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Microscopic Theory of the Two-Dimensional Quantum Antiferromagnet in a Paramagnetic Phase

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We have developed a consistent theory of the Heisenberg quantum antiferromagnet in the disordered phase with a short range antiferromagnetic order on the basis of the path integral for spin coherent states. In the framework of our approach we have obtained the response function for the spin fluctuations for all values of the frequency ω and the wave vector $\mathbf{k}$ and have calculated the free energy of the system. We have also reproduced the known results for the spin correlation length in the lowest order in $1/N$. We have presented the Lagrangian of the theory in a form which is explicitly invariant under rotations and found natural variables in terms of which one can construct a natural perturbation theory. The short wave spin fluctuations are similar to those in the spin wave theory and they are on the order of the smallness parameter $1/2s$ where s is the spin magnitude. The long-wave spin fluctuations are governed by the nonlinear sigma model and are on the order of the smallness parameter $1/N$, where N is the number of field components. We also have shown that the short wave spin fluctuations must be evaluated accurately and the continuum limit in time of the path integral must be performed after the summation over the frequencies ω.

1. INTRODUCTION

The theory of the two-dimensional Heisenberg antiferromagnet (AF) has attracted a great deal of interest over the past several years in connection with the problem of the spin fluctuations in the copper oxides [1]. We especially call the attention of the reader to the reviews of Manousakis [2], Auerbach [3], and Sachdev [4] in which a general situation of the quantum AF (QAF) has been elucidated. The main point of interest was the QAF for spin 1/2 in a disordered state where the average spin on the lattice site equals zero. The main investigations have used two models of the spin short range order (SRO): (1) spin liquid type SRO order, which was proposed by Anderson [5] and developed by many other authors [6]; (2) antiferromagnetic SRO (AFSRO) which was also proposed by many other authors, including Chakravarty *et al*. [8] and, from a different standpoint, Pines [7]. In this paper, we will concentrate on the theory of the QAF with AFSRO.

The most advanced approach to the description of the QAF with AFSRO is based on the path integral for the spin coherent states [10, 11]. The modern approach to the QAF with AFSRO is based

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on papers of Haldane [9], in which he obtained the action of the QAF in an explicitly rotational invariant form, in the lowest order in the ferromagnetic fluctuations, and deduced, in the same approximation, the long-wave (LW) sigma model. He also investigated the role of the topological term in the action.

The sigma model for the case of the QAF is the continuum model for the unit vector $\mathbf{n}(t, \mathbf{r})$, $\mathbf{n}^2 = 1$ in the $1 + 2$ time and space dimensions [14, 15]. We note that the three-dimensional sigma model is not a renormalizable theory. Very interesting and important results were obtained by Chakravarty *et al*. [8], Hasenfratz and Nieder mayer [13], and Sachdev and co-workers [12]. For example, when the correlation length ξ was calculated, a very skillful treatment was required in order to absorb some divergent quantities in the parameters of the sigma model such as the spin rigidity ρ_s and the velocity of sound c_s. These parameters were calculated independently in the framework of the spin wave theory at the temperature $T = 0$ [16].

It is more or less obvious that, for an unrenormalizable field theory in the continuum, it is not possible to include all divergences in some simple observable quantities. The recent result of Hasenfratz [17] on the calculation of the correlation length, in which he goes beyond the continuum approximation, confirms this point of view.

A consistent theory of the spin fluctuations of the QAF with AFSRO for all space scales (not only for LW lengths) was, up to now, absent. In our opinion, it is not simple to develop the ideas suggested by Haldane [9] to the full scale theory. It is necessary to overcome some nontrivial technical difficulties. This is precisely the topic of this paper. As a result we can describe spin fluctuation of the QAF with AFSRO in $1 + 2$ dimensions at any temperature and for any space and time scales of the spin fluctuations in a regime of weak coupling with respect to the expansion parameters $1/2s$ and $1/N$. This is the main physical result of this paper.

The spin correlation function, which is a very important physical characteristic of the QAF, was calculated in all values of the wave vector $\mathbf{k}$ and the frequency ω. This is a new result. As $\mathbf{k}$ approaches the antiferromagnetic vector this result converges to known LW length results [2]. An expression for the free energy of the system, valid not only at low temperatures T [12] but also at T on the order of the exchange constant J, when short-wave (SW) spin excitations are essential, was also obtained.

This paper has the following structure.

(1) A form of spin coherent states (Appendix A) invariant under rotations was proposed. It allows the derivation of the Berry phase and of the Lagrangian of the QAF in forms which are explicitly invariant under rotations (Section 2.2).

(2) Variables $\mathbf{\Omega}$ and $\mathbf{M}$, which describe AF and ferromagnetic spin fluctuations, have been introduced. The Faddev–Popov trick allows the fluctuation of these fields to be made independent in the leading approximation and a convenient quadratic form for perturbation theory (Section 2.3) in the parameters $1/2s$ and $1/N$ to be obtained.

(3) We have integrated the action over the $\mathbf{M}$ field in the leading approximation in $1/2s$, and we have obtained (Section 2.6) some sort of quantum lattice rotator model (QLRM) [2, 8]. We shall call this model the spin-rotator (SR) model. It can be useful in the calculations in the leading approximation in $1/2s$.

(4) Since it is not possible to construct a perturbation theory based on the time continuum, a method of calculations at the final time step was developed (Section 3.1). After that we have calculated the free energy (Section 3.2) and the first order corrections to the leading approximation (Section 3.3).

(5) The separation of scales was performed on the basis of the Pauli–Villars transformation. As a result, we have obtained the LW nonlinear sigma model with additional contributions from SW fluctuations. In the lowest order in $1/N$, these SW contributions can be included in the renormalization of the spin stiffness and the velocity of sound. In higher orders, this is not possible.

2. BASIC TIME CONTINUUM APPROXIMATION

2.1. *Magnetic Fluctuations and 1/2s Approximation*

We consider the spin system which is described by the following Heisenberg Hamiltonian:

$$\hat{H}_{Hei} = \frac{J}{2} \sum_{l,l'=\langle l \rangle} \hat{\mathbf{S}}_l \cdot \hat{\mathbf{S}}_{l'}, \qquad \hat{\mathbf{S}}_l \cdot \hat{\mathbf{S}}_l = s(s+1), \tag{1}$$

where $\hat{\mathbf{S}}_l$ are the spin operators; the index l runs over a two-dimensional square lattice; the index l' runs over the nearest neighbors of the site l; $J > 0$ is the exchange constant which, since it is positive, corresponds to the AF spin interaction; and s is the magnitude of spin. The most efficient method of dealing with a spin system is based on the representation of the generalized partition function (GPF) Z or the generating functional of the spin Green functions (GF) in the form of the functional integral over spin coherent states z, z^* [11, 18] or over the unit vector $\mathbf{n}$, $\mathbf{n}^2 = 1$, on a sphere [2]:

$$\begin{gathered} Z = Tr[e^{-\beta \hat{H}}], \qquad Z = \int \cdots \int_{-\infty}^{\infty} D\mu(\mathbf{n}) \exp(A(\mathbf{n})), \\ D\mu(\mathbf{n}) = \prod_{\tau l} \frac{2s+1}{2\pi} \delta\left(\mathbf{n}_{\tau l}^2 - 1\right) d\mathbf{n}_{\tau l}, \end{gathered} \tag{2}$$

where $\beta = 1/T$, T is the temperature, τ is the imaginary time, and $A(\mathbf{n})$ is the action of the system. In the continuum approximation, which is valid in the leading order in $1/2s$, the expression of the action $A(\mathbf{n})$ is simplified [11]

$$A(\mathbf{n}) = -\int_0^{\beta} \sum_l [\mathcal{L}_{kin}(\tau, l) + \mathcal{H}(\tau, l)]\, d\tau, \tag{3}$$

$$B(\tau, l) = \langle \mathbf{n} | \frac{\partial}{\partial \tau} | \mathbf{n} \rangle = is(1 - \cos\theta_{\tau l}) \dot{\varphi}_{\tau l}, \tag{4}$$

$$\mathcal{L}_{kin}(\tau, l) = B(\tau, l), \quad \mathcal{H}(\tau, l) = \frac{Js^2}{2} \sum_{l'=\langle l \rangle} \mathbf{n}_{\tau l} \cdot \mathbf{n}_{\tau l'},$$

where $B(\tau, l)$ is the Berry phase, θ, φ are the Euler angles of the unit vector $\mathbf{n} = (\cos\varphi \sin\theta, \sin\varphi \sin\theta, \cos\theta)$, and $\dot{\varphi}_{\tau l}$ is the time derivative of this angle. The kinetic part of the action $\mathcal{L}_{kin}$ is highly nonlinear and it is not clear how to proceed with it consistently. Essential transformations of the Berry phase of the QAF were made by Haldane [9] but they do not have a final character (see also [2–4]).

Further in this paper we use the idea of the near AF order. Following this fundamental hypothesis, we split our square lattice into two AF sublattices a and b. In sublattice a the spins $\mathbf{S}$ are directed along some axis $\mathbf{\Omega}$, and in sublattice b they are directed in the opposite direction. In this way, we obtain a new square lattice with two spins a and b in the elementary cell with a volume $b^2 = 2a^2$, where a is the space distance between spins. The axes of this new lattice are rotated by 45° with respect to the primary axes. We assume that this AF order is only defined locally and any global AF order is absent. As a result, the summation over the lattice sites l and l' can be expressed as a summation over $l \in$ a and $l' \in$ b. Thus, the Lagrangian $\mathcal{L}_{kin}$ is a sum of two such Lagrangians, one for sublattice a and another for sublattice b, which are expressed in terms of two vectors $\mathbf{n}_a(\tau, l)$ and $\mathbf{n}_b(\tau, l')$, respectively. The Hamiltonian $\mathcal{H}$ retains its form if $l \in$ a and $l' \in$ b but $J/2 \to J$ because the double summation is then absent.

In this way we have two spins in each AF elementary cell which are defined in different space positions l and l'. This circumstance is not convenient for subsequent nonlinear changes of variables. One can introduce new variables $\mathbf{n}_{a,b}(\tau, l)$ which are both defined at sublattice a (or at the center of the AF elementary cell).

For that we pass to the Fourier image $\mathbf{n}_{a,b}(\tau, \mathbf{k})$ of the original vectors $\mathbf{n}_a(\tau, l)$ and $\mathbf{n}_b(\tau, l')$, where the momentum vector $\mathbf{k}$ runs over the AF Brillouin band. We can return to the space representation and consider the coordinate $\boldsymbol{\rho}$ as a continuum variable. As a result we have the definition

$$\mathbf{n}_{a,b}(\tau, \boldsymbol{\rho}) = \sqrt{1/N_s} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\boldsymbol{\rho}} \mathbf{n}_{a,b}(\tau, \mathbf{k}), \tag{5}$$

where $2N_s$ is the total number of sites in the space lattice. Of course, we assume periodic boundary conditions. We can now place the variable $\boldsymbol{\rho}$ on sublattice a (or in a specific center of the AF elementary cell). One can check that the Lagrangian $\mathcal{L}_{kin}$ will be the same in terms of the new variables $\mathbf{n}_{a,b}(\tau, \boldsymbol{\rho}) \equiv \mathbf{n}_{a,b}(\tau, l)$. In the same manner one can change the measure of integration (2) and write it out in terms of $\mathbf{n}_{a,b}(\tau, l)$. The Hamiltonian $\mathcal{H}$ retains its simple form in the momentum representation. To be valid, this procedure supposes that the action can be expanded in a power series in the vectors $\mathbf{n}_{a,b}$ [9].

2.2. *Invariant Lagrangian*

The form of the Lagrangian $\mathcal{L}_{kin}$ is not invariant under rotations although the physical problem itself is invariant. The reason for this situation is explained in detail in Appendix A.1. In Appendix A.2 an invariant form of the Lagrangian $\mathcal{L}_{kin}$ is proposed (84). For the two sublattices a and b it has the form

$$\mathcal{L}_{kin} = -is\ \mathbf{n}_a \cdot [\mathbf{m}_a \times \dot{\mathbf{m}}_a] - is\ \mathbf{n}_b \cdot [\mathbf{m}_b \times \dot{\mathbf{m}}_b]. \tag{6}$$

Equation (6) for $\mathcal{L}_{kin}$ is valid for any choice of the unit vectors $\mathbf{m}_{a,b}$ if they satisfy the conditions $\mathbf{m}_{a,b}^2 = 1$, $\mathbf{n}_{a,b} \cdot \mathbf{m}_{a,b} = 0$. For the problem of the quantum AF with two sublattices we can choose the following expression for the vectors $\mathbf{m}_{a,b}$

$$\mathbf{m}_{a,b} = \frac{\mathbf{n}_{b,a} - x\mathbf{n}_{a,b}}{\sqrt{1-x^2}}, \qquad x = \mathbf{n}_a \cdot \mathbf{n}_b. \tag{7}$$

Substituting these expressions for $\mathbf{m}_{a,b}$ into Eq. (6) we get invariant forms under rotation for $\mathcal{L}_{kin}$ and also for $\mathcal{H}$ (see (4))

$$\begin{aligned} \mathcal{L}_{kin} &= B(\tau, l) = \frac{is(\dot{\mathbf{n}}_{a\tau l} - \dot{\mathbf{n}}_{b\tau l}) \cdot [\mathbf{n}_{a\tau l} \times \mathbf{n}_{b\tau l}]}{1 - \mathbf{n}_{a\tau l} \cdot \mathbf{n}_{b\tau l}}, \\ \mathcal{H} &= Js^2 \sum_{l'=\langle l \rangle} \mathbf{n}_{a\tau l} \cdot \mathbf{n}_{b\tau l'}, \qquad \mathbf{n}_{a\tau l} \in a, \qquad \mathbf{n}_{b\tau l} \in b. \end{aligned} \tag{8}$$

Now we can introduce new variables which are more convenient: $\boldsymbol{\Omega}(\tau, l)$ and $\mathbf{M}(\tau, l)$. These variables realize the stereographic mapping of a sphere

$$\mathbf{n}_{a,b} = \frac{\pm\boldsymbol{\Omega}(1 - \mathbf{M}^2/4) - [\boldsymbol{\Omega} \times \mathbf{M}]}{1 + \mathbf{M}^2/4}, \tag{9}$$

where $\mathbf{\Omega}^2 = 1$ and $\mathbf{\Omega} \cdot \mathbf{M} = 0$. In terms of these variables the total Lagrangian $\mathcal{L}_{\Omega M} = \mathcal{L}_{kin} + \mathcal{H}$ has the final form

$$\mathcal{L}_{kin} = \frac{2\,i s\,\dot{\mathbf{\Omega}} \cdot \mathbf{M}}{1 + \mathbf{M}^2/4}, \qquad \mathcal{H} = J s^2 \sum_{l' = \langle l \rangle} H_{ll'},$$
$$H_{ll'} = \{\mathbf{\Omega} \cdot \mathbf{\Omega}'[(1 - \mathbf{M}^2/4)(1 - \mathbf{M}'^2/4) - \mathbf{M} \cdot \mathbf{M}'] + \mathbf{\Omega} \cdot \mathbf{M}' \mathbf{\Omega}' \cdot \mathbf{M}\}(1 + \mathbf{M}^2/4)^{-1}(1 + \mathbf{M}'^2/4)^{-1}, \tag{10}$$

where $\mathbf{\Omega} \equiv \mathbf{\Omega}_{\tau l}$, $\mathbf{\Omega}' \equiv \mathbf{\Omega}_{\tau l'}$, $\mathbf{M} \equiv \mathbf{M}_{\tau l}$, and $\mathbf{M}' \equiv \mathbf{M}'_{\tau l}$. This Lagrangian determines the quadratic Lagrangian and nonlinear terms which give the amplitudes of the magnon scatering in the tree approximation which is valid in the lowest order in $1/2s$. After this change of variables the measure of integration $D\mu(\mathbf{n})$ (2) becomes

$$\prod_{\tau l} \frac{(2s+1)^2(1 - \mathbf{M}^2/4)}{2\pi^2(1 + \mathbf{M}^2/4)^3} \delta(\mathbf{\Omega}^2 - 1)\delta(\mathbf{\Omega} \cdot \mathbf{M})\, d\mathbf{\Omega}\, d\mathbf{M}, \tag{11}$$

where the index l runs over the AF (double) lattice cells.

2.3. *Gauge Transformation*

The variable $\mathbf{\Omega}$ is responsible for the AF fluctuations and the variable $\mathbf{M}$ for the ferromagnetic ones. The ferromagnetic fluctuations are small according to the smallness parameter $1/2s$ and therefore one can expand the Lagrangian $\mathcal{L}_{\Omega M}$ (10) in powers of $\mathbf{M}$. The vector of the ferromagnetic fluctuations $\mathbf{M}$ plays the role (up to a factor 2s) of the canonical momentum conjugate to the canonical coordinate $\mathbf{\Omega}$. The term, in the Berry phase, of first order in $\mathbf{M}$ coincides (after change of variables), with previous results of Haldane [9] (see also [2–4]).

From Eq. (10) one can easily extract the quadratic part, $\mathcal{L}_{quad}$, of the total Lagrangian,

$$\mathcal{L}_{quad} = 2\,i s\,(\mathbf{M} \cdot \dot{\mathbf{\Omega}}) + J s^2 \sum_{l'} [\mathbf{\Omega}^2 - \mathbf{\Omega} \cdot \mathbf{\Omega}' + \mathbf{M}^2 + \mathbf{M} \cdot \mathbf{M}']. \tag{12}$$

We stress again that this quadratic form is very close to the 1988 result of Haldane [9], but is different to the extent that Haldane's result involves the variable $\mathbf{L} = [\mathbf{M} \times \mathbf{\Omega}]$. As a result we have a quite simple quadratic form.

The Lagrangian $\mathcal{L}_{quad}$ (12) is very simple but the measure $D\mu(\mathbf{n})$ (11) is not simple due to the presence of two delta functions. Therefore we cannot simply perform the Gaussian integration over the fields $\mathbf{\Omega}$ and $\mathbf{M}$.

To solve this problem we shall use the method of Lagrange multipliers together with the saddle point approximation [14, 15] to eliminate the delta function $\delta(\mathbf{\Omega}^2 - 1)$,

$$\delta(\mathbf{\Omega}^2 - 1) = (2\pi)^{-1} \int_{-\infty}^{\infty} \exp(A_\lambda)\, d\lambda,$$
$$-A_\lambda = \mathcal{L}_\lambda = (i\lambda + c_\mu)(\mathbf{\Omega}^2 - 1), \tag{13}$$

where λ is a Lagrange multiplier and c_μ is a constant which will be fixed with the help of the saddle point condition [14, 15].

To eliminate the delta function $\delta(\mathbf{\Omega} \cdot \mathbf{M})$ we shall use a form of the Faddev–Popov trick which was proposed in [20]. Let us consider the integral

$$I(f) = \int f(\mathbf{M})\delta(\mathbf{\Omega}\cdot\mathbf{M})\,d\mathbf{M}, \tag{14}$$

where $f(\mathbf{M})$ is an arbitrary function of $\mathbf{M}$. Let us insert in the right hand side of (14) the identity

$$1 = Z_{ga}\int \exp\left(-\frac{1}{2}\varphi\hat{B}_{ga}\varphi\right)\frac{d\varphi}{\sqrt{2\pi}}, \qquad Z_{ga}^2 = \det(\hat{B}_{ga}), \tag{15}$$

where $\hat{B}_{ga}$ is a positive number or a positive definite operator for some multidimensional generalization. After changing the orders of integration over $\mathbf{M}$ and φ we can make the change of variables $\mathbf{M}\colon \mathbf{M} \to \mathbf{M} - \mathbf{\Omega}\varphi$. After that, due to the delta function, we have $\varphi = (\mathbf{\Omega}\cdot\mathbf{M})$ so that the delta function disappears from integral (14),

$$\begin{aligned} I(f) &= Z_{ga}\int f(\mathbf{M}_{tr})\exp(A_{ga})\,d\mathbf{M}/\sqrt{2\pi}, \\ -A_{ga} &= \mathcal{L}_{ga} = \frac{1}{2}(\mathbf{\Omega}\cdot\mathbf{M})\hat{B}_{ga}(\mathbf{\Omega}\cdot\mathbf{M}), \end{aligned} \tag{16}$$

where $\mathbf{M}_{tr} \equiv \mathbf{M} - \mathbf{\Omega}(\mathbf{\Omega}\cdot\mathbf{M})$. With the help of identity (16) we can remove the delta function $\delta(\mathbf{\Omega}\cdot\mathbf{M})$ from measure (11). As a result we must substitute $\mathbf{M} \to \mathbf{M}_{tr}$ in the Lagrangian $\mathcal{L}_{\Omega M}$ (10) and add the gauge fixing Lagrangian $\mathcal{L}_{ga}$ due to the additional exponential in (16). It is convenient to choose the Lagrangian $\mathcal{L}_{ga}$ in the form

$$\mathcal{L}_{ga} = Js^2\sum_{l'\in\langle l\rangle}[(\mathbf{\Omega}\cdot\mathbf{M})^2 + (\mathbf{\Omega}\cdot\mathbf{M})(\mathbf{\Omega}'\cdot\mathbf{M}')]. \tag{17}$$

Such choice removes the major dependence on $\mathbf{\Omega}$ from the Lagrangian (12) which appears due to substitution $\mathbf{M} \to \mathbf{M}_{tr}$. We can also replace $\mathbf{M}_{tr} \to \mathbf{M}$ in the first term of the Lagrangian $\mathcal{L}_{quad}$ (12) due to the identity $(\mathbf{\Omega}\cdot\dot{\mathbf{\Omega}}) = 0$. In this way, the expression (12) for $\mathcal{L}_{quad}$ is valid in the leading order in the small parameter $1/2s$.

The final expression for the GPF of the QAF is

$$\begin{aligned} Z &= \int\cdots\int \exp(A(\mathbf{\Omega},\mathbf{M},\lambda))Z_{ga}D\mu((\mathbf{\Omega},\mathbf{M})D\mu(\lambda), \\ D\mu(\mathbf{\Omega},\mathbf{M}) &= \prod_{\tau l}\frac{(2s+1)^3(1-\mathbf{M}^2/4)}{(2\pi)^3(1+\mathbf{M}^2/4)^3}\,d\mathbf{\Omega}(\tau,l)\,d\mathbf{M}(\tau,l), \\ D\mu(\lambda) &= \prod_{\tau l} 2\,d\lambda(\tau,l)/\big[(2s+1)(2\pi)^{1/2}\big]. \end{aligned} \tag{18}$$

Here $D\mu(\mathbf{\Omega},\mathbf{M},\lambda) = Z_{ga}D\mu(\mathbf{\Omega},\mathbf{M})D\mu(\lambda)$ is the measure of integration, and the action $A(\mathbf{\Omega},\mathbf{M},\lambda)$ is determined by the total Lagrangian $\mathcal{L}_{tot} = \mathcal{L}_{\Omega M} + \mathcal{L}_{ga} + \mathcal{L}_{\lambda}$.

2.4. *Properties of the Basic Approximation*

One can change to the $q = (\omega, \mathbf{k})$ momentum representation (ω is the frequency, $\mathbf{k}$ is the wave vector) and write out the total quadratic part of the Lagrangian in the matrix form

$$\begin{gathered}\mathcal{L}_{quad}(q) = s\mathbf{X}_q^*\hat{\Lambda}(q)\mathbf{X}_q, \quad \mathbf{X}_q^* = (\mathbf{\Omega}_q^*, \mathbf{M}_q^*),\\ \hat{\Lambda}(q)\mathbf{X}_q = \begin{pmatrix} P'_{\mathbf{k}}, & \omega \\ -\omega, & Q_{\mathbf{k}} \end{pmatrix}\begin{pmatrix} \mathbf{\Omega}_q \\ \mathbf{M}_q \end{pmatrix}, \quad P'_{\mathbf{k}} = P_{\mathbf{k}} + c_\mu,\\ c_\mu = \mu_0^2/2\mathcal{J}, \quad Q_{\mathbf{k}} = \mathcal{J}(1+\gamma_{\mathbf{k}}), \quad P_{\mathbf{k}} = \mathcal{J}(1-\gamma_{\mathbf{k}}),\\ \mathcal{J} = jsz, \quad \gamma_{\mathbf{k}} = (1/2)(\cos(k_x a) + \cos(k_y a)).\end{gathered} \tag{19}$$

Here $\mathbf{X}_q$ is a two component vector field which combines the vector fields $\mathbf{\Omega}_q$ and $\mathbf{M}_q$; the constant c_μ (13) is expressed through the constant μ_0 which is the mass of the $\mathbf{\Omega}$ field in the lowest order of perturbation theory. One can invert the 2×2 matrix $\hat{\Lambda}(q)$ and get the bare Green function (GF) $\hat{G}_q$ of the $\mathbf{\Omega}_q$ and $\mathbf{M}_q$ fields

$$\begin{gathered}\hat{G}_q = \frac{1}{2s}(\hat{\Lambda}(q))^{-1} = \frac{1}{2sL_q}\begin{pmatrix} Q_{\mathbf{k}}, & -\omega \\ \omega, & P'_{\mathbf{k}} \end{pmatrix}\\ L_q = \omega^2 + \omega_{0\mathbf{k}}^2, \qquad \omega_{0\mathbf{k}}^2 = \left(1-\gamma_{\mathbf{k}}^2\right)\mathcal{J}^2 + (1+\gamma_{\mathbf{k}})\mu_0^2/2,\end{gathered} \tag{20}$$

where $\omega_{0\mathbf{k}}$ is the primary magnon frequency in the paramagnetic phase. Below we shall use the notations $G_q^{\Omega} = G_q^{11}$, $G_q^d = G_q^{21}$, $G_q^u = G_q^{12}$, and $G_q^M = G_q^{22}$ for the matrix elements of the matrix GF $\hat{G}_q$.

First let us discuss the parameter of perturbation theory. One can see from the explicit form of the Lagrangian (10) that the spin wave nonlinearity of the theory is due to the term $\mathbf{M}_{tr}$ and its modifications. Its average value $\langle \mathbf{M}_{tr}^2 \rangle$ is

$$(N-1)\sum_q G_q^M = \frac{(N-1)T}{2s}\sum_{\omega=2\pi nT,\mathbf{k}} \frac{P_{\mathbf{k}}}{\omega^2+\omega_{0\mathbf{k}}^2}, \tag{21}$$

where $N=3$ is the number of components of the $\mathbf{\Omega}$ field. The summation over ω is obtained by standard methods [15] and we have

$$\left\langle \mathbf{M}_{tr}^2 \right\rangle = \frac{(N-1)}{2s}\sum_{\mathbf{k}} \frac{P_{\mathbf{k}}}{2\omega_{0\mathbf{k}}}(1+2n_{0\mathbf{k}}) = \frac{(N-1)}{4s}\begin{cases} C_{M0}, & T \ll \mathcal{J} \\ (T/\mathcal{J})C_{M\infty}, & T \gg \mathcal{J}. \end{cases} \tag{22}$$

Here, $n_{0\mathbf{k}} = (\exp(\omega_{0\mathbf{k}}/T)-1)^{-1}$ is the Planck function, and summation over $\mathbf{k}$ means the normalized integration over the AF Brillouin band. The constants C_{M0} and $C_{M\infty}$ are defined by the relations

$$\begin{aligned} C_{M0} &= \sum_{\mathbf{k}} \sqrt{\frac{1-\gamma_{\mathbf{k}}}{1+\gamma_{\mathbf{k}}}} = c_0 - c_1 = 0.65075,\\ C_{M\infty} &= \sum_{\mathbf{k}} \frac{2}{1+\gamma_{\mathbf{k}}} = 1.48491,\end{aligned} \tag{23}$$

where all sums of type (23) are calculated by the following method

$$\begin{gathered} c_n = \sum_{\mathbf{k}} \frac{\gamma_{\mathbf{k}}^n}{\sqrt{1-\gamma_{\mathbf{k}}^2}}, \qquad \sum_{\mathbf{k}} f(\gamma_{\mathbf{k}}) = \int_0^1 f(\epsilon)\rho(\epsilon)\,d\epsilon,\\ \rho(\epsilon) = \sum_{\mathbf{k}} \delta(\epsilon - \gamma_{\mathbf{k}}) = \frac{4}{\pi^2}K(1-\epsilon^2).\end{gathered} \tag{24}$$

Here $K(x)$ is the complete elliptic integral of the first kind. In the same manner one can calculate the average at different time and space points.

$$\langle M_i(\tau+\delta, \mathbf{1}+\mathbf{r})\mathbf{\Omega}_j(\tau, \mathbf{1})\rangle = \frac{i}{4s}\delta_{ij}\epsilon(\delta)\sum_{\mathbf{k}}\frac{\exp(i\mathbf{k}\cdot\mathbf{r}-|\delta|\omega_{0\mathbf{k}})}{1-\exp(-\beta\omega_{0\mathbf{k}})}. \tag{25}$$

Here $\epsilon(\delta)$ is the sign function: $\epsilon(\delta)=1$ for $\delta>0$, $\epsilon(\delta)=-1$ for $\delta<0$. For $\mathbf{r}=0$ and $\delta\mathcal{J}\ll 1$ we have an explicit expression

$$\langle M_i(\delta)\mathbf{\Omega}_j(0)\rangle = \frac{i}{4s}\delta_{ij}\epsilon(\delta)\begin{cases}1, & T\ll\mathcal{J}\\ T\mathcal{J}/C_0, & T\gg\mathcal{J}.\end{cases} \tag{26}$$

From Eqs. (22) and (25) we clearly see that the smallness parameter of perturbation theory is $1/2s$ at low temperatures $T\ll\mathcal{J}$ and $T/(2s\mathcal{J})$ at high temperatures $T\geq\mathcal{J}$. Thus, perturbation theory is working when $1/2s$ is a small parameter and the temperature is not high. We remind the reader that this is just the applicability condition of the spin wave theory.

Now we can consider the saddle point condition for the λ field $\langle\mathbf{\Omega}^2\rangle=1$ which is the basic constraint (BC) of the theory which determines its phase state:

$$1=\langle\mathbf{\Omega}^2\rangle = N\sum_q G_q^{\Omega} = \frac{N}{2s}\sum_{\mathbf{k}}\frac{Q_{\mathbf{k}}}{2\omega_{0\mathbf{k}}}(1+2n_{0\mathbf{k}}). \tag{27}$$

The right hand side of Eq. (27) contains two terms. The first term $Q_{\mathbf{k}}/2\omega_{0\mathbf{k}}$ is responsible for the quantum fluctuations of the $\mathbf{\Omega}$ field. The second term $Q_{\mathbf{k}}n_{0\mathbf{k}}/\omega_{0\mathbf{k}}$ is responsible for the classical thermal fluctuations of the $\mathbf{\Omega}$ field. The role of these two terms is quite different. The quantum fluctuations are small with respect to the smallness parameter of perturbation theory $1/2s$ and in the leading approximation they can be neglected. The thermal fluctuations can be considered in the continuum approximation for which $Q_{\mathbf{k}}\simeq 2\mathcal{J}$ and $\omega_{0\mathbf{k}}^2\simeq c_{0s}^2\mathbf{k}^2+\mu_0^2$, where c_{0s} is the primary velocity of sound and $c_{0s}^2=2J^2s^2za^2/\hbar^2$. The integration over the two-dimensional momentum $\mathbf{k}$ can be easily performed [12]. The integration over the angle is trivial, and the integration over the modulus $|\mathbf{k}|$ is performed if we introduce a new variable of integration $x=\beta\omega_{0\mathbf{k}}$. As a result we have the BC

$$1=-\frac{TN}{2\pi Js^2}\ln\bigl(1-e^{-\mu_0/T}\bigr)\simeq-\frac{TN}{2\pi Js^2}\ln(\mu_0/T). \tag{28}$$

The coefficient before the logarithm in this equation is always small when the regime of weak coupling is valid. At small temperatures $T\ll\mathcal{J}$ this is obvious. At the temperature $T\simeq\mathcal{J}$ this coefficient coincides with the parameter of perturbation theory (22) and also must be considered as small. This means the logarithm in (28) must be negative and large is modulus. This leads to the condition $\mu_0/T\ll 1$ which justifies the last simplification in (28). As a result we have the well known [2, 8, 12] zero order expression for μ_0

$$\mu_0 = T\exp(-2\pi Js^2/TN). \tag{29}$$

The quantity $\xi_0=\hbar c_{0s}/\mu_0$ is the correlation length [2, 12]. This relation can be easily obtained if we find Green function $G^{\mathbf{\Omega}}(\mathbf{k})=\sum_\omega G_q^{\Omega}$ and change to coordinate representation for it. From Eq. (29), the very important conclusion follows: in the regime of the weak coupling the correlation length ξ is much larger than the lattice constant a. This conclusion enables the scale separation for the problem of disordered QAF [8] to be accomplished.

To close the theory it is helpful to define the polarization operator $\Pi(q)$ of the $\mathbf{\Omega}$ field

$$A_{\lambda quad} = -\frac{1}{2}\sum_{q} \lambda^*(q)\Pi(q)\lambda(q), \tag{30}$$

which is the dressed loop, and the GF of the λ field is $\Pi(q)^{-1}$. In the lowest approximation $\Pi(q)$ is simply the loop from two GF's G^{Ω}

$$\Pi_0(q) = 2NT\sum_{q'} G^{\Omega}(q')G^{\Omega}(q-q'). \tag{31}$$

Using the GF $G^{\Omega}(q)$ from (20) we can perform the summation over ω and have the expression for the simple loop.

$$\Pi_0(q) = \frac{N}{4s^2}\sum_{\mathbf{k}'}(1+2n_1)\frac{Q_1Q_2}{\omega_1\omega_2}\left[\frac{\omega_2+\omega_1}{\omega^2+(\omega_2+\omega_1)^2}+\frac{\omega_2-\omega_1}{\omega^2+(\omega_2-\omega_1)^2}\right],$$
$$Q_i \equiv Q_{\mathbf{k}_i}, \qquad \omega_i \equiv \omega_{0\mathbf{k}_i}, \qquad n_i \equiv n_{0\mathbf{k}_i}, \tag{32}$$

where the index $i := 1, 2$, corresponding, respectively, to the momenta $\mathbf{k}_1 \equiv \mathbf{k}'$ and $\mathbf{k}_2 \equiv \mathbf{k} - \mathbf{k}'$. The main contribution in $1/2s$ in (32) is from the thermal fluctuations even at low temperatures T, because the integral strength of the thermal fluctuations does not depend on the temperature. It is fixed by the saddle point condition (27), in spite of the temperature entering into this condition. The explicit form for $\Pi_0(q)$ may be obtained in two limiting cases $\hbar q \gg T$ and $\hbar q \ll T$, where $q^2 = \omega^2 + c_s^2k^2$. In the first case the momentum $k' \sim T/c_s \ll q$, and we can separate the integration over $\mathbf{k}'$ and put $\mathbf{k}' = 0$ in all places in (32) affected by the factor $n_1 \equiv n(\mathbf{k}')$. The result is extremely simple

$$\Pi_0(q) = 4G^{\Omega}(q) = \frac{2\mathcal{J}(1+\gamma_{\mathbf{k}})}{s\left(\omega^2+\omega_{0\mathbf{k}}^2\right)}, \qquad q \gg k_T, \tag{33}$$

where $k_T = T/c_{0s}$. At small $q \ll c_{0s}/a$ a similar result was obtained in [12]. Notice that it exceeds the quantum contribution in (32) $\Pi_0(q) = N/4q$ in the large parameter $16s\mathcal{J}/Nq$. The second limiting case $\hbar q \ll T$ lies in the purely continuum region. It corresponds to the pure classical two-dimensional case: $\omega = 0$ and $\omega' = 0$. Integration over $\mathbf{k}'$ can be easily performed as the result for $\Pi_0(k)$ coincides with [12] up to the normalization factor

$$\Pi_0(k) = \frac{8NT}{\pi s^2 q\sqrt{q^2+4\mu_0^2}}\ln\left(\frac{q+\sqrt{q^2+4\mu_0^2}}{2\mu_0}\right), \tag{34}$$

where $q = c_{0s}k$.

2.5. *The Spin Correlation Functions*

The approach of this paper enables us to find the spin correlation functions for all values of ω and $\mathbf{k}$. The dynamical spin susceptibility is determined by the relation

$$\chi(\omega,\mathbf{k})\delta_{ij} = -\frac{i}{\hbar}\int_0^{\infty} d\tau \sum_{\mathbf{l}} Tr\{[\hat{S}_i(\tau,\mathbf{l}),\hat{S}_j(0,\mathbf{0})]\exp(\beta(F-\hat{H}))\}\exp(i\omega\tau - ia\mathbf{k}\cdot\mathbf{l}), \tag{35}$$

where $F = -T\ln(Z)$ is the free energy, and the wave vector $\mathbf{k}$ runs without limitations over the Brillouin band. It is well known that the dynamical spin susceptibility $\chi(\omega, \mathbf{k})$ coincides with the temperature GF continued on the imaginary frequency ω. It can be calculated on the basis of the functional integral (18)

$$\chi(\omega, \mathbf{k})\delta_{ij}\delta(\omega - \omega')\delta(\mathbf{k} - \mathbf{k}') = -\frac{is^2}{\hbar}\langle n_i^*(\mathbf{\Omega}, \mathbf{M}, \omega', \mathbf{k}')n_j(\mathbf{\Omega}, \mathbf{M}, \omega, \mathbf{k})\rangle. \tag{36}$$

Here, the unit vector $\mathbf{n}(\mathbf{\Omega}, \mathbf{M}, \omega, \mathbf{k})$ is a function of the fields $\mathbf{\Omega}(\tau, l), \mathbf{M}(\tau, l)$ according to (9); the brackets $\langle \ldots \rangle$ mean averaging over the $\mathbf{\Omega}(\tau, l), \mathbf{M}(\tau, l)$ fields according to (18). Equation (36) reduces the problem of the calculation of the spin GF to the problem of the calculation of the averages of the $\mathbf{\Omega}$ and $\mathbf{M}$ fields. In the lowest order in $1/2s$ it is sufficient to use the lowest order relation

$$\mathbf{n}(\mathbf{\Omega}, \mathbf{M}, \tau, l) \simeq \exp(ia\mathbf{l}\cdot\mathbf{q}_{AF})\mathbf{\Omega} - [\mathbf{\Omega}\times\mathbf{M}], \tag{37}$$

where $\mathbf{\Omega} \equiv \mathbf{\Omega}(\tau, l), \mathbf{M} \equiv \mathbf{M}(\tau, l)$, and $\mathbf{q}_{AF} = (\pi/a, \pi/a)$ is the AF vector (9). Substituting the vector $\mathbf{n}$ from (37) into (36) we get the dynamical spin susceptibility as a sum of two terms $\chi(\omega, \mathbf{k}) = \chi_A(\omega, \mathbf{k}) + \chi_F(\omega, \mathbf{k})$. The spin susceptibility $\chi_A(\omega, \mathbf{k})$ is responsible for the AF fluctuations. It is proportional to the GF G_q^{Ω} analytically continued and shifted by the AF vector $\mathbf{q}_{AF}$

$$\chi_A(\omega, \mathbf{k}) = -\frac{Js^2z(1+\gamma_{\mathbf{k}^*})}{2\left(\omega^2 - \omega_{0\mathbf{k}^*}^2 + i\omega\delta\right)}, \tag{38}$$

where $\mathbf{k}^* = \mathbf{k} - \mathbf{q}_{AF}$, and $\omega_{0\mathbf{k}}$ is the magnon frequency (20). For the spin susceptibility $\chi_F(\omega, \mathbf{k})$ we have the loop expression

$$2s^2\sum_{q'}[G^{\Omega}(q')G^M(q-q') - G^u(q')G^d(q-q')]. \tag{39}$$

In the leading approximation in $1/2s$ the first term gives the main contribution in the same manner as in (31) when the contribution from the Planck fuction n_1 was dominant

$$\chi_F(\omega, \mathbf{k}) \simeq -\sum_{\mathbf{k}'} n_1\frac{Q_1P_2'}{2\omega_1\omega_2}\left[\frac{\omega_2+\omega_1}{\omega^2-(\omega_2+\omega_1)^2+i\omega\delta} + \frac{\omega_2-\omega_1}{\omega^2-(\omega_2-\omega_1)^2+i\omega\delta}\right], \tag{40}$$

where the notation is the same as in (31). In the case of $q = \sqrt{\omega^2 - c_s^2k^2} \gg k_T$ the expression (40) is substantially simplified on the basis of the idea of dominant small $k' \simeq k_T$,

$$\chi_F(\omega, \mathbf{k}) \simeq -\frac{2s^2}{N}G^M(q) = -\frac{Js^2z(1-\gamma_{\mathbf{k}})}{N\left(\omega^2 - \omega_{0\mathbf{k}}^2 + i\omega\delta\right)}. \tag{41}$$

For the case $q \leq k_T$ the expression for $\chi_F(\omega, \mathbf{k})$ is not so simple and we give as the result the limit $\mu \ll \omega$, $\omega_{\mathbf{k}} \ll k_T$

$$\chi_F(\omega, \mathbf{k}) = -\frac{a^2T^2}{\pi c_s^2 q}\xi(2) + i\epsilon(\omega)\frac{a^2T}{16\pi c_s^2|q|^2}(2\pi\theta(q^2)\omega(4\omega - 3|q|) + \theta(-q^2)T|q|\xi(2)), \tag{42}$$

where $\xi(n)$ is the Riemann zeta function, and $\epsilon(\omega)$ is the sign function. The two terms in (42) which are proportional to $\xi(2)$ are generated by the integral which is cut at large k by the Planck

distribution function $n(\mathbf{k}')$. The ferromagnetic spin susceptibility (43) is suppressed in comparison with the antiferromagnetic one (38) by the parameter $(qa)^2$.

2.6. *The Spin-Rotator Model*

In the leading approximation in $1/2s$ the Lagrangian is quadratic in the $\mathbf{M}$ field and one can integrate over this field and obtain the final action for the $\mathbf{\Omega}$ field and the Lagrange multiplier λ,

$$\mathcal{L}_{\Omega\lambda} = s(\dot{\mathbf{\Omega}}\hat{Q}^{-1}\dot{\mathbf{\Omega}}) + s(\mathbf{\Omega}\hat{P}'\mathbf{\Omega}) + i\lambda(\mathbf{\Omega}^2 - 1), \tag{43}$$

where the quantities $\hat{Q}$ and $\hat{P}'$ are defined in the $\mathbf{k}$ representation in (20). As a result of this integration the $\mathbf{M}$ field becomes a function of the $\mathbf{\Omega}$ field: $\mathbf{M} = \hat{Q}^{-1}\dot{\mathbf{\Omega}}$. One can easily recognize in (21) the Lagrangian of a QLRM kind [8]. However, this model is different from the standard model due to the momentum dependence of the kinetic term in Eq. (21). We shall call these kinds of models SR models. The SR model describes a quantum antiferromagnet in the limit $s \to \infty$. The QLRM is also well defined and does not contain any divergences. It allows all calculations to be performed accurately because all physical quantities are well defined in the framework of this model.

3. BEYOND THE APPROXIMATION OF THE TIME CONTINUUM

3.1. *Basic Approach*

When we try to construct the perturbation corrections to the basic approach discussed in the previous section we meet a fundamental difficulty: the integrals arising from the GF (20), over the frequency ω, are not well defined. This is obvious from the consideration of the average $\langle M_i(\tau + \delta, \mathbf{l})\mathbf{\Omega}_j(\tau, \mathbf{l})\rangle$. The result essentially depends on the time shift δ (25) which reflects the phase space nature of the $\mathbf{\Omega}$ and $\mathbf{M}$ variables: the GF $G^{u,d}(q) \sim \omega^{-1}$ at large ω. Moreover some doubts may arise that the calculation of the quantity $\langle \mathbf{M}_{tr}^2 \rangle$ was indeed correct. Actually, at low temperature

$$\langle \mathbf{M}_{tr}^2 \rangle \sim \sum_{\mathbf{k}} \int_{-\pi/\Delta}^{\pi/\Delta} \frac{d\omega}{2\pi} \frac{\mathcal{J}(1-\gamma_{\mathbf{k}})}{\omega^2 + \omega_{0\mathbf{k}}^2} = C_{M0}, \tag{44}$$

where Δ is the time step in the accurate definition of the GPF and the interval $(-\pi/\Delta, \pi/\Delta)$ gives the one-dimensional Brillouin band for the final time step Δ. The limit $\Delta \to 0$ gives a correct value of this average. At first sight this limit is trivial because the integral over ω in (44) is well defined. Suppose that we were not so accurate and the numerator of (44) contains in fact a small correction $\mathcal{J}(1-\gamma_{\mathbf{k}}) \Rightarrow \mathcal{J}(1-\gamma_{\mathbf{k}}) + \Delta\omega^2$. If now we at first calculate the integral (44) with this numerator and after that pass to the limit $\Delta \to 0$ the result will be different: $C_{M0} \to C_{M0} + 1$. This example should convince the reader that for a spin system the continuum limit of the path integral for the GPS (2) must be performed with proper accuracy: at first it is necessary to formulate the theory at finite Δ and one can put $\Delta = 0$ only after the calculation of all integrals over ω has been done. Notice also that the accurate version of the GPF, discrete in time (2), is necessary when we calculate the free energy.

We obtain now, on the basis of the results of Appendix A, an accurate expression for the quadratic part of the action. Instead of expression (3) for the action $A(\mathbf{n})$ we shall use a more accurate expression

$$A(\mathbf{n}) = -\sum_{j=0}^{N_\tau} \sum_{l} \Delta[\mathcal{L}_{kin}(j,l) + \mathcal{H}(j,l)], \tag{45}$$

where $\tau = j\Delta$ and $\Delta N_\tau = \beta$. According to the results of Appendix A, $\mathcal{L}_{kin}(j, l)$ consist of two parts $\mathcal{L}_{kin} = \mathcal{L}_{mod} + \mathcal{L}_{pha}$. The first term is purely real and the second term is purely imaginary.

According to Eq. (80) the Lagrangian $\mathcal{L}_{mod}$ can be written for two sublattices a and b in the form

$$\Delta\mathcal{L}_{mod} = -s \ln[(1 + \underline{\mathbf{n}}_a \cdot \mathbf{n}_a)(1 + \underline{\mathbf{n}}_b \cdot \mathbf{n}_b)/4], \tag{46}$$

where $\mathbf{n}_a = \mathbf{n}_a(j, l)$, $\underline{\mathbf{n}}_a = \mathbf{n}_a(j + 1, l)$, $\underline{\mathbf{n}}_b = \mathbf{n}_b(j + 1, l)$, and $\mathbf{n}_b = \mathbf{n}_b(j, l)$. It is assumed that the vectors $\underline{\mathbf{n}}_a$, $\mathbf{n}_a$, $\underline{\mathbf{n}}_b$, and $\mathbf{n}_b$ are functions of the dynamical variables $\mathbf{\Omega}$ and $\mathbf{M}$ according to Eq. (9).

The Lagrangian $\mathcal{L}_{pha}$ is not so simple and according to Appendix A (86) it is

$$\Delta\mathcal{L}_{pha} = -\frac{s}{2} \ln\left(\frac{T_a \underline{T}_a^* T_b \underline{T}_b^*}{T_a^* \underline{T}_a T_b^* \underline{T}_b}\right), \tag{47}$$

where the quantity $T_{a,b}$ is defined in (88) and has a rather complicated form. The expansion of $\Delta\mathcal{L}_{pha}$ in powers of the $\mathbf{M}$ field contains only odd powers of $\mathbf{M}$.

The Hamiltonian $\mathcal{H}(\mathbf{n})$ can be obtained on the basis of Eq. (77) for the matrix element of the spin operator $\mathbf{S}$ if we substitute them in the Heisenberg Hamiltonian

$$\mathcal{H}(\mathbf{n}) = Js^2 \sum_{l' \in \langle l \rangle} \boldsymbol{\mathcal{S}}(\underline{\mathbf{n}}, \mathbf{n}) \cdot \boldsymbol{\mathcal{S}}(\underline{\mathbf{n}}', \mathbf{n}'), \tag{48}$$

where $\underline{\mathbf{n}} = \mathbf{n}_a(j+1, l)$, $\mathbf{n} = \mathbf{n}_a(j, l)$, $\underline{\mathbf{n}}' = \mathbf{n}_b(j+1, l')$, and $\mathbf{n}' = \mathbf{n}_b(j, l')$. All these vectors are also functions of the dynamical variables $\mathbf{\Omega}$ and $\mathbf{M}$ according to Eq. (9). The vector $\mathcal{S}(\underline{\mathbf{n}}, \mathbf{n})$ is determined by the relation

$$\mathbf{S}(\underline{\mathbf{n}}, \mathbf{n}) = \frac{\langle \underline{\mathbf{n}} | \hat{\mathbf{S}} | \mathbf{n} \rangle}{\langle \underline{\mathbf{n}} | \mathbf{n} \rangle} = \frac{\underline{\mathbf{n}} + \mathbf{n} - i[\underline{\mathbf{n}} \times \mathbf{n}]}{1 + \underline{\mathbf{n}} \cdot \mathbf{n}}. \tag{49}$$

This quantity transforms indeed as a vector under rotations according to the discussion in Appendix A.

Expanding the Lagrangians $\mathcal{L}_{mod}$ (46), $\mathcal{L}_{pha}$ (47), and the Hamiltonian (48) in powers of the vector $\mathbf{M}$ up to second order we get

$$\begin{aligned} \Delta\mathcal{L}_{kin} &= s[1 - \underline{\mathbf{\Omega}} \cdot \mathbf{\Omega} + \mathbf{M}^2 - \underline{\mathbf{M}} \cdot \mathbf{M} + i(\underline{\mathbf{\Omega}} \cdot \mathbf{M} - \mathbf{\Omega} \cdot \underline{\mathbf{M}})], \\ \mathcal{H} &= Js^2 \sum_{l' \in \langle l \rangle} [\underline{\mathbf{\Omega}} \cdot \mathbf{\Omega} - \mathbf{\Omega} \cdot \mathbf{\Omega}' + \underline{\mathbf{M}} \cdot \mathbf{M} + \mathbf{M} \cdot \mathbf{M}' - i(\underline{\mathbf{\Omega}} \cdot \mathbf{M} - \mathbf{\Omega} \cdot \underline{\mathbf{M}})], \end{aligned} \tag{50}$$

where the regular quantities $\mathbf{\Omega}$ and M are defined for the value j, l of the arguments; the underlined ones are defined for $j+1, l$; those with a prime are defined for j, l'; the ones which are simultaneously underlined and have a prime are defined for $j + 1, l'$.

According to the analysis performed in Section 2.3 it is necessary to add to the Lagrangian (50) the gauge Lagrangian $\mathcal{L}_{ga}$ generalizing (17) in the case of a finite time step

$$\Delta\mathcal{L}_{ga} = s[(\mathbf{\Omega} \cdot \mathbf{M})^2 - (\underline{\mathbf{\Omega}} \cdot \underline{\mathbf{M}})(\mathbf{\Omega} \cdot \mathbf{M})] + \Delta Js^2 \sum_{l' \in \langle l \rangle} [(\underline{\mathbf{\Omega}} \cdot \underline{\mathbf{M}})(\mathbf{\Omega} \cdot \mathbf{M}) + (\mathbf{\Omega} \cdot \mathbf{M})(\mathbf{\Omega}' \cdot \mathbf{M}')]. \tag{51}$$

This Lagrangian $\mathcal{L}_{ga}$ cancels most of the interaction between the $\mathbf{\Omega}$ and $\mathbf{M}$ fields.

In this step we can change to the $q = (\omega, \mathbf{k})$ representation

$$\begin{aligned} \mathbf{X}(q)) &= \sqrt{2/N_t} \sum_{j,l} \exp(ib\mathbf{k} \cdot \mathbf{1} - i\Delta\omega j)\mathbf{X}(j, l), \\ \omega &= 2\pi T j, \qquad \mathbf{k} = (2\pi m_a/bN_a, 2\pi m_b/bN_b), \end{aligned} \tag{52}$$

where $N_t = N_\tau N_s$, $-(N_\tau - 1)/2 < j < (N_\tau - 1)/2$, and $-(N_{a,b} - 1)/2 < m_{a,b} < (N_{a,b} - 1)/2$, we choose N_τ, N_a, and N_b as odd numbers, $N_s = N_a N_b$ is the number of sites on one sublattice, and j, m_a, m_b are natural numbers.

Now one can write the action in the form $A(\mathbf{\Omega}, \mathbf{M}) = \sum_q \mathcal{L}_{quad}(q)$ where the Lagrangian $\mathcal{L}_{quad}(q)$ is given in (19) but the matrix $\hat{\Lambda}(q)$ acting on $\mathbf{X}_q = (\mathbf{\Omega}_q, \mathbf{M}_q)$ is now different

$$\begin{aligned} \hat{\Lambda}(q) &= \begin{pmatrix} \Lambda^{\Omega}(q), & \Lambda^{u}(q) \\ -\Lambda^{u}(q), & \Lambda^{M}(q) \end{pmatrix}, & c_\omega &= \cos(\omega\Delta) \\ & & s_\omega &= \sin(\omega\Delta) \\ \Lambda^{M}(q) &= u_\omega + \Delta\mathcal{J}(c_\omega + \gamma_{\mathbf{k}}), & \Lambda^{u}(q) &= s_\omega(1 - \Delta\mathcal{J}), \\ \Lambda^{\Omega}(q) &= u_\omega + \Delta\mathcal{J}(c_\omega - \gamma_{\mathbf{k}}) + \Delta\mu_0^2/2\mathcal{J}, & u_\omega &= 1 - c_\omega. \end{aligned} \tag{53}$$

Inverting the matrix $\hat{\Lambda}(q)$ we get the GF generalizing (20) in the case of a finite time step Δ

$$\begin{aligned} \hat{G}_q &= \frac{1}{2s\bar{L}(q)} \begin{pmatrix} \Lambda^{M}(q), & -\Lambda^{u}(q) \\ \Lambda^{u}(q), & \Lambda^{\Omega}(q) \end{pmatrix}, \\ \bar{L}(q) &\simeq \left(1 - \Delta\mathcal{J} + \Delta\mu_0^2/4\mathcal{J}\right)\left[2u_\omega + \Delta^2\omega_{0\mathbf{k}}^2\right], \end{aligned} \tag{54}$$

where the quantities $Q_{\mathbf{k}}$, $P'_{\mathbf{k}}$, and the bare frequency $\omega_{0\mathbf{k}}$ were defined in (20). At small ω when $\omega\Delta \ll 1$, if we neglect small terms of order $\Delta\mathcal{J}$ and $\Delta\mu_0^2/\mathcal{J}$, the matrices $\hat{\Lambda}(q)$ and $\hat{G}_q$ are replaced (up to normalization factors Δ and Δ^{-1}) by their continuum analogues (19) and (20).

Of course, the difference between the continuum expressions (19) and (20) for $\hat{\Lambda}(q)$ and $\hat{G}_q$ and the precise values (53) and (54) are only essential for the intermediate steps of the calculations. We want to stress that the amplitudes of the magnon scattering in the skeleton approximation are determined by the continuum action (18) and the continuum Green function (20) only.

At first we demonstrate that the simple calculation of the averages performed in Section 2.4 was not in fact done with the required accuracy. The result at low $T \ll \mathcal{J}$ is:

$$\begin{aligned} \langle M_i M_j \rangle &= \delta_{ij}(1 + c_0 - c_1)/4s, \\ \langle \underline{M}_i M_j \rangle &= \delta_{ij}(c_0 - c_1)/4s. \end{aligned} \tag{55}$$

This calculation was performed with formulae similar to (21), (25), and (27), but expression (54) was used for the GF $\hat{G}$, and summation over ω was restricted by N_τ terms. The tricks necessary to carry out the calculation are discussed in Appendix C. Notice, that the presence of the term u_ω in the numerator of the GF (54) leads to the difference of the underlined and non-underlined averages. This difference is due to the contribution of large $\omega \sim \pi/\Delta$. In particular the average $\langle \mathbf{M}_{tr}^2 \rangle$ calculated in (22) coincides in fact with the average $\langle \underline{\mathbf{M}}_{tr} \cdot \mathbf{M}_{tr} \rangle$ but the actual value of $\langle \mathbf{M}_{tr}^2 \rangle$ is different and differs from the result of (22) by the constant $(N - 1)/4s$. All other averages, $\langle \underline{M}_i M'_j \rangle$, $\langle \mathbf{\Omega}'_i \underline{M}_j \rangle$, $\langle \underline{\mathbf{\Omega}}_i \mathbf{\Omega}_j \rangle$, and so on, can be calculated in a similar manner. We stress that the result crucially depends on time τ or $\tau + \Delta$.

3.2. *Free Energy*

After the formulation of the theory for a finite time step Δ one can calculate the GPF and the free energy of the QAF in the paramagnetic phase. We can perform the calculation in the leading approximation in $1/2s$. The free energy has three contributions as it follows from Eq. (18) for the GPF Z: $F_{AF} = -T \ln(Z) = F_{\Omega M} + F_\lambda + F_{ga}$. In the lowest approximation in $1/2s$, $Z_{\Omega M}$, Z_λ, and Z_{ga} are powers of determinants. The explicit form of these determinants follows from (50), (53), and

(51) and (30) and (31)

$$F_{\Omega M} = \frac{TNN_s}{2}\sum_{\omega\mathbf{k}} \ln[\bar{L}(q)],$$
$$F_{ga} = -\frac{TN_s}{2}\sum_{\omega\mathbf{k}} \ln[2s\bar{Q}(q)], \qquad F_{\lambda} = \frac{TN_s}{2}\sum_{\omega\mathbf{k}} \ln[s^2\Pi_0(q)], \tag{56}$$

where all notation was given in (53). Let us consider these three free energies separately. One can check that $F_{\Omega M}$ has a finite limit when $\Delta \to 0$, $\Delta N_\tau = \beta$. F_{ga} and F_λ do not have finite limits when $\Delta \to 0$, $\Delta N_\tau = \beta$ separately, but their sum has a finite limit.

Consider at first F_λ. It may be written in the form $F_\lambda = F_{\lambda l} + F_{\lambda h}$,

$$F_{\lambda l} = \frac{TN_s}{2}\sum_{\omega\mathbf{k}} \ln[\Pi_n(q)], \qquad F_{\lambda h} = \frac{TN_s}{2}\sum_{\omega\mathbf{k}} \ln[s^2\Pi_\infty(q)],$$

where $\Pi_n(q) = \Pi_0(q)/\Pi_\infty(q)$, $\Pi_\infty(q) = 4G^{\mathbf{\Omega}}(q)$ is the polarization operator at large frequencies $\omega \gg T$ (33) and the GF $G^{\mathbf{\Omega}}(q)$ is taken from Eq. (54). The summation over ω in the equation for $F_{\lambda l}$ is convergent because the function $\ln[\Pi_n(q)]$ tends to zero at large frequencies ω as $1/\omega^2$. Therefore the summation over ω can be extended to infinity in the limit $\Delta \to 0$. It is reasonable to combine the free energy $F_{\lambda h}$ with F_{ga}

$$\delta F = F_{\lambda h} + F_{ga} = \frac{TN_s}{2}\sum_{\omega\mathbf{k}} \ln[2sG^{\mathbf{\Omega}}(q)/\tilde{Q}(q))] = -\frac{TN_s}{2}\sum_{\omega\mathbf{k}} \ln[\bar{L}(q)] = -\frac{1}{N}F_{\Omega M}. \tag{57}$$

The summation over the frequencies ω for $F_{\Omega M}$ can be performed as in [21] and we have the total free energy $F_{AF} = ((N-1)/N)F_{\Omega M} + F_{\lambda l}$, where $F_{\Omega M}$ and $F_{\lambda l}$ are

$$F_{\Omega M} = -NN_s\mathcal{J}/2 + NN_s\sum_{\mathbf{k}}\{\omega_{0\mathbf{k}}/2 + T\ln[1-\exp(-\omega_{0\mathbf{k}}/T)]\},$$
$$F_{\lambda l} = \frac{TN_s}{2}\sum_{\omega\mathbf{k}} \ln\left[\frac{s\left(\omega^2+\omega_{0\mathbf{k}}^2\right)\Pi_0(q)}{2\mathcal{J}(1+\gamma_{\mathbf{k}})}\right], \tag{58}$$

where the polarization operator $\Pi_0(q)$ is defined in (32). In this formula we neglect a small contribution of the order $\mu^2/\mathcal{J}^2$.

The first term in the free energy F_{AF} represents the free energy of the ordered antiferromagnet, which consists of the ground state energy and the free energy of the magnon gas with two degenerate degrees of freedom.

The temperature dependent part of the free energy (58) at low temperatures $T \ll \mathcal{J}$ is proportional to $F_{AF} \approx N_s T^3/\mathcal{J}$. This contribution has two origins: one from $F_{\Omega M}$ and the other one from $F_{\lambda l}$.

3.3. *Perturbative Corrections*

In this section we present the result of the calculation of corrections to the mass operators of the $\mathbf{\Omega}$ and $\mathbf{M}$ fields. The detailed analysis of such corrections is far beyond the scope of this paper. We restrict ourselves to the lowest order of perturbation theory in $1/2s$. In this case these corrections can be presented as a renormalization of the initial quadratic Lagrangian (50). It is necessary to have the Lagrangian $\mathcal{L}_{mod}$ and the Hamiltonian $\mathcal{H}$ up to fourth order in the field $\mathbf{M}$ and the Lagrangian $\mathcal{L}_{pha}$ up to third order.

From Eq. (46) for $\mathcal{L}_{mod}$ we have

$$\Delta\mathcal{L}^{(4)}_{mod} = s\{2K^2 - (\mathbf{M}^2)^2 - \mathbf{M}^2\underline{\mathbf{M}}^2 + 2K(\mathbf{M}^2 + \underline{\mathbf{M}}^2 - 2\mathbf{M}\cdot\underline{\mathbf{M}}) - 2(\mathbf{\Omega}\cdot\underline{\mathbf{M}} - \underline{\mathbf{\Omega}}\cdot\mathbf{M})^2\}/8, \quad K = 1 - \mathbf{\Omega}\cdot\underline{\mathbf{\Omega}}. \tag{59}$$

From Eq. (47) for $\mathcal{L}_{pha}$ we have

$$\Delta\mathcal{L}^{(3)}_{pha} = isU[(\mathbf{\Omega}\cdot\underline{\mathbf{M}})\underline{\mathbf{M}}^2 - (\underline{\mathbf{\Omega}}\cdot\mathbf{M})\mathbf{M}^2 - 2U(1-K)(\mathbf{\Omega}\cdot\underline{\mathbf{M}} - \underline{\mathbf{\Omega}}\cdot\mathbf{M})(\mathbf{M}^2 + \underline{\mathbf{M}}^2 - 2(\mathbf{M}\cdot\underline{\mathbf{M}}))]/2 + 2isU^3(\mathbf{\Omega}\cdot\underline{\mathbf{M}} - \underline{\mathbf{\Omega}}\cdot\mathbf{M})^3/8, \quad U = (1 + \mathbf{\Omega}\cdot\underline{\mathbf{\Omega}})^{-1}. \tag{60}$$

The expression for the Hamiltonian $\mathcal{H}$ (48) depends on the scalar products of the fields $\mathbf{\Omega}$, $\underline{\mathbf{\Omega}}$, $\mathbf{\Omega}'$, $\underline{\mathbf{\Omega}}'$, $\mathbf{M}$, $\underline{\mathbf{M}}$, $\mathbf{M}'$, $\underline{\mathbf{M}}'$. The term of fourth order in $\mathbf{M}$ is rather cumbersome and we will not present its explicit form. We only note that its evaluation is a purely algebraic technical problem. For its derivation it is enough to substitute the expression (9) for the vectors $\mathbf{n}_{a,b}$ in Eq. (49) for the matrix element of the spin operator $\hat{\mathbf{S}}$. After that the result must be substituted into the expression for the Hamiltonian $\mathcal{H}$ (48). After expanding this expression in powers of the field $\mathbf{M}$ up to fourth order we get $\mathcal{H}^{(4)}$.

At this step one can perform the averaging of the Lagrangians $\mathcal{L}^{(4)}_{mod}$, $\mathcal{L}^{(3)}_{pha}$, and the Hamiltonian $\mathcal{H}^{(4)}$ over the fields $\mathbf{\Omega}$ and $\mathbf{M}$. We observe that the averaging of the fourth and higher powers of the $\mathbf{\Omega}$ field is a little more sophisticated. It requires taking into account the fluctuation of the λ field in the skeleton approximation. To avoid this complication we have given the result in the $1/N$ approximation where this complication is not essential.

The effective kinetic Lagrangian and the Hamiltonian in the leading approximation in $1/2s$ are

$$\begin{aligned}\Delta\mathcal{L}_{kin} &= s[a_0(1 - \mathbf{\Omega}\cdot\underline{\mathbf{\Omega}}) + b_0(\mathbf{M}^2 - \mathbf{M}\cdot\underline{\mathbf{M}}) - ie_0(\mathbf{\Omega}\cdot\underline{\mathbf{M}} - \underline{\mathbf{\Omega}}\cdot\mathbf{M})],\\ \mathcal{H} &= Js^2\sum_{l'\in\langle l\rangle}[a_1(1 - \mathbf{\Omega}\cdot\underline{\mathbf{\Omega}}) + a_2(1 - \mathbf{\Omega}\cdot\mathbf{\Omega}') + a_3(1 - \mathbf{\Omega}'\cdot\underline{\mathbf{\Omega}}) + b_1\mathbf{M}^2 + b_2\mathbf{M}\cdot\underline{\mathbf{M}}\\ &\quad + b_3\mathbf{M}\cdot\mathbf{M}' + b_4\mathbf{M}'\cdot\underline{\mathbf{M}} - ie_1(\mathbf{\Omega}\cdot\underline{\mathbf{M}} - \underline{\mathbf{\Omega}}\cdot\mathbf{M}) - ie_2(\mathbf{\Omega}'\cdot\underline{\mathbf{M}} - \underline{\mathbf{\Omega}}\cdot\mathbf{M}')],\end{aligned} \tag{61}$$

where the notation is the same as in (50), and the constants $a_0, \ldots, e_2$ are

$$\begin{aligned}&a_i = a_i^0 + g\alpha_i, \qquad b_i = b_i^0 + g\beta_i, \qquad e_i = e_i^0 + g\gamma_i,\\ &a_0^0 = 1, \qquad b_0^0 = 1, \qquad e_0^0 = 1, \qquad a_1^0 = -1,\\ &a_2^0 = 1, \qquad a_3^0 = 0, \qquad b_1^0 = 0, \qquad b_2^0 = 1, \qquad b_3^0 = 1, \qquad b_4^0 = 0,\\ &e_1^0 = -1, \qquad e_2^0 = 0, \qquad \alpha_0 = 2, \qquad \beta_0 = (3 - c_0 + c_1)/2,\\ &\gamma_0 = (7 - c_0 + c_1)/4, \qquad \alpha_1 = 2(1 + c_1 - c_2),\\ &\alpha_2 = 3 + 8/\pi^2 - 3c_0 + 2c_1 + c_2,\\ &\alpha_3 = -4/\pi^2 + 2c_0 - 2c_1 - c_2,\\ &\beta_1 = (5 - 12/\pi^2 + c_1 - c_2)/2,\\ &\beta_2 = (-4 + 8/\pi^2 + c_0 - 5c_1 + 4c_2)/2,\\ &\beta_3 = (2 - 24/\pi^2 - 3c_0 + c_1 + 2c_2)/2, \qquad \gamma_2 = 1,\\ &\beta_4 = 3/\pi^2, \qquad \gamma_1 = (-6 + 16/\pi^2 + 9c_0 - c_1 - 8c_2)/4,\end{aligned} \tag{62}$$

where $g=(N-1)/4s$, $i:=0,1,2,3$. The reason why the number of the components N enters in the effective coupling constant as $N-1$ is as follows. The short range fluctuations are directed perpendicularly to the long wave fluctuations and their number of independent components is $N-1$.

Now one can write out the effective quadratic form for the Lagrangian (61) in the ω, $\mathbf{k}$ representation and find the GF which can be given in the form (54) with the quantities $\Lambda^i(q)$ for $i:=\mathbf{\Omega}, M, u, d$ obtained from Eq. (61),

$$\begin{aligned}\bar{L}(q) &= \left(e_0^2+\Delta\mathcal{J}x_1\right)\left[2(u_\omega)+u_\omega^2\Delta\mathcal{J}x_2+\Delta^2\omega_{\mathbf{k}}^2\right],\\ \omega_{\mathbf{k}}^2 &= \mathcal{J}^2\left[e_0^{-2}a_{23}(1-\gamma_{\mathbf{k}})+\mu^2/(\mathcal{J}^2b_{1234})\right](b_{12}+b_{34}\gamma_{\mathbf{k}}),\end{aligned} \tag{63}$$

where $a_{ij}=a_i+a_j$, $b_{ij}=b_i+b_j$, $b_{1234}=b_{12}+b_{34}$, and the explicit form of the coefficients x_1, x_2 follows from (61). From (9), (54), and (63) one can find the spin correlation function up to this order in $1/2s$. For that it is necessary to take into account nonlinear corrections to Eq. (37) which follow from (9) and also corrections to the GF in the framework of this formula.

We shall give the explicit result for the correlation radius up to this order in $1/2s$ on the basis of Eq. (27). The contribution of different frequencies ω and momenta $\mathbf{k}$ in this BC relation can be separated into two parts. The first part is the high frequency and momentum part. To calculate this contribution it is enough to take the GF $G^{\Omega}(q)$ in the bare approximation (54) because this contribution is of the order $1/2s$. The second contribution which is proportional to the distribution function $n_{\mathbf{k}}$ can be considered in the continuum approximation but with $1/2s$ corrections taken into account,

$$G^{\Omega}(q)\simeq\frac{1}{2a^2\Delta}\frac{\chi_\perp^{-1}}{\omega^2+\omega_{\mathbf{k}}^2},\qquad \omega_{\mathbf{k}}^2=c_s^2\mathbf{k}^2+\mu^2, \tag{64}$$

where $c_s^2=e_0^{-2}a_{23}b_{1234}\mathcal{J}^2a^2/x$, $\chi_\perp=\bar{\rho}_s/c_s^2$, and $\bar{\rho}_s=Js^2a_{23}$. Now, instead of Eq. (27) we have

$$(N/4s\bar{\rho}_s)\sum_{\mathbf{k}}\frac{n_{\mathbf{k}}}{\omega_{\mathbf{k}}}=R,\qquad R=1-g(1+c_0+c_1). \tag{65}$$

The factor R includes the direct SW renormalizations. Performing the integration in the same manner as in (28) we have

$$\mu=T\exp(-2\pi\rho_s/TN),\qquad \rho_s=\tilde{\rho}_sR,\qquad \xi=\hbar c_s/\mu. \tag{66}$$

The actual temperature dependence of the factor in front of the exponential changes ($T\to\mathcal{J}$) if we take into account the LW fluctuations in the next order in $1/N$ [12].

4. SEPARATION OF SCALES: DESCRIPTION OF LONG-WAVE FLUCTUATIONS

When the correlation length ξ is much larger than the lattice constant a one can separate the LW and SW spin fluctuations. If we are interested in the LW spin fluctuations we can construct an effective LW theory with some cut-off. In our case this theory is the sigma model (see for example [12]). The LW theory with a cut-off is well defined at least in the sense of perturbation theory but the results depend on this cut-off. This dependence on the cut-off is totally artificial. It may be absorbed into some observable quantities. It is not easy to consistently perform this program if the theory is nonrenormalizable as in our case. Another option is to take into account additional contributions to the LW theory which cancel the dependece on the cut-off and introduce the dependence on the

observable quantities or on natural parameters of the theory such as the exchange constant J. Our treatment of this problem has a qualitative character and we only sketch a possible approach to it.

The fluctuations of the M field are SW and the GF $G^M(q)$, $G^{u,d}(q)$ are regular in the LW limit. Therefore the separation of scales is actually important for the $\mathbf{\Omega}$ field or the GF $G^{\Omega}(q)$. This dressed GF $G^{\Omega}(q)$ determines the action of the LW sigma model. This action is universal and can easily be obtained from the SR Lagrangian (43) or from the GF (54) by the naive LW limit [4]

$$\mathcal{L}_{cont} = \frac{\chi_{\perp}}{2}\left[\dot{\mathbf{n}}^2 + c_s^2(\partial_i \mathbf{n} \cdot \partial_i \mathbf{n}) + \mu^2 \mathbf{n}^2\right] + i\lambda(\mathbf{n}^2 - 1), \tag{67}$$

where ∂_i is the space derivative for $i := x, y$. At the characteristic low-energy scale, the mass of the Ω field μ is much less than the exchange constant J and the LW AF fluctuations contain many universal properties [12]. The connection of the constants which determine these universal properties with parameters of the original Heisenberg model was obtained not in a direct manner but by some calculations in the ordered phase [13, 16].

We will use the scale separation based on some sort of Pauli–Villars transformation because it is well defined in comparison with the scale separation in $\mathbf{k}$ space. Suppose that we have some theory for the field φ. The GF $\hat{G}$ of the field φ can be separated into two parts $\hat{G} = \hat{G}_1 + \hat{G}_2$, which correspond to two new fields $\varphi_{1,2}$. The interaction $V(\varphi)$ changes into $V(\varphi_1 + \varphi_2)$. This transformation can be perfomed in a precise manner. Let us choose $\hat{G} = p^{-2}$ and $\hat{G}_1 = (p^2(1 + p^2/\Lambda^2))^{-1}$, $\hat{G}_2 = (p^2 + \Lambda^2)^{-1}$. The achieved splitting of the Green function of a scalar field φ into two parts provides the scale separation because the field φ_1 is dominant at small p and the field φ_2 at large p.

Let us apply this method to the Lagrangian $\mathcal{L}_{tot}$ (45). The field $\mathbf{\Omega}$ may be written as a sum of two new fields $\mathbf{n}$ and $\mathbf{v}$: $\mathbf{\Omega} = \mathbf{n} + \mathbf{v}$. The operators $\hat{G} \equiv \hat{G}^{\Omega}(q)$, $\hat{G}_1 \equiv \hat{G}^{n}(q)$, and $\hat{G}_2 \equiv \hat{G}^{v}(q)$, in this case in the (ω, k) representation, may be chosen in the form (53), (54)

$$\begin{aligned} G^{\Omega}(q) &= \Lambda^M(q)/2s\bar{L}(q) \equiv F(q)/\bar{L}(q), \\ \tilde{L}(q) &= 2u_{\omega} + \Delta^2\omega_{0\mathbf{k}}^2, \qquad F(q) = [u_{\omega} + \Delta\mathcal{J}(1 + \gamma_{\mathbf{k}})]/2s, \\ G^{n}(q) &= \frac{F(q)\Lambda^2}{\tilde{L}(q)(\Lambda^2 + \tilde{L}(q))}, \qquad G^{v}(q) = \frac{F(q)}{\Lambda^2 + \tilde{L}(q)}, \end{aligned} \tag{68}$$

where the primary dispersion law $\omega_{0\mathbf{k}}$ is defined in (20). We omit in (68) some small terms of the order Δ which can be essential only for the calculation of the primary free energy (3.2). We assume that $\max(T, \mu) \ll \Lambda \ll \mathcal{J}$. Only in this case the cut-off momentum Λ has a clear meaning.

The fluctuations of the field $\mathbf{n}$ are of LW and low frequency (LF) type. This leads to the rapid decrease of the GF $G^n(q)$ with an increase of the three-dimensional momentum $q = (\omega, c_s\mathbf{k})$, $q^2 = \omega^2 + c_s^2\mathbf{k}^2$. As a result, the Lagrangian $\mathcal{L}_{\Omega\lambda}$ reduces to $\mathcal{L}_{n\nu\lambda}$ and has the form

$$\mathcal{L}_{n\nu\lambda} = [s/2\mathcal{J}\Lambda^2][\mathbf{n} \cdot (\hat{q}^2 + \mu^2)(\Lambda^2 + \hat{q}^2)\mathbf{n}] + [\mathbf{v} \cdot (1/2F(\hat{q})(\Lambda^2 + \tilde{L}(\hat{q}))\mathbf{v}] + i\lambda(\mathbf{n} + \mathbf{v})^2. \tag{69}$$

The LW and the LF fluctuations of the field $\mathbf{v}$ are suppressed due to its big mass Λ, and only the LW and LF fluctuations of the fields Ω and λ are essential. One can check that the LW theory for the fields Ω and λ does not contain practically any ultraviolet divergencies due to the cut-off Λ. Actually the GF of the λ field is determined by the polarization operator $\Pi_0(q)$ (33) and in the continuum limit has the form

$$G^{\lambda}(q) = (\Pi_0(q))^{-1} = sq^2/4\mathcal{J}, \qquad q \geq k_T. \tag{70}$$

Now we have the following large momentum behavior of the elements of the diagram technique

$G^n(q) \sim q^{-4}$, $G^\lambda(q) \sim q^2$, and $\Gamma(q) \sim q^0$, where $\Gamma(q)$ is the vertex. The only divergent diagram is the diagram for the mass operator in the lowest order but it is naturally subtracted once [14] and after that it is convergent. The next order of perturbation theory leads to (a) two additional GF $G^n(q)$, (b) additional GF $G^\lambda(q)$, (c) additional vertex $\Gamma(q)$, and (d) additional integration over q. As a result we have the renormalization factor $R(q) = (G^n(q))^2 G^\lambda(q)\Gamma(q)q^3 \sim q^{-3}$ and the general convergence is improved. This means that the Pauli–Villars regularization is working. It is necessary to stress that without the regularization factor $\Lambda^2/(q^2+\Lambda^2)$ in the **n** field GF we have $R \sim q$. This means that the original long-wave and low frequency theory is unrenormalizable, and it is not possible to include all divergences in the finite number of objects of the theory. Of course, the parameter Λ is artificial and must be canceled when we calculate any observable properties due to the compensation of the dependence on Λ from long-wave and short-wave contributions.

Let us demonstrate how this scheme works for the example of the BC of the theory $\langle \mathbf{\Omega}^2 \rangle = 1$. Substituting $\mathbf{\Omega} = \mathbf{n} + \mathbf{v}$ we have $\langle \mathbf{n}^2 \rangle = 1 - \langle \mathbf{v}^2 \rangle$ and

$$\begin{aligned} \langle \mathbf{n}^2 \rangle &= N \sum_q G^n(q) \equiv NT \sum_{\omega - 2\pi jT} \sum_{\mathbf{k}} G^n(q) \\ \langle \mathbf{v}^2 \rangle &= N \sum_q G_v(q) \equiv N \lim_{\Delta \to 0} \int_{-\pi/\Delta}^{\pi/\Delta} \frac{d\omega}{2\pi} \sum_{\mathbf{k}} G_v(q), \end{aligned} \tag{71}$$

where GF $G^n(q)$ and $G_v(q)$ are defined in Eq. (68), and the continuum form of the GF $G^n(q)$ follows from (69). Here the summation over j for the GF $G^n(q)$ is performed in the limits $\pm\infty$. The main contributions in the integrals in (71) arising from the Green function G^n come from momenta $\mathbf{k} \le \Lambda$ and those arising from the GF G^v come from momenta $\mathbf{k} \ge \Lambda$. The left hand side of Eq. (71) can be calculated if we reformulate accurately the summation over the frequencies $\omega = 2\pi j$ and the integration over the momentum $\mathbf{k}$ can be extended to infinity (see [2, 12]). When we calculate the right hand side of Eq. (71) we can put the temperature T equal to zero and replace the summation over ω by an integration and the integration over ω can be easily performed. The integration over $\mathbf{k}$ can be performed treating $\Lambda/\mathcal{J} \ll 1$ as a small parameter. In the part of the integral depending on Λ, the integration over $\mathbf{k}$ can be extended to infinity. The other part is independent of Λ and can be calculated in the same manner as the constant c_{M0} in Eq. (22). As a result, the BC has the form

$$\frac{N}{4\pi J s^2}\left(\Lambda + 2T \ln\left(\frac{\mu}{T}\right)\right) = 1 + \frac{N\Lambda}{4\pi J s^2} - \frac{N}{4s}(1 + c_0 - c_1).$$

We can see that the dependence on Λ is canceled in both sides of the BC and for μ we obtain expression (29) if we take into account the leading order contribution in $1/2s$.

We have demonstrated some general properties of the QAF with separation of scales $\xi \ll a$. The role of the classical and quantum spin fluctuations is essentially different. The separation of the spin fluctuation into quantum and classical ones in perturbation theory is determined by the summation over the frequencies ω. The Sommerfeld–Watson transformation gives us the characteristic contributions proportional to $1 + 2n(\mathbf{k})$, where $n(\mathbf{k})$ is the Planck distribution function, and determines the separation of fluctuations. The quantum fluctuations are independent from the temperature T. From the point of view of the LW theory the quantum fluctuations are divergent in the ultraviolet region. The main contribution to the quantum fluctuations comes from the region in the momentum space $ka \sim 1$. The contributions of the order $k \sim \Lambda$ are small. Actually the second term in the right hand side of the BC is lower than the last one by the small parameter $\hbar c_s \Lambda/\mathcal{J}$. This illustrates the idea that the quantum fluctuations in the LW region are not essential and can be neglected. In this LW region only the classical fluctuations with the Planck distribution function are essential. In this way we arrive at the "renormalized classical region"

picture [8, 12] for the classical fluctuations. The classical LW fluctuations possesses some nice properties.

(1) They are convergent in the ultraviolet region due to a natural cut-off at $k \sim k_T$ due to the Planck functions.

(2) The parameters which determine these fluctuations are the renormalized $\rho_s, c_s^2, \chi_\perp = \rho_s/c_s^2$ that enter in the action (67).

The previous discussion clarifies the formula (66) for the mass μ of the Ω field: all the quantum renormalizations are included in the renormalized spin stiffness ρ_s.

Whether this result remains valid in higher order of $1/N$ is an open question because the interaction between the LW $\mathbf{n}$ and the λ fields is not renormalizable. In the recent paper of Hasenfratz [17] there is a direct confirmation of this point of view.

5. DISCUSSION

Our approach to the theory of the QAF is based on an explicitly rotational invariant formulation of the path integral in terms of the spin coherent states. A nontrivial choice of variables enables the formulation of the theory on the basis of the saddle point approximation for the fields $\mathbf{\Omega}$, $\mathbf{M}$, and λ. As a result we were able to obtain the spin fluctuations at short and at long distances, and for short and long times. This is the main result of the present paper.

We have worked out the method of construction of perturbation theory in relation to this saddle point. This program is not trivial because it requires taking an accurate limit when the time step Δ tends to zero. This permits developing a theory which in some sense is similar to the spin wave theory for the calculation of the short distance and short time fluctuations and is similar to the sigma model when we consider long distance and long time fluctuations. We have obtained the free energy and the first corrections to the Green functions of the theory.

We have performed the separation of scales with the help of Pauli–Villars transformation. This permits us to separate out the quantum and the thermal fluctuations. The quantum fluctuations are short waves and the thermal fluctuations are long waves. The fluctuations of the Largrange multiplier λ contain short wave as well as long wave contributions.

We believe that the present approach to the QAF will be fruitful in the theory of the AF fluctuations in HTSC superconductors.

A. INVARIANT COHERENT STATES FOR THE ROTATIONAL GROUP

A.1. *Transformation Properties of the Spin Coherent States*

At first we discuss why the Lagrangian (4) is not explicitly rotational invariant, although the physical problem related to the Heisenberg Hamiltonian (1) possesses obvious rotational symmetry. The reason lies in the transformation properties of the state $|z\rangle$ under rotations. For further discussion it is more convenient to use the state $|\mathbf{n}\rangle$ which coincides with the state $|z\rangle$ up to a phase factor $\exp(is\varphi)$ [11, 18]

$$|\mathbf{n}\rangle = \exp(-i\varphi\hat{S}_z)\exp(-i\theta\hat{S}_y)\,|ref\rangle. \tag{72}$$

In Eq. (72) it is assumed that the complex number z and the unit vector $\mathbf{n}$ are connected by the relation $z = \tan(\theta/2)\exp(i\varphi)$. One can easily check that the state $|\mathbf{n}\rangle$ satisfies the equation

$$(\hat{\mathbf{S}}\cdot\mathbf{n})|\mathbf{n}\rangle = s|\mathbf{n}\rangle. \tag{73}$$

We may consider Eq. (72) as a solution of Eq. (73). Although Eq. (73) is explicitly rotational invariant, its solution is not. This circumstance was clarified by Perelomov in [10] where the coherent states for an arbitrary Lee group were introduced. The rotational group has three parameters: the Euler angles φ, θ, and ψ. However, a point on the sphere is parameterized by two parameters φ, θ only. Due to this circumstance there is an invariance up the phase factor

$$|\mathbf{n}'\rangle = \exp(i\Phi(\mathbf{n}, \hat{a}))\hat{U}(\hat{a})|\mathbf{n}\rangle, \qquad n_i = a_{ij}n_j. \tag{74}$$

Here $\hat{a}$ is the 3×3 orthogonal matrix of the three-dimensional rotations; $\Phi(\mathbf{n}, \hat{a})$ is the phase function which depends on the vector $\mathbf{n}$ and the matrix $\hat{a}$; $\hat{U}(\hat{a})$ is the operator (matrix) of the $2s+1$ dimensional representation of the rotation $\hat{a}$. The situation with respect to the invariance under three-dimensional rotations is clarified by Eq. (74). The vector $|\mathbf{n}\rangle$ is not invariant but the projector $|\mathbf{n}\rangle\langle\mathbf{n}|$ is invariant. Now it is obvious why the total action and the partition function are invariant under rotations. Notice that the invariance of the measure of integration over z is obvious if we change the variable to $\mathbf{n}$. However, the kinetic part of the Lagrangian $\mathcal{L}_{kin}(j, \mathbf{n})$ is not invariant under rotations

$$\Delta\mathcal{L}_{kin}(j, \mathbf{n}) \Rightarrow \Delta\mathcal{L}_{kin}(j, \mathbf{n}) - i\Phi(\mathbf{n}_j) + i\Phi(\mathbf{n}_{j+1}). \tag{75}$$

The transformation (75) is a kind of Abelian lattice gauge field transformation.

From this discussion it is obvious that the modulus of the scalar product of two states $|\mathbf{n}\rangle$ and $|\underline{\mathbf{n}}\rangle$ is an invariant under rotations

$$|\langle\underline{\mathbf{n}}|\mathbf{n}\rangle| = [(1 + \underline{\mathbf{n}} \cdot \mathbf{n})/2]^s. \tag{76}$$

A nontrivial scalar, vector, tensor, etc. under rotations is, in general, determined by the ratio

$$A_{ij\ldots} = \langle\underline{\mathbf{n}}|\hat{A}_{ij\ldots}|\mathbf{n}\rangle/\langle\underline{\mathbf{n}}|\mathbf{n}\rangle, \tag{77}$$

where $\hat{A}_{ij\ldots}$ is a tensor operator acting on the spin Hilbert space. When a rotation is performed the additional phase factors from the numerator and the denominator cancel each other. One obtains an invariant vector if one takes $\hat{\mathbf{S}}$ for $\hat{A}_{ij\ldots}$ (see Eq. (49)).

A.2. *Invariant Coherent States*

It seems that the noninvariance under rotations of the spin coherent states $|\mathbf{n}\rangle$ is an intrinsic property of them. However, it is possible to define formally invariant states if we introduce some additional unit vector $\mathbf{m}$, $\mathbf{m}^2 = 1$ which is orthogonal to the vector $\mathbf{n}$, $\mathbf{n} \cdot \mathbf{m} = 0$. Together with the vector $\mathbf{k} = [\mathbf{n} \times \mathbf{m}]$, these unit vectors determine a reference frame. One can determine the components of these unit vectors in the initial reference frame: $\mathbf{m}_0 = (1, 0, 0)$, $\mathbf{k}_0 = (0, 1, 0)$, $\mathbf{n}_0 = (0, 0, 1)$. Instead of the transformation (72) which defines the state $|\mathbf{n}\rangle$ we define the state $|\mathbf{n}; \mathbf{m}\rangle$ with the help of the general rotation from the reference state

$$|\mathbf{n}; \mathbf{m}\rangle = e^{-i\varphi\hat{S}_z}e^{-i\theta\hat{S}_y}e^{-i\psi\hat{S}_z}|ref\rangle. \tag{78}$$

Due to our choice of reference state $|ref\rangle = |ss\rangle$ the last exponential operator in (78) is in fact a numerical factor. One can easily find that $\tan\psi = -k_z/m_z$. For that it is sufficient to find the three-dimensional matrix which rotates the vectors $\mathbf{n}_0, \mathbf{m}_0$ into the vectors $\mathbf{n}, \mathbf{m}$.

Now one can find the Lagrangian $\mathcal{L}_{kin}(j, \mathbf{n})$ which is simply given by

$$\Delta\mathcal{L}_{kin}(j, \mathbf{n}) = -\ln(\langle\underline{\mathbf{n}}; \underline{\mathbf{m}}|\mathbf{n}; \mathbf{m}\rangle), \tag{79}$$

where we use the notation $\underline{x} \equiv x(j+1)$, $x \equiv x(j)$. It is convenient to separate the Lagrangian $\mathcal{L}_{kin}$ into its real and imaginary parts, $\mathcal{L}_{kin} = \mathcal{L}_{mod} + i\mathcal{L}_{pha}$,

$$\begin{aligned} \langle \underline{\mathbf{n}}; \underline{\mathbf{m}} | \mathbf{n}; \mathbf{m} \rangle &= [(1 + \underline{\mathbf{n}} \cdot \mathbf{n})/2]^s Y(\underline{\mathbf{n}}, \underline{\mathbf{m}}, \mathbf{n}, \mathbf{m}), \\ \Delta\mathcal{L}_{mod} &= -s \ln[(1 + \underline{\mathbf{n}} \cdot \mathbf{n})/2)], \\ \Delta\mathcal{L}_{pha} &= i \ln(Y(\underline{\mathbf{n}}, \underline{\mathbf{m}}, \mathbf{n}, \mathbf{m})), \end{aligned} \tag{80}$$

where $|Y(\underline{\mathbf{n}}, \underline{\mathbf{m}}, \mathbf{n}, \mathbf{m})| = 1$. Thus, according to Eq. (76), Y is a pure phase factor.

The explicit form of Y can be found from Eq. (78) in terms of the Euler angles

$$Y^2 = \exp(is(\underline{\psi} - \psi))\langle ref| \exp(i\underline{\theta}\hat{S}_y) \exp(i(\underline{\varphi} - \varphi)\hat{S}_z) \exp(-i\theta\hat{S}_y)|ref\rangle/(H.C.). \tag{81}$$

The matrix element in (81) can be calculated using Wigner d-functions [11, 19] or with the help of the z-representation of the spin coherent state [11, 18], $Y = \underline{P}^*_{\psi} P_{\psi} \underline{P}^*_{\varphi} P_{\varphi} P_n$, where

$$\begin{aligned} P_{\varphi} &= \left(\frac{n_x - in_y}{n_x + in_y}\right)^{s/2}, \qquad P_{\psi} = \left(\frac{m_z + ik_z}{m_z - ik_z}\right)^{s/2}, \\ P_n &= [(1 + \underline{\mathbf{n}} \cdot \mathbf{n} + \underline{n}_z + n_z + i[\underline{\mathbf{n}} \times \mathbf{n}]_z)/H.C.]^s. \end{aligned} \tag{82}$$

The Y factor must be an invariant under rotations but this invariance is not obvious from the form (82). In fact Y is a function of the scalar products $\underline{\mathbf{n}} \cdot \mathbf{n}$, $\underline{\mathbf{n}} \cdot \mathbf{m}$, and $\underline{\mathbf{m}} \cdot \mathbf{k}$ so on. To find this function we shall use the following trick. We calculate the Y factor in a special reference frame where $\mathbf{m} = (1, 0, 0)$, $\mathbf{k} = (0, 1, 0)$, and $\mathbf{n} = (0, 0, 1)$. In this reference frame $P_{\psi} = P_{\varphi} = P_n = 1$ and $\underline{n}_x = \underline{\mathbf{n}} \cdot \mathbf{m}$, $\underline{\mathbf{n}}_y = \mathbf{n} \cdot \mathbf{k}$, $\underline{m}_z = \underline{\mathbf{m}} \cdot \mathbf{n}$, and $\underline{k}_z = \underline{\mathbf{k}} \cdot \mathbf{n}$. Finally we obtain for $\mathcal{L}_{pha}$ the expression

$$\Delta\mathcal{L}_{pha} = (is/2) \ln[R\underline{R}^*/R^*\underline{R}], \qquad R = \underline{\mathbf{n}} \cdot \mathbf{m} + i\underline{\mathbf{n}} \cdot \mathbf{k}. \tag{83}$$

In (83) and below we suppose that a double underlined quantity x corresponds to a nonunderlined quantity x. Another form for the Lagrangian $\mathcal{L}_{pha}$ can be obtained if one changes to the reference frame where $\mathbf{n} = (1, 0, 0)$, $\mathbf{k} = (0, 1, 0)$, and $\mathbf{m} = (0, 0, -1)$.

Now one can obtain an expression for the Lagrangian $\mathcal{L}_{kin}$ in the continuum limit. The magnitude of $\mathcal{L}_{mod}$ is a small quantity of the order Δ. Using the obvious decomposition $\underline{\mathbf{x}} \simeq \mathbf{x} + \Delta\dot{\mathbf{x}}$ for $\mathbf{x} := \mathbf{n}, \mathbf{m}, \mathbf{k}$ we get from (83) a simple expression for $\mathcal{L}_{pha}$

$$\mathcal{L}_{pha} = -s\mathbf{n} \cdot [\mathbf{m} \times \dot{\mathbf{m}}]. \tag{84}$$

We obtain the well-known form for $\mathcal{L}_{pha}$ if we choose $\mathbf{m} = (\mathbf{e}_z - n_z\mathbf{n})/\sqrt{1 - n_z^2}$, with $\mathbf{m}^2 = 1$, and $\mathbf{n} \cdot \mathbf{m} = 0$: $\mathcal{L}_{pha} = s(1 - \cos\theta)\dot{\varphi}$, where $\mathbf{e}_z$ is the unit vector along the z-axis.

B. INVARIANT LAGRANGIAN FOR THE QUANTUM ANTIFERROMAGNET

The invariant Lagrangian $\mathcal{L}_{mod}(\mathbf{n})$ and Hamiltonian $\mathcal{H}(\mathbf{n})$ were given in Eqs. (46) and (48) but the form of the Lagrangian $\mathcal{L}_{pha}(\mathbf{n})$ is more complicated and will be discussed in detail below.

The Lagrangian $\mathcal{L}_{pha}$ cannot be expressed in terms of the vectors $\mathbf{n}$ alone (83). Its expression also involves the vectors $\mathbf{m}$ and $\mathbf{k}$. These vectors are expressed in terms of the vectors $\mathbf{\Omega}$, $\mathbf{M}$ as

$$\mathbf{n}_{a,b} = \pm c_m \mathbf{\Omega} + s_m \mathbf{l}, \qquad \mathbf{m}_{a,b} = c_m \mathbf{l} \mp s_m \mathbf{\Omega}, \qquad \mathbf{k}_{a,b} = \pm[\mathbf{\Omega} \times \mathbf{l}],$$
$$c_m = \frac{1 - M^2/4}{1 + M^2/4}, \qquad s_m = \frac{M}{1 + M^2/4}, \qquad c_m^2 + s_m^2 = 1, \tag{85}$$
$$\mathbf{l} = -M^{-1}[\mathbf{\Omega} \times M], \qquad |\mathbf{l}| = 1, \qquad \mathbf{f} = s_m \mathbf{l}, \qquad \mathbf{g} = [\mathbf{\Omega} \times \mathbf{f}].$$

These expressions for $\mathbf{m}$ and $\mathbf{k}$ are not analytic in the vector $\mathbf{M}$: they do not have a well-defined limit independent from the direction of the vector $\mathbf{M}$ when it tends to zero. But the auxiliary vectors $\mathbf{f}$ and $\mathbf{g}$ have definite limits as $\mathbf{M}$ tends to zero. However, if the partial contributions of sublattices a and b are combined, it may be shown that $\mathcal{L}_{pha}$ is expressed in terms of the scalars c_m and s_m and the vectors $\mathbf{f}$ and $\mathbf{g}$ which are analytic in $\mathbf{M}$. Therefore $\mathcal{L}_{pha}$ is also analytic in $\mathbf{M}$. According to (83) we have

$$\Delta\mathcal{L}_{pha} = \frac{is}{2} \ln\left(\frac{R_a \underline{R}_a^* R_b \underline{R}_b^*}{R_a^* \underline{R}_a R_b^* \underline{R}_b}\right). \tag{86}$$

Substituting Eqs. (85) for $\mathbf{n}$, $\mathbf{m}$, and $\mathbf{k}$ in Eq. (83) for R we get $R_{a,b} = D_{a,b} + E_{a,b}$ with

$$D_{a,b} = \underline{c}_m[\pm c_m(\underline{\mathbf{\Omega}} \cdot \mathbf{l}) + i(\underline{\mathbf{\Omega}} \cdot \mathbf{k})], \tag{87}$$
$$E_{a,b} = -\underline{c}_m s_m(\underline{\mathbf{\Omega}} \cdot \mathbf{\Omega}) \mp s_m(\underline{\mathbf{f}} \cdot \mathbf{\Omega}) + c_m(\underline{\mathbf{f}} \cdot \mathbf{l}) \pm i(\underline{\mathbf{f}} \cdot \mathbf{k}).$$

The quantities $D_{a,b}$ and $E_{a,b}$ are not analytic in $\mathbf{M}$ because they contain the nonanlytic vectors $\mathbf{l}$ and $\mathbf{k}$ explicitly. However, one can introduce new quantities $T_{a,b} = D_{a,b}^* R_{a,b}$. Using the identity $D_a = -D_b^*$ one can check that the expression (86) for $\mathcal{L}_{pha}$ will not change if we make the replacement $R_{a,b} \Rightarrow T_{a,b}$. This property is valid due to the compensation of the D-factors coming from sublattices a and b. Finally we obtain, for the quantities $T_{a,b}$,

$$T_{a,b} = A_{a,b} + B_{a,b}, \qquad A_{a,b} = D_{a,b}^* D_{a,b}, \qquad B_{a,b} = D_{a,b}^* E_{a,b},$$
$$A_{a,b} = \underline{c}_m^2[1 - (\underline{\mathbf{\Omega}} \cdot \mathbf{\Omega})^2 - (\underline{\mathbf{\Omega}} \cdot \mathbf{f})^2],$$
$$\begin{aligned} B_{a,b} = \underline{c}_m\{&\pm \underline{c}_m c_m(\underline{\mathbf{\Omega}} \cdot \mathbf{\Omega})(\underline{\mathbf{\Omega}} \cdot \mathbf{f}) + c_m(\underline{\mathbf{\Omega}} \cdot \mathbf{f})(\underline{\mathbf{\Omega}} \cdot \mathbf{f}) \\ &\pm (\underline{\mathbf{f}} \cdot \mathbf{f})(\underline{\mathbf{\Omega}} \cdot \mathbf{f}) \mp (\mathbf{\Omega} \cdot \mathbf{f}) \pm (\underline{\mathbf{\Omega}} \cdot \mathbf{\Omega})(\mathbf{\Omega} \cdot \underline{\mathbf{f}}) \\ &+ i[\underline{c}_m(\underline{\mathbf{\Omega}} \cdot \mathbf{\Omega})(\underline{\mathbf{\Omega}} \cdot \mathbf{g}) \pm c_m(\mathbf{\Omega} \cdot \underline{\mathbf{f}})(\underline{\mathbf{\Omega}} \cdot \mathbf{g}) + c_m(\mathbf{\Omega} \cdot \underline{\mathbf{g}})]\}. \end{aligned} \tag{88}$$

One can see that $T_{a,b}$ (88) depend only on the vectors $\mathbf{\Omega}$, $\mathbf{f}$, and $\mathbf{g}$ and the scalar c_m which are analytic in $\mathbf{M}$.

C. CALCULATION OF INTEGRALS AND SUMS OVER ω

The calculation of integrals and sums over the frequency ω for a finite time step Δ can be performed in the following manner. The function to be summed over (integrated over), $f(\omega)$, can be split into two parts, $f(\omega) = f_p(c_\omega) + f_{np}(c_\omega)$, where $f_p(c_\omega)$ is the polynomial part in $c_\omega = \cos(\omega\Delta)$ and $f_{np}(c_\omega)$ is the nonpolynomial part of the function which decreases for $\omega \to \infty$. The sum (integral) of the function $f_p(c_\omega)$ over ω, within the limits $\pm\pi/\Delta$, can be easily performed. The sum (integral) of the function $f_{np}(c_\omega)$ can be converted into the contour integral as shown in Fig. 1 with the help of the Sommerfeld–Watson transformation. The contour integration is possible because the integral over the vertical line $C1$ and the vertical lines $C2$ cancel each other due to the periodicity of the function f: $f(\omega + 2\pi/\Delta) = f(\omega)$. The result of the summation is the sum of the residues of the function

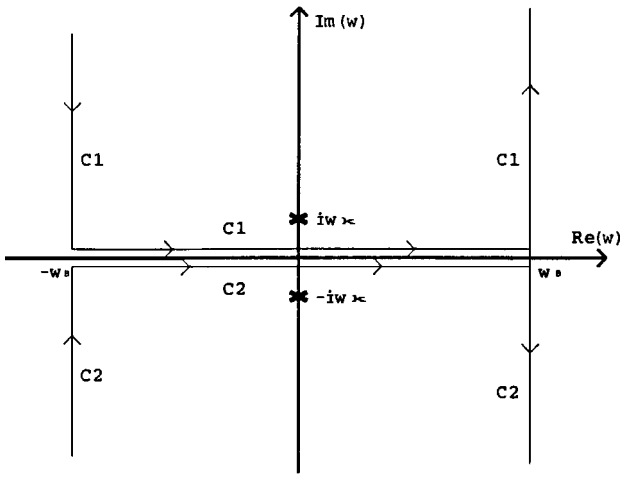

FIG. 1. Contours of integration in the complex ω plane for the calculation of the integral of the function $f_{np}(c_\omega)$. On the picture $w \equiv \omega$ and $w_B = \pi/\Delta$. The points $\pm i w_k$ show the typical poles of the function $f_{np}(c_\omega)$.

$0.5\beta \cot(\beta\omega/2) f_{np}(c_\omega)$ as shown in Fig. 1. For $T = 0$ one can simply convert the integral of the function $f_{np}(c_\omega)$ over $-\pi/\Delta < \omega < \pi/\Delta$ into the contour integral over $C1$ or $C2$.

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