Static and Dynamic Spin Structure Factors of Frustrated Heisenberg Antiferromagnet

O. P. Sushkov

School of Physics, The University of New South Wales, Sydney 2052, Australia

Abstract

Using the modified spin-wave theory we calculate static and dynamic spin structure factors in spin-liquid state of the $J_1-J_2$ model. The spectrum of excitations in the vector channel is discussed. The developed technique can also be applied to the $t-J$ model describing copper oxide superconductors.

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Magnetically disordered states in quantum spin models are of considerable interest. Much of this interest stems from the connection of this problem to high-\(T_c\) superconductivity. The ground state of an undoped compound has long range antiferromagnetic order, which is well described by the Heisenberg model and has been studied by numerous methods. However introducing a small number of holes leads to destruction of long range order.

Destruction of long range order can be studied by introducing some frustration into the Heisenberg model. This simplified mechanism of the destruction is certainly far from the reality for cuprates, but the investigation of this relatively simple model allows us to develop approaches to more realistic models. From this point of view the main purpose of the present work is to develop a technique applicable to the \(t-J\) model.

We will focus on the simplest frustrated Heisenberg model. It is the \(J_1-J_2\) model defined by

\[
H = J_1 \sum_{NN} \mathbf{S}_r \cdot \mathbf{S}_{r'} + J_2 \sum_{NNN} \mathbf{S}_r \cdot \mathbf{S}_{r'}. \tag{1}
\]

In this Hamiltonian, the \(J_1\) term describes the usual Heisenberg interaction of the nearest neighbor spins (\(S = \frac{1}{2}\)) on a square lattice, while the \(J_2\) term introduces a frustrating interaction between the next nearest neighbor sites. For convenience, we set \(J_1 = 1\) and denote \(\alpha \equiv J_2/J_1\).

For small \(\alpha\), the ground state is Néel ordered. For large \(\alpha\) the system is decomposed into two Néel ordered sublattices which, however, have the same quantization axis. This is so called collinear state. Whether or not the Néel and collinear states are separated in parameter space by a spin liquid state has been a subject of many discussions. Besides the spin-wave calculations, the model has been studied by the Schwinger boson mean field theory, analysis of small lattices, a series expansion, a mean field theory of bond operators, and other methods. The majority of these works including most recent exact finite lattice diagonalizations and series expansion indicate the existence of a different intermediate phase for \(0.4 < \alpha < 0.6\). Therefore in this work we assume that the system undergoes a second order quantum phase transition at \(\alpha = \alpha_c \approx 0.4\) from the Néel to a spin-liquid state. We are interested in this spin liquid phase close to the transition point, so \(\alpha > \alpha_c\) and \(\alpha - \alpha_c \ll 1\). In our previous work for description of this state we used modified spin-wave theory originally suggested by Takahashi for the Heisenberg model at nonzero temperature. In the present work we use same approach.
We remind the reader that for spin-wave description it is convenient to use Dyson-Maleev
transformation\(^1\) (see also review\(^2\)) for localized spin \(S = 1/2\),
\[ S^+_{l} = a^\dagger_{l}, \quad S^-_{l} = (2S - a^\dagger_{l}a_{l}), \]
\[ S^z_{l} = S - a^\dagger_{l}a_{l}, \quad \text{for } l \in \text{up sublattice}; \]
\[ S^+_{m} = b^\dagger_{m}, \quad S^-_{m} = b^\dagger_{m}(2S - b^\dagger_{m}b_{m}), \]
\[ S^z_{m} = -S + b^\dagger_{m}b_{m}, \quad \text{for } m \in \text{down sublattice}, \]
and Fourier representation for \(a_{l}\) and \(b_{m}\)
\[ a_{l} = \sqrt{\frac{2}{N}} \sum_{k} e^{i k \mathbf{r}_{l} \cdot \mathbf{a}} a_{k}, \]
\[ b_{m} = \sqrt{\frac{2}{N}} \sum_{k} e^{i k \mathbf{r}_{m} \cdot \mathbf{b}} b_{k}. \]

Here \(N\) is number of sites on square lattice. The summation over \(k\), here and everywhere
below is restricted to the inside magnetic Brillouine zone \((|k_x| + |k_y| \leq \pi)\). There are two
simple ways to find an effective Hamiltonian quadratic in the operators \(a\) and \(b\). First way is
just dropping the quartic terms, and this is the linear spin-wave theory (LSWT). Second way
 corresponds to the mean field treating of the quartic terms \(a^\dagger a b^\dagger b \rightarrow \langle a^\dagger a \rangle b^\dagger b + \langle a^\dagger b^\dagger \rangle a b + ...\),
and this is mean field spin-wave theory (MFSWT). Both approximations give very similar
results (see e. g. Ref\(^3\)). Therefore as soon as we believe that spin-liquid phase exists, it
does not matter which approximation is used for calculations of the properties of this phase.
However LSWT gives the value of \(\alpha_c \approx 0.4\) very close to that found from exact numerical
computations. Therefore in the present work we will use linear spin-wave theory.

Using Bogoliubov transformation one can easily find spectrum of spin-waves and
staggered magnetization of sublattice in the Néel state
\[ \omega_k = 2\sqrt{[1 - \alpha(1 - \eta_k)]^2 - \gamma_k^2}; \]
\[ m \equiv |\langle S_z \rangle| = 1 - \frac{2}{N} \sum_{k} \frac{1 - \alpha(1 - \eta_k)}{\omega_k}. \]

As usually we have defined
\[ \gamma_k = \frac{1}{2}(\cos k_x + \cos k_y) \quad \text{and} \quad \eta_k = \cos k_x \cos k_y. \]

At \(\alpha = 0\) the staggered magnetization \(m = 0.3\). It decreases with increasing of \(\alpha\) and
vanishes at \(\alpha = \alpha_c \approx 0.4\) where the system undergoes a second order transition into the
liquid state. Zero sublattice magnetization means that the ground state is a condensate of many spin waves \( a_k \) and \( b_k \). To describe the emerging phase we must take into account their non-linear interaction. We cannot do this exactly. However, there is an approximate method originally suggested by Takahashi for the Heisenberg model at nonzero temperature. Following Takahashi, we impose an additional condition that sublattice magnetization is zero

\[
\langle S_u^z - S_d^z \rangle = \langle \frac{1}{2} - a^+_1a_1 + \frac{1}{2} - b^+_mb_m \rangle = 0,
\]

where \( u \) and \( d \) are the spin up and down sublattices. The constraint (5) gives an effective cutoff of unphysical states in Dyson-Maleev transformation. This question is discussed in the paper.

The constraint (5) is introduced into the Hamiltonian via a Lagrange multiplier \( \frac{1}{8} \nu^2 \).

Now we must diagonalize

\[
H_\nu = H_{LSWT} - \frac{1}{8} \nu^2 (S_u^z - S_d^z) \rightarrow 2 \sum_k \left( A_k (a^+_ka_k + b^+_kb_k) + \gamma_k (a_kb_{-k} + a^+_kb^-_{-k}) \right),
\]

where \( A_k = 1 - \alpha (1 - \eta_k) + \frac{1}{8} \nu^2 \). The simple (linear) second term in (6), taken together with Eq. (5), takes account of non-linear interaction of spin waves. Diagonalizing Eq. (6) by Bogoliubov transformation

\[
a_k = U_k \alpha_k + V_k \beta^+_k,
\]

\[
b_{-k} = V_k \alpha^+_k + U_k \beta_{-k},
\]

we get the spectrum of excitations

\[
\omega_{\nu k} = 2 \sqrt{A_k^2 - \gamma_k^2}.
\]

This spectrum has a gap \( \nu \sqrt{1 + \frac{\nu^2}{16}} \approx \nu \), so the meaning of Lagrange multiplier is elucidated.

Taking also into account that in thermal equilibrium

\[
n_k \equiv \langle a_k^+a_k \rangle = \langle \beta_k^+\beta_k \rangle = \frac{1}{\exp(\omega_{\nu k}/T) - 1}
\]

we get from (6) the equation for \( \nu \)

\[
0 = 1 - \frac{2}{N} \sum_k \frac{A_k}{\omega_{\nu k}} (1 + 2n_k).
\]
The spin-wave velocity does not vanish at critical point \( c = \sqrt{2(1 - 2\alpha)} \approx 0.7 \). Therefore for \( \nu, k \ll 1 \) the spectrum is of the form \( \omega_{\nu k} = \sqrt{\nu^2 + c^2k^2} \) and equation (10) can be rewritten as

\[
m + \frac{2}{N} \sum_k \left[ \frac{1}{ck} - \frac{1}{\sqrt{\nu^2 + c^2k^2}} \coth \left( \frac{\sqrt{\nu^2 + c^2k^2}}{2T} \right) \right] = 0, \quad (11)
\]

where \( m < 0 \) is given by Eq.(4). We would like to stress that the condition \( c \neq 0 \) is not crucial for the validity of the method. Moreover for \( t - J \) model, which we are mainly interested in, the speed vanishes, or even \( c^2 < 0 \). Nevertheless the method works for \( J_1 - J_2 \) model \( c > 0 \) and we will use the simplification \( \omega_{\nu k} \rightarrow \sqrt{\nu^2 + c^2k^2} \), but from comparison with exact numerical solution of equation (10) we know that it is valid only for very small \( \nu \) and \( T: \nu, T \ll \frac{1}{10} \). Solution of equation (11) at zero temperature is straightforward

\[
\nu_0 = \pi|m|c^2 = \pi Bc^2(\alpha - \alpha_c) \approx 3.7(\alpha - \alpha_c). \quad (12)
\]

We took into account that near critical point \( m = B(\alpha_c - \alpha) \) with slope \( B \approx 2.4 \) according to LSWT and most recent exact finite lattice diagonalizations and series expansions. Index 0 in \( \nu_0 \) indicates that it is a gap at zero temperature. Equation (11) can be also written as

\[
2T \ln \left( 2 \sinh \frac{\nu}{2T} \right) = -\pi mc^2 = \nu_0. \quad (13)
\]

Similar equation has been obtained in the Ref. for the non-linear \( \sigma \)-model in the limit when the number of components of the order parameter \( N = \infty \). Solution of equation (13) at low and high temperature looks like

\[
\nu \approx \nu_0(1 + e^{-\nu_0/T}), \quad T \ll \nu_0, \quad (14)
\]
\[
\nu \approx \Theta T + \frac{1}{\sqrt{5}}\nu_0, \quad T \gg \nu_0,
\]

where \( \Theta = 2 \ln \frac{1 + \sqrt{5}}{2} = 0.9624 \). We follow the notations of Ref.

Now we can proceed to the calculation of spin structure factor in spin-liquid state. It is quite similar to the Takahashi’s calculation for Heisenberg model at nonzero temperature. Using Dyson-Maleev representation, constraint (3) \( \langle a_l^\dagger(t)a_l(t) \rangle = \langle b_m^\dagger(t)b_m(t) \rangle = \frac{1}{2} \), and mean field procedure for averaging of the quartic terms \( \langle a^L a b^L b \rangle \rightarrow \langle a^L a \rangle (b^L b) + \langle a^L b^L \rangle \langle ab \rangle \) one finds
\[ \langle S_m(t)S_l(0) \rangle = -\langle b_m^\dagger(t)a_l^\dagger(0) \rangle \langle b_m(t)a_l(0) \rangle, \] (15)
\[ \langle S_{l'}(t)S_l(0) \rangle = \langle a_{l'}^\dagger(t)a_l(0) \rangle \langle a_{l'}(t)a_l^\dagger(0) \rangle, \]

where \(l, l' \in \text{ up sublattice} \), and \(m \in \text{ down sublattice} \). Further calculation gives

\[ \langle S_i(t)S_j(0) \rangle = f^2(t, r_{ij}) - \frac{1}{4} \delta^2(t, r_{ij}), \quad i, j \in \text{ same sublattice}, \] (16)
\[ \langle S_i(t)S_j(0) \rangle = -g^2(t, r_{ij}), \quad i, j \in \text{ different sublattices}. \]

where

\[ f(t, r) = \frac{2}{N} \sum_k e^{ikr} A_k \frac{A_{k+q}}{\omega_k} [e^{-i\omega_k t}(1+n_k) + e^{i\omega_k t}n_k], \]
\[ \delta(t, r) = \frac{2}{N} \sum_k e^{ikr} \left[ e^{-i\omega_k t}(1+n_k) - e^{i\omega_k t}n_k \right], \] (17)
\[ g(t, r) = -\frac{2}{N} \sum_k e^{ikr} \frac{\gamma_k}{\omega_k} \left[ e^{-i\omega_k t}(1+n_k) + e^{i\omega_k t}n_k \right], \]

\( \delta \) from (15) and (17) one can easily find explicitly spin-spin correlator at large separation \( r = (m, n), r = \sqrt{m^2 + n^2} \)

\[ \langle S(t, r)S(t, 0) \rangle = (-1)^{m+n} \exp \left( -\frac{2\nu}{c} r \right) \times \begin{cases} 1/(\pi c r)^2, & 1 \ll r \ll c\nu/T^2; \\ 2T/(\pi c^3 \nu r), & r \gg c\nu/T^2. \end{cases} \] (18)

So the magnetic correlation length equals \( \xi_M = 0.5c/\nu \).

Using (16) and (17) we can also find static and dynamic spin structure factors

\[ S_M(q) = \sum_r e^{iqr} \langle S(t, r) \cdot S(t, 0) \rangle = \] (19)
\[ = \frac{2}{N} \sum_k \left[ -\frac{1}{4} + \frac{A_k A_{k+q} - \gamma_k \gamma_{k+q}}{\omega_k \omega_{k+q}} (1 + 2n_k)(1 + 2n_{k+q}) \right], \]

\[ S_M(\omega, q) = \int \frac{dt}{2\pi} e^{i\omega t} \sum_r e^{iqr} \langle S(t, r) \cdot S(0, 0) \rangle = \] (20)
\[ = \frac{2}{N} \sum_k \left\{ \left[ -\frac{1}{4} + \frac{A_k A_{k+q} - \gamma_k \gamma_{k+q}}{\omega_k \omega_{k+q}} \right] \times \right. \]
\[ \times \left[ (1 + n_k)(1 + n_{k+q})\delta(\omega - \omega_{k+q} - \omega_k + \omega_{k+q}) + n_k n_{k+q}\delta(\omega + \omega_{k+q} - \omega_k + \omega_{k+q}) \right] + \]
\[ + \left[ \frac{1}{4} + \frac{A_k A_{k+q} - \gamma_k \gamma_{k+q}}{\omega_k \omega_{k+q}} \right] 2n_k (1 + n_{k+q})\delta(\omega + \omega_k - \omega_{k+q}) \right\}. \]

We would like to stress that the dynamic structure factor \( S_M(\omega, q) \) at \( T = 0 \) contains only two-quasiparticle intermediate states. It is similar to the situation in one dimensional...
Heisenberg chain where elementary excitation is spinon. We will discuss this point in conclusion. Now let us calculate the structure factors $S_M(q)$ and $S_M(\omega, q)$ for $q = 0$ and $q = Q \equiv (\pm \pi, \pm \pi)$. Taking into account Eq.(8) we find from (20)

$$S_M(\omega, 0) = \delta(\omega) \frac{2}{N} \sum_k n_k(1 + n_k) = \frac{1}{\pi c^2} \delta(\omega) \times \left\{ \begin{array}{ll} \nu_0 T \exp(-\nu_0/T), & T \ll \nu_0; \\ 1.04 T^2, & 1 \gg T \gg \nu_0. \end{array} \right.$$ (21)

One can easily obtain static factor $S_M(0)$ integrating (21) by $\omega$. The calculation at $q = Q$ is also very simple. It gives

$$S_M(\omega, Q) \approx \frac{2}{\pi c^2} \ln \frac{1}{\nu},$$

with function $F$ defined as

$$F\left(\frac{\nu}{T}\right) = \int_{\nu/T}^{\infty} \frac{dx}{x \sinh^2(x/2)} = \left\{ \begin{array}{ll} 4T/\nu_0 \exp(-\nu_0/T), & T \ll \nu_0; \\ 1.67, & 1 \gg T \gg \nu_0. \end{array} \right.$$ (23)

The $\omega$-distribution at $q = 0$ and $q = Q$ contains infinitely sharp $\delta(\omega)$-function and step function $\theta(\pm \omega - 2\nu)$. However at $q \neq 0, Q$ the $\omega$-distribution is smooth.

Average energy $E = \langle H \rangle$ can be easily calculated using Eqs. (1) and (17)

$$E/N = 2[-g^2(0, r_1) + \alpha f^2(0, r_2)],$$ (24)

where $r_1 = (1, 0)$ and $r_2 = (1, 1)$. As an example, at Fig.1, we present the plot of energy as a function of temperature at $\alpha \approx \alpha_c \approx 0.4$. The value of $\alpha - \alpha_c$ is chosen in such a way that the gap at zero temperature equals $\nu_0 = 0.05$. In this case our calculation gives for energy per site at zero temperature the value $E(T = 0)/N = -0.513$. This is slightly above the value $E/N \approx -0.520$ found in Ref.12 by finite lattice diagonalization and in Ref.13 by series expansion.

**Discussion**

In the present work using modified spin-wave theory we calculated static and dynamic spin structure factors in spin-liquid state of $J_1$-$J_2$ model. We believe that similar technique can be applied to the $t$-$J$ model describing copper oxide superconductors. Let us point out the strong and weak sides of the modified spin-wave theory. It gives a very simple description of the spin liquid state, and this is definitely a strong side. However the description
explicitly violates the rotational symmetry, and this is drawback of the approach. We would like to stress that violation of exact symmetry quite often appears in approximate description of a strongly interacting system. For example Hartree-Fock method in atoms violates gauge-invariance of the electromagnetic transition amplitudes, and unrestricted Hartree-Fock method in atoms and nuclei violates rotational symmetry. Usually the symmetry is approximately restored in the final answer despite the violation on the way. We hope that the situation is similar in Takahashi’s modified spin-wave theory.

In our approach the dynamic structure factor $S_M(\omega, \mathbf{q})$ contains only two-quasiparticle intermediate states. It means that there is no simple vector excitation which would give $C_q \delta(\omega - \Omega_q)$ contribution to the dynamic structure factor. In this sense the picture is similar to that in one dimensional Heisenberg chain where elementary excitation is spinon. We stress that the number of dynamic degrees of freedom is also similar to the $S = 1/2$ case because only doublets $S_z = \pm 1$ are involved in the dynamics. However it would be probably wrong to say that the spin of elementary excitation $S = 1/2$, because still $S_z = \pm 1$. More close analogy to the present situation is a gauge vector field in the axial gauge. In this sense the violation of the rotational symmetry is similar to the fixing of gauge. There are two separate questions in this situation

1) Is the structure of spectrum in vector channel without narrow $\delta$-functions valid for $J_1 - J_2$ model, or it is just a byproduct of the approximation?

2) Is this technique applicable to $t - J$ model?

The answer to first question is not clear. I hope that further numerical simulations can elucidate this question. The answer to second question is more clear. In $t - J$ model narrow structures in $\omega$-distribution are much less important due to the very strong damping of spin-waves. In this situation the most important point is to avoid double counting of low-energy spin degrees of freedom. Takahashi’s modified spin-wave theory definitely provides a correct count of these degrees of freedom. Therefore in my opinion this approach is reasonably justified for $t - J$ model.

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Figure caption, Fig.1
Energy per site at $J_2/J_1 \equiv \alpha \approx \alpha_c \approx 0.4$. The value of $\alpha - \alpha_c$ is chosen in such a way that the gap at zero temperature equals $\nu_0 = 0.05$. 

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Fig. 1