Spin-wave Hamiltonian in double-exchange systems

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Abstract

A simple derivation of the effective spin-wave Hamiltonian for a double-exchange system with infinitely large Hund's-rule coupling is demonstrated. The formalism can be applied to models with arbitrary range of hopping as well as those with randomness. The result shows that, within the leading order of the $1/S$ expansion, one magnon excitation spectrum can be described by the Heisenberg model.

Key words: double exchange; spin-wave; colossal magnetoresistance

Double-Exchange (DE) model [1,2] has been introduced to study the metallic ferromagnetism in perovskite manganese oxides. One-magnon excitation spectrum has been investigated using the spin-wave approximation [3–5]. Recently, spin excitation spectrum of the DE systems with randomness has been studied using the Green's-function formalism [6].

In this paper, we demonstrate a simple derivation of the effective spin-wave Hamiltonian for the DE systems, which can be applied to generic cases with arbitrary hopping range or with randomness. Within the leading order of the $1/S$ expansion, the results are equivalent to those by the Green's function formalism. The advantage of this derivation is that it provides an intuitive understanding of the ferromagnetic exchange coupling mediated by the DE interactions, compared to the Green's-function formalism.

We begin with the DE model in the limit of large Hund's-rule coupling with localized spins being treated as classical spins. For the moment, we consider a system without randomness. In this limit, local spin quantization axes for conduction electrons are taken parallel to the localized spin in each site, and electrons with antiparallel spin states to localized spins are projected out. Then, the transfer integral between sites i and j depends on the relative angle of localized spins at corresponding sites S_i and S_j as [2]

$$t_{ij}(\mathrm{S}_i,\mathrm{S}_j) = {t_{ij}}^0 \left\{ \cos\frac{\theta_i}{2}\cos\frac{\theta_j}{2} + \sin\frac{\theta_i}{2}\sin\frac{\theta_j}{2} e^{-\mathrm{i}(\phi_i-\phi_j)} \right\}. \quad (1)$$

Here θ and ϕ are defined by the direction of the localized spin S as

$$\begin{aligned} S_i^x &= S\sin\theta_i\cos\phi_i, \\ S_i^y &= S\sin\theta_i\sin\phi_i, \\ S_i^z &= S\cos\theta_i, \end{aligned} \quad (2)$$

while ${t_{ij}}^0 = {t_{ji}}^0$ is the transfer integral between sites i and j in the absence of the DE interaction. The Hamiltonian is given by

$$H = -\sum_{ij}\left[t_{ij}(S_i,S_j) c_i^\dagger c_j + t_{ji}(S_j,S_i) c_j^\dagger c_i \right]. \quad (3)$$

Note that we explicitly treat the complex transfer integral in this formalism.

The absolute value of the transfer integral is rewritten as

$$\frac{|t_{ij}(\mathrm{S}_i,\mathrm{S}_j)|}{{t_{ij}}^0} = \sqrt{\frac{1}{2} + \frac{1}{2S^2}\mathrm{S}_i\cdot\mathrm{S}_j}. \quad (4)$$

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On the other hand, the imaginary part becomes as

$$\frac{Im\, t_{ij}}{{t_{ij}}^0} = \frac{1}{2}\sqrt{\frac{S^2}{(S+S_i^z)(S+S_j^z)}}\,\frac{S_i^y S_j^x - S_i^x S_j^y}{S^2}. \tag{5}$$

Note that $Im\, t_{ij}$ is antisymmetric with respect to the exchange of i and j, as expected from $t_{ij} = t_{ij}^*$.

Now, we apply the spin-wave approximation to this Hamiltonian. We consider the spin-wave excitation from the perfectly-polarized ferromagnetic ground state where the spins align along the z direction. Namely, we replace the spin variables S_i by the Holstein-Primakoff transformation

$$\begin{aligned} S_i^x &\simeq \sqrt{\frac{S}{2}}\left(a_i^\dagger + a_i\right), \\ S_i^y &\simeq \mathrm{i}\sqrt{\frac{S}{2}}\left(a_i^\dagger - a_i\right), \\ S_i^z &= S - a_i^\dagger a_i, \end{aligned} \tag{6}$$

and take account of the expansion by $1/S$ up to the leading order $O(1/S)$. By substituting Eqs. (6) into Eq. (4), we obtain

$$\frac{|t_{ij}|}{{t_{ij}}^0} = 1 + \frac{1}{4S}(a_i^\dagger a_j + a_j^\dagger a_i - a_i^\dagger a_i - a_j^\dagger a_j) + O(\frac{1}{S^2}). \tag{7}$$

In the same manner, we obtain the imaginary part as

$$\frac{Im\, t_{ij}}{{t_{ij}}^0} = \frac{1}{4S}\left(a_i^\dagger a_j - a_j^\dagger a_i\right) + O(\frac{1}{S^2}). \tag{8}$$

Since the imaginary part is $O(1/S)$, if we denote $t_{ij} = |t_{ij}|\exp(\mathrm{i}\Phi_{ij})$, we obtain

$$\begin{aligned} \mathrm{e}^{\mathrm{i}\Phi_{ij}} &= 1 + \mathrm{i}\Phi_{ij} + O(\frac{1}{S^2}) \\ &= 1 + \mathrm{i}\frac{Im\, t_{ij}}{|t_{ij}|} + O(\frac{1}{S^2}). \end{aligned} \tag{9}$$

Therefore, we obtain the magnon-electron Hamiltonian in the spin-wave approximation up to $O(1/S)$ as

$$\begin{aligned} H \simeq &-\sum_{ij} {t_{ij}}^0 \left[1 + \frac{1}{4S}(a_i^\dagger a_j + a_j^\dagger a_i - a_i^\dagger a_i - a_j^\dagger a_j)\right] \\ &\qquad\qquad \times \left(c_i^\dagger c_j + c_j^\dagger c_i\right) \\ &+ \frac{1}{4S}\sum_{ij} {t_{ij}}^0 \left(a_i^\dagger a_j - a_j^\dagger a_i\right)\left(c_i^\dagger c_j - c_j^\dagger c_i\right). \end{aligned} \tag{10}$$

To obtain the effective Hamiltonian for magnons, we trace out the fermion degrees of freedom in Eq. (10). Up to $O(1/S)$, the result is given by replacing terms $c_i^\dagger c_j$ by $\langle c_i^\dagger c_j\rangle$. Here, the expectation value should be taken for the ferromagnetic ground state without any magnon, whose Hamiltonian is described by

$$H_0 = -\sum_{ij} {t_{ij}}^0 \left(c_i^\dagger c_j + c_j^\dagger c_i\right). \tag{11}$$

In the perfectly-polarized ground state without degeneracies, the relation $\langle c_i^\dagger c_j\rangle = \langle c_j^\dagger c_i\rangle$ generally holds since the expectation value is real. Then, the second term in Eq. (10) vanishes and we finally obtain the effective spin-wave Hamiltonian as

$$\begin{aligned} H_{\rm eff} = &-\frac{1}{2S}\sum_{ij} {t_{ij}}^0 \langle c_i^\dagger c_j\rangle \\ &\times \left(a_i^\dagger a_j + a_j^\dagger a_i - a_i^\dagger a_i - a_j^\dagger a_j\right), \end{aligned} \tag{12}$$

up to irrelevant constants. In the uniform system with nearest neighbor hoppings where $\langle c_i^\dagger c_j\rangle$ is constant, this Hamiltonian gives a cosine-like dispersion as previously obtained by the different method [3].

Let us discuss the relation with the Heisenberg model. Comparing with the spin-wave approximation (6) of the Heisenberg model $H_{\rm Heis} = -2\sum J_{ij}\mathrm{S}_i\cdot\mathrm{S}_j$, we see that the magnon Hamiltonian (12) can be reproduced by the Heisenberg model with exchange couplings

$$J_{ij} = \frac{{t_{ij}}^0}{4S^2}\langle c_i^\dagger c_j\rangle, \tag{13}$$

within the leading order of $1/S$ expansion. Since ${t_{ij}}^0\langle c_i^\dagger c_j\rangle$ describes the local kinetic energy, Eq. (13) gives the relation between the DE ferromagnetic interaction and the kinetics of conduction electrons.

Finally, we note that Eq. (13) has been derived for generic electronic hoppings ${t_{ij}}^0$, which includes the cases with arbitrary hopping range or with random hopping integrals. Let us consider the case with site-diagonal random potential for conduction electrons. Since this type of potential does not couple to the spin-wave operators within the leading terms of $1/S$, the spin-wave Hamiltonian can be similarly obtained. Namely, the Hamiltonian (11) should be replaced by that with random potential, and expectation values $\langle c_i^\dagger c_j\rangle$ should be taken by the ground state of the replaced Hamiltonian. We also see that $J_{ij} \neq 0$ for Anderson-localized insulating systems where $\langle c_i^\dagger c_j\rangle \neq 0$. Namely, DE ferromagnetism can also exist in such non-metallic systems.

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