Spin wave spectrum of a disordered double exchange model

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A double exchange model with quenched disorder for conduction electrons is studied by field theoretical methods. By using a path integral formalism and replica techniques based on it, an ensemble-averaged spin wave dispersion of the localized spins is derived. It is shown that the spectrum of the spin wave has gaps at the multiple of the Fermi wavenumber of the conduction electrons in the presence of disorder, and hence, quenched disorder for electrons adds a striking effect to the dynamics of the localized spins. In the strong disorder limit, the present results suggest spin-glass like behavior due to the frustration of the exchange coupling.

The double exchange (DE) model [1] has been attracting much renewed interest due to the discovery of colossal magnetoresistance of perovskite manganites [2][3][4]. These materials show a variety of phases, in which spin, charge, orbital, and lattice degrees of freedom and their interplay provide rich and complex behavior. Although a lot of experimental and theoretical studies have been clarifying some aspects of complex physics of manganites, they still remain fascinating and incompletely understood phenomena [5].

It is believed that the DE mechanism is essential to the metallic ferromagnetism of manganites. However, several authors have pointed out the importance of disorder, which is inevitably included in the materials [13][14][15][16]. Especially, recent experiments have reported anomalous behavior of spin wave spectrum, which cannot be explained by a simple DE theory [2][10][11][12]. Motome and Furukawa [17] have numerically studied DE model with quenched disorder and found that the model successfully describe the anomalies of spin wave dispersion. They have suggested that the origin of the anomalies is the Friedel oscillation.

Motivated by their work, we study, in this paper, the effects of quenched disorder on the spin wave by field theoretical method. Using the replica approach for the ensemble average over disorder and integrating out the electrons, we derive an effective action for the localized spins. The equation of motion derived from this action leads us to the usual one for the Heisenberg ferromagnets spins. The equation of motion derived from this action is given by

$$ S[j] = -\sum_{j} \left( \sum_{\sigma} \left( c_{j}^{\dagger} \sigma \cdot c_{j+1} \sigma + \text{h.c.} \right) - J_{H} \sum_{j} s_{j} \cdot S_{j} \right) $$

where $s_{j} = \frac{1}{2} c_{j}^{\dagger} \sigma_{\sigma_{s}} c_{j+\sigma_{s}}$ denotes a spin operator of the conduction electron, $S_{j}$ a localized spin which we treat as a classical object $S_{j} = S n_{j}$ with a unit vector $n_{j}$ defined by $n_{j} = (\sin \theta_{j} \cos \phi_{j}, \sin \theta_{j} \sin \phi_{j}, \cos \theta_{j})$, and $\epsilon_{j}$ is on-site disorder potential with the gaussian distribution $P[\epsilon] = \exp \left[-\frac{1}{2} \epsilon_{j}^{2}/\eta \right]$.

We start with the canonical DE model without disorder to have a path integral formalism convenient for taking disorder into account. The Hund’s-rule coupling term can be written as $J_{H} \sum_{j} s_{j} \cdot S_{j} = (J_{H} S/2)c_{j}^{\dagger} S_{j} c_{j}$, where $c_{j}^{\dagger} = (c_{j,\uparrow}^{\dagger}, c_{j,\downarrow}^{\dagger})$ and

$$ S_{j}(\theta_{j}, \phi_{j}) \equiv \left( \begin{array}{c} \cos \theta_{j} \\ \sin \theta_{j} e^{-i\phi_{j}} \end{array} \right). $$

The partition function is then represented by a path integral form $Z = \int Dc Dc^{\dagger} e^{-S}$, where the action is given by

$$ S = \int_{0}^{\beta} d\tau \left( \sum_{j} c_{j}^{\dagger} \partial_{\tau} c_{j} - H - \mu \sum_{j} c_{j}^{\dagger} c_{j} \right) $$

The matrix $S_{j}$ in Eq. (2) is diagonalized by a local unitary matrix $U_{j}(\tau) \equiv S_{j}(\theta_{j}/2, \phi_{j})$ as $U_{j}^{\dagger}(\tau) S_{j} U_{j}(\tau) = \sigma_{3}$. Let us define a fermion field $\tilde{c}_{j} = U_{j} c_{j}$ in the locally rotated frame. For a large $J_{H}$, only up-spin fermions survive, and we have an effective action described solely by fermions $\tilde{c}_{j,\uparrow} \equiv c_{j}$ in this limit,

$$ S = \int_{0}^{\beta} d\tau \sum_{j} \left[ c_{j,\uparrow}^{\dagger} \partial_{\tau} + \langle n_{j} | \partial_{\tau} n_{j} \rangle \right] c_{j,\uparrow} - t \left( c_{j,\uparrow}^{\dagger} \langle n_{j} | n_{j+1} \rangle c_{j,\uparrow+1} + \text{h.c.} \right) - \mu c_{j,\uparrow}^{\dagger} c_{j,\uparrow} \right]. $$

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The Hamiltonian we study is given by [17]

$$ H = -t \sum_{j} \sum_{\sigma} \left( c_{j,\sigma}^{\dagger} c_{j+1,\sigma} + \text{h.c.} \right) - J_{H} \sum_{j} s_{j} \cdot S_{j} $$

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It should be noted that in this projection the nonlocal transformation yields nontrivial additional terms such as $\langle U_{j} \partial_{\tau} U_{j+1} \rangle$ and $\langle U_{j} U_{j+1} \rangle$ in the canonical and hopping terms, respectively. To describe these, we have introduced a bracket notation

$$ \langle U_{j} U_{j+1} \rangle \equiv \langle n_{j} | n_{j+1} \rangle $$

since this is actually equivalent to the inner product of the spin coherent state, $\langle n_{j} | n_{j+1} \rangle \equiv \langle n_{j} | n_{j+1} \rangle$. Therefore, $\langle n_{j} | \partial_{\tau} n_{j} \rangle \equiv A_{j}(\tau)$ can be
interpreted as the Berry phase, playing an important role in the dynamics of the localized spins.

Assume that the localized spins are almost aligned to one direction, \( \langle n_j | n_j \rangle \approx 1 \). In this case we introduce a small field variable \( \langle n_j | n_j \rangle = \langle n_j | n_j \rangle - 1 \), and then the action can be divided into two pieces \( S = S_0 + S_n \), where

\[
S_0 = \int_0^\beta d\tau \sum_j \left[ c_j^\dagger \partial_\tau c_j - t \left( c_j^\dagger c_{j+1} + \text{h.c.} \right) - \mu c_j^\dagger c_j \right],
\]

\[
S_n = \int_0^\beta d\tau \sum_j \left[ c_j^\dagger A_j c_j - t \left( c_j^\dagger (n_j | n_{j+1}) c_{j+1} + \text{h.c.} \right) \right].
\]

These equations are basis of our perturbative calculations. At the leading order, an effective action \( W[n] \) for the localized spins, defined by \( e^{-W[n]} = \langle e^{-S_n} \rangle \), is given by

\[
W[n] = \int_0^\beta d\tau \sum_j \left[ g_j A_j - \frac{1}{2} J_j n_j \cdot n_{j+1} \right]
\]

except for some irrelevant constant terms, where

\[
g_j \equiv \langle c_j^\dagger (\tau) c_j(\tau) \rangle, \quad J_j \equiv t \langle c_j^\dagger (\tau) c_{j+1}(\tau) \rangle,
\]

and we have used the fact that \( \langle n_j | n_j \rangle = \frac{1}{2} (1 + n_j \cdot n_j) \), namely, \( \langle n_j | n_j \rangle + \text{c.c.} \approx \frac{1}{2} (n_j \cdot n_j - 1) \). In the pure model under consideration, \( g_j = 1 - x \equiv g_0 \) and \( J_j = 2t \sum_{k>0} f(\varepsilon_k) \cos k = J_0 \) are uniform constants, where \( x \) is the hole concentration, \( \varepsilon_k = -2t \cos k - \mu \) is the transfer energy of electrons, and \( f(\varepsilon) = 1/(e^{\beta \varepsilon} + 1) \) is the Fermi distribution function. It should be noted that in Eq. (6), \( n_j \cdot n_{j+1} \approx 1 \) is implicitly assumed.

The classical equation of motion for the localized spins \( n_j \) can be derived from the effective action Eq. (6): The variation of the action \( W[n] \) with respect to \( n_j \), \( \delta W/\delta n_j(\tau) = 0 \), leads us to

\[
g_j \frac{dn_j}{dt} = n_j \times (J_j - \frac{1}{2} J_j n_{j-1} + J_j n_{j+1})
\]

after the replacement \( \tau \to -it \). In deriving this, the Berry phase is involved in the time derivative of the spin variable \( n_j \). In the pure case, this equation is just the one for the Heisenberg ferromagnets, giving dispersion relation \( \omega_k = (2J_0/g_0)(1 - \cos k) \).

Now let us take account of disorder effects on the spin wave spectrum. Since the disorder potential in Eq. (1) is invariant under the unitary transformation \( U_j(\tau) \), it gives rise to \( H_d = \sum_i c_i^\dagger c_i \) in the projected action \( 4 \). We now introduce \( m \) replicas to take quenched average over disorder. Ensemble average yields the following term

\[
S_d = -\frac{g}{2} \int_0^\beta d\tau \int_0^\beta d\tau' \sum_{a,b=1}^m c_{i\omega}^\dagger(\tau) c_{a\omega}(\tau) c_{b\omega}(\tau') c_{ia}(i\omega) c_{b\omega}(i\omega')
\]

\[
\times c_{b\omega}(i\omega') c_{i\omega}^\dagger(\tau')
\]

where \( a, b = 1, 2, \ldots, m \) denote replica species. Although the fermions in the present replica theory are spinless (fully-polarized), this inter-replica coupling in \( S_d \) as well as the spin-fermion coupling in \( S_n \) are reminiscent of the theory of the spin density wave (SDW): They are expected to play similar roles to the Coulomb interaction and phonons in SDW, respectively. The wisdom obtained so far tells that \( 2k_F \) oscillating mode of phonons makes a gap in the fermion sector, where \( k_F \) denotes the Fermi wavenumber. On the analogy of this, we expect that the \( 2k_F \) mode of localized spins in \( S_n \) would be potentially involved with a gap formation of fermions, although we will treat \( S_n \) separately from \( S_0 + S_d \), in what follows. Based on these observations, let us first examine the mean field ground state of the fermions within the action \( S_0 + S_d \), and next compute the coupling constants of the localized spins, \( g_j \) and \( J_j \) in Eq. (7). We have to mention here that \( S_d \) is nonlocal with respect to \( \tau \), and therefore careful treatment of the inter-replica interaction is needed. Namely, we divide the summation over the Matsubara frequencies into two parts:

\[
S_d = \frac{g}{2} \sum_{a \neq b} \sum_{\omega \omega_1' \omega_2' \omega_1} \sum_{q,k,k'} c_{k+q,a}(i\omega_1 + i\omega) c_{b}(i\omega) c_{k',a}(i\omega_2 - i\omega) c_{k',b}(i\omega_2')
\]

\[
+ \frac{g}{2} \sum_{a,b} \sum_{\omega \omega_1' \omega_2'} \sum_{q,k,k'} c_{k+q,a}(i\omega_1 + i\omega) c_{a}(i\omega) c_{k',a}(i\omega_2 - i\omega) c_{k',b}(i\omega_2').
\]

Here, \( \omega_n = 2\pi n/\beta \) is bosonic Matsubara frequency. It should be noted that \( a = b \) terms of the first line of the right hand side above vanish identically due to the Fermi statistics. Introducing two kinds of auxiliary fields leads us to the action which is bilinear in the Fermi fields,

\[
S_d = \frac{1}{2g} \sum_{\omega_n} \sum_q \sum_{a \neq b} Q_{q,ba}(i\omega_n) Q_{q,ab}(-i\omega_n) + \frac{1}{2g} \sum_{\omega_n \neq 0} \sum_q P_q(i\omega_n) P_{-q}(-i\omega_n)
\]
Let us now assume a static \((i\omega_n = 0)\) saddle point solution with the following replica symmetric form

\[
Q_{q,ab}(i\omega_n) = 2i\Delta \delta_{n,0} \delta_{q,2k_F},
\]

where \(P_q(i\omega_n) = 0\) since \(i\omega_n = 0\) is prohibited in the summation in Eq. \((11)\). This form of the mean field solution is similar to the one in the replica theory for spin glass models \([19]\). Although we have mentioned the similarity to the theory of SDW, the present replica coupling is repulsive. Therefore, we cannot expect a stable mean field ground state if the number of species \(m\) is an integer \(m \geq 1\): This is the reason we assume an imaginary \(Q\) in Eq. \((12)\). Substituting Eq. \((12)\) into Eq. \((11)\), we have

\[
S_d = - \sum_{a \neq b} \sum_{\omega_n} \sum_k \Delta \left[ c_{k+2k_F,a}^\dagger (i\omega_n) c_{k,b}(i\omega_n) + h.c \right] - \frac{2m(m-1)}{g} \Delta^2.
\]

Due to the assumption of imaginary \(Q\), the \(\Delta^2\) potential above has actually a wrong sign. Nevertheless, in the replica limit \(m \to 0\), we have a mean field solution, as we shall see momentarily.

Now let us determine the parameter \(\Delta\) by minimizing the effective action for \(\Delta\). To this end, we decompose the Fourier modes into several pieces,

\[
c_{j,a}(i\omega_n) = \sum_{|k| < k_F - \Lambda} e^{ikj} c_{k,a}(i\omega_n) + \sum_{|k| > k_F + \Lambda} \mathbf{u}_{k,j}^\dagger c_{k,a}(i\omega_n),
\]

where \(c_{k,a}^\dagger \equiv (c_{k+k_F,a}^\dagger, c_{k-k_F,a}^\dagger)\) and \(\mathbf{u}_{k,j}^\dagger \equiv (e^{i(k+k_F)j}, e^{i(k-k_F)j})\). Then the fermion action becomes

\[
S_0 + S_d = - \sum_{a,b} \sum_{\omega_n} \left[ \sum_{|k| < k_F - \Lambda} \left( c_{k,a}^\dagger (i\omega_n) - \varepsilon_k \right) c_{k,b}(i\omega_n) - \sum_{|k| < \Lambda} c_{k,a}^\dagger (i\omega_n) \left[ D_k(i\omega_n) \delta_{ab} + M(1 - \delta_{ab}) \right] c_{k,b}(i\omega_n) \right],
\]

where

\[
D_k(i\omega_n) \sim \begin{pmatrix} i\omega_n - v_F k & 0 \\ 0 & i\omega_n + v_F k \end{pmatrix},
\]

\[
M = \begin{pmatrix} 0 & \Delta \\ \Delta & 0 \end{pmatrix}.
\]

Here we have linearized the transfer energy of electrons as \(\varepsilon_{k\pm k_F} \sim \pm v_F k\) with \(v_F \equiv 2\sin k_F\). Note that the matrix \(D_k \delta_{ab} + M(1 - \delta_{ab})\) can be diagonalized in the replica space by a global unitary transformation, giving \((m-1)\) eigenvalues \(D_k - M\) and 1 eigenvalue \(D_k - (1 - m)M\). Therefore, integrating out the Fermi fields yields

\[
e^{-F(\Delta)} = \int \mathcal{D}c \mathcal{D}c^\dagger e^{-(S_0 + S_d)},
\]

where

\[
F(\Delta) = - \frac{2m(m-1)\beta}{g} \Delta^2 - (m-1) \ln \det \left( D - (1 - m)M \right).
\]

It is readily seen that \(D_k(i\omega_n) - M\) has eigenvalues

\[
i\omega_n \pm E_k(\Delta)\] with \(E_k(\Delta) = \sqrt{(v_F k)^2 + \Delta^2}\). Then, the variation with respect to \(\Delta\) gives

\[
\frac{\partial F}{\partial \Delta} = m \Delta \left\{ \frac{4(1 - m)}{g} \right\} - \frac{1}{v_F} \ln \left[ \frac{\pi v_F \Lambda}{\Delta} + \sqrt{1 + \left( \frac{v_F \Lambda}{\Delta} \right)^2} \right] + O(m),
\]

where we have assumed that the temperature of the system is much lower than \(\Delta\), i.e., \(\beta \Delta \ll 1\). This equation gives no solution in the normal case with \(m \geq 1\), since the inter-replica interaction is repulsive, as mentioned above. However, it turns out that we obtain non trivial stable solution in the replica limit \(m \to 0\),

\[
\Delta = 2v_F \Lambda \frac{e^{4\pi v_F}}{e^{4\pi v_F} - 1} \sim 2v_F \Lambda e^{-4\pi v_F}.
\]
This is due to the change of the sign of the $\Delta^2$ potential at $m = 1$.

Now we calculate the effective action Eq. (6) in the presence of disorder by using ensemble-averaged correlation functions in Eq. (17). To this end, we need $\langle c_j^\dagger(\tau)c_j(\tau) \rangle = \lim_{m \to 0} \langle c_{1,j}^\dagger(\tau)c_{1,j}(\tau) \rangle$ in the replica approach. In order to calculate this in the replica-diagonal frame introduced previously, we have to note that the above correlation function is equivalent to $\lim_{m \to 0} \frac{1}{m} \sum_a \langle c_{1,a}^\dagger(\tau)c_{1,a}(\tau) \rangle$, and therefore, invariant under the global transformation. As we mentioned already, this transformation yields $m - 1$ eigenvalues $D + M$ and 1 eigenvalue $D + (1 - m)M$, the latter of which approaches the former in the replica limit $m \to 0$, and therefore, this observation enables us to keep just one replica species, say, $a = 1$ with $D + M$ to calculate the above correlation function. To simplify the notation, we will suppress the replica indices hereafter.

Based on

$$\langle c_j(\tau)c_j(\tau) \rangle = \sum_{\omega_n} \left[ \sum_{|k|<k_F} e^{ik(j-j')} \frac{-1}{\omega_n - \varepsilon_k} + \sum_{|k|>k_F} \right],$$

and assume that $\Delta$ is much smaller than the temperature under consideration, we end up with

$$g_j = g_0 - g_0^{\text{osc}} \cos(2k_F j),$$
$$J_j = J_0 - \delta J - J_0^{\text{osc}} \cos[k_F(2j + 1)],$$

where each term can be computed as

$$g_0^{\text{osc}} = 2 \sum_{0<k<k_F} \frac{\Delta}{E_k} \arcsinh \left( \frac{\Delta v_F}{\varepsilon_0} \right),$$
$$\delta J = 2t \sin k_F \sum_{0<k<k_F} \sin k \left( 1 - \frac{v_F k}{E_k} \right),$$
$$J_0^{\text{osc}} = 2t \sum_{0<k<k_F} \cos k \frac{\Delta}{E_k}.$$ (22)

Thus we have derived a classical ferromagnetic spin-wave action [8] with Eqs. (21) and (22), which yields the equation of motion [8]. Eq. (21) tells us that nonmagnetic impurities of conduction electrons give rise to a $2k_F$ oscillating component to the exchange coupling of the localized spins. This results in the gap opening in the spin wave dispersion $\omega_q$ at $q = k_F, 2k_F, \cdots \mod(\pi)$, which are controlled by the Fermi wavenumber $k_F$ of conduction electrons. We show in Fig. 1 a schematic spin wave spectrum for a $x = 1/3$ doping case. As expected from the exchange coupling with the $2k_F$ oscillation, there appears a gap at $q = (2/3)\pi$. In addition, the dispersion relation has a small gap at $q = 2k_F = (1/3)\pi \mod \pi$. In general, when the Fermi wavenumber is commensurate, $k_F = (m/n)\pi$, there appears $n$ gaps in the spin wave dispersion. It should be noted that $2k_F$ oscillation is included not only in the exchange coupling but also in the Berry phase term, both of which determine the size of gaps. As far as we have studied the equation of motion numerically, $g_j$ tends to make the gap at $q = k_F$ larger and the other gaps smaller. Details will be published elsewhere.

In a strong disorder limit, we expect relatively large $\Delta$ of order $\Lambda$. Although the present formalism is a weak disorder approach, it may be suggestive to consider the case $\Delta \to \infty$. Setting $\Lambda \sim k_F$, we have $g_j \sim 2(1-x)\sin^2(k_F j)$ and $J_j \sim \frac{\pi}{2}\sin[k_F(j + 1)]\sin(k_F j)$. These equations tell that the exchange coupling could be frustrated, which may be responsible for the glass phase of the manganites observed actually by experiments [24]. However, in this case, quantum treatments of the localized spins would be required.

So far we have studied a spin wave dispersion in one dimension, which has gaps for any disorder strength $g$. In higher dimensions, there exists a critical value $g_c(>0)$, below which the dispersion has no gaps. Details will be published elsewhere.

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