Spin dynamics in the two-dimensional spin-$\frac{1}{2}$ Heisenberg antiferromagnet

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We present low-temperature dynamic properties of the quantum two-dimensional antiferromagnetic Heisenberg model with spin $S=1/2$. The calculation of the dynamic correlation function is performed by combining a projection operator formalism and the modified spin-wave theory, which gives a gap in the dispersion relation for finite temperatures. The so calculated dynamic correlation function shows a double peak structure. We also obtain the spin-wave damping and compare our results to some experimental data and theoretical results obtained by other authors using different approaches.

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I. INTRODUCTION

Interest in quantum antiferromagnetism is old and can be traced back to the early years of quantum theory, with Bethe's solution for the Heisenberg antiferromagnetic chain.[1] However, research in this field remains very active and was further triggered by the discovery of high-temperature superconductivity in copper-oxide compounds. Superconductivity in the cuprates is attained upon doping the stoichiometric parent compounds, such as La_2CuO_4, which are believed to be experimental realizations of the two-dimensional (2D) quantum Heisenberg antiferromagnet (QHAF) with spin $S=1/2$, described by the model Hamiltonian

$$\mathcal{H} = J\sum_{\langle i,j\rangle} \vec{S}_{\vec{r}_i} \cdot \vec{S}_{\vec{r}_j}, \tag{1}$$

where $J>0$; $\langle i,j\rangle$ denotes the nearest neighbor (NN) sites on a square lattice, without double counting of bonds. The 2DQHAF can be mapped into the 2D quantum nonlinear σ model[2] (2DQNLSM) and many theoretical works have been dedicated to the investigation of the properties of this last model. However, the mapping is rigorously valid only in the large S continuum limit,[3] although it can be justified on general grounds for the extreme quantum limit[4] $S=1/2$.

The widely held belief that antiferromagnetism plays a central role in high-temperature superconductivity has contributed to a noticeable proliferation of theoretical, numerical, and experimental works devoted to the investigation of the magnetic properties of the stoichiometric parent compounds, as described by Eq. (1) and by the 2DNLSM.[5,6] However, despite this connection with high-T_c superconductivity, the understanding of the properties of the system is important by itself.

Some early theoretical investigations of the 2DQHAF (Ref. 7) raised doubts about the nature of the ground state of the model, suggesting that it would be a disordered quantum spin-liquid state with correlations decaying exponentially with distance.[8] Later, further investigations ruled out this possibility and the system is known to exhibit a broken symmetry Néel ground state,[5] which is destroyed by thermal fluctuations[9] when $T>0$. In fact, at low temperatures, the system is in a renormalized classical (RC) regime, that is, it behaves as a classical 2D system with coupling constants simply renormalized by quantum fluctuations, as showed by Chakravarty, Halperin, and Nelson[4] in their renormalization-group analysis of the 2DQNLSM. This approach was improved by Hasenfratz and Niedermayer[10] who obtained an expression for the correlation length ξ of the 2DQNLSM in the RC regime which agrees very well with experimental data[11] for the monolayer cuprate $Sr_2CuO_2Cl_2$ over a certain temperature range.

At higher temperatures, $T/J\sim 0.5$, the 2DQNLSM shows a crossover into a quantum critical (QC) region,[12] with correlation length linear in $1/T$. Although this prediction is difficult to be experimentally tested in cuprates such as $Sr_2CuO_2Cl_2$ and La_2CuO_4, given the high value of J in these compounds ($J\sim 130$ meV), recent experiments on copper formiate tetradeuterate (CFTD),[13,14] which is also described as a 2DQHAF (Refs. 15 and 16) and whose much smaller value of J ($J\sim 6$ meV) allows measurements up to higher temperatures, found no evidence for a crossover into a QC phase. It should be remarked that the 2DQNLSM is expected to model the 2DQHAF in the limit of low temperatures, when the correlation length is very large, and the above mentioned experiments seem to settle an upper temperature limit for the applicability of this approach. In fact, the validity of the 2DQNLSM approach was shown to be inadequate to describe the behavior of the 2DQHAF with spin value greater than or equal to 1 in the experimentally acessible temperature region.[17] For spin $S=1/2$, a series of experiments[11,18] and Monte Carlo simulations[19–21] showed that the length scale at which the renormalized 2DQNLSM description becomes valid is surprisingly long. The low-energy spectrum of the $S=1/2$ Heisenberg model, obtained by quantum Monte Carlo on finite size lattices,[22] disagrees rather strongly with the prediction of the nonlinear σ model even when the size of the system is not too small. All these results show that it is important to work directly with Hamiltonian (1) instead of using the 2DQNLSM if one wants to make comparisons with experimental data.

Nowadays, it is believed that the available experimental data for *static* properties is well described by a combination

of low-temperature static properties,[4] QMC simulations[19,20] at an intermediate range, and at higher temperatures, by high-T expansion[21] and pure-quantum self-consistent harmonic approximation (PQSCHA).[23] So, the attention has turned to the dynamical properties of the 2DQHAF at finite temperatures, since the intrinsic nonlinearities in the equations of motion for a spin system give room for stronger quantum effects in the dynamics, particularly at higher excitation energies. Therefore, further microscopic calculations of the dynamic structure factor for Eq. (1) are still very welcome in order to allow a better understanding about the system's behavior at finite temperatures.

Many of the interesting phenomena and experimental measurements in strongly correlated quantum systems are related to the dynamics of the system. Despite the considerable progress in many-body theory, available exact results on quantum dynamics in many-body systems are rather scarce. Indeed, even a systematic framework for approximate calculations is not well established.[24]

In this paper, we calculate the dynamical correlation function for the 2DQHAF with $S=1/2$ using the equation of motion approach in conjunction with projection operator methods, following a procedure proposed originally by Reiter[25] and further developed by other authors.[26] This method has proven successful in the study of the classical and quantum Heisenberg models in one[27] and two[28] dimensions showing good agreement with experimental data, molecular dynamic simulations, and with other theories.

The calculation of the memory function, which plays a central role in the formalism, does not require long-range order to be valid because it depends only on correlations between nearest neighbors. The frequency of the local spin-wave modes is also used as input in the method. The calculation of the static correlations and spin-wave frequency needed in the formalism we are using, is done within the context of the modified spin-wave (MSW) theory proposed by Takahashi[29] and Hirsch and Tang.[30] The MSW theory applied to antiferromagnets imposes a constraint on the total staggered magnetization to be zero in an isotropic system, as required by Mermin-Wagner theorem.[9] It has been shown[5] that the results obtained via the MSW approximation are identical to the ones obtained by Arovas and Auerbach[32] using a path integral formulation in the Schwinger boson representation. Also, the correlation length, as calculated within MSW theory, agrees with one-loop order in renormalization-group theory for the 2DQNLσM.[4] The combination of these two techniques, the projection operator method and the MSW theory was already applied by some of us[31] to study the low-temperature properties of the quantum one-dimensional Heisenberg model with spin $S=1$, where a gap is expected to occur.

The dynamical structure function of Eq. (1) at finite temperature was first calculated by Auerbach and Arovas[33] as the Fourier transform of the imaginary part of the spin-density correlation function

$$S(\vec{q},\omega,T)=\frac{1}{\pi}\langle S^z(\vec{q},\omega)S^z(-\vec{q},\omega)\rangle, \tag{2}$$

using the Schwinger boson mean-field representation. The procedure includes processes where the incident particle creates quasiparticle excitations as well as scattering from thermally excited particles. However, the projection operator method, in the approximation proposed by Reiter,[25] goes beyond a mean-field theory and, thus, the effects due to magnon scattering are more properly incorporated in the calculation of the dynamical structure factor. This procedure was applied to the 2DQHAF model by Becher and Reiter,[34] using a standard spin-wave formalism for the calculation of the static quantities, however, as it is well known, conventional spin-wave theory predicts a zero gap value for finite temperatures, i.e., it does not take into account the inexistence of long-range order (LRO) for $T>0$. Tyc and Halperin[35] used the Dyson-Maleev formalism to calculate the damping of spin-waves for the 2DQHAF but they did not calculate the dynamical correlation function which is, by far, the most important quantity when the target is to make comparisons to experimental data. More recently, the spin dynamics of the 2DQHAF was investigated by Nagao and Igarashi[36] by using the self-consistent theory of Blume and Hubbard.[37] Their method is expected to work well at high temperatures, although the authors claim that the results obtained for relatively low temperatures, $T/J\sim 0.4$, are reliable because the relaxation function is found to satisfy a dynamical scaling relation consistent with the nonlinear σ model analysis and, also, Monte Carlo simulations.[38] Therefore, a calculation of the spin dynamical correlation function for Hamiltonian (1) at low temperatures and in a wide wave vector range, as proposed in this work, is still valuable.

The outline of this paper is as follows. Section II gives a brief overview of the MSW results for the spin-wave energy, as obtained by Takahashi.[29] The steps leading to the calculation of the dynamical structure factor are also given in thas section. In Sec. III, we discuss our numerical results and, finally, in Sec. IV we present our conclusions.

II. THE MODIFIED SPIN-WAVE THEORY AND THE PROJECTION OPERATOR METHOD

It is well known that the standard spin-wave theory is not applicable to low-dimensional quantum magnets at finite temperatures without modifications.[9] The consequence of the Mermin-Wagner theorem is enforced by hand in a variational density-matrix approach proposed by Takahashi,[29] which we will shortly review here. We start our calculations, writing Eq. (1) in the form

$$\mathcal{H}=J\sum_{\langle i,j\rangle}\vec{S}_{\vec{r}_i}\cdot\vec{T}_{\vec{r}_j}, \tag{3}$$

where we divide the lattice into two sublattices A and B: spins in sublattice A (B) are denoted as $\vec{S}_{\vec{r}_i}$ ($\vec{T}_{\vec{r}_j}$) and the sum runs over all $\vec{r}_i\in A$ sublattice sites and its NN on the B sublattice, avoiding double counting of bonds. We now apply a Dyson-Maleev transformation to represent the spin operators in each antiferromagnetic sublattice in terms of bosonic operators

$$S^-_{\vec{r}_i}=a^\dagger_{\vec{r}_i},\quad S^\dagger_{\vec{r}_i}=(2S-a^\dagger_{\vec{r}_i}a_{\vec{r}_i})a_{\vec{r}_i},\quad S^z_{\vec{r}_i}=S-a^\dagger_{\vec{r}_i}a_{\vec{r}_i},$$

$$T^-_{\vec{r}_j}=-b_{\vec{r}_j},\quad T^\dagger_{\vec{r}_j}=-b^\dagger_{\vec{r}_j}(2S-b^\dagger_{\vec{r}_j}b_{\vec{r}_j}), \tag{4}$$

$$T^z_{\vec{r}_j} = -S + b^\dagger_{\vec{r}_j} b_{\vec{r}_j}, \tag{5}$$

following the canonical commutation relations. In terms of these creation and annihilation operators, the Hamiltonian (3) becomes

$$\mathcal{H} = -2NJS^2 + J\sum_{\langle i,j\rangle}\left\{ S(a^\dagger_{\vec{r}_i} a_{\vec{r}_i} + b^\dagger_{\vec{r}_j} b_{\vec{r}_j} - a_{\vec{r}_i} b_{\vec{r}_j} - a^\dagger_{\vec{r}_i} b^\dagger_{\vec{r}_j}) + \frac{1}{2} a^\dagger_{\vec{r}_i} (a_{\vec{r}_i} - b^\dagger_{\vec{r}_j})^2 b_{\vec{r}_j} \right\}. \tag{6}$$

We then introduce an ideal spin-wave ansatz for the density matrix of the system

$$\rho = \exp\left\{ \frac{1}{T}\sum_{\vec{q}}{}' \omega_{\vec{q}} (\alpha^\dagger_{\vec{q}} \alpha_{\vec{q}} + \beta^\dagger_{-\vec{q}} \beta_{-\vec{q}}) \right\}, \tag{7}$$

where $\Sigma'_{\vec{q}}$ indicates summation over half of the first Brillouin zone, and $\alpha_{\vec{q}}$ and $\beta^\dagger_{-\vec{q}}$ are given by the Bogoliubov transformation

$$\alpha_{\vec{q}} = \cosh(\theta_{\vec{q}}) a_{\vec{q}} - \sinh(\theta_{\vec{q}}) b^\dagger_{-\vec{q}},$$

$$\beta^\dagger_{-\vec{q}} = -\sinh(\theta_{\vec{q}}) a_{\vec{q}} + \cosh(\theta_{\vec{q}}) b^\dagger_{-\vec{q}}. \tag{8}$$

We have also introduced the Fourier transform of the original boson operators

$$a_{\vec{q}} = \frac{1}{\sqrt{N_A}} \sum_{\vec{r}_i \in A} e^{-i\vec{q}\cdot\vec{r}_i} a_{\vec{r}_i},$$

$$b^\dagger_{-\vec{q}} = \frac{1}{\sqrt{N_B}} \sum_{\vec{r}_j \in B} e^{-i\vec{q}\cdot\vec{r}_j} b^\dagger_{\vec{r}_j}, \tag{9}$$

where $N_A + N_B = N$ is the number of sites in the lattice. The dispersion relation $\omega_{\vec{q}}$ is obtained after minimizing the free energy with the constraint that the magnetization on each sublattice is zero, $\langle S^z_{\vec{r}}\rangle = 0$ and $\langle T^z_{\vec{r}}\rangle = 0$, as required by Mermin-Wagner theorem. In this way, we get

$$\omega_{\vec{q}} = \lambda(1 - \eta^2 \gamma^2_{\vec{q}})^{1/2}, \quad \gamma_{\vec{q}} = \frac{1}{2}(\cos q_x + \cos q_y). \tag{10}$$

We write the wave vector $\vec{q} = (q_x, q_y)$ in units of the inverse lattice spacing. The parameters η and λ can be determined by solving the following set of self-consistent equations:

$$S + \frac{1}{2} = \frac{2}{N}\sum_{\vec{q}}{}' \frac{1}{(1-\eta^2\gamma^2_{\vec{q}})^{1/2}} \frac{1}{2} \coth\left\{ \frac{\lambda}{2T}(1-\eta^2\gamma^2_{\vec{q}})^{1/2} \right\},$$

$$\frac{\eta\lambda}{4J} = \frac{2}{N}\sum_{\vec{q}}{}' \frac{\eta\gamma^2_{\vec{q}}}{(1-\eta^2\gamma^2_{\vec{q}})^{1/2}} \frac{1}{2} \coth\left\{ \frac{\lambda}{2T}(1-\eta^2\gamma^2_{\vec{q}})^{1/2} \right\}. \tag{11}$$

As noticed in the review by Manousakis,[5] the same equations were obtained by Hirsch and Tang,[30] and by Arovas and Auerbach.[32] The procedure adopted by Hirsch and Tang is also a MSW theory and it is not surprizing to find such agreement. However, Arovas and Auerbach applied a quite different approach using a path-integral formulation in the Schwinger representation. As mentioned in the Introduction, other results obtained via MSW, such as, for example, the correlation length, agree with results obtained from other approximate theories. Many times, due to the lack of exact results, theoreticians are obliged to make use of approximate methods to advance in their knowledge about the behavior of a specific model. However, even the approximate methods are not completely transparent and it is often difficult to evaluate which of the essential features of the model were captured or not. Therefore, it is always very reassuring to obtain equivalent results by using quite different methods because this may indicate that the most important ingredients were taken into account.

TABLE I. Results for the η and λ parameters for some temperatures T used in our calculations. The values were obtained by solving Eq. (11) numerically.

T/J	η	λ
0.05	0.999999993	2.609963279
0.10	0.999995178	2.609876929
0.15	0.999939299	2.599595679
0.20	0.999709621	2.562049716
0.25	0.999280433	2.567211935
0.30	0.998523449	2.558794763

Takahashi[29] was able to find out the asymptotic forms of Eq. (11) in the $T \to 0$ limit and, also, to evaluate the η parameter for the spin $S = 1/2$ case for 4×4 and 64×64 lattices. However, for the calculation of the dynamical structure factor according to the projection operator procedure, we need to know the spin-wave energy for the infinite square lattice model at finite temperatures and, thus, we solved Eqs. (11) using an iterative numerical model obtaining the results displayed in Table I.

As is well known, there is no gap in the 2DQHAF with $S = 1/2$ at $T = 0$. Indeed, when $T \to 0$, we can see that $\eta \to 1$. However, for finite temperatures, η becomes smaller than unity and so a gap opens in the system, reflecting the fact that the correlation length ξ becomes finite and the long wavelength, low-energy spin-waves cannot propagate. So, spin-wave excitations are well defined only for wavelengths significantly smaller than ξ.

In antiferromagnets, spin-waves have two flavors, one associated with the conventional magnetization $\mathcal{M}^\alpha_{\vec{q}} = S^\alpha_{\vec{q}} + T^\alpha_{\vec{q}}$ and another to the staggered magnetization $\mathcal{R}^\alpha_{\vec{q}} = S^\alpha_{\vec{q}} - T^\alpha_{\vec{q}}$ with $\alpha = x, y, z$. At low temperature, the $\mathcal{R}^\alpha_{\vec{q}}$ correlation function is the leading contribution to the structure factor near the antiferromagnetic wave vector. As in classical systems, the staggered $\mathcal{R}^\alpha_{\vec{q}}$ and the usual $\mathcal{M}^\alpha_{\vec{q}}$ correlation functions will be quite different. This can be easily seen from the expressions for the first-order term of the z components of $\mathcal{R}$ and $\mathcal{M}$,

$$\mathcal{R}^z_{\vec{q}} = 2S\sqrt{N}\delta_{\vec{q}=\mathbf{0}} + \cdots,$$

$$\mathcal{M}_{\vec{q}}^{z}=\frac{1}{\sqrt{N}}\sum_{\vec{r}_i} e^{-i\vec{q}\cdot\vec{r}_i}(b_{r_i}^{\dagger}b_{r_i}^{\sim}-a_{r_i}^{\dagger}a_{r_i}^{\sim})+\cdots. \tag{12}$$

The expressions for $\mathcal{R}_{\vec{q}}^{x,y}$ and $\mathcal{M}_{\vec{q}}^{x,y}$ contain sum and differences of the $a_{\vec{q}}$, $a_{\vec{q}}^{\dagger}$, $b_{\vec{q}}$, and $b_{\vec{q}}^{\dagger}$ operators. Thus, we see that the staggered magnetization is linear in magnon creation and annihilation operators while the uniform magnetization is a two-magnon operator process. In fact, the calculation of the $\mathcal{M}_{\vec{q}}$ correlation function could be performed by using the same procedure applied in this work, but the calculation would require us to go to a higher order in magnon operators.

It is important to emphasize that we only calculate rotationally invariant quantities such as $\mathcal{R}_{\vec{q}}=\frac{1}{3}(\mathcal{R}_{\vec{q}}^{x}+\mathcal{R}_{\vec{q}}^{y}+\mathcal{R}_{\vec{q}}^{y})$. Obviously, we expect that, for the isotropic Heisenberg model, each of the three spin components gives the same contribution to the dynamical behavior of the model. However, the Dyson-Maleev transformation breaks the symmetry of the spin space giving a privileged rule to the z-spin component. Therefore, we restore the model's symmetry by computing rotationally invariant quantities.

Now, we describe only the main steps leading to the calculation of the dynamic structure factor following the projection operator method. A complete description of the theory can be found in Refs. 25 and 26. One of the advantages of this procedure is that it allows us to obtain the structure factor for all values of the wave vector $\vec{q}$, while calculations based on the nonlinear σ model are restricted to the long wavelength limit $\vec{q}\to(0,0)$. The Fourier transform of the relaxation function is given by[39]

$$R(\vec{q},\omega)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}dt e^{-i\omega t}\frac{(\mathcal{R}_{\vec{q}}(t),\mathcal{R}_{\vec{q}}(0))}{(\mathcal{R}_{\vec{q}},\mathcal{R}_{\vec{q}})}. \tag{13}$$

Here, (A,B) is the Kubo inner product of two operators A and B defined as[40]

$$(A,B)=\frac{1}{\beta}\int_0^{\beta}\langle e^{\lambda H}A^{\dagger}e^{-\lambda H}B\rangle d\lambda, \tag{14}$$

where $\langle\cdots\rangle$ denotes the usual thermal average and $\beta=1/k_BT$. One can show that, after some analytical work, the dynamical correlation function $R(\vec{q},\omega)$ is given by

$$R(\vec{q},\omega)=(\mathcal{R}_{\vec{q}},\mathcal{R}_{\vec{q}})\langle\omega_{\vec{q}}^2\rangle\frac{\Sigma_{\vec{q}}''(\omega)}{[\omega^2-\langle\omega_{\vec{q}}^2\rangle+\omega\Sigma_{\vec{q}}'(\omega)]^2+[\omega\Sigma''_{\vec{q}}(\omega)]^2}, \tag{15}$$

where $\Sigma_{\vec{q}}'(\omega)$ and $\Sigma_{\vec{q}}''(\omega)$ are the real and imaginary parts of the second order memory function $\Sigma_{\vec{q}}(\omega)$, respectively. In time space, this memory function is expressed by

$$\Sigma_{\vec{q}}(t)=\frac{(QL^2\mathcal{R}_{\vec{q}},e^{-iQLQt}QL^2\mathcal{R}_{\vec{q}})}{(L\mathcal{R}_{\vec{q}},L\mathcal{R}_{\vec{q}})}, \tag{16}$$

where Q is a projection operator that projects out any term proportional to $\mathcal{R}_{\vec{q}}$ and $L\mathcal{R}_{\vec{q}}$, and L is the Liouville operator, defined by the relation $LA=-i[A,H]=-i\dot{A}$. Reiter[25] has shown that, to leading order in temperature, the projection operator Q in the exponential function in Eq. (16) can be dropped and we can also write

$$QL^2\mathcal{R}_{\vec{q}}=L^2\mathcal{R}_{\vec{q}}-\langle\omega_{\vec{q}}^2\rangle\mathcal{R}_{\vec{q}}. \tag{17}$$

In Eq. (15), we also need to define the second frequency moment $\langle\omega_{\vec{q}}^2\rangle$, which is given by

$$\langle\omega_{\vec{q}}^2\rangle=\frac{(L\mathcal{R}_{\vec{q}},L\mathcal{R}_{\vec{q}})}{(\mathcal{R}_{\vec{q}},\mathcal{R}_{\vec{q}})}. \tag{18}$$

The second time derivatives needed to evaluate the numerator of the memory function (16) are directly obtained from the definition of the Liouville operator and from Eq. (3). Since this calculation is very straightfoward and the expressions are enormous, we will not show them here. We then apply the Dyson-Maleev (4) and Bogoliubov (8) transformations for the spin operators in those expressions. Doing so, we can simply replace the time evolution $\exp(-iLt)$ by the harmonic time evolution

$$\alpha_{\vec{q}}(t)=e^{-i\omega_{\vec{q}}t}\alpha_{\vec{q}}(0), \tag{19}$$

$$\alpha_{\vec{q}}^{\dagger}(t)=e^{i\omega_{\vec{q}}t}\alpha_{\vec{q}}^{\dagger}(0), \tag{20}$$

with similar equations for $\beta_{\vec{q}}(t)$ and $\beta_{\vec{q}}^{\dagger}(t)$. So, we are left with a number of Kubo products of four bosonic operators which can be decoupled by means of Wick's theorem. After a tedious but simple calculation, we get

$$\Sigma_{\vec{q}}(t)=\frac{4}{N}\sum_{\vec{p}}{}'\{A_+(\vec{q},\vec{p})\cos(\Omega_+t)+A_-(\vec{q},\vec{p})\cos(\Omega_-t)\}. \tag{21}$$

$A_+(\vec{q},\vec{p})$ and $A_-(\vec{q},\vec{p})$ are given by

$$A_+(\vec{q},\vec{p})=\frac{\lambda^2Tn_{\vec{q}_+}n_{\vec{q}_-}(e^{\beta\Omega_+}-1)}{4\Omega_+\omega_{\vec{q}_+}\omega_{\vec{q}_-}(L\mathcal{R}_{\vec{q}},L\mathcal{R}_{\vec{q}})}[s(\vec{q},\vec{p})-t(\vec{q},\vec{p})]^2, \tag{22}$$

$$A_-(\vec{q},\vec{p})=\frac{\lambda^2Tn_{\vec{q}_+}n_{\vec{q}_-}(e^{\beta\omega_{\vec{q}_+}}-e^{\beta\omega_{\vec{q}_-}})}{4\Omega_-\omega_{\vec{q}_+}\omega_{\vec{q}_-}(L\mathcal{R}_{\vec{q}},L\mathcal{R}_{\vec{q}})}[s(\vec{q},\vec{p})+t(\vec{q},\vec{p})]^2, \tag{23}$$

where we introduced the notation $\vec{q}_{\pm}=\vec{q}/2\pm\vec{p}$, and

$$\begin{aligned}s(\vec{q},\vec{p})&=[4J^2(\gamma_{\vec{q}_+}+\gamma_{\vec{q}_-})(\gamma_{\vec{q}_+}+\gamma_{\vec{q}_-}-2)+\langle\omega_{\vec{q}}^2\rangle]\\&\times(1+\eta\gamma_{\vec{q}_+})^{1/2}(1+\eta\gamma_{\vec{q}_-})^{1/2},\\ t(\vec{q},\vec{p})&=[4J^2(\gamma_{\vec{q}_+}+\gamma_{\vec{q}_-})(\gamma_{\vec{q}_+}+\gamma_{\vec{q}_-}+2)+\langle\omega_{\vec{q}}^2\rangle]\\&\times(1-\eta\gamma_{\vec{q}_+})^{1/2}(1-\eta\gamma_{\vec{q}_-})^{1/2}.\end{aligned} \tag{24}$$

In the expressions above, $n_{\vec{q}}=(\exp(\beta\omega_{\vec{q}})-1)^{-1}$ is the boson occupation number and $\Omega_{\pm}(\vec{q},\vec{p})$ is defined as

$$\Omega_{\pm}(\vec{q},\vec{p})=\omega_{\vec{q}_+}\pm\omega_{\vec{q}_-}. \tag{25}$$

The second moment is readily evaluated from its definition (18). It is given by the ratio of the following expressions:

$$(L\mathcal{R}_{\vec{q}}, L\mathcal{R}_{\vec{q}}) = \frac{4JT}{N}\sum_{\vec{k}}{}'(2\gamma_{\vec{k}} + \gamma_{\vec{k}+\vec{q}} + \gamma_{\vec{k}-\vec{q}}) \times \frac{\eta\gamma_{\vec{k}}}{(1-\eta^2\gamma_{\vec{q}}^2)^{1/2}} \coth\left\{\frac{\lambda}{2T}(1-\eta^2\gamma_{\vec{q}}^2)^{1/2}\right\} \tag{26}$$

and

$$(\mathcal{R}_{\vec{q}}, \mathcal{R}_{\vec{q}}) = \frac{T}{\lambda}\frac{1}{(1-\eta\gamma_{\vec{q}})}. \tag{27}$$

We note that Eq. (26) is also needed in the evaluation of Eq. (22).

If we take the Laplace transform of the memory function (21) and then apply the Cauchy formula we finally get the real and imaginary parts of the memory function as given by

$$\Sigma'_{\vec{q}}(\omega) = \frac{1}{2\pi^2}\mathcal{P}\left\{\int d^2p\left[\frac{A_+(\vec{q},\vec{p})}{\omega+\Omega_+(\vec{q},\vec{p})} + \frac{A_+(\vec{q},\vec{p})}{\omega-\Omega_+(\vec{q},\vec{p})} + \frac{A_-(\vec{q},\vec{p})}{\omega+\Omega_-(\vec{q},\vec{p})} + \frac{A_-(\vec{q},\vec{p})}{\omega-\Omega_-(\vec{q},\vec{p})}\right]\right\}, \tag{28}$$

and

$$\Sigma''_{\vec{q}}(\omega) = \frac{1}{2\pi}\int d^2p\{A_+(\vec{q},\vec{p})\,\delta[\omega+\Omega_+(\vec{q},\vec{p})] + A_+(\vec{q},\vec{p})\,\delta[\omega-\Omega_+(\vec{q},\vec{p})] + A_-(\vec{q},\vec{p})\,\delta[\omega+\Omega_-(\vec{q},\vec{p})] + A_-(\vec{q},\vec{p})\,\delta[\omega-\Omega_-(\vec{q},\vec{p})]\}. \tag{29}$$

Comparing Eq. (21) with the corresponding one obtained by Becher and Reiter [see Eq. (9) in their paper[34]], we can note that they are very similar if we assign to η and λ their zero temperature values in our expressions. But there are some slight differences between our definitions for $s(\vec{q},\vec{p})$ and $t(\vec{q},\vec{p})$, Eqs. (24), and their equivalent ones due to the fact that, in this work, we considered two sublattices for the antiferromagnet.

At this point, we should comment on the domain validity for the method employed in this paper. The method is restricted to the low temperature regime, that is, $T \ll J$, but, as discussed by Reiter,[25] it is exact to leading order in temperature. The extension of the wavevector region depends on how precise are the expressions to be used for the static quantities required by the memory function formalism. If we had *exact* expressions for, say, the second moment, the whole wavevector range would be covered by this technique. However, as we are using the MSW theory in our calculations, we are bound to the same domain of that theory, that is, $q > \xi^{-1}$, where ξ is the correlation length. In the next section we discuss our numerical results for the dynamic structure factor calculated from the above expressions.

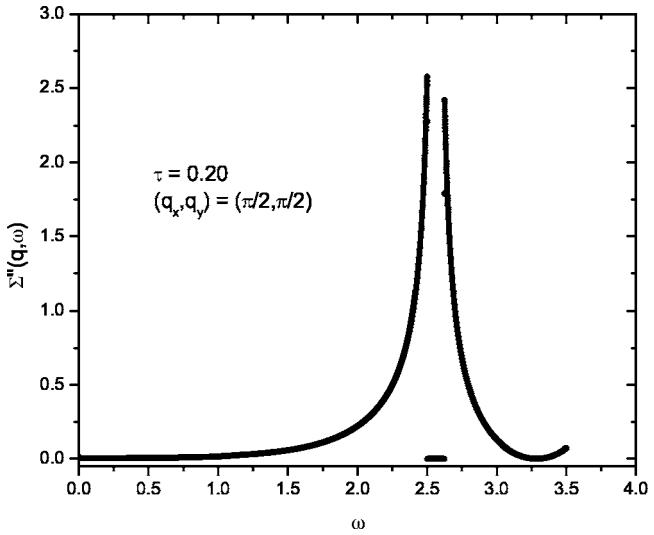

FIG. 1. Imaginary part of the memory function, $\Sigma''_{\vec{q}}(\omega)$, as a function of ω for $(q_x, q_y)=(\pi/2, \pi/2)$ and $\tau=0.20$.

III. DISCUSSION OF THE NUMERICAL RESULTS

The evaluation of the imaginary part of the memory function is far from trivial. For this purpose, we adopt a numerical method introduced by Gilat and co-workers[41] and further developed by Wysin.[42] A typical result is shown in Fig. 1, for $(q_x, q_y)=(\pi/2, \pi/2)$, $\tau=T/J=0.20$; the frequency is given in units of JS^2 (throughout this paper, $k_B=\hbar=1$). A prominent feature displayed in that figure is that $\Sigma''_{\vec{q}}(\omega)$ vanishes in a finite interval approximately centered at the zero-temperature spin-wave energy. At $T=0$, the parameter η is equal to 1, describing the absence of an energy gap at zero temperature. However, for the wave vector $(\pi/2, \pi/2)$ used to generate Figs. 1 and 2, the spin-wave energy depends only on λ, which, as indicated in Table I, approaches the value $2.61J$ as $T \to 0$, and, then, $\omega_{T=0}(\pi/2, \pi/2) \approx 2.61J$. The behavior shown in Fig. 1 can be understood if we look at Eq. (29). We see that we only have contributions when the argument of the delta functions, given by differences or sums of the fre-

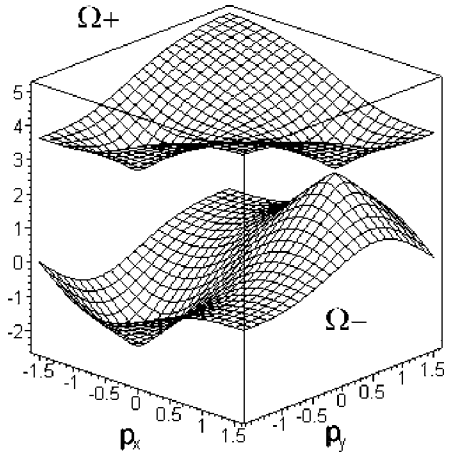

FIG. 2. $\Omega_-(\vec{q},\vec{p})$ and $\Omega_+(\vec{q},\vec{p})$ as a function of (p_x, p_y) for $(q_x, q_y)=(\pi/2, \pi/2)$ and $\tau=0.20$.

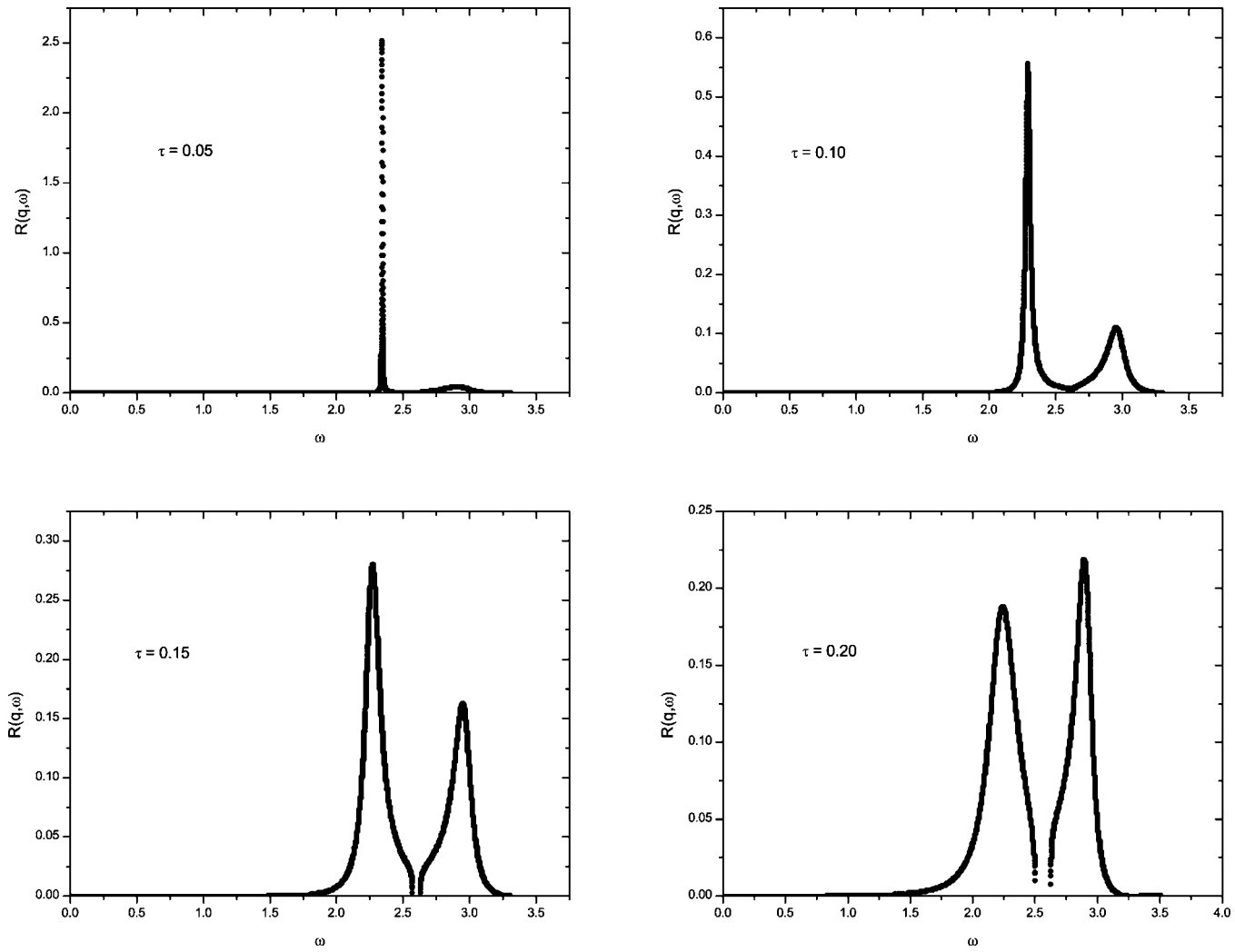

FIG. 3. Dynamic structure factor $R(q,\omega)$ for $(q_x,q_y)=(\pi/2,\pi/2)$ and $\tau=0.05$, 0.10, 0.15, and 0.20.

quency and the functions $\Omega_-(\vec{q},\vec{p})$ (which accounts for processes involving an absorption followed by the reemission of a magnon with a lower energy) and $\Omega_+(\vec{q},\vec{p})$ (that describes the decay of a magnon into two others), vanishes. The shape of these two functions is shown in Fig. 2, also for $(q_x,q_y)=(\pi/2,\pi/2)$ and $\tau=0.20$. We note that the nonunitary value of η at finite temperatures, a consequence of the absence of long-range order, imposes the opening of a small gap between $\Omega_-(\vec{q},\vec{p})$ and $\Omega_+(\vec{q},\vec{p})$, as we can see in the figure. This gap is close to the zero-temperature spin-wave frequency. So, as we raise the frequency, the two terms involving $\Omega_-(\vec{q},\vec{p})$ cease to contribute to the integral in a region where the term in $\delta[\omega-\Omega_+(\vec{q},\vec{p})]$ still does not contribute, and $\Sigma''_{\vec{q}}(\omega)$ is zero within it. A similar behavior was obtained by some of us in a previous work regarding the dynamics of the $S=1$ antiferromagnetic chain.[31]

The real part of the memory function is readily evaluated by a generalization[43] of a numerical method used in one-dimensional cases. In this way, we can directly compute the dynamical correlation function by means of Eq. (15). In Fig. 3, we show the results obtained for $(q_x,q_y)=(\pi/2,\pi/2)$ at $\tau=0.05$, 0.10, 0.15, and 0.20. The results for other values of $\vec{q}$ are very similar, except for small wave vectors [such as $(q_x,q_y)=(\pi/64,\pi/64)$] at the highest temperatures studied. In this case, we observe that the imaginary part of the memory function changes its shape, from the *normal* one as displayed in Fig. 1 at the lowest temperature investigated ($\tau=0.05$), into an anomalous one in higher temperatures. This leads to a *blurrying* of the peaks observed in $R(q,\omega)$. However, this region—small wave vector and high temperature—is outside the validity range of the method employed in this work.

We can note that the cancellation of the imaginary part of the memory function in an interval, as discussed above, leads to the vanishing of the dynamic structure factor in the same region. In particular, this feature prevents us to investigate the $\vec{q}\to(0,0)$ limit, since the gap remains relatively large and there are no peaks in $R(q,\omega)$. So, we cannot compare our results to those obtained by Becher and Reiter,[34] who found that the damping of the magnons is zero at $T=0$.

But, what is remarkable in the curves obtained for $R(q,\omega)$ is the presence of a double-peak structure. It is interesting to note that the low-energy peak follows the behavior expected for a spin-wave peak, that is, it becomes broader as the temperature increases and its intensity decreases. However, the

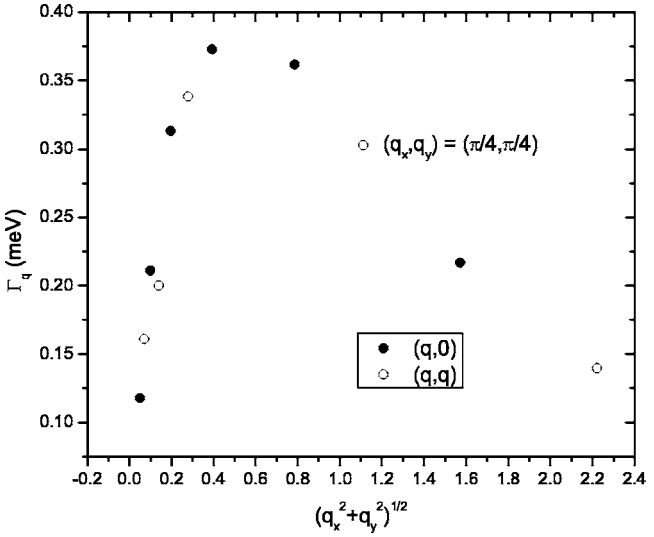

FIG. 4. Results obtained in our work (as explained in the text) for the spin-wave damping, $\Gamma(\vec{q},\tau)$, as a function of $(q_x^2+q_y^2)^{1/2}$ for $\tau=0.05$. Filled circles are for wavectors along the direction $(q,0)$ and open circles for (q,q). Wave vector $(q_x,q_y)=(\pi/4,\pi/4)$ is indicated.

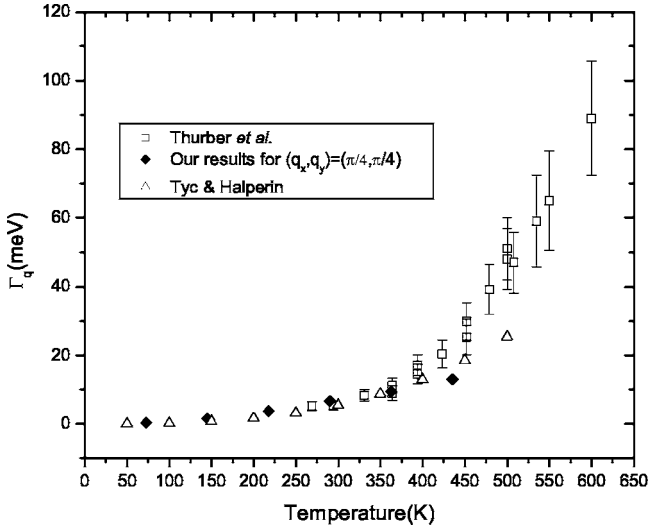

FIG. 5. Spin-wave damping $\Gamma(\vec{q},\tau)$, as a function of temperature for $(q_x,q_y)=(\pi/4,\pi/4)$ (filled-diamonds). Open squares are the experimental results from Thurber *et al.* (Ref. 44), and open triangles are theoretical results from Tyc and Halperin (Ref. 35).

high-energy peak surprisingly has its intensity *increased* when we turn up the temperature. One can be tempted to relate this peak to two-magnon excitations, which should become more important when the temperature raises. It is hard to imagine that such a sharp structure defining a double-peak structure will be destroyed if we take into account higher order processes, which are expected to give important contributions only at high temperatures.

A similar structure was also obtained by Auerbach and Arovas[33] in their Schwinger boson treatment of Eq. (1). It is indeed possible that the double peak structure is an artifact of the approximations done in each of the two different procedures. However, we *do* believe that it is due to the fact that both treatments included only up to two-magnon processes. In this way, we obtain a region where these processes do not contribute, as explained in the discussion of Fig. 2, and, there, higher order processes may dominate. We intend, in the near future, to investigate the effect of three magnons processes. Nevertheless, at the moment, we cannot discard the possibility that the present result, obtained by two different appraches, deserves some credit and must be verified by other means such as numerical simulation and/or experimental data. The same suggestion was made by Auerbach and Arovas.

In order to calculate the damping of the spin-waves, $\Gamma(\vec{q},\tau)$, we fit Lorentzians to the data points obtained for $R(\vec{q},\omega)$. $\Gamma(\vec{q},\tau)$ is so obtained as the half width of the low-energy peak, with no use of adjustable parameters. In Fig. 4, we show $\Gamma(\vec{q},\tau)$ as a function of the wave-vetor magnitude along two high symmetry directions in the antiferromagnetic Brillouin zone, for $\tau=0.05$. We see that the half width varies appreciably with the wave vector in the region near $\vec{q}=0$ and near the edge of the Brillouin zone; in most of the Brillouin zone the dependence of Γ on q is smoother. This result is in agreement with Monte Carlo results obtained by Makivic and Jarrell.[38]

The temperature dependence of Γ for the 2DQHAF was experimentally observed by Thurber *et al.*[44] in the $Sr_2CuO_2Cl_2$ compound. The estimated value for the exchange interaction in this 2DAF compound is $J=1450$ K and the magnetic anisotropy is so weak ($J_{xy}/J\approx 10^{-4}$) that the isotropic 2D Heisenberg behavior is robust even down to $\approx$280 K. Thurber *et al.* performed NMR studies in a broad range of temperatures ($0.2\leqslant T/J\leqslant 0.5$) and measured the nuclear spin lattice relaxation rate $1/T_1$. As is well known, the relaxation rate is related to the dynamical spin correlation function $S(\vec{q},\omega)$. Assuming that the elementary excitations in 2DQHAF are spin waves, those authors obtained an expression for $S(\vec{q},\omega)$ that depends on $\Gamma(\vec{q})$. However, they considered $\Gamma(\vec{q})=\Gamma$ as independent of $\vec{q}$ in most of the Brillouin zone, and, then, Γ is taken as a wave vector averaged damping.

In order to compare our results to the experimental data obtained by Thurber *et al.*, we chose the wave vector $(q_x,q_y)=(\pi/4,\pi/4)$, indicated in Fig. 4, since this has an intermediate value for the damping. The temperature dependence of the half width is shown in Fig. 5: our results were obtained for $J=1450$ K and with use of no normalization or fitting procedure. We can see an excelent agreement between our data, indicated by filled diamonds, and the experimental ones, up to a temperature of $T\sim 350$ K. Also shown in the figure are the previous results by Tyč and Halperin[35] in their self-consistent calculations and we also see a good agreement between our results. In Ref. 35, the spin-wave damping is calculated via perturbation theory, and, as in the procedure applied in this work, their theory is expected to be valid in the limit of low temperatures and long wavelengths. In order to extend their results to the $S=1/2$ case, they used renormalized quantum values for the zero-temperature spin-stiffness constant and magnon frequencies. However, whereas the two theoretical estimates for the temperature dependence of the spin wave damping do not differ appreciably

in the temperature range they are valid, it is important to emphasize, that only the present work gives a calculation of the $S(\vec{q},\omega)$ function which is, indeed, the important quantity for the understanding of the dynamical properties of the model.

IV. CONCLUSIONS

In summary, we have calculated the dynamic structure factor for the antiferromagnetic Heisenberg model with $S=1/2$ using a projection operator technique. This approach was also followed by Becher and Reiter,[34] but they used conventional spin-wave theory in order to calculate the static correlations needed as an input. Instead, we combined the method with the MSW theory, which goes beyond the linear one in the sense that it takes into account the inexistence of long-range order in the model at any finite temperature. We obtained a double-peak structure, as in a previous work of Auerbach and Arovas.[33] The damping, calculated by fitting lorentzians to our data points, agrees well with experimental data[44] and with previous theoretical calculations by Tyč and Halperin[35] up to a temperature $T\sim 350$ K.

It is worth remarking that, in the classical limit, the gap will vanish and the double peak struture will disappear. So, the double peak structure found here is a quantum effect.

Huberman *et al.*[45] probed the low-temperature magnetic excitations of the 2D $S=5/2$ AF compound Rb_2MnF_4 using pulsed inelastic neutron scattering and found a dominant sharp peak that can be identified with one-magnon excitations. However, in addition to this one magnon peak, he was able to observe a relatively weak continuum scattering at higher energies. This continuum scattering was attributed to scattering by pairs of magnons as expected to happen for the $\mathcal{M}_q$ correlation function. This will be the subject of a future work.

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