Two-dimensional classical Heisenberg model with easy-plane anisotropy at low temperatures: Out-of-plane dynamics

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Correlation functions of the two-dimensional classical Heisenberg model with easy-plane anisotropy are calculated at low temperatures and compared with simulation data. The out-of-plane static correlation function is found to have an exponential decay with a temperature-independent correlation length. The normalized out-of-plane spin-wave energy is found to have the same temperature dependence as the square root of the nearest-neighbor in-plane static correlation function.

I. INTRODUCTION

In the last few years, great effort has been dedicated to experimental and theoretical study of low-dimensional magnetism. For one-dimensional (1D) magnetic systems, the combined theoretical and experimental work has been extremely successful, and nowadays, there is some agreement that most of the important features required for a thorough understanding of the problem are known. Two-dimensional (2D) magnetism appears then as a natural extension of the work done, a good candidate for the application of tools and models so carefully elaborated and tested during the 1D analysis. Also 2D magnetic systems have been thought as ideal vehicles to test results obtained from other disciplines as, for example, from quantum field theories. Besides, there is the rare opportunity to study dynamical aspects intrinsically associated with two dimensions such as vortex unbinding, instantons, etc. And, last but not least, the exciting discovery of high-t_c superconductivity in 2D antiferromagnets has attracted a lot of attention to this area. For all these reasons, the amount of experimental data (and also numerical simulation data) at our disposal is now large enough to serve as a test or a guide to the methods and theories used in the 2D analysis. However, in spite of all effort that has been done, a consistent understanding of 2D magnetism is far from being achieved, and it is important to make a complete discussion of the approximations done in each theoretical method and/or model.

In this paper we consider the two-dimensional classical easy-plane Heisenberg model

$$H=\pm\frac{J}{2}\sum_{\mathbf{r},\mathbf{u}}(S_{\mathbf{r}}^{x}S_{\mathbf{r}+\mathbf{u}}^{x}+S_{\mathbf{r}}^{y}S_{\mathbf{r}+\mathbf{u}}^{y}+\lambda S_{\mathbf{r}}^{z}S_{\mathbf{r}+\mathbf{u}}^{z}) , \qquad (1)$$

where $S_{\mathbf{r}}^x$, $S_{\mathbf{r}}^y$, and $S_{\mathbf{r}}^z$ are the three spin components localized at site $\mathbf{r}=a(n_x,n_y)$, with n_x and n_y integers, in the square lattice with lattice parameter a and $0\le\lambda<1$. $\pm J$ corresponds to antiferromagnetic (+) and ferromagnetic (−) nearest-neighbor couplings. This model admits vortexlike configurations that lead to the well-known Kosterlitz-Thouless transition[1] at some critical temperature $T_c(\lambda)$.[2] Vortex effects becomes important only near $T_c(\lambda)$ and will not be considered here. It is interesting to note that while static correlation functions for the XY model [$\lambda=0$ in Eq. (1)] have been fully studied (for reviews, see Refs. 3 and 4), the same is not true for the anisotropic model ($0<\lambda<1$). From the dynamical point of view, there have been only few theoretical studies[5–10] of dynamic correlation functions below T_c. We report here both "in-plane" and "out-of-plane" static correlation functions and the out-of-plane dynamical correlation function at low temperature for $0\le\lambda<1$.

Our approach uses an expansion of spin operators in boson operators (for convenience, we have worked mostly within the quantum-mechanical framework and then the classical limit will be taken as appropriate). For the static calculations, the statistical average has been done by considering only the lowest-order nontrivial term of the Hamiltonian's expansion. The projection-operator technique was used for the out-of-plane dynamical correlation function calculation: Through this formalism spin-wave interaction effects are considered in a rather simple way. Previously, Villain[6] proposed a method, the self-consistent harmonic approximation (SCHA), to address the same problem, but his approach turned out to be very difficult to apply. Besides, the method we use here provides a better agreement with simulation data, and for these reasons, a critical analysis of the approximations and details involved in its elaboration deserve attention.

In Sec. II we present a standard method for obtaining a diagonal form for the lowest-order nontrivial term of Hamiltonian (1) and calculate the static correlations. The main results reported there are the following: (a) The in-plane static correlation function has the same polynomial decay as the planar model. However, its amplitude is smaller because of out-of-plane spin fluctuations. (b) The out-of-plane static correlation function has an exponential decay with a temperature-independent correlation length at low temperatures. The projection-operator technique is briefly described in Sec. III where we also give an asymptotic form for the out-of-plane dynamical correlation function. We argue that the normalized out-of-plane spin-wave energy $\omega_{\mathbf{q}}^{\perp}(T)/\omega_{\mathbf{q}}$ has the same temperature dependence as the square root of the nearest-neighbor in-plane static correlation function.

II. STATIC CORRELATIONS

By making use of the polar representation for the spin at site $\mathbf{r}$,

$$\mathbf{S}_\mathbf{r}=(S[1-(S_\mathbf{r}^z/S)^2]^{1/2}\cos\varphi_\mathbf{r}\,,\quad S[1-(S_\mathbf{r}^z/S)^2]^{1/2}\sin\varphi_\mathbf{r},S_\mathbf{r}^z)\,, \tag{2}$$

with $\{\varphi_\mathbf{r},S^z_{\mathbf{r}'}\}=\delta_{\mathbf{r},\mathbf{r}'}$, Hamiltonian (1) becomes

$$H=\pm(J/2)\sum_{\mathbf{r},\mathbf{u}}\{S^2[1-(S_\mathbf{r}^z/S)^2]^{1/2}\times[1-(S^z_{\mathbf{r}+\mathbf{u}}/S)^2]^{1/2}\times\cos(\varphi_\mathbf{r}-\varphi_{\mathbf{r}+\mathbf{u}})+\lambda S^z_\mathbf{r}S^z_{\mathbf{r}+\mathbf{u}}\}\,. \tag{3}$$

For the antiferromagnet we redefine $\varphi_\mathbf{r}$ according to

$$\varphi'_\mathbf{r}=\varphi_\mathbf{r}+[1-(-1)^{n_x+n_y}]\pi/2\,, \tag{4}$$

so that the new angular variable $\varphi'_\mathbf{r}$ refers to fluctuations about a fundamental state in which the spins are parallelly aligned along some arbitrary direction in the easy plane. It is convenient to introduce transformation (4) because, at low temperatures, $\varphi'_\mathbf{r}$ is a smoothly varying function of $\mathbf{r}$, and then Hamiltonian (1) for the antiferromagnetic case can be expanded into the small powers of $(\varphi'_\mathbf{r}-\varphi'_{\mathbf{r}+\mathbf{u}})^2$, as can be done for the ferromagnetic case. Henceforth in this section as well as in Sec. III, all results are valid for both antiferromagnetic and ferromagnetic couplings. In order to simplify the notation, we shall use the same symbol $\varphi_\mathbf{r}$ for both cases and adopt the following convention: Whenever the $\pm$ or $\mp$ symbol appears, the upper signal refers to antiferromagnetic and the lower one refers to ferromagnetic coupling. If only one sign appears, the same formula is valid for both cases.

Carrying out the expansion into powers of $(S_\mathbf{r}^z/S)^2$ and $(\varphi_\mathbf{r}-\varphi_{\mathbf{r}+\mathbf{u}})^2$, we obtain

$$H=E_0+H_0+H_I\,, \tag{5}$$

where $E_0=-2NJS^2$ is the energy of the ground state, H_I represents higher-order terms, and H_0 is the harmonic Hamiltonian, which, after a Fourier transformation, is given by

$$H_0=2J\sum_\mathbf{q}\{S^2[1-\gamma(\mathbf{q})]\varphi_\mathbf{q}\varphi_{-\mathbf{q}}+[1\pm\lambda\gamma(\mathbf{q})]S^z_\mathbf{q}S^z_{-\mathbf{q}}\}\,, \tag{6}$$

where

$$\gamma(\mathbf{q})=\tfrac{1}{2}(\cos q_x+\cos q_y)\,, \tag{7}$$

and we have taken the lattice parameter $a=1$, for simplicity of notation. By introducing the canonical transformation (setting $\hbar=1$)

$$\varphi_\mathbf{q}=\frac{1}{(2S)^{1/2}}\left[\frac{1\pm\lambda\gamma(\mathbf{q})}{1-\gamma(\mathbf{q})}\right]^{1/4}(a^\dagger_\mathbf{q}+a_{-\mathbf{q}})\,, \tag{8}$$

$$S^z_\mathbf{q}=i\left[\frac{S}{2}\right]^{1/2}\left[\frac{1-\gamma(\mathbf{q})}{1\pm\lambda\gamma(\mathbf{q})}\right]^{1/4}(a^\dagger_\mathbf{q}-a_{-\mathbf{q}})\,, \tag{9}$$

where $a^\dagger_\mathbf{q}$ and $a_\mathbf{q}$ are the boson-creation and -annihilation operators, respectively, H_0 becomes

$$H_0=\sum_\mathbf{q}\omega_\mathbf{q}(a^\dagger_\mathbf{q}a_\mathbf{q}+\tfrac{1}{2})\,, \tag{10}$$

where

$$\omega_\mathbf{q}=4JS\{[1-\gamma(\mathbf{q})][1\pm\lambda\gamma(\mathbf{q})]\}^{1/2}\,. \tag{11}$$

We remark here that, for the antiferromagnet, two dispersion relations symmetrically related to each other by $\omega_1(\mathbf{q})=\omega_2(\mathbf{q}_0)$, where $\mathbf{q}_0=(\pi-q_x,\,\pi-q_y)$, are expected. Apparently, then, Eq. (11) fails in giving these two magnon modes for the antiferromagnet. However, this is not the case, as can be seen if one calculates the dynamical functions $\langle\varphi_\mathbf{q}(t)|\varphi_\mathbf{q}\rangle$ and $\langle S^z_\mathbf{q}(t)|S^z_\mathbf{q}\rangle$. Because of the $(-1)^{n_x+n_y}$ term in Eq. (4), we shall get $\omega_{\mathbf{q}_0}$ in the temporal evolution of $\langle\varphi_\mathbf{q}(t)|\varphi_\mathbf{q}\rangle$ and $\omega_\mathbf{q}$ for $\langle S^z_\mathbf{q}(t)|S^z_\mathbf{q}\rangle$.

We can now calculate the static correlations in the harmonic approximation context. The out-of-plane static correlation function is obtained from Eq. (9) and is given by

$$S^z(\mathbf{r})\equiv\langle S^z_0S^z_\mathbf{r}\rangle=\frac{\tau S^2}{4}\frac{1}{(2\pi)^2}\int d^2k\frac{\cos(\mathbf{k}\cdot\mathbf{r})}{1\pm\lambda\gamma(\mathbf{k})}\,, \tag{12}$$

where $\tau=T/JS^2$ is the reduced temperature. For $\lambda=0$ it is easy to see that

$$S^z(\mathbf{r})=\begin{cases}\tau S^2/4 & \text{for } \mathbf{r}=\mathbf{0}\,,\\ 0 & \text{for } |\mathbf{r}|>0\,.\end{cases} \tag{13}$$

For $0<\lambda<1$, by numerically solving the integral in (12), we can see that $S^z(\mathbf{r})$ has an exponential decay[11] with a temperature-independent correlation length. This exponential decay has been found by Kawabata and Bishop[2,12] through Monte Carlo simulation for all temperatures ($T\geq T_c$ as well as $T<T_c$). Their data also suggest a temperature-independent correlation length at low temperatures. For large distances a good fitting for the numerical results is

$$\frac{S^z(\mathbf{r})}{S^z(\mathbf{0})}\approx(\mp1)^{n_x+n_y}A\frac{e^{-r/\xi}}{\sqrt{r}}\quad\text{for } r\gg1\,, \tag{14}$$

where A and ξ are fitting parameters whose λ dependence is shown in Fig. 1. For $\lambda\simeq1$ we can evaluate the integral in (12) and then obtain

$$\frac{S^z(\mathbf{r})}{S^z(\mathbf{0})}\approx(\mp1)^{n_x+n_y}\frac{1}{\ln\xi_A^2}(2\pi\xi_A)^{1/2}\frac{e^{-r/\xi_A}}{\sqrt{r}}\quad\text{for } r\gg\xi_A \text{ and } \lambda\approx1\,, \tag{15}$$

where

$$\xi_A=\frac{1}{2}\left[\frac{\lambda}{1-\lambda}\right]^{1/2}. \tag{16}$$

ξ_A is also plotted in Fig. 1, where we can see that it compares very well with ξ in the $\lambda\to1$ limit.

It is straightforward to calculate the out-of-plane susceptibility $\beta^{-1}\kappa_z=\sum_\mathbf{r}|S^z(\mathbf{r})|$. From Eq. (9) we get

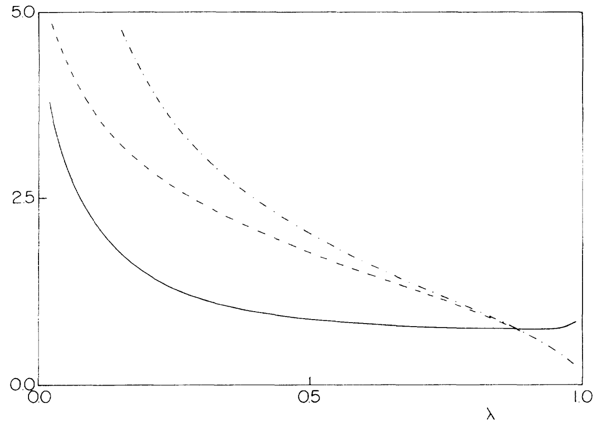

FIG. 1. Fitting parameters A (solid curve) and $1/\xi$ (dashed curve) of $S^z(\mathbf{r})/S^z(\mathbf{0})$ for $0<\lambda<1$ and, for comparison with $1/\xi$, the inverse correlation length $1/\xi_A$ (dot-dashed curve) of $S^z(\mathbf{r})/S^z(\mathbf{0})$ for $\lambda \approx 1$ as a function of the anisotropy λ. Note that, for $\lambda > 0.70$, $1/\xi$ is very close to $1/\xi_A$.

$$\kappa_z = \frac{1}{4J(1-\lambda)} \ . \tag{17}$$

Therefore we see that there is a temperature-independent susceptibility associated with the temperature-independent correlation length of the out-of-plane correlation.

For calculating the in-plane static correlation function, we use the fact that $\varphi_{\mathbf{r}}$ and $S^z_{\mathbf{r}}$ are, in the static case, uncoupled variables and that the out-of-plane fluctuations are exponentially decreasing in $\mathbf{r}$ with a temperature-independent correlation length, to obtain

$$\begin{aligned} S''(\mathbf{r}) &\equiv \langle S_0^x S_{\mathbf{r}}^x \rangle + \langle S_0^y S_{\mathbf{r}}^y \rangle \\ &= (\mp 1)^{n_x+n_y} S^2 [1 - \langle (S_0^z/S)^2 \rangle] \\ &\quad \times \langle \cos(\varphi_{\mathbf{r}} - \varphi_0) \rangle \ , \end{aligned} \tag{18}$$

at first order in temperature. The term $\langle (S_0^z/S)^2 \rangle$ is given by Eq. (12). It describes a decrease in the in-plane correlation due to out-of-plane fluctuations. The term $\langle \cos(\varphi_{\mathbf{r}} - \varphi_0) \rangle$ can be obtained by calculating the functional integral of $\exp(-\beta H_0)$ over $\varphi_{\mathbf{r}}$ and $S^z_{\mathbf{r}'}$ as has been done by Wegner[13] and Berezinskii.[14] Because of strong fluctuation effects, it falls off as a power law, and a first-order expansion in temperature fails in describing its long-distance behavior. Alternatively, this result can be obtained from the boson canonical representation of $\varphi_{\mathbf{r}}$ [Eq. (8)]. In the harmonic approximation, the average of a certain number of operators $\varphi_{\mathbf{r}}$ product decomposes into a sum of all products of average of separate pair of operators $\langle \varphi_{\mathbf{r}} \varphi_{\mathbf{r}'} \rangle$ (Wick's theorem). Thus we obtain

$$\begin{aligned} \langle \cos(\varphi_{\mathbf{r}} - \varphi_0) \rangle &= \sum_{n=0}^{\infty} \frac{\langle (\varphi_{\mathbf{r}} - \varphi_0)^{2n} \rangle}{2n!} \\ &= \exp(\langle \varphi_0 \varphi_{\mathbf{r}} \rangle - \langle \varphi_0^2 \rangle) \ . \end{aligned} \tag{19}$$

From Eq. (8) we get

$$\langle \varphi_0 \varphi_{\mathbf{r}} \rangle - \langle \varphi_0^2 \rangle = -\frac{\tau}{4} g(\mathbf{r}) \ , \tag{20}$$

where

$$g(\mathbf{r}) = \frac{1}{(2\pi)^2} \int d^2k \frac{1-\cos(\mathbf{k}\cdot\mathbf{r})}{1-\gamma(\mathbf{k})} \ . \tag{21}$$

This integral can be carried out.[15] For the special case $n_x = n_y = n$, we have a particularly simple result:

$$g(\mathbf{r}) = \frac{2}{\pi} \sum_{k=0}^{n-1} \frac{1}{k+\frac{1}{2}} \ . \tag{22}$$

An excellent approximation for $g(\mathbf{r})$, in the general case, is

$$g(\mathbf{r}) \cong \frac{2}{\pi} \ln \left[\frac{r}{r_0} \right] \quad \text{for } r \gg 1 \ , \tag{23}$$

where

$$r_0 = \frac{e^{-\gamma}}{2\sqrt{2}} \cong 0.2 \ , \tag{24}$$

where γ is Euler's constant. This is a good approximation even for $r \gtrsim 1$. Then the in-plane static correlation function becomes

$$S''(\mathbf{r}) = (\mp 1)^{n_x+n_y} S^2 [1 - \langle (S_0^z/S)^2 \rangle] \left[\frac{r_0}{r} \right]^{\tau/2\pi} \ . \tag{25}$$

Because of this polynomial decay, the in-plane susceptibility, $\beta^{-1}\kappa_{,,} = \sum_{\mathbf{r}} |S''(\mathbf{r})|$, diverges at low temperatures (up to T_c). In order to compare our results with simulation data, we introduce here the short-range order (SRO) defined as the square root of the nearest-neighbor in-plane static correlation function, i.e. $[S''(r=1)/S^2]^{1/2}$. This quantity is specially interesting because, as we shall see in the following section, it is related to the temperature dependence of the spin-wave energy. In Fig. 2 we present our calculations at first order in temperature for

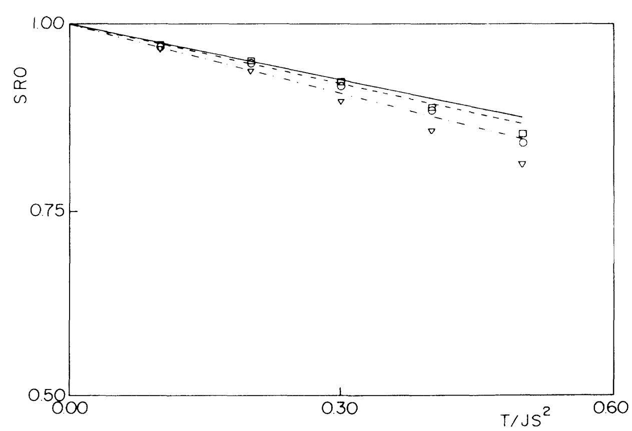

FIG. 2. SRO, defined as $[S''(r=1)/S^2]^{1/2}$, given as a function of the reduced temperature T/JS^2 for the ferromagnet. The marks correspond to numerical simulation results (Ref. 16), and the lines are our first-order calculations: $\lambda=0$ (□, solid curve), $\lambda=0.6$ (○, dashed curve), and $\lambda=0.9$ (∇ dot-dashed curve).

the ferromagnet and compare them with the results of Shirakura, Matsubara, and Inawashiro,[16] which have been obtained by means of numerical simulations based on Langevin equations. As we expected, the spin-wave theory is successful in describing the short-distance behavior at low temperatures. In fact, there is a good agreement up to $T \approx T_c/2$. For higher temperatures vortex effects become important and must be included in order to make an improved description.

III. OUT-OF-PLANE DYNAMICS

In studying the dynamics of a system, the quantity we are interested in calculating is the normalized two-spin relaxation function

$$R_{\mathbf{q}}^{\alpha}(t)=\langle S_{\mathbf{q}}^{\alpha}(t)|S_{\mathbf{q}}^{\alpha}\rangle\langle S_{\mathbf{q}}^{\alpha}|S_{\mathbf{q}}^{\alpha}\rangle^{-1} , \tag{26}$$

where the inner product between two operators A and B is defined by

$$\langle A|B\rangle=\frac{1}{\beta}\int_0^{\beta}\langle e^{\lambda H}Ae^{-\lambda H}B^{\dagger}\rangle d\lambda . \tag{27}$$

For a classical system, the inner product is an ordinary thermal average, such as $\langle S_{\mathbf{q}}^{\alpha}(t)|S_{\mathbf{q}}^{\alpha}\rangle=\langle S_{\mathbf{q}}^{\alpha}(t)S_{-\mathbf{q}}^{\alpha}\rangle$.

The well-known formalism of Mori[17] leads us to

$$R_{\mathbf{q}}^{\alpha}(z)=\frac{i}{z-\langle\omega_{\mathbf{q}}^2\rangle^{\alpha}/[z+\Sigma_{\mathbf{q}}^{\alpha}(z)]} , \tag{28}$$

where $R_{\mathbf{q}}^{\alpha}(z)$ is the Laplace transform of $R_{\mathbf{q}}^{\alpha}(t)$, $\langle\omega_{\mathbf{q}}^2\rangle^{\alpha}$ is the second moment, and $\Sigma_{\mathbf{q}}^{\alpha}(z)$ is the memory function defined as

$$\langle\omega_{\mathbf{q}}^2\rangle^{\alpha}=\langle LS_{\mathbf{q}}^{\alpha}|LS_{\mathbf{q}}^{\alpha}\rangle\langle S_{\mathbf{q}}^{\alpha}|S_{\mathbf{q}}^{\alpha}|\rangle^{-1} , \tag{29}$$

$$\Sigma_{\mathbf{q}}^{\alpha}(z)=-\langle QL^2S_{\mathbf{q}}^{\alpha}|(z-QLQ)^{-1}|QL^2S_{\mathbf{q}}^{\alpha}\rangle \times\langle LS_{\mathbf{q}}^{\alpha}|S_{\mathbf{q}}^{\alpha}\rangle^{-1} . \tag{30}$$

Here L is the Liouville operator and Q is the projection operator, which projects on nonsecular variables. Q is defined by $Q=1-P$, where

$$P=\frac{|S_{\mathbf{q}}^{\alpha}\rangle\langle S_{\mathbf{q}}^{\alpha}|}{\langle S_{\mathbf{q}}^{\alpha}|S_{\mathbf{q}}^{\alpha}\rangle}+\frac{|LS_{\mathbf{q}}^{\alpha}\rangle\langle LS_{\mathbf{q}}^{\alpha}|}{\langle LS_{\mathbf{q}}^{\alpha}|LS_{\mathbf{q}}^{\alpha}\rangle} . \tag{31}$$

We have, further,

$$QL^2S_{\mathbf{q}}^{\alpha}=L^2S_{\mathbf{q}}^{\alpha}-\langle\omega_{\mathbf{q}}^2\rangle^{\alpha}S_{\mathbf{q}}^{\alpha} , \tag{32}$$

which can be obtained using Eq. (31) and the identity

$$\langle A|L|B\rangle=(1/\beta)\langle[A^{\dagger},B]\rangle . \tag{33}$$

Concerning out-of-plane dynamics, it is cumbersome but straightforward to show, with help of Eqs. (32) and (33), that $\Sigma_{\mathbf{q}}^{z}(t)\propto T^2$. This should be expected because easy-plane systems exhibit a very narrow peak associated with the out-of-plane dynamical correlation function,[7] and the width of this peak, from analysis of Eq. (28), is expected to be just proportional to the imaginary part of $\Sigma_{\mathbf{q}}^{z}(\omega)$. In fact, a perturbative quantum calculation[18] shows that a finite width of the magnon peak of the z component of the spectral function appears only at a two-loop level. Therefore, as far as a first order in the temperature calculation is concerned, $\Sigma_{\mathbf{q}}^{z}(t)=0$, and from Eq. (28), the following low-temperature asymptotical form of the normalized spectral function is obtained:

$$R_{\mathbf{q}}^{z}(\omega)=(1/\pi)[\delta(\omega+(\langle\omega_{\mathbf{q}}^2\rangle^{z})^{1/2}) +\delta(\omega-(\langle\omega_{\mathbf{q}}^2\rangle^{z})^{1/2})] . \tag{34}$$

Evidently, through this form we cannot say much about the linewidth, except that it is expected to be very narrow. But we can obtain, at first order in temperature, the out-of-plane spin-wave energy as

$$\omega_{\mathbf{q}}^{\perp}(T)=(\langle\omega_{\mathbf{q}}^2\rangle^{z})^{1/2} . \tag{35}$$

Here "out-of-plane spin-wave energy" refers to the energy (or frequency) where the peak of the z component of the spectral function occurs. Using the identity (33), $\langle\omega_{\mathbf{q}}^2\rangle^{z}$ can be put in a more convenient form:

$$\langle\omega_{\mathbf{q}}^2\rangle^{z}=\frac{4J^2S^2[1-\gamma(\mathbf{q})]}{\langle S_{\mathbf{q}}^{z}|S_{\mathbf{q}}^{z}\rangle}|S''(r=1)| . \tag{36}$$

In order to evaluate this expression, we shall make use of the static correlations obtained in Sec. II through the harmonic approximation. This approximation, for $S''(r=1)$, was discussed there. For $\langle S_{\mathbf{q}}^{z}|S_{\mathbf{q}}^{z}\rangle$ we argue that, since the out-of-plane static correlation function is a "pulse-shaped" function of $\mathbf{r}$, an improved calculation of this correlation at large distances should have a small effect in the reciprocal space at low temperatures. Then, with this approximation, we obtain

$$\omega_{\mathbf{q}}^{\perp}(T)=\omega_{\mathbf{q}}|S''(r=1)/S^2|^{1/2} , \tag{37}$$

where the last term is given in Sec. II. Therefore the normalized out-of-plane spin-wave energy $\omega_{\mathbf{q}}^{\perp}(T)/\omega_{\mathbf{q}}$ is just equal to SRO and, consequently, does not depend on $\mathbf{q}$ at low temperatures. In Fig. 3 we compare our calculation of $\omega_{\mathbf{q}}^{\perp}(T)$ for the antiferromagnet with the molecular-

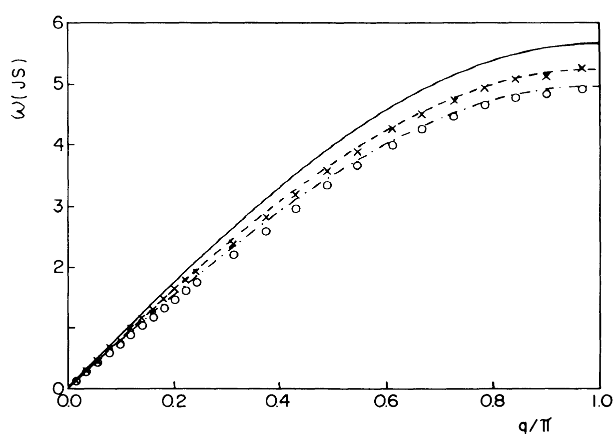

FIG. 3. Energy of the out-of-plane spin wave $\omega_{\mathbf{q}}^{\perp}(T)$ as a function of $\mathbf{q}=(q,q)$ for the antiferromagnet with $\lambda=0$. The marks correspond to numerical simulation results (Ref. 19), and the lines are our first-order calculations: $T=0$ (solid curve), $T=0.3JS^2$ (×, dashed curve), and $T=0.5JS^2$ (○, dot-dashed curve).

dynamics results of Völkel *et al.*[19] at two values of temperature, namely, $\tau=0.3$ and 0.5. We see that there is an excellent agreement at $\tau=0.3$ for all values of **q**. It is interesting to note that even at a temperature as high as $\tau=0.5$, our first-order calculation presents only a small deviation from the simulation data.

In conclusion, we observe that Eq. (34) is valid for all **q**, and then we expect well-defined spin-wave peaks in the z component of the spectral function for any transferred momentum. We also remark that spin-wave theory, as presented here, does not describe as successfully in-plane dynamics, at least quantitatively, because, since in this case the long-distance behavior is a determinant factor, an improved calculation of the static correlations is required.

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