Spin Fluctuations in an Itinerant Heisenberg System

--- Naive RPA Treatment ---

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The dynamical spin fluctuations in a two-dimensional square lattice in its paramagnetic phase are examined within the framework of Random Phase Approximation (RPA). Itinerant carriers with spin interact with each other via an antiferromagnetic Heisenberg interaction.

Then there appear three fundamental scattering processes; a) scattering with spin-flip, b) scattering between parallel spins and c) scattering between antiparallel spins. To examine how these scattering processes affect the dynamical spin fluctuations, we pick up carefully all possible combination of RPA diagrams in a consistent manner and take the spin rotational symmetry into account. Then it becomes clear that we have to take up a sequence of the irreducible single loop which in itself is modified due to the particle-hole ladder type vertex correction. We set up the Bethe-Salpeter equation for the vertex correction and show that this can be solved in a closed form due to separable nature of the antiferromagnetic interaction. We evaluated numerically the effect of the vertex correction and found that the correction is negligibly small.

Therefore we propose that in an itinerant Heisenberg system, including the $t$-$J$ model as its derivative, the simplified RPA, where the irreducible single loop is unrenormalized, works very well. This conclusion strongly supports the simplified treatment which is widely used in High-$T_c$ problem. Moreover the present formalism enables us to proceed further microscopic calculations on the magnetic properties in the current High-$T_c$ problem.

§ 1. Introduction

The purpose here is to explore the dynamical spin fluctuations in a paramagnetic state of a two-dimensional square lattice electron system in terms of the itinerant Heisenberg model within the framework of the naive random phase approximation (RPA). In this model the free motion of the itinerant carrier, electron or hole with spin, is modified by scattering processes via an antiferromagnetic Heisenberg interaction.*> Then there appear three fundamental scattering processes; a) scattering between carriers with parallel spins, b) scattering between carriers with antiparallel spins and c) scattering between carriers with spin-flip. These processes affect each other and appear in the renormalized spin fluctuating processes in all possible ways. So far, however, little attention has been given to the naive treatment of this problem.

A similar problem has been studied, in connection with current High-$T_c$ problems, in terms of the $t$-$J$ model which can be regarded as the derivative of the present model. In the $t$-$J$ model where the effect of non-double occupancy condition due to the strong correlation is incorporated and consequently the magnetic processes

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*1 Although the present work was motivated by the usual treatment of the $t$-$J$ model. We thought it better to avoid calling the present model "$t$-$J$" model, since the present model neglects the non-double occupancy condition due to the strong correlation. Our standpoint is similar to Ref. 1) in which the spinon loop is regarded as an ordinary hole and the effect of the non-double occupancy condition is not taken into account.
are governed by the spinon's degree of freedom. Then there exist scattering processes between the free spinons via an antiferromagnetic Heisenberg interaction. In this sense the same problem occurs concerning the spin fluctuating processes as in the case of the present model.

Indeed, within the framework of a mean field picture of the $t$-$J$ model, the spin fluctuations have been intensively studied by Tanamoto, Kohno and Fukuyama (T.K.F)\(^4\) where the dynamical spin-spin correlation function, $\chi_{t.K.F}(q) = \chi_{\text{spinon}}[1 + J_q \chi_{\text{spinon}}(q)]^{-1}$, plays a central role. Here $\chi_{\text{spinon}}(q)$ is the irreducible single loop of a free spinon and $J_q=2J(\cos q_x a + \cos q_y a)$ is an antiferromagnetic Heisenberg interaction in a momentum space.

However the form of the correlation function $\chi_{t.K.F}(q)$ includes only one single scattering channel and, from a diagrammatic point of view, consists of a sequence of the irreducible single loop which is unrenormalized. Moreover this form of the susceptibility does not contain the spin indices as $\chi^{a\theta}$. The simple form similar to $\chi_{t.K.F}(q)$ has been widely used in the context of the High-$T_c$ problem.

The present work is motivated by a naive question; "when we consider all the possible scattering processes within RPA, what kind of the scattering processes contributes to the dynamical spin fluctuations and consequently the simplified structure of $\chi_{t.K.F}(q)$ should be modified or not?".

In the present paper we put aside the effect of the strong correlation and concentrate only on the structure of possible scattering processes which produce the dynamical spin fluctuations within the framework of RPA.

Generally the naive RPA corresponds to picking up the so-called ring diagram which is a sequence of the irreducible single loop. Then the irreducible single loop naturally includes the particle-hole exchange scattering processes as the lowest order vertex correction.\(^5\) This treatment fully reproduces an equation of motion method.

However, in specific problems, how to choose the proper diagrams is model-dependent. For example, in the paramagnon theory based on the Hubbard model,\(^6\) the transverse spin fluctuations consist of one renormalized single loop incorporating the particle-hole exchange scattering and the longitudinal spin fluctuations consist of a sequence of the unrenormalized single loop. This situation comes from the short-range nature of the Hubbard interaction.

As another example, in the Coulomb gas problem, the paramagnetic susceptibility contains a single loop modified due to the exchange scattering.\(^7\)

It will be shown that in the present case both of the transverse and longitudinal spin fluctuations consist of a sequence of the irreducible single loop modified due to the particle-hole exchange scattering processes.

Since we consider a paramagnetic phase, it is also important to pay our attention to the spin rotational symmetry of the theory.

In § 2 we present the model. In § 3 we review the general formalism for the spin fluctuation and construct the naive RPA. Then we show that the Bethe-Salpeter equation for the vertex correction can be solved in a closed form due to the separable form of the exchange interaction. We obtain the expression for the spin fluctuations in a closed form, which is different from the form where the irreducible single loop is unrenormalized. In § 4 we discuss the spin rotational symmetry in the present treat-
ment. Finally in § 5 we present the numerical results and discuss quantitative difference between the present treatment and the simplified one.

As a result we propose that the simplified treatment for the spin fluctuations of a square lattice which has been widely used works fairly well in the present framework.

§ 2. Model

We start from the itinerant Heisenberg model,
\[ \mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\text{int}}, \]  
Here
\[ \mathcal{H}_0 = \sum_k \xi_k \sigma_k c_{k, \sigma} c_{k, \sigma}, \]  
is the kinetic Hamiltonian where \( c_{k, \sigma}(c_{k, \sigma}^\dagger) \) is a creation (annihilation) operator of an itinerant carrier with the momentum \( k \) and the spin projection \( \sigma \).

Further
\[ \mathcal{H}_{\text{int}} = 2 \sum_q J_q S_q \cdot S_{-q} \]  
represents the antiferromagnetic Heisenberg interaction between the nearest neighbor spins where
\[ J_q = 2J (\cos q_x a + \cos q_y a) \]  
denotes the momentum dependent spin-spin interaction. The spin fluctuation operator with momentum \( q \) is defined by
\[ S_q = \frac{1}{2} \sum_{k, a, \sigma} c_{k+q, \sigma} \sigma_{ab} c_{k, \sigma}, \]  
where \( \sigma \) denotes the usual Pauli matrixes and we set \( \hbar = 1 \).

Bearing the high-\( T_c \) problem in mind, we include not only the nearest-neighbor hopping, \( t \), but also the next-nearest-neighbor hopping, \( t' \), and then we have
\[ \xi_k = \epsilon_k - \mu = -2t (\cos k_x a + \cos k_y a - \cos k_x a \cos k_y a) - \mu, \]  
where \( a \) is the lattice constant and \( \alpha = -2t'/t \). Here \( 0 \leq \alpha \leq 1 \) is a parameter which characterizes the geometry of the Fermi contour. Furthermore \( \mu \) denotes the chemical potential.

The dispersion (6) produces the density of states (DOS),
\[ \mathcal{D}(\epsilon) = \frac{1}{2\pi^2 t} \frac{1}{\sqrt{1 + \alpha \epsilon / 2t}} K\left[ \frac{1 - (\alpha / 2 - \epsilon / 4t)^2}{1 + \alpha \epsilon / 2t} \right], \]  
where \( K(x) \) denotes the elliptic integral of the first kind. The derivation of (7) will be presented in Appendix A. The carrier density in the electron picture is determined by
where \( f(\varepsilon) = (e^{(\varepsilon - \mu)/T} + 1)^{-1} \). \( N_c \) and \( N \) represent the number of carrier and lattice sites respectively. Then \( n=1 \) corresponds to the half filling.

This type of DOS shows the logarithmic van-Hove singularity at \( \varepsilon = -2a \) for \( 0 \leq a < 1 \) and the square root singularity for \( a=1 \), which originates from the saddle points located at the four points \((\pm \pi, 0), (0, \pm \pi)\) in the first Brillouin zone. The case \( a=0 \) which corresponds to LSCO compounds leads to the perfect nesting. As the parameter \( a \) becomes nearer to \( a=1 \), the curvature of the convex along the \( \Gamma - Y \) line near the saddle point becomes flatter. Then \( a=1 \) corresponds to the perfectly flat curvature of the convex. This type of the saddle point is called “the extended saddle point” which produces the power singularity in DOS. In the case of YBCO, \( a=0.9 \) corresponds to the real data, which is very near the case of the extended saddle point.

In Fig. 1, we show the energy contour, corresponding DOS, and the structure of the saddle point near the \( Y \) point \((0, \pi)\) for typical values of \( a \).

(a) \( a=0 \)

(b) \( a=0.5 \)

(c) \( a=1 \)

Fig. 1. From left to right, the energy contour, the structure of the saddle point near the \( Y \)-point, and corresponding DOS for (a) \( a=0 \), (b) \( a=0.5 \), (c) \( a=1 \).

The thick line in each figure represents the Fermi contour at the half filling and the broken line corresponds to the energy level at which the DOS becomes divergent.
§ 3. Transverse spin fluctuation

3.1. General formalism

We consider the magnetic response in a square lattice electron system within the framework of the present model. Whole information on spin dynamics is contained in the dynamical wave number dependent magnetic susceptibility,

\[ \chi_{\alpha\beta}(q) = \int_0^\beta d\tau e^{i\omega_\tau} \langle T_\tau [S_\alpha^\mu(q,\tau)S_\beta^\nu(0)] \rangle = \frac{1}{4} \sum_{\mu\nu\lambda\rho} \sigma^\mu_{\alpha\beta} \Gamma^{\mu\nu;\lambda\rho}(q) \sigma^\nu_{\lambda\rho}, \]  

(9)

where

\[ \Gamma^{\mu\nu;\lambda\rho}(q) = \int_0^\beta d\tau e^{i\omega_\tau} \frac{1}{N} \sum_{\mathbf{k},\mathbf{k}'} \langle T_\tau [c_{\mathbf{k},\alpha}(\tau)c_{\mathbf{k}+\mathbf{q},\beta}(\tau)c_{\mathbf{k}',\beta}(0)c_{\mathbf{k}',\alpha}(0)] \rangle \]  

(10)

denotes the spin dependent polarization function where \( \alpha, \beta = +, -, z \) and \( \mu, \nu, \lambda, \rho = \uparrow, \downarrow \) and \( \omega_n = 2\pi T n \) is a bosonic Matsubara frequency. Throughout the present paper \( q \) denotes a four vector \( q = (q, i\omega_n) \).

Furthermore

\[ c_{\mathbf{k},\alpha}(\tau) = \exp(\tau\mathcal{H})c_{\mathbf{k},\alpha}(0)\exp(-\tau\mathcal{H}) \]  

(11)

represents imaginary time dependent creation operator where we set \( \hbar=1 \) and \( k_B=1.\)

\[ \langle \cdots \rangle = \text{Tr}(e^{-\mathcal{H}/T}\cdots) / \text{Tr}(e^{-\mathcal{H}/T}) \]  

denotes the thermal average under the full Hamiltonian.

By noting

\[ \sigma^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \sigma^- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \]  

(12)

the longitudinal and transverse spin susceptibility can be obtained as

\[ \chi^{\sigma\sigma'}(q) = \frac{\Gamma^{\sigma\sigma';\sigma\sigma'}(q)}{4}, \]  

(13)

\[ \chi^{\sigma\sigma'}(q) = \frac{\Gamma^{\sigma\sigma';\sigma\sigma'}(q)}{4}, \]  

(14)

\[ \chi^{zz}(q) = \frac{1}{4} \left[ \Gamma^{\uparrow\downarrow;\downarrow\downarrow}(q) + \Gamma^{\downarrow\uparrow;\downarrow\downarrow}(q) - \Gamma^{\uparrow\downarrow;\uparrow\uparrow}(q) - \Gamma^{\downarrow\uparrow;\uparrow\uparrow}(q) \right] \]  

\[ = \frac{1}{2} [\chi^{zz}(q) - \chi^{zz}(q)], \]  

(15)

where \( \chi^{\sigma,\sigma}(q) \equiv \Gamma^{\sigma,\sigma;\sigma,\sigma}(q). \)

Throughout this paper we consider the paramagnetic phase and therefore the dynamic spin susceptibilities must satisfy the rotational symmetry relation in spin space,

\[ 2\chi^{zz} = \chi^{zz}. \]  

(16)

The dynamical susceptibility of a free carrier system can be given by

\[ \chi_{\text{free}}(q) = -\frac{T}{N} \sum_{\mathbf{k}} \mathcal{G}_0(k+q) \mathcal{G}_0(k). \]  

(17)
Here

\[ G_0(k) = \frac{1}{i\varepsilon_n - \xi_k} \]  

is a thermal Green's function of a free carrier where \( \varepsilon_n = (2n+1)\pi T \) is a fermionic Matsubara frequency. Furthermore from now on the summation over the four momentum means

\[ \frac{1}{N}\sum_{k'=\pm \pi} \int \frac{dk_x da}{2\pi} \int \frac{dk_y a}{2\pi} . \]

By taking the Matsubara summation we obtain

\[ \chi_{\text{tree}}(q) = \frac{1}{2N} \sum_{n=\pm \pi} \Lambda_{k,q}(T)(\xi_{k+q} - \xi_k) \]

where \( \varepsilon_n \) is a fermionic Matsubara frequency and

\[ \Lambda_{k,q}(T) = \tanh\left(\frac{\xi_{k+q}}{2T}\right) - \tanh\left(\frac{\xi_k}{2T}\right) \]

denotes the thermal extinction factor.

3.2. RPA

Now we consider the dynamical susceptibility which is modified due to \( J_q \). We calculate the dynamical susceptibility within the framework of RPA.

The fundamental processes induced by \( J_q \) are produced through

\[ S_q \cdot S_q = \frac{1}{2}(S_q^+ S_q^- + S_q^- S_q^+) + S_q^z S_q^z . \]  

By rewriting this expression in a second quantized form, we get three fundamental vertexes for the scattering processes between propagating carriers with spin.

The first term of (22) produces the scattering process with spin flip (type-a). The second term of (22) produces two fundamental processes; scattering processes between parallel spins (type-b) and anti-parallel spins (type-c). These processes are shown in the diagrams below.

![Fig. 2. The fundamental processes induced by \( J_q \). (a) The scattering process with spin flip (type-a), (b) the scattering processes between parallel spins (type-b) and (c) the scattering processes between anti-parallel spins (type-c). Here the straight line and the wavy line represent respectively the Green's function of an itinerant carrier and the antiferromagnetic interaction.](https://academic.oup.com/ptp/article-abstract/94/4/543/1934694)
Fig. 2.

Here we first consider the transverse spin fluctuation. The problem of the rotational symmetry in spin space will be taken up in the next section. The string type summation as shown in Fig. 3 produces the form,

$$\chi^+(q) = \frac{\tilde{\chi}_d(q)}{1 + J_q \tilde{\chi}_d(q)} ,$$

(23)

where $$\tilde{\chi}_d(q)$$ is the irreducible single fermion loop which cannot be cut into two pieces by removing an interaction line and which can be written in the form

$$\tilde{\chi}_d(q) = -\sum_{k} G(k) \Gamma(k, k+q) G(k+q) ,$$

(24)

where $$\Gamma(k, k+q)$$ is the triangle vertex inserted in a single loop.

Furthermore $$G(k)$$ is a dressed Green's function determined through the Dyson equation

$$G(k)^{-1} = G_0(k)^{-1} - \Sigma(k) ,$$

(25)

where $$\Sigma(k)$$ denotes the self-energy part.

We can see that in Fig. 3 only the type-a processes can contribute to the ring diagram for the transverse susceptibility within RPA. Here we should note that, even within the framework of RPA, the type-c processes can produce the exchange scattering between an electron and a hole inside a single loop. Consequently we have to include the particle-hole ladder process in the vertex $$\Gamma(k+q, k)$$. These types of diagrams are characteristic to the present model while in the Hubbard model the string type summation cannot appear in the transverse fluctuation.

Therefore we have to include the string type summation and the ladder type summation simultaneously to get the naive result within RPA.

To treat the compatibility of the self-energy and the vertex correction, it is sufficient to consider only the Fock term to ensure the Ward-Takahashi identity. This procedure corresponds to the simplest case of Baym and Kadanoff's conserving approximation. Then $$\Sigma(k)$$ can simply be written by

$$\Sigma(k) = -\frac{3}{2} \frac{T}{N} \sum_{k'} J(k-k') G(k') ,$$

(26)

which can be reduced to the form
\[
\Sigma(k) = -\frac{3}{2} J X(T) (\cos k_x a + \cos k_y a),
\]

where

\[
X(T) = \sum_{k'} \frac{\cos k_x a + \cos k_y a}{i \varepsilon - \varepsilon_k + \mu - \Sigma(k')}
= -\frac{1}{2} \int \frac{dk'}{(2 \pi)^2} \left[ (\cos k_x a + \cos k_y a) \tanh \left( \frac{(\varepsilon_k - \mu + \Sigma(k'))}{2T} \right) \right].
\]

Here we have performed the Matsubara summation and taken into account the $D_4$ symmetry of the system. We can obtain the self-energy by solving (28) in a self-consistent manner. $X(T)$ depends weakly on the temperature $T$ and turns out to have a positive value. It follows from this situation that the Fock term, as usual, enhances the effective mass. Now the energy dispersion of a single carrier is slightly modified from (6) to the form

\[
\varepsilon_k = -2 \left[ t - \frac{3}{4} J X(T) \right] (\cos k_x a + \cos k_y a) + 2at \cos k_x a \cos k_y a.
\]

The triangle vertex $\Gamma(k, k+q)$ satisfies the Bethe-Salpeter equation for a particle-hole channel as shown in Fig. 4,

\[
\Gamma(k+q, k) = 1 + \frac{T}{N} \sum_{k'} \Gamma(k, k'+q) \mathcal{G}(k', k'+q).
\]

We can solve (30) in the closed form as

\[
\Gamma(k, k+q) = 1 + JC(q) (\cos k_x a + \cos k_y a) + JS(q) (\sin k_x a + \sin k_y a),
\]

where

\[
C(q) = -\frac{1}{2} \chi_1(q) \left[ 1 + \frac{1}{2} J x_3(q) \right] + J \left[ \frac{1}{2} \chi_3(q) \right] \left[ \frac{1}{2} \chi_3(q) \right] \left[ 1 + \frac{1}{2} J x_3(q) \right] - \left[ \frac{1}{2} J x_3(q) \right]^2,
\]

\[
S(q) = -\frac{1}{2} \chi_2(q) \left[ 1 + \frac{1}{2} J x_3(q) \right] + J \left[ \frac{1}{2} \chi_3(q) \right] \left[ \frac{1}{2} \chi_3(q) \right] \left[ 1 + \frac{1}{2} J x_3(q) \right] - \left[ \frac{1}{2} J x_3(q) \right]^2.
\]

We may leave the details of the derivation of this formula to Appendix B. Here $\chi_1(q), \ldots, \chi_3(q)$ are defined by

![Fig. 4. The Bethe-Salpeter equation for the triangle vertex.](https://academic.oup.com/ptp/article-abstract/94/4/543/1934694)
\[ \chi_1(q) = -\frac{T}{N} \sum_k (\cos k_x a + \cos k_y a) \mathcal{G}(k) \mathcal{G}(k + q), \]
\[ \chi_2(q) = -\frac{T}{N} \sum_k (\sin k_x a + \sin k_y a) \mathcal{G}(k) \mathcal{G}(k + q), \]
\[ \chi_3(q) = -\frac{T}{N} \sum_k (\cos k_x a + \cos k_y a)^2 \mathcal{G}(k) \mathcal{G}(k + q), \]
\[ \chi_4(q) = -\frac{T}{N} \sum_k (\cos k_x a + \cos k_y a)(\sin k_x a + \sin k_y a) \mathcal{G}(k) \mathcal{G}(k + q), \]
\[ \chi_5(q) = -\frac{T}{N} \sum_k (\sin k_x a + \sin k_y a)^2 \mathcal{G}(k) \mathcal{G}(k + q). \] (34)

Therefore we can obtain the result
\[ \tilde{\chi}_0(q) = \chi_0(q) + J \mathcal{C}(q) \chi_1(q) + J \mathcal{S}(q) \chi_2(q), \] (35)
where
\[ \chi_0(q) = -\frac{T}{N} \sum_k \mathcal{G}(k + q) \mathcal{G}(k). \] (36)

We note here that for the commensurate spin-fluctuation with \( q = Q = (\pi/a, \pi/a) \), \( \chi_2 = \chi_4 = 0 \) due to the \( D_4 \) symmetry of the square lattice, and then consequently \( S(q) = 0 \).

Directly from the above expressions (34), we can expect the correction terms in (35) are negligibly small. Therefore we expect in our scheme the vertex correction coming from the exchange scattering processes can be neglected. We will confirm this situation numerically in § 5.

\section*{§ 4. Rotational symmetry in spin space}

When we consider the spin fluctuations in a paramagnetic phase, to ensure the consistency of the theory, the dynamical spin susceptibilities have to satisfy the symmetry relation (16) in spin space. Here we prove the rotational symmetry of the theory in the present scheme. Our concern is to show the relation (16),

\[ 2\chi^{\alpha z} = \chi^{+-}. \] (37)

First we show that the spin rotational symmetry is satisfied in a single loop level. Namely,
\[ 2\tilde{\chi}_0^{\alpha z} = \tilde{\chi}_0^{+-} = \tilde{\chi}_0, \] (38)
where \( \tilde{\chi}_0 \) was given by (24). Then we have to include various intermediate spin configurations between a given initial and final spin configuration. We consider a single loop of the \( n \)-th order term, \( \tilde{\chi}_0^{\alpha z(n)} \), with respect to \( J_q \). There can appear the type-a and the type-b vertexes in all the possible manners, as is shown in Fig. 5. We have to take summation with respect to all the possible intermediate spin configurations and pick up a lot of diagrams. Fortunately we can obtain the relation between \( \tilde{\chi}_0^{\alpha z(n)}, \tilde{\chi}_0^{\alpha z(n)} \) and \( \tilde{\chi}_0^{+-(n)} \) by order-by-order consideration. The results are as...
When \( n=2m \),
\[
\tilde{\chi}^0(2m) = \tilde{\chi}^0(2m) \sum_{k=0}^{m} \omega^{2k} C_{2k},
\]
(39)
\[
\tilde{\chi}^1(2m) = \tilde{\chi}^1(2m) \sum_{k=0}^{m-1} \omega^{2k+1} C_{2k+1},
\]
(40)

where \( \omega = k! / [(k-1)!1!] \) is a binomial coefficient. Here, for example, we derive the formula (39). In this case \( n=2m \) and therefore the single loop can include the even number of the type-a processes. Then all the other vertices are the type-b vertexes. We consider the case when there are \( 2k \) type-a processes and \( 2m-2k \) type-b vertexes. Since the type-a vertex gives the factor \( J_q \) and the type-b vertex gives the factor \( J_q/2 \), if we replace all the type-a vertexes simply by the type-b vertexes, there appears the factor \( 2^{2k} \). On the other hand, there are \( 2m C_{2k} \) ways of locating the type-a vertexes inside a loop. As a result the corresponding expression has a factor \( 2^{2k} 2m C_{2k} \) and therefore we obtain (39). Here \( \tilde{\chi}^0(2m) \) is a single loop corresponding to the transverse fluctuation of the same order with respect to \( J_q \). Now by noting that
\[
\sum_{k=0}^{m} \omega^{2k} C_{2k} = \sum_{k=0}^{m-1} \omega^{2k+1} C_{2k+1} = (1-2)^{2m} = 1
\]
and
\[
\sum_{k=0}^{m} \omega^{2k} C_{2k} = \sum_{k=0}^{m-1} \omega^{2k+1} C_{2k+1} = (1-2)^{2m+1} = -1,
\]
we can see that for arbitrary order,
\[
\tilde{\chi}_0^{1\dagger} - \tilde{\chi}_0^{1\dagger} = \tilde{\chi}_0^{1\dagger} = \tilde{\chi}_0^{1\dagger}
\]
(43)
and consequently
\[
\tilde{\chi}_0^{1\dagger} - \tilde{\chi}_0^{1\dagger} = \tilde{\chi}_0^{1\dagger} = \tilde{\chi}_0.
\]
(44)
Therefore we obtain the result (38) which would be expected.

Next we consider the string type series for the longitudinal spin fluctuations. In the string processes, in this case, there can appear the type-b and type-c vertexes. Then the \( m \)-th order term with respect to \( J_q \) can be expressed by
\[
C_m ^{\sigma_\tau} = \left(-\frac{J_q}{2}\right)^m \sum_{\sigma_1,\sigma_2,\ldots,\sigma_m} (-1)^{\sigma_1 - \sigma_2} (-1)^{\sigma_3 - \sigma_4} \cdots (-1)^{\sigma_{2m-1} - \sigma_{2m}} \tilde{\chi}_0^{\sigma_1} \tilde{\chi}_0^{\sigma_2} \cdots \tilde{\chi}_0^{\sigma_m \sigma_\tau},
\]
(45)
This process is shown in Fig. 6.

By using (15) we can obtain the longitudinal spin susceptibility as

$$\chi^{zz} = \frac{1}{2} \sum_{m=0}^{\infty} (C_m^{zz} - C_m^{zz}).$$

First we take the summation over $\sigma_1$ and $\sigma_2$ in (45) to get

$$C_m^{zz} = (-\frac{J_0}{2})^m \sum_{\sigma_1,..,\sigma_{2m}} (-1)^{\sigma_1-\sigma_2} ... (-1)^{\sigma_{2m-1}-\sigma_{2m}} \times (\tilde{X}_0^{\sigma_1} - \tilde{X}_0^{-\sigma_1}) (\tilde{X}_0^{\sigma_2} - \tilde{X}_0^{-\sigma_2}) \tilde{X}_0^{\sigma_3} ... \tilde{X}_0^{\sigma_{2m}}. \tag{46}$$

Here we used the relation (44).

By repeating the summation procedures over the pair $(\sigma_{2i-1}, \sigma_{2i})$, we get the result for the $i$-th procedure as

$$C_m^{zz} = (-\frac{J_0}{2})^m \sum_{\sigma_{2i+1},..,\sigma_{2i+2m}} (-1)^{\sigma_{2i+1}-\sigma_{2i+2}} ... (-1)^{\sigma_{2m-1}-\sigma_{2m}} \times (\tilde{X}_0^{\sigma_{2i+1}} - \tilde{X}_0^{-\sigma_{2i+1}}) ... \tilde{X}_0^{\sigma_{2m}}. \tag{47}$$

Finally we obtain the relation

$$C_m^{zz} = \frac{1}{2} (-J_0)^m \tilde{X}_0^{m} (\tilde{X}_0^{\sigma^2} - \tilde{X}_0^{-\sigma^2}). \tag{48}$$

Therefore we get

$$\chi^{zz} = \frac{1}{2} \sum_{m=0}^{\infty} (C_m^{zz} - C_m^{zz}) = \frac{1}{2} \sum_{m=0}^{\infty} (-J_0)^m \tilde{X}_0^{m+1} = \frac{1}{2} \frac{\tilde{X}_0}{1 + J_0 \tilde{X}_0}, \tag{49}$$

which is just one half of the result for the corresponding transverse susceptibility (23). Thus we have proven the expected relation (37).
§ 5. Numerical results and conclusion

In this section we show numerically that the correction terms in (35) can be neglected and justify the anticipation that a simplified treatment where the irreducible single loop is unrenormalized works well.

For this purpose we concentrate on evaluation of the terms $JC(q)\chi(q)$ and $JS(q)\pi(q)$ in (35).

From now on, to proceed numerical work, we set the parameters $J=t/4$.

1. Self-energy

First we present the numerical results of the self-consistent equation for the self-energy; (28). We performed the integration over the first Brillouin zone divided into $64 \times 64$ uniform mesh. We set the carrier density $n=0.85$. In Fig. 7(a) we show the temperature dependence of the factor $X(T)$ in (28) for $a=0$ and $a=1$. We can see that the self-energy depends very weakly on the temperature over the wide range $0 < T < 200[K]$.

Next in Fig. 7(b) we show the carrier density dependence of $X(T)$. It follows from this that in case $a=0$ the effective mass becomes monotonically heavier as the system approaches the perfect nesting. On the other hand in case $a=1$ the effective mass has the highest value near the carrier density $n \sim 0.7$.

In any event the Fock term gives rise to the negative correction to the hopping integral $t$ of the order $(3/4)JX(T) \sim 10^{-2} t$ which can safely be neglected. It is true that we should take the Fock term into account to ensure the consistency of the theory, but it becomes negligibly small in magnitude and can be neglected.

2. Irreducible single loop $\tilde{Z}_0(q)$

Next we are concerned with the correction terms in the single loop. If the single

![Graph](attachment:image.png)

Fig. 7. Temperature dependence of $X(T)$ in the self-energy, $\Sigma(k) = -(3/4)JX(T)(\cos k_x a + \cos k_y a)$, for $a=0$; $n=0.85$ and $a=1$; $n=0.85$. We set $J=t/4$.

(b) Carrier density dependence of $X(T)$ at $T=0.06 t \sim 100[K]$.

* Here we put $t \sim 130[\text{meV}]$. 
Fig. 8. Scan of $\chi_0, \cdots, \chi_5$ along the $\Gamma \rightarrow X \rightarrow M \rightarrow \Gamma$ line in the first Brillouin zone for (a) $\alpha=0$; $n=0.75$ and (b) $\alpha=1$; $n=0.75$. We set $T=0.04t\sim60$[K].

loop can well be approximated by the unrenormalized one, $\chi_0(q)$, we can replace the irreducible polarization by the polarization for the free carrier system (17), since as shown above the self-energy correction can be neglected.* In such a case our treatment reproduces the effective RPA in Ref. 4).

Here we fix the temperature to $T=0.04t\sim60$[K] and take the corresponding lowest Matsubara frequency $\omega_1\sim37$[meV]. The integration is performed over the first Brillouin zone divided into $128 \times 128$ uniform mesh.

First in Fig. 8 we present the numerical results for the modified polarizations (34) in the first Brillouin zone for the fixed carrier density $n=0.75$. Figures 8(a) and (b) correspond to the cases $\alpha=0$ and $\alpha=1$ respectively.

In case $\alpha=0$, $\chi_0, \chi_2$ and $\chi_5$ exhibit the well-known incommensurate peaks around the nesting vector $q=(\pi, \pi)$, since these two terms directly reflect the symmetry of the Fermi contour. On the other hand $\chi_2$ and $\chi_4$ vanish at $q=(\pi, \pi)$, as was suggested in § 3. The reason why $\chi_1$ also vanishes at $q=(\pi, \pi)$ is that then the integrand of the $\chi_1$ becomes odd function with respect to the energy.

In case $\alpha=1$, the overall structures and magnitudes of the modified polarizations are similar to the case $\alpha=0$.

It should be noted that in any case $\chi_1$ and $\chi_4$ which appear in the numerators of $C(q)$ and $S(q)$ in the expressions (32) and (33) become very small in comparison with the $\chi_3$ and $\chi_5$ which appear in the denominators. It follows from this observation that we expect the terms $JC\chi_1$ and $JS\chi_2$ to become negligibly small in comparison with $\chi_0$.

Indeed as shown in Fig. 9, $JC\chi_1$ and $JS\chi_2$ have a very small value in the whole region of the first Brillouin zone. However we can say for certain that these terms have a tendency to reduce the magnetic fluctuation, because these terms have negative values in the whole region.

We can see directly from the results shown in Fig. 9 that in case $\alpha=0$, the nesting condition strongly suppresses both of $JC\chi_1$ and $JS\chi_2$. This means the exchange scattering processes are strongly suppressed due to the nesting condition.

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* We note that if we discard the vertex correction, it is no longer necessary to include the self-energy correction to ensure the Ward-Takahashi identity.
On the other hand, in case \( a = 1 \), the exchange scattering is enhanced as the system becomes nearer to the half-filling. Furthermore we note that the absolute value of these terms are smaller than that in case \( a = 0 \). We can say this difference comes from the different geometry of the Fermi contour.

Finally we compare \( \chi_0 \) and \( \chi_0 = \chi_0 + JC_1 + JS_2 \). As shown in Fig. 10, we can see that we cannot distinguish these two quantities. This situation is just what we expect and therefore we can certainly say that we can work well only by taking \( \chi_0 \) into account. This means in the present model that the spin fluctuations of the system can fairly well be described in terms of the simplified, or effective RPA, which include only the string type processes in Fig. 3 in which the single loop can be replaced by the bare one.

We can expect that this situation can survive in case of the \( t-J \) model. In the \( t-J \) model the free carrier in the present work is replaced by the free spinon and, in the mean field level, the bare hopping parameters \( t \) and \( t' \) are replaced by \( \tilde{t} \) and \( \tilde{t}' \) which depend on carrier concentration. However fundamental scattering processes are
Spin Fluctuations in an Itinerant Heisenberg System

In the present paper we have established the consistent formalism to treat the spin fluctuations by an itinerant Heisenberg model within the framework of RPA. Here the conservation law of the spin and the rotational symmetry of the system was carefully treated. As a result of this careful consideration, the simplified version of RPA turns out to work fairly well even in the real High-$T_c$ problems.

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Appendix A

—— Density of States ——

Here we derive an analytic expression for the density of states per spin.

\[
\mathcal{D}_\alpha(\epsilon) = \alpha^2 \int_{-\pi/\alpha}^{\pi/\alpha} \frac{dk_x}{2\pi} \int_{-\pi/\alpha}^{\pi/\alpha} \frac{dk_y}{2\pi} \delta(\epsilon - \epsilon_k)
\]

\[
= \frac{1}{\pi} \int_0^\pi dx \int_0^\pi dy \delta(\epsilon + 2t(\cos x + \cos y - \alpha \cos x \cos y))
\]

\[
= \frac{1}{\pi^2 t} \int_{-1}^{1} \frac{d\xi}{\sqrt{1 - \xi^2}} \int_{-1}^{1} \frac{d\eta}{\sqrt{1 - \eta^2}} \delta[\epsilon/t - 2(\xi + \eta - \alpha \xi \eta)]
\]

\[
= \frac{1}{2\pi^2 t} \int_{-1}^{1} \frac{d\xi}{\sqrt{(1 - \xi^2)((1 + \epsilon/2) + (1 - a)\xi)((1 - \epsilon/2) - (1 + a)\xi)}}
\]

\[
= \frac{1}{2\pi^2 t} \frac{1}{\sqrt{1 + a\epsilon/2t}} K\left[\frac{1 - (a/2 - \epsilon/4t)^2}{1 + a\epsilon/2t}\right],
\]

where \(K(x)\) denotes the elliptic integral of the first kind. Here we make use of a formula,\(^{12}\)

\[
\int_u^b \frac{dx}{\sqrt{(a-x)(b-x)(x-c)(x-d)}}
\]

\[
= \frac{2}{\sqrt{(a-c)(b-d)}} F\left[\sin^{-1}\sqrt[4]{(a-c)(b-u)}, \sqrt[4]{(b-c)(a-u)}, \sqrt[4]{(a-c)(b-d)}\right]
\]

and the relation \(F(\pi/2, q) = K(x)\) where \(F(\kappa, x)\) denotes the elliptic integral of the second kind. Here \(a > b > u > c > d\).
Appendix B

--- Bethe-Salpeter Equation for Particle-Hole Channel ---

Here we present the derivation of the solution of the Bethe-Salpeter equation for particle-hole channel (30). The equation to be solved is

\[ \Gamma(k + q, k) = 1 + \frac{1}{2} \frac{T}{N} \sum_{k'} J_{k' - k'} \mathcal{G}(k' + q) \Gamma(k' + q, k') \mathcal{G}(k'). \]  

(51)

By noting that

\[ J_{k' - k} = 2J(\cos k_x a \cos k'_x a + \sin k_x a \sin k'_x a + \cos k_y a \cos k'_y a + \sin k_y a \sin k'_y a), \]  

(52)

we can rewrite (51) in the form

\[ \Gamma(k + q, k) = 1 + JC(q)(\cos k_x a + \cos k_y a) + JS(q)(\sin k_x a + \sin k_y a). \]  

(53)

Here

\[ C(q) = \frac{1}{2} (\cos k_x a + \cos k_y a), \quad S(q) = \frac{1}{2} (\cos k'_x a + \cos k'_y a), \]  

(54)

where

\[ (\ldots) = \frac{T}{N} \sum_{k'} (\ldots) \mathcal{G}(k' + q) \Gamma(k' + q, k') \mathcal{G}(k'), \]  

(55)

and \( C(q) \) and \( S(q) \) are to be determined self-consistently. By inserting (54) back into (51), we obtain the following equations,

\[ C(q) = -\frac{1}{2} \chi_1(q) - \frac{1}{2} JC(q) \chi_3(q) - \frac{1}{2} JS(q) \chi_5(q), \]  

(56)

\[ S(q) = -\frac{1}{2} \chi_2(q) - \frac{1}{2} JC(q) \chi_4(q) - \frac{1}{2} JS(q) \chi_6(q), \]  

(57)

where \( \chi_1, \ldots, \chi_6 \) have been defined in (34). Finally by solving these simultaneous equations, we obtain (32) and (33).

References

1) H. Won and K. Maki, Phys. Rev. B49 (1994), 15305.
2) P. W. Anderson, Science 235 (1987), 1197.
   F. C. Zhang and T. M. Rice, Phys. Rev. B37 (1988), 3754.
3) G. Baskaran, Z. Zou and P. W. Anderson, Solid State Commun. 63 (1987), 973.
4) T. Tanamoto, H. Kohno and H. Fukuyama, J. Phys. Soc. Jpn. 60 (1991), 3072; 62 (1993), 717; 63 (1994), 2739.
5) P. W. Anderson, Phys. Rev. 110 (1958), 827.
6) N. F. Berk and J. R. Schrieffer, Phys. Rev. Lett. 17 (1966), 433.
   S. Doniach and S. Engelsberg, Phys. Rev. Lett. 17 (1966), 750.
   P. W. Anderson and W. F. Brinkmann, Phys. Rev. Lett. 30 (1973), 1108.
   S. Nakajima, Prog. Theor. Phys. 50 (1973), 1101.
7) P. A. Wolff, Phys. Rev. 120 (1960), 814; and as a review, e.g.,
   G. D. Mahan, Many-Particle Physics, Sec. 5.8 (Plenum Press, 1990).
8) A. A. Abrikosov, J. C. Campuzano and K. Gofron, Physica C214 (1993), 73.
9) J. Yu and A. J. Freeman, J. Chem. Solids 52 (1991), 1351.
10) B. S. Shastry, J. of Phys. F9 (1979), 1367.
11) G. Baym and L. P. Kadanoff, Phys. Rev. 124 (1961), 287.
12) I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series and Products* (Academic Press, Inc., 1980).