are shown in Fig.2. It is found that the Néel temperature shows a monotonic increase with increasing \( J \).

![Fig.2. Néel temperature \( T_N \) as a function of Kondo coupling. The solid and broken lines represent the present and the mean-field results, respectively. The inset shows that the Néel temperature is linear to \( J^2 \ln(1/J) \) in the weak-coupling region.](image)

From the asymptotic behavior shown in the inset of Fig.2, we obtain the expression of \( T_N \) in the weak-coupling limit as follows:

\[ T_N = 0.087 J^2 \ln \left( \frac{1}{J} \right). \tag{19} \]

The mean-field theory also predicts the \( J \)-dependence similar to (19) in the limit \( J \to 0 \). However \( T_N \) in our theory is smaller than that in the mean-field theory by a factor 0.71. The
deviation from 1 is due to the quantum fluctuations between localized spins. This is to be compared with the corresponding ratio 0.66 in Heisenberg antiferromagnet.

It should be pointed out that the ratio of the spin-wave velocity and the Néel temperature $v_s/T_N$ is enhanced as the Kondo coupling becomes small. This is because the long-range nature of effective interactions between localized spins suppresses collective excitations at low temperatures.

In summary, the spin excitations of the AFO phase in half-filled KLM were studied by means of the decoupling approximation for spin Green’s function. The spin-wave spectrum and the Néel temperature were calculated as a function of Kondo coupling, and their asymptotic behaviors in the weak-coupling limit were discussed in detail. It was shown that the collective spin excitations in weak-coupling KLM are considerably suppressed in comparison with those in the Heisenberg antiferromagnet, reflecting the long-range nature of effective interactions between localized spins.

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[9] It seems that these formulas could be applied if $T < v_s$. However this criterion overestimates the region in which these low-temperature approximations valid. The correct criterion is derived by comparing the contribution from the collective excitations given by eqs. (15) and (16) with that from the local excitations given by the mean-field theory. Thus the crossover temperature (below which the collective excitations dominantly govern the thermodynamic properties of the system) can be estimated as $T^* = [\ln(v_s/T_N)]T_N$. 