Perturbative calculation of the spin-wave dispersion in a disordered double-exchange model

Taeko Semba and Takahiro Fukui

Department of Mathematical Sciences, Ibaraki University, Mito 310-8512, Japan
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We study the spin-wave dispersion of localized spins in a disordered double-exchange model using the perturbation theory with respect to the strength of the disorder potential. We calculate the dispersion up to the next-leading order, and extensively examine the case of one-dimension. We show that in that case, disorder yields anomalous gapped-like behavior at the Fermi wavenumber of the conduction electrons.

KEYWORDS: colossal magnetoresistance manganites, double-exchange model, randomness, spin-wave dispersion, perturbation

Colossal magnetoresistance manganites\(^1\)\(^-\)\(^3\) have been providing hot topics owing to their rich magnetic and electronic properties.\(^4\)\(^-\)\(^6\) Recent studies have clarified that the double-exchange (DE) mechanism\(^7\)\(^-\)\(^10\) alone is not enough to understand a variety of phases of these materials, which is actually induced by the interplay between spin, charge and orbital degrees of freedom.

Recently, the softening of the spin-wave dispersion,\(^11\)\(^-\)\(^15\) observed in R\(_{1-x}\)D\(_x\)MnO\(_3\) (R=La, Pr, Nd and D=Ba, Sr, Ca, etc.), has suggested that a random potential also plays a crucial role in magnetic properties of these materials.\(^16\)\(^-\)\(^21\) Although some other mechanism\(^22\)\(^-\)\(^26\) have been proposed to describe the softening phenomena, recent numerical calculations by Motome and Furukawa\(^27\)\(^-\)\(^29\) have shown that a simple DE model with a random potential can explain the anomalous behavior of the spin-wave spectrum including broadening, gap formation as well as softening.

Motivated by their work, we study a disordered DE model by the use of the perturbation with respect to the strength of a random potential. Based on a general formula we derived, we show that in the case of 1-dimensional (1D) systems randomness yields a singularity of the spin-wave dispersion at the Fermi wavenumber of conduction electrons. It turns out that such anomalous behavior is mainly due to the nesting of the Fermi surface in 1D models. We then discuss the higher dimensional systems, based on the results of 1D systems.

We start with the following Hamiltonian:

\[
H = -t \sum_{\langle i,j \rangle} \sum_{\sigma} c_{i\sigma}^\dagger c_{j\sigma} - J_H \sum_i s_i \cdot S_i + \sum_i \epsilon_i c_{i\sigma}^\dagger c_{i\sigma},
\]

where \(s_i = \frac{1}{2} c_{i\sigma}^\dagger \sigma_{\sigma\sigma'} c_{i\sigma'}\) and \(S_i\) denotes, respectively, the electron spin and the localized spin in
the spin-\(S\) representation, and \(\epsilon_i\) is the quenched random potential with statistical properties \(\langle \epsilon_j \rangle = 0\) and \(\epsilon_i \epsilon_j = g \delta_{i,j}\). This model includes two large parameters, \(S\) and \(J_H\). Assuming that localized spins are almost aligned to the \(z\)-direction, we first take into account the leading terms with respect to the series of \(1/S\). To this end, we utilize the Holstein-Primakoff mapping for localized spins:

\[
S_i^+ = \sqrt{2S} a_i, \quad S_i^- = \sqrt{2S} a_i^\dagger, \quad S_i^z = S - a_i^\dagger a_i, \tag{2}
\]

which leads us to the following truncated Hamiltonian up to \(O(1/S^0)\):

\[
H = -t \sum_{\langle i,j \rangle, \sigma} c_i^\dagger \sigma c_j \sigma - \frac{J_H S}{2} \sum_{i, \sigma} \sigma c_i^\dagger \sigma c_i^\dagger \sigma c_i \sigma + \frac{J_H}{2} \sum_{i, \sigma} a_i^\dagger \sigma c_i^\dagger \sigma + \sum_{i, \sigma} \epsilon_i c_i^\dagger \sigma c_i \sigma. \tag{3}
\]

Based on this Hamiltonian, we calculate the spin-wave dispersion perturbatively with respect to the strength of disorder \(g\), collecting the leading terms with respect to \(J_H\).

Previously, Furukawa\(^{30}\) calculated the magnon dispersion in the clean DE model, according to the diagrams (a) in Fig.1. In the presence of disorder, these diagrams should be evaluated by the use of the electron propagator with the self-energy induced by the scattering of electrons by impurities. Since down-spin electrons are located in the momentum space far above the Fermi energy in the large \(J_H\) limit, it is readily seen that disorder yields the self-energy to up-spin electrons only, which is evaluated as

\[
\Sigma^\uparrow_{\text{disp}}(i\epsilon_n) = \sum_k \frac{-g}{i\epsilon_n - \epsilon_k} \sim \frac{i}{\tau} \text{sgn}(\epsilon_n) \tag{4}
\]

in a weak disorder limit, where \(\epsilon_n = (2n+1)\pi/\beta\) is the fermionic Matsubara frequency, \(\epsilon_k = -2t \sum \mu \cos k \mu - \epsilon_F\) is the bare electron dispersion, and the relaxation time \(\tau\) is given by \(1/\tau = \pi g D(\epsilon_F)\).

Fig. 1. (a) The leading self-energy of the spin-wave. Thin-lines denotes the down-spin propagator, whereas the thick-line denotes the up-spin propagator with the self-energy induced by disorder. (b) The propagator of up-spin electrons used in the diagrams (a). The thin-line and dotted-line denotes the bare up-spin propagator and impurity potential, respectively.
Using the propagator with the self-energy above, the diagrams in Fig.1 (a) are calculated as

\[ \Pi^{(0)}(0, q) = \frac{J_H^2 S}{2} \sum_{\varepsilon_n} \sum_{\varepsilon_k} \frac{-1}{i\varepsilon_n - \varepsilon_k + \Sigma_\uparrow(i\varepsilon_n)} \frac{-1}{i\varepsilon_n + \omega_n - \varepsilon_{k+q} - J_H S} \]

\[ - \frac{J_H}{2} \sum_{\varepsilon_n} \sum_{\varepsilon_k} \frac{-1}{i\varepsilon_n - \varepsilon_k + \Sigma_\uparrow(i\varepsilon_n)} \]

\[ \rightarrow \frac{1}{2S} \sum_{k} f_\tau(\varepsilon_k)(\varepsilon_{k+q} - \varepsilon_k), \quad (5) \]

where

\[ f_\tau(\varepsilon) = \frac{1}{2} \left( 1 - \frac{2}{\pi} \arctan \tau \varepsilon \right), \quad (6) \]

and the arrow in eq.(5) implies the large \( J_H \) limit. This equation indicates that disorder merely smears the Fermi surface at the leading order and hence, does not give rise to anomalous behavior for the magnon spectrum.

In order to calculate the self-energy of the spin-wave at the next leading order, let us consider the diagrams in Fig.2. Each diagram is evaluated as follows:

\[ \Pi^{(1a)}_{q+p,q}(i\omega_n; \epsilon_p) = \frac{J_H^2 S}{2} \sum_{\varepsilon_n} \sum_{\varepsilon_k} \frac{-1}{i\varepsilon_n - \varepsilon_k + \Sigma_\uparrow(i\varepsilon_n)} \frac{-1}{i\varepsilon_n + \omega_n - \varepsilon_{k+q} - J_H S} \]

\[ \times \frac{-1}{i(\varepsilon_n + \omega_n) - \varepsilon_{k+p+q} - J_H S} \]

\[ \rightarrow \frac{J_H}{2} \epsilon_p \chi_p + \frac{1}{2S} \sum_{k} f_\tau(\varepsilon_k) \frac{2i\omega_n + 2\varepsilon_k - \varepsilon_{k+p+q} - \varepsilon_{k-q}}{\varepsilon_k - \varepsilon_{k+p}}, \quad (7) \]
\[ \Pi(q+p,q;i\omega_n;\epsilon_p) = \frac{J_H^2 S}{2\epsilon_p} \sum_{\epsilon_n} \sum_k \frac{-1}{i\epsilon_n - \epsilon_k + \Sigma^\dagger(i\epsilon_n)} \frac{-1}{i(\epsilon_n + \omega_n) - \epsilon_{k+q} - J_H S} \times \frac{-1}{i(\epsilon_n + \omega_n) - \epsilon_{k+p+q} - J_H S} \rightarrow -\frac{1}{2S} \epsilon_p \sum_k f_\tau(\epsilon_k), \] (8)

and

\[ \Pi^{(1c)}_{q+p,q}(i\omega_n;\epsilon_p) = -\frac{J_H}{2} \epsilon_p \sum_{\epsilon_n} \sum_k \frac{-1}{i\epsilon_n - \epsilon_k + \Sigma^\dagger(i\epsilon_n)} \frac{-1}{i\epsilon_n - \epsilon_{k+p} + \Sigma^\dagger(i\epsilon_n)} \rightarrow -\frac{J_H}{2} \epsilon_p \chi_p, \] (9)

where \( \epsilon_p \) stands for the impurity potential in eq.(3) in the momentum representation, \( \chi_p \) is defined by

\[ \chi_p = \sum_k \frac{f_\tau(\epsilon_k) - f_\tau(\epsilon_{k+p})}{\epsilon_k - \epsilon_{k+p}}, \] (10)

and \( \omega_n \) is the bosonic Matsubara frequency \( \omega_n = 2n\pi/\beta \). Collecting these diagrams, we obtain

\[ \Pi^{(1)}_{q+p,q}(i\omega_n;\epsilon_p) = \frac{\epsilon_p}{2S} \sum_k f_\tau(\epsilon_k) \frac{\Sigma^\dagger(2i\omega_n + \epsilon_k - \epsilon_{k-q} + \epsilon_{k+p} - \epsilon_{k+p+q})}{\epsilon_k - \epsilon_{k+p}}. \] (11)

As already claimed, the contractions of the impurity lines in the same electron loop in Fig.2, which corresponds to Fig.1, do not give any anomalies in the magnon spectrum. Therefore, one can expect singular behavior in another type of diagrams, in which impurity lines are contracted among different electron loops in such a way as induces the correlations among up-spin electrons through the disorder potential. One of such simplest diagrams is given in Fig.3. To calculate this diagram explicitly, we use the quadratic dispersion \( \epsilon_k \sim t k^2 - \epsilon_F \).

![Fig. 3. The next-leading self-energy of the spin-wave.](image)

In 1D systems, this approximation works basically without loss of generality, whereas in the case of higher dimensional systems, it is well-known that the above self-energy, the function \( \chi_p \) in particular, is quite sensible to the form of the dispersion relation of bare electrons. Therefore, we restrict our calculations to 1D systems to reveal the mechanism of gap opening in a disordered DE model. As to higher dimensional systems, we will discuss what we expect at the end of the calculation based on the results of the 1D model.
The use of the quadratic dispersion leads to the following expression of the self-energy in Fig.3 for the 1D system,

$$\Pi_q^{(1)}(i\omega_n) = \frac{gt^2}{S^2} \sum_p \frac{(pq + q^2)^2 \chi_p^2}{i\omega_n - \Pi_q^{(0)}(i\omega_n)}.$$  \hspace{1cm} (12)

Here, we have neglected the Matsubara frequency in the numerator, since it merely gives rise to small effects. The total self-energy is now given by $$\Pi_q^{(0)}(i\omega_n) + \Pi_q^{(1)}(i\omega_n),$$ and the spin-wave dispersion relation can be determined by solving $$\omega = \Pi_q^{(0)}(\omega) + \Pi_q^{(1)}(\omega).$$ In what follows, we solve this nonlinear equation iteratively.

At the first step, one finds the spectrum given by

$$\omega_q = \Pi_q^{(0)} = 2t'(1 - \cos q),$$  \hspace{1cm} (13)

where \(t' = t/(2S)\sum_k f_\tau(\epsilon_k) \cos k\). Next, substituting this into \(\Pi_q^{(1)}(\omega)\), we have

$$\omega_q = \Pi_q^{(0)} - \frac{gt^2}{S^2} \sum_p \frac{(pq)^2}{p^2 + 2pq} \chi_p^2,$$  \hspace{1cm} (14)

where we have used the quadratic dispersion approximation for the spin-wave, \(\Pi_q^{(0)} \sim t'q^2\).

The second term above should exhibit singular behavior in the spin-wave spectrum. To observe this, we first calculate the function \(\chi_p\) with the smeared distribution function \(f_\tau(\epsilon)\) in eq.(6). We obtain

$$\chi_p = -\frac{1}{2\pi t} \frac{1}{2p} \ln \left( \frac{(p^2/2)^2 + \overline{k}_F \cos \theta + \overline{k}_F^2}{(p^2/2) - pk_F \cos \theta + \overline{k}_F^2} \right),$$  \hspace{1cm} (15)

where \(\overline{k}_F\) and \(\theta\) is defined, respectively, \(\overline{k}_F = (k_F^4 + \epsilon^2)^{1/4}\) with \(\epsilon = 1/(t\tau)\) and \(\tan \theta = \epsilon/k_F^2\).

It may be instructive to take the zero disorder limit, \(g \rightarrow 0\) \((\epsilon \rightarrow 0)\) in this function: It then becomes the well-known form,

$$\chi_p \rightarrow -\frac{1}{2\pi t} \frac{1}{2p} \ln \left| \frac{p + 2k_F}{p - 2k_F} \right|.$$  \hspace{1cm} (16)

This function plays a crucial role in the spin-density-wave (SDW) in 1D systems due to the divergence at \(p = 2k_F\) in the absence of disorder. However, in the system under consideration, it shows just a peak at \(p = 2k_F\) due to the self-energy of electrons, i.e., the scattering of up-spin electrons by the disorder potential. In Fig.4, we show examples of this function in two kinds of the hole densities (of the lower band) \(x\) defined by \(k_F = \pi(1 - x)\). One can see that the height of the peak depends weakly on \(x\), since \(g\) enters \(\chi_p\) through \(\theta\).

Having derived the function \(\chi_p\), we next calculate the dispersion of the spin-wave. The \(p\)-integration in eq.(14) is rewritten as

$$\sum_p \frac{(pq^2 + q^4)}{p^2 + 2pq} \chi_p^2 = \frac{1}{(2\pi t)^2} \overline{k}_F Q \left[ g_Q^{(2)} + \frac{Q^2}{4} g_Q^{(0)} \right],$$  \hspace{1cm} (17)
Fig. 4. The function $\chi$ in eq.(15) computed for two kinds of hole-densities: $x = 0.5$ and $x = 0.3$. The parameters used are $g/t^2 = 0.1$ and $S = 3/2$ in both cases.

where $Q = q/\tilde{k}_F$ and $g^{(n)}_Q$ for $n = 0, 2$ is defined by

$$g^{(n)}_Q = \frac{1}{2\beta} \int_{-\infty}^{\infty} dx \left( \frac{1}{x + Q} + \frac{1}{x - Q} \right) \frac{1}{x^{3-n}} \ln \left( \frac{1 + 2 \cos \frac{\theta}{2} + x^2}{1 - 2 \cos \frac{\theta}{2} + x^2} \right). \quad (18)$$

Using the contour integral in the complex plane, this integral can be converted into

$$g^{(n)}_Q = \frac{\pi \theta \cos \frac{\theta}{2}}{Q^2} \delta_{n,0} - \frac{\pi}{Q^{3-n}} \ln \left| \frac{e^{-i\theta/2} - Q}{e^{i\theta/2} + Q} \right| \left[ \arg \left( \frac{e^{-i\theta/2} - Q}{e^{i\theta/2} + Q} \right) \right] + \pi \int_{\cos \frac{\theta}{2}}^{\infty} dx \Im \left[ \left( \frac{1}{x + Q + i \sin \frac{\theta}{2}} + \frac{1}{x - Q + i \sin \frac{\theta}{2}} \right) \ln \left( \frac{\cos \frac{\theta}{2} - 2i \sin \frac{\theta}{2} + x}{\cos \frac{\theta}{2} - 2i \sin \frac{\theta}{2} - x} \right) \right]. \quad (19)$$

This expression is convenient for numerical computation as well as to take the $g \to 0$ limit, as we shall see momentarily. The dispersion of the spin-wave is finally given by

$$\omega_q = t'q^2 - \frac{g}{S^2 t' (2\pi)^2} \tilde{k}_F Q^2 \left[ g^{(2)}_Q + \frac{Q^2}{4} g^{(0)}_Q \right]. \quad (20)$$

Computing $g^{(n)}_Q$ in eq.(19) numerically, we show in Fig.5 examples of the spin-wave dispersion for the same systems as those in Fig.4. One can indeed find an anomalous dispersion at the Fermi wavenumber of electrons. Although gap opening is not observed, a sharp jump appears just at the Fermi wavenumber. Therefore, we can conclude that the diagram in Fig.3, which includes the correlations among up-spin fermions through disorder, plays an important role in the dynamics of localized spins, even though the disorder is nonmagnetic.

So far we have derived the spin-wave dispersion in the presence of disorder by the use of $f_\tau(\varepsilon)$ in the calculation of $\chi_p$ and hence, of $g^{(n)}_Q$. To clarify the origin of such anomalous behavior, let us take $g \to 0$ limit in eq.(19), as has been done for $\chi_p$ in eq.(16), yielding

$$g^{(n)}_Q = \frac{2\pi^2}{Q^2} \delta_{n,0} \pm \frac{\pi^2}{Q^{3-n}} \ln \left| \frac{1 + Q}{1 - Q} \right| \quad \text{for} \quad \left\{ \begin{array}{l} |Q| < 1 \nonumber \\ |Q| > 1 \end{array} \right. . \quad (21)$$
Fig. 5. The dispersion in eq. (20). The dotted-line denotes the quadratic dispersion in the $g = 0$ limit (i.e., $\omega_q = t'q^2$). The down-arrows denote the positions of the Fermi wavenumbers.

If one uses this formula instead of eq. (19), one reaches the following spin-wave dispersion:

$$\omega_q = (t' + 2g\alpha)q^2 \mp 5k_Fg\alpha q \ln \frac{q + k_F}{q - k_F}$$

for

$$\begin{cases} |q| < k_F \\ |q| > k_F \end{cases}$$

where the constant $\alpha$ is given by $\alpha = 1/(64\pi k_F S^2 t')$. The dispersion in eq. (22) now diverges at $q = k_F$. Therefore, the present result reveals that an enhancement in $\chi_p$ at the nesting vectors is responsible for the anomalous gapped-like behavior of the spin-wave dispersion of localized spins. However, it should be stressed that even though the divergence in $\chi_p$ is suppressed by disorder, which is due to the smearing of the Fermi surface, singular behavior of spin-wave dispersion seems robust.

So far we have demonstrated that nonmagnetic impurities of conduction electrons actually induce the anomalous behavior of localized spins at the Fermi wavenumbers of electrons, as suggested by Motome and Furukawa, by using the leading order perturbation theory. In models with small $J_H$, the diagrams in Fig. 1 leads to interesting physics such as SDW or spin glass (RKKY exchange interaction). Contrary to these, the same diagram merely yields the canonical dispersion of the spin-wave in the present systems with large $J_H$ because of weak correlations between electrons with different spins. Even in such systems, however, disorder induces correlations among up-spin electrons, and strongly affects the magnetic properties, even if disorder is weak and nonmagnetic.

Finally, we would like to discuss the models in higher dimensions. The chief ingredient in a step-function-like behavior in the dispersion is the function $\chi_p$, which has a sharp peak at $p = 2k_F$ in 1D. This reflects the nesting of the Fermi surface. In higher dimensions, however, this function is continuous if we use the free electron (quadratic) dispersion. Therefore, in such an approximation, one cannot expect any anomalous dispersions in the spin-wave excitation. On the other hand, the tight-binding electron dispersion gives rise to an enhancement around the nesting wavevectors of electrons near half-filling. Therefore, one can expect similar anomalous
behavior of spin-waves there even in higher dimensions. The question is how robust such anomalous behavior is away from half-filling. Unfortunately, cosine dispersion of electrons does not allow analytic calculations in higher dimensions, and therefore, the details, including numerical results, will be published elsewhere.

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