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Dimensional crossover in the magnetic properties of highly anisotropic antiferromagnets

N. Majlis and S. Selzer
Scuola Normale Superiore, I-56100 Pisa, Italy
and Instituto de Física, UFF, Outeiro de São Joao Batista S/N, 24020 Niterói, Rio de Janeiro, Brazil

G. C. Strinati
Scuola Normale Superiore, I-56100 Pisa, Italy
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Magnetic properties of highly anisotropic perovskites based on copper oxide planes have commonly been interpreted in terms of the free-spin-wave approximation to a Heisenberg model. For this model, we calculate the Néel temperature, the magnetic moment, the spin-wave velocity, and the first-nearest-neighbor instantaneous spin correlator by varying the anisotropy ratio $\epsilon = J_\perp / J_\parallel$ between the intraplane and interplane effective exchange couplings at three different levels of approximation: the ordinary free-spin-wave, the Tyablikov random-phase approximation (RPA), and a modified RPA obtained by adapting Callen original decoupling procedure. In all cases, we find that the crossover from three to two dimensions occurs at $\epsilon \approx 10^{-3}$. By interpreting the available experimental data for La_2CuO_4 with our calculations, we also find that the value of ϵ verges on the two-dimensional side, although it can vary by a factor 10^2 depending on the approximation. Our results call for more accurate experimental determination and theoretical interpretation of the temperature-dependent magnetic excitations in the perovskite compounds. Their two-dimensional character favors, in fact, the existence of local magnetic excitations that outlive the disappearance of long-range order, as shown by the calculated behavior of the first-nearest-neighbor instantaneous spin correlator.

I. INTRODUCTION

There has been lately considerable interest in highly anisotropic magnetic compounds which are parent systems of high-T_c superconducting perovskites. In particular, La_2CuO_4 and $YBa_2Cu_3O_6$ show fairly large Néel temperatures T_N and strongly anisotropic antiferromagnetic correlations, indicating that the effective exchange coupling $J_\parallel$ within the CuO_2 planes is unusually large ($\simeq 0.1$ eV) while the anisotropy ratio $\epsilon = J_\perp / J_\parallel$ is quite small.[1-4] The ratio ϵ controls the dimensional crossover from three to two dimensions, and accordingly determines the thermodynamic behavior of the anisotropic antiferromagnet. A reliable estimate of ϵ is thus required to make contact between the experimental data and the results of the two-dimensional ($T=0$) calculations which are commonly used to study the magnetic properties of these systems.

Interpretation of the magnetic properties of La_2CuO_4 and $YBa_2Cu_3O_6$ has been done with the assumption that the magnetic moments reside in the spin-$\frac{1}{2}$ Cu atoms, although a detailed three-dimensional spin arrangement has not been unambiguously determined on the basis of NMR, NQR, and neutron diffraction experiments. For this reason, it has been common practice to model the three-dimensional magnetic arrangement by a simple tetragonal bipartite (A and B) lattice with two distinct antiferromagnetic couplings, the intraplane $J_\parallel$ and the interplane $J_\perp$. In this paper we shall follow this common practice.

Within such geometry, the magnetic dynamics has usually been described via an anisotropic quantum Heisenberg model. Neutron and light scattering data have been fitted by resorting to a free-spin-wave approximation to this model.[1-4] Typical fits for ϵ have given values in the range 10^{-5}–10^{-4} for La_2CuO_4, thereby supporting the strongly two-dimensional character for this magnetic system.[3,5] The value $\epsilon \cong 10^{-5}$ has been obtained by relying on a purely two-dimensional description of the magnetic excitations and on a general scaling relation for T_N in terms of ϵ.[3] The value of $\epsilon \cong 10^{-4}$ has been obtained instead by treating the full three-dimensional coupling within the free-spin-wave approximation which is known to be valid when $T \ll T_N$.[5]

In this context, it appears worthwhile to undertake a more systematic study of the dependence of accessible physical quantities (such as the magnetic moment μ, the spin-wave velocity v, and the first-nearest-neighbor instantaneous spin correlator F) in terms of ϵ and T, by relying on theoretical treatments which can extend the validity of the ordinary free-spin-wave approximation up to temperatures below, but comparable with, T_N. One of the purposes of this paper is then to compare theoretical results obtained for the anisotropic Heisenberg model at different levels of approximation and to clarify to what extent the estimates of ϵ from measured quantities depend on the underlying theoretical approximation. We shall, in particular, compare results of the ordinary free-spin-wave approximation with two more elaborate approximations, namely, (i) the Tyablikov random-phase approximation (RPA)[6] which takes into account the self-consistent temperature-dependent renormalization of the magnetic moment μ due to large transverse spin fluctuations, and (ii) the Callen modified RPA approximation[7]

(MRPA) which includes also the self-consistent renormalization of the first-nearest-neighbor instantaneous spin correlator F. For our purposes, we have adapted both approximations to the case of an anisotropic antiferromagnet.

We shall find that, apart from the Néel temperature that has to scale to zero with $\ln 1/\epsilon$ when $\epsilon \rightarrow 0$, the quantities μ, v, and F saturate at their two-dimensional value when $\epsilon \approx 10^{-3}$, a value that thus corresponds to the actual crossover from three ($\epsilon \cong 1$) to two ($\epsilon = 0$) dimensions. [We consistently assume that the system is in an ordered state at $T=0$ even for $\epsilon = 0$ (cf. Ref. 8, and references therein).] We shall also find that T_N and v depend considerably on the chosen approximation while μ does not. In particular, the dependence of T_N on ϵ obtained within the RPA approximation is scaled by a factor 2/3 from that obtained by both free-spin-wave and MRPA approximations. Similarly, the values of v near $T=0$ almost coincide in the free-spin-wave and the MRPA approximations while the RPA gives a smaller value (typically, by a factor 2/3 when $\epsilon = 0$). However, the free-spin-wave and MRPA values for μ and v differ markedly in their temperature dependence owing to the self-consistent renormalizations required by the MRPA approximation. Our analysis thus warns against a simple-minded use of the free-spin-wave approximation and indicates that a cautious interpretation of the experimental data on La_2CuO_4 and $YBa_2Cu_3O_6$ is required in order to extract reliable information on the macroscopic parameters of these anisotropic antiferromagnets.[9]

We mention finally that we have successfully tested our calculation for the first-nearest-neighbor instantaneous spin correlator F at T_N with the available experimental data on the isotropic ($\epsilon = 1$) $GdAlO_3$ doped with Cr^{3+} from fluorescence measurements,[10] and found very good agreement with experiment to within our estimated 15% error.

The plan of the paper is the following. In Sec. II we set up the relevant finite-temperature formalism via the Matsubara Green's functions technique and discuss the three alternative approximations (free spin waves, RPA, and MRPA) to calculate the physical quantities of interest. Details of the calculations are given in the Appendix. In Sec. III we describe the numerical procedure and the results. Section IV contains our conclusions.

II. DECOUPLING PROCEDURES FOR THE DYNAMIC TRANSVERSE SPIN CORRELATION FUNCTION IN AN ANISOTROPIC ANTIFERROMAGNET

In this section we calculate the wave vector and frequency-dependent finite-temperature transverse spin correlation function in the broken symmetry phase for an anisotropic antiferromagnet. We assign a spin-$\frac{1}{2}$ operator $\mathbf{S}$ to each site of a tetragonal lattice with lattice constants $\Delta_\parallel$ in the basal plane and $\Delta_\perp$ along the tetragonal symmetry axis. The Hamiltonian we consider is the Heisenberg model

$$H = \sum_{i,j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j \tag{2.1}$$

with spatial anisotropy defined by the first-nearest-neighbor effective exchange coupling

$$J_{ij} = \begin{cases} J_\parallel, & \text{for } (i,j) \text{ on the basal plane,} \\ J_\perp, & \text{for } (i,j) \text{ on adjacent planes.} \end{cases} \tag{2.2}$$

Dynamic properties of this system can be characterized by the transverse spin temperature correlation function

$$\chi_{ij}^{+-}(\tau) = \langle T_\tau [S_i^+(\tau) S_j^-(0)] \rangle , \tag{2.3}$$

where τ is the Matsubara imaginary time, T_τ denotes the time-ordering operator, $\langle \cdots \rangle$ stands for the thermal average, and ($\hbar = 1$)

$$S_i^\pm(\tau) = \exp(H\tau) S_i^\pm \exp(-H\tau) \tag{2.4}$$

evolve in the modified Heisenberg picture.[6] The equation of motion for $\chi_{ij}^{+-}(\tau)$ can be readily derived from the τ evolution of $S_i^+(\tau)$. One obtains

$$\begin{aligned} \frac{\partial}{\partial \tau} \chi_{ij}^{+-}(\tau) = & -2J_\parallel \sum_{\Delta_\parallel} \{ \langle T_\tau [S_{i+\Delta_\parallel}^+(\tau) S_i^z(\tau) S_j^-(0)] \rangle - \langle T_\tau [S_{i+\Delta_\parallel}^z(\tau) S_i^+(\tau) S_j^-(0)] \rangle \} \\ & -2J_\perp \sum_{\Delta_\perp} \{ \langle T_\tau [S_{i+\Delta_\perp}^+(\tau) S_i^z(\tau) S_j^-(0)] \rangle - \langle T_\tau [S_{i+\Delta_\perp}^z(\tau) S_i^+(\tau) S_j^-(0)] \rangle \} + 2\delta_{ij} \delta(\tau) \langle S_i^z \rangle . \end{aligned} \tag{2.5}$$

Here and below the sums over $\Delta_\parallel$ and $\Delta_\perp$ are restricted to the "star" of first-nearest-neighbor atoms on the basal plane and on the tetragonal symmetry axis, respectively.

The appearance of a three-spin correlation function in Eq. (2.5) and the difficulties in implementing an equivalent to Wick theorem for spin operators suggest, as usual, that one resorts to *ad hoc* decoupling procedures in order to solve Eq. (2.5) for $\chi_{ij}^{+-}(\tau)$ in a closed form. In the following, we adapt to the present context two decoupling procedures which have been originally developed for isotropic ferromagnets. For completeness, some material other than ours will be reported.

A. Free-spin-wave and Tyablikov RPA approximations

The conventional free-spin-wave approximation[11] (FSWA) and the Tyablikov RPA approximation[6] for the spin correlation function result form Eq. (2.5) by replacing the operator $S_i^z(\tau)$ whenever it occurs by $\pm\frac{1}{2}$ (depending on the sublattice) and by $\langle S_i^z \rangle$, respectively. In what follows we thus sketch the calculation for the RPA approximation only.[12]

It is convenient to exploit at the outset the periodicity in τ and the translational symmetry of the lattice by introducing the Fourier decomposition

$$\chi^{+-}(\mathbf{q},\mathbf{q}';\Omega_\lambda)=\frac{1}{N}\sum_{i,j}\int_0^\beta d\tau\, e^{i\Omega_\lambda\tau}e^{-i\mathbf{q}\cdot\mathbf{R}_i}\chi_{ij}^{+-}(\tau)e^{i\mathbf{q}'\cdot\mathbf{R}_j}\ , \tag{2.6}$$

where N is the number of atomic unit cells, $\beta=(k_BT)^{-1}$ is the inverse temperature, $\Omega_\lambda=2\pi\lambda/\beta$($\lambda$ integer) is a Matsubara frequency, and $\mathbf{R}_i$ is a lattice vector. The (Néel) antiferromagnetic ansatz can be imposed at this point by setting

$$\langle S_i^z\rangle=\langle S_A^z\rangle\exp(-i\mathbf{Q}\cdot\mathbf{R}_i)\ , \tag{2.7}$$

where the wave vector $\mathbf{Q}$ is such that

$$\exp(-i\mathbf{Q}\cdot\mathbf{\Delta}_\parallel)=\exp(-i\mathbf{Q}\cdot\mathbf{\Delta}_\perp)=-1 \tag{2.8}$$

and $\langle S_A^z\rangle$ is associated with any site of the A (up) sublattice. Equation (2.5) thus becomes in Fourier space:

$$-i\Omega_\lambda\chi^{+-}(\mathbf{q},\mathbf{q}';\Omega_\lambda)+[\omega_0-\omega_1(\mathbf{q})]\chi^{+-}(\mathbf{q}+\mathbf{Q},\mathbf{q}';\Omega_\lambda)=2\langle S_A^z\rangle\delta(\mathbf{q}+\mathbf{Q}-\mathbf{q}')\ , \tag{2.9}$$

where we have set

$$\omega_0=2\langle S_A^z\rangle(J_\parallel z_\parallel+J_\perp z_\perp)\ ,\qquad \omega_1(\mathbf{q})=2\langle S_A^z\rangle[J_\parallel z_\parallel\gamma_\parallel(\mathbf{q})+J_\perp z_\perp\gamma_\perp(\mathbf{q})]\ . \tag{2.10}$$

In these expressions, $z_\parallel$ and $z_\perp$ are the coordination numbers in the basal plane and along the tetragonal symmetry axis, respectively, and

$$\gamma_\parallel(\mathbf{q})=\frac{1}{z_\parallel}\sum_{\mathbf{\Delta}_\parallel}e^{i\mathbf{q}\cdot\mathbf{\Delta}_\parallel}\ ,\qquad \gamma_\perp(\mathbf{q})=\frac{1}{z_\perp}\sum_{\mathbf{\Delta}_\perp}e^{i\mathbf{q}\cdot\mathbf{\Delta}_\perp} \tag{2.11}$$

are the normalized structure factors. Equation (2.9) can be readily solved, to yield the desired transverse spin correlation function

$$\chi^{+-}(\mathbf{q},\mathbf{q}';\Omega_\lambda)=-2\langle S_A^z\rangle\frac{i\Omega_\lambda\delta(\mathbf{q}+\mathbf{Q}-\mathbf{q}')+[\omega_0-\omega_1(\mathbf{q})]\delta(\mathbf{q}-\mathbf{q}')}{(i\Omega_\lambda)^2-[\omega_0^2-\omega_1(\mathbf{q})^2]}\ . \tag{2.12}$$

Analytic continuation to real frequencies can be performed at this point by letting $i\Omega_\lambda\to\omega+i\delta$ with $\delta=0^+$.

Notice that the correlation function (2.12) has poles for $\omega=\pm\Omega(\mathbf{q})$ with

$$\Omega(\mathbf{q})=\sqrt{\omega_0^2-\omega_1(\mathbf{q})^2}\ . \tag{2.13}$$

Notice also that the residue of the second term in the numerator of Eq. (2.12) only survives when $\omega\to0$, provided we take $\mathbf{q}=\mathbf{q}'=\mathbf{Q}+\delta\mathbf{q}$ (reflecting the fact that only the staggered transverse correlation function diverges in the static limit for an antiferromagnet.) For this function we obtain

$$\chi^{\pm}(\mathbf{Q}+\delta\mathbf{q},\mathbf{Q}+\delta\mathbf{q}';\omega)=-2\langle S_A^z\rangle\frac{[\omega_0+\omega_1(\delta\mathbf{q})]}{[\omega-\Omega(\delta\mathbf{q})][\omega+\Omega(\delta\mathbf{q})]}\delta(\delta\mathbf{q}-\delta\mathbf{q}')\ , \tag{2.14}$$

where $\omega_0+\omega_1(\delta\mathbf{q})\to2\omega_0$ for $\delta\mathbf{q}\to0$.

The spin-wave spectrum for the ordinary FSWA is obtained by replacing $\langle S_A^z\rangle$ with $\frac{1}{2}$ in Eq. (2.10). Within the RPA, however, $\langle S_A^z\rangle<\frac{1}{2}$ for any value of the anisotropy ratio ϵ and even at $T=0$ owing to quantum fluctuations; the effect of thermal fluctuations at finite temperature is to further reduce $\langle S_A^z\rangle$, making it vanish at a critical temperature which is identified with the Néel temperature T_N.[6] In this context, we recall that the low-temperature series expansion by the Dyson method[13] for an isotropic ferromagnet yields a spin-wave spectrum renormalization with temperature that can be reasonably reproduced by the RPA effective interpolation procedure.[14] For an antiferromagnet, on the other hand, it seems more appropriate to consider the renormalized value of $\langle S_A^z\rangle$ even at $T=0$, as in the RPA, instead of its nominal saturated value 1/2, as in the FSWA.

To evaluate $\langle S_A^z\rangle$ within the RPA from the staggered correlation function (2.14) we exploit, as usual, the operator identity

$$S_i^z+\frac{1}{2}=S_i^+S_i^-\ , \tag{2.15}$$

which holds for spin $\frac{1}{2}$ at any given lattice site. We obtain:

$$\langle S_A^z\rangle=\frac{1/2}{1+2\psi} \tag{2.16}$$

with the notation

$$\psi=\frac{1}{N}\sum_{\mathbf{q}}{}'\left[\frac{\omega_0}{\Omega(\mathbf{q})}\coth\left[\frac{\beta}{2}\Omega(\mathbf{q})\right]-1\right] \tag{2.17}$$

and the understanding that the primed sum extends over the antiferromagnetic Brillouin zone. In the ordinary FSWA,[11,12] one would obtain instead

$$\langle S_A^z\rangle=\frac{1}{2}-\psi'\ , \tag{2.18}$$

where ψ' results from ψ given by Eq. (2.17) by replacing $\langle S_A^z\rangle$ with 1/2 in the expressions (2.10) and (2.13) for ω_0 and $\Omega(\mathbf{q})$. Notice that, with this provision, Eq. (2.18) is obtained formally by expanding the denominator in Eq. (2.16) to first order in ψ. Notice also that, at zero temperature, $\psi=\psi'$ because the prefactor of the spin-wave spectrum cancels out: the integral (2.17) is of geometric character and depends on the dynamics only through the anisotropy ratio ϵ.

The Néel temperature T_N is obtained, by definition, within the RPA by taking $\langle S_A^z \rangle$ given by Eq. (2.16) to vanish. One obtains

$$\frac{k_B T_N^{(\mathrm{RPA})}}{J_\parallel} = \frac{z_\parallel + \epsilon z_\perp}{2W_\epsilon} \tag{2.19}$$

with the notation

$$W_\epsilon = \frac{2}{N} \sum_{\mathbf{q}}{}' \frac{1}{1-\gamma_\epsilon(\mathbf{q})^2} , \tag{2.20}$$

$$\gamma_\epsilon(\mathbf{q}) = \frac{z_\parallel \gamma_\parallel(\mathbf{q}) + \epsilon z_\perp \gamma_\perp(\mathbf{q})}{z_\parallel + \epsilon z_\perp} . \tag{2.21}$$

The dominant contribution to the sum in Eq. (2.20) originates from the neighborhood of $\mathbf{q}=0$ where $\gamma_\epsilon(\mathbf{q})$ tends to unity. Quite generally, a $\ln\epsilon$ term can be isolated from W_ϵ to yield

$$\frac{k_B T_N^{(\mathrm{RPA})}}{J_\parallel} = \frac{A}{B_\epsilon + \ln 1/\epsilon} , \tag{2.22}$$

where A is a numerical constant and B_ϵ is a smooth function of ϵ. The singular ln term in Eq. (2.22), which represents the contribution of the neighborhood of $\mathbf{q}=0$, restores in the two-dimensional limit ($\epsilon=0$) the correct thermodynamic behavior which is violated at the mean-field level, where

$$\frac{k_B T_N^{(\mathrm{MF})}}{J_\parallel} = \frac{1}{2}(z_\parallel + \epsilon z_\perp) \tag{2.23}$$

has a finite value for $\epsilon=0$. Our numerical results, to be presented in the next section, confirm the behavior (2.22) for W_ϵ, with $B_\epsilon \simeq$ constant within numerical error over a wide range of ϵ. Notice that the ratio B/A controls the crossover from the three-dimensional to the two-dimensional case.

An expression similar to (2.22) is also obtained within the FSWA with, in general, different coefficients A and B.

B. Callen Modified RPA

The Tyablikov RPA approximation discussed above neglects the correlation between longitudinal and transverse fluctuations, by replacing the operator S_i^z in Eq. (2.5) with its average value $\langle S_i^z \rangle$. It is thus expected that an improved approximation would retain the operator character of S_i^z, at least through its connection with the transverse operators S_i^+ and S_i^-. In this spirit, Callen[7] has proposed to take *a weighted average* between the operator identity (2.15) and the alternative one

$$S_i^z - \frac{1}{2} = -S_i^- S_i^+ \tag{2.24}$$

for spin-$\frac{1}{2}$ operators, in the form

$$S_i^z = \left[\frac{1-\alpha}{2}\right]\left[-\frac{1}{2} + S_i^+ S_i^-\right] + \left[\frac{1+\alpha}{2}\right]\left[\frac{1}{2} - S_i^- S_i^+\right] . \tag{2.25}$$

The value of the parameter α can be suitabley chosen to fulfill some conditions. Callen[7] has shown that the choice

$$\alpha = 2\langle S_i^z \rangle \tag{2.26}$$

improves the agreement with Dyson's low-temperature expansion over the RPA approximation for an isotropic ferromagnet, provided one suitably decouples the higher-order correlators among transverse spin operators which result from Eq. (2.25).[15] Lacking a corresponding comparison for an (anisotropic) antiferromagnet, we take over Callen's procedure to the present case in the same spirit as what has been done above for the RPA approximation.

Callen's procedure for the anisotropic antiferromagnet replaces the equation of motion (2.5) by the following one:

$$\begin{aligned}\frac{\partial}{\partial\tau}\chi_{ij}^{+-}(\tau) = & -2J_\parallel \langle S_i^z \rangle \sum_{\Delta_\parallel} [\chi_{ij}^{+-}(\tau)(1-2\langle S_{i+\Delta_\parallel}^+ S_i^- \rangle) + \chi_{i+\Delta_\parallel j}^{+-}(\tau)(1-2\langle S_{i+\Delta_\parallel}^- S_i^+ \rangle)] \\ & -2J_\perp \langle S_i^z \rangle \sum_{\Delta_\perp} [\chi_{ij}^{+-}(\tau)(1-2\langle S_{i+\Delta_\perp}^+ S_i^- \rangle) + \chi_{i+\Delta_\perp j}^{+-}(\tau)(1-2\langle S_{i+\Delta_\perp}^- S_i^+ \rangle)] + 2\delta_{ij}\delta(\tau)\langle S_i^z \rangle .\end{aligned} \tag{2.27}$$

Notice that Eq. (2.27) contains, besides the local average $\langle S_i^z \rangle$, also the *first-nearest-neighbor instantaneous correlator* $\langle S_i^+ S_j^- \rangle$ which must be determined self-consistently.

For symmetry reasons, there are only two such independent correlators when $0 < \epsilon < 1$ (but only one when either $\epsilon = 1$ or 0.) We set in general

$$\langle S_{i+\Delta_\parallel}^+ S_i^- \rangle = F_\parallel^{(1)} + e^{i\mathbf{Q}\cdot\mathbf{R}_i} F_\parallel^{(2)} , \tag{2.28}$$

$$\langle S_{i+\Delta_\perp}^+ S_i^- \rangle = F_\perp^{(1)} + e^{i\mathbf{Q}\cdot\mathbf{R}_i} F_\perp^{(2)} , \tag{2.29}$$

where the dependence on ϵ is understood. It can be readily shown that $F_\parallel^{(1)}$ and $F_\perp^{(1)}$ are real while $F_\parallel^{(2)}$ and $F_\perp^{(2)}$ are purely imaginary whenever the lattice has an inversion symmetry such as in the present case. Accordingly, it can further be shown that $F_\parallel^{(2)}$ and $F_\perp^{(2)}$ must vanish (cf. the Appendix). In the following we shall thus drop the labels 1 and 2 on the F.

Equation (2.9) in Fourier space is now replaced by

$$-i\Omega_\lambda \chi^{+-}(\mathbf{q},\mathbf{q}';\Omega_\lambda)+\{[\omega_0-\omega_1(\mathbf{q})]-[\Gamma_0-\Gamma(\mathbf{q})]\}\times\chi^{+-}(\mathbf{q}+\mathbf{Q},\mathbf{q}';\Omega_\lambda)=2\langle S_A^z\rangle\delta(\mathbf{q}+\mathbf{Q}-\mathbf{q}') , \quad (2.30)$$

where

$$\Gamma(\mathbf{q})=4\langle S_A^z\rangle[J_\parallel z_\parallel F_\parallel \gamma_\parallel(\mathbf{q})+J_\perp z_\perp F_\perp \gamma_\perp(\mathbf{q})] \quad (2.31)$$

and $\Gamma_0=\Gamma(\mathbf{q}=0)$. The solution of Eq. (2.30) is

$$\chi^{+-}(\mathbf{q},\mathbf{q}';\Omega_\lambda)=-2\langle S_A^z\rangle\frac{i\Omega_\lambda\delta(\mathbf{q}+\mathbf{Q}-\mathbf{q}')+\{(\omega_0-\Gamma_0)-[\omega_1(\mathbf{q})-\Gamma(\mathbf{q})]\}\delta(\mathbf{q}-\mathbf{q}')}{(i\Omega_\lambda)^2-\tilde{\Omega}(\mathbf{q})^2} \quad (2.32)$$

with the modified dispersion relation for spin waves

$$\tilde{\Omega}(\mathbf{q})=\sqrt{(\omega_0-\Gamma_0)^2-[\omega_1(\mathbf{q})-\Gamma(\mathbf{q})]^2} . \quad (2.33)$$

The complete solution of the problem has thus been reduced to solving (for given ϵ and T) a system of three coupled nonlinear integral equations for $\langle S_A^z\rangle$, $F_\parallel$, and $F_\perp$ which are obtained in the Appendix. Numerical solutions to these equations will be discussed in the next section.

It is worthwhile to comment at this point on the analytical results one obtains for the spin-wave velocity in the linear dispersion region near the *center* of the Brillouin zone. For simplicity, we report only the results for the isotropic limits ($\epsilon=1$ or 0), since the general trends are preserved between these two limits. For the three approximations, we obtain

$$v=\sqrt{2z}J\Delta\begin{cases}1 & \text{(FSWA)},\\ 2\langle S_A^z\rangle & \text{(RPA)},\\ 2\langle S_A^z\rangle(1-2F) & \text{(MRPA)},\end{cases} \quad (2.34)$$

with the understanding that the values of $z,J,\Delta,\langle S_A^z\rangle$, and F correspond properly to either one of the two limits. At zero temperature, $\langle S_A^z\rangle$ and F are readily obtained in both limits in terms of known integrals from the ordinary spin-wave theory of antiferromagnets.[11] One obtains for $2\langle S_A^z\rangle$ the values 0.865 and 0.718 when $\epsilon=1$ and 0, respectively; and for $2\langle S_A^z\rangle$ $(1-2F)$ the values 1.054 and 1.002 when $\epsilon=1$ and 0, respectively.

The occurrence of three different renormalization factors on the right-hand side of Eq. (2.34) can intuitively be understood as follows. Within the RPA one allows the transverse fluctuations to develop without being dynamically correlated to the longitudinal ones, the only effect retained being the average reduction of $\langle S_A^z\rangle$ from its saturated value $\frac{1}{2}$. The effective stiffness of the transverse fluctuations is self-consistently weakened in this way. Within the MRPA, on the other hand, the dynamical coupling between transverse and longitudinal fluctuations is retained at the lowest level, thereby yielding an effective hardening of the transverse fluctuations through the factor $(1-2F)$.[16] As it turns out, at zero temperature there results an almost complete compensation of the two effects associated with the two factors $2\langle S_A^z\rangle$ and $(1-2F)$. Notice finally that, contrary to the FSWA result which is appropriate to the zero-temperature limit, both the RPA and the MRPA expressions for *v vanish at the critical temperature.*

III. NUMERICAL RESULTS AND DISCUSSION

Our numerical task consists in evaluating, at various T and ϵ, the quantities ψ and W_ϵ given by Eqs. (2.17) and (2.20), respectively, within the RPA (and similar quantities with the FSWA), and in evaluating $F_\parallel$, $F_\perp$, and $\langle S_A^z\rangle$ given in the Appendix within the MRPA. Both ψ for the RPA and the coupled $F_\parallel$,$F_\perp$, and $\langle S_A^z\rangle$ for the MRPA have been determined self-consistently by a multidimensional Newton-Raphson method. The convergence of the integrals over the wave vector in the magnetic Brillouin zone has been checked *a posteriori* by refining the integration mesh.

Figure 1 shows the dependence of the Néel temperature on the anisotropy parameter ϵ for the three approximations we have considered. In all cases, T_N can be expressed in the form (2.22) with coefficients A and B different for the three cases, as shown in Table I. From the comparison given in Fig. 1 between T_N in the RPA and in the MRPA, we see that there is a general tendency of the renormalization of $\langle S_A^z\rangle$ and of the F's to compensate each other. This feature has also been derived analytically in the Appendix for the isotropic ($\epsilon=1$) and the two-dimensional ($\epsilon=0$) cases, and agrees with Callen's findings for the isotropic ferromagnet.[7] One may again argue that the indirect coupling of transverse to longitudinal spin fluctuations, which is effectively introduced by the MRPA procedure, makes the transverse fluctuations stiffer, thereby increasing the critical temperature and bringing it closer to the FSWA result. Because

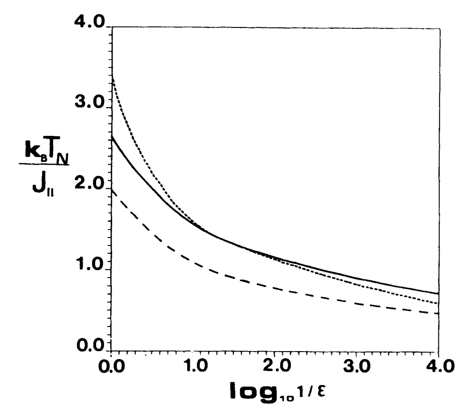

FIG. 1. Néel temperature in units of $J_\parallel/k_B$ vs. $\log_{10}1/\epsilon$ for the three approximations adopted in the text: dotted line (FSWA); broken line (RPA); solid line (MRPA).

TABLE I. Coefficients of Eq. (2.22) of the text for the three approximations considered. In the ϵ range of Fig. 1, $B_\epsilon \cong$ constant to within a 5% fitting of those curves.

	A	B
FSWA	7.7	2.3
RPA	6.0	3.0
MRPA	9.7	3.6

of the two compensating effects, within the MRPA the end result is closer to what is obtained by naively extrapolating the FSWA to high temperatures. The same compensating effects show up in the spin-wave velocity, to be discussed below.

In Fig. 2 the ($T=0$) local moment $\mu = 2\langle S_A^z \rangle$ is shown vs ϵ for the three approximations. This figure clearly indicates that the crossover from the three- to the two-dimensional behavior has already been exhausted at $\epsilon \approx 10^{-3}$ with a negligible variation for smaller ϵ. Notice that the values of $\langle S_A^z \rangle$ within the RPA and MRPA coincide (at $T=0$) in the two extreme limits $\epsilon=1$ and 0, while there is an appreciable (up to 10%) difference with the FSWA value. As already discussed in Sec. II, the coincidence between the RPA and the MRPA results in this case stems from the canceling out of the dynamical prefactor in the spin-wave spectrum, while the difference with the FSWA is due to the lack of self-consistency in the latter approach.

As the temperature increases, or when $0<\epsilon<1$, the dynamical differences in the RPA or MRPA show up in the magnitude of the local moment $\langle S_A^z \rangle$. This can be seen in Fig. 3 where $\mu = 2\langle S_A^z \rangle$ vs T is reported for the three approximations at the crossover anisotropy value $\epsilon = 10^{-3}$.

Dynamical differences among the three approximations are most evident in the behavior of the spin-wave velocity (at $\mathbf{q}=0$) as a function of ϵ and/or T. In Fig. 4 we report the two independent components ($v_\parallel, v_\perp$) vs ϵ at $T=0$. We notice that $v_\parallel$ saturates to its two-dimensional value when $\epsilon \gtrsim 10^{-3}$, showing that the dimensional crossover occurs simultaneously for all relevant physical quantities.

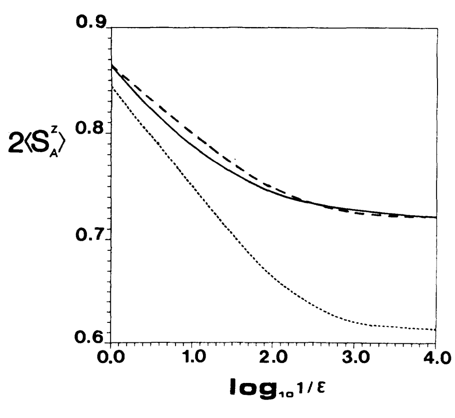

FIG. 2. Local magnetic moment $2\langle S_A^z \rangle$ vs. $\log_{10} 1/\epsilon$ at $T=0$ for the three approximations (conventions are as in Fig. 1).

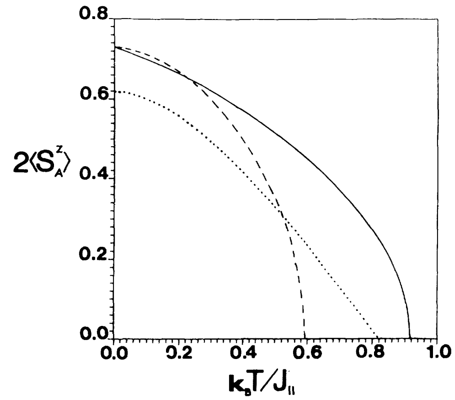

FIG. 3. Local magnetic moment $2\langle S_A^z \rangle$ vs $k_B T/J_\parallel$ at $\epsilon=10^{-3}$ for the three approximations (conventions are as in Fig. 1).

$v_\perp$, on the other hand, vanishes like $\sqrt{\epsilon}$ when $\epsilon \to 0$, for the three approximations.

The behavior of $v_\parallel$ and $v_\perp$ vs T for two significant values of ϵ is shown in Fig. 5. These quantities are normalized to the corresponding values within the FSWA which do not depend on T. The vanishing of $v_\parallel$ and $v_\perp$ at T_N is controlled by the order parameter $\langle S_A^z \rangle$ and is a consequence of the self-consistent renormalization of the

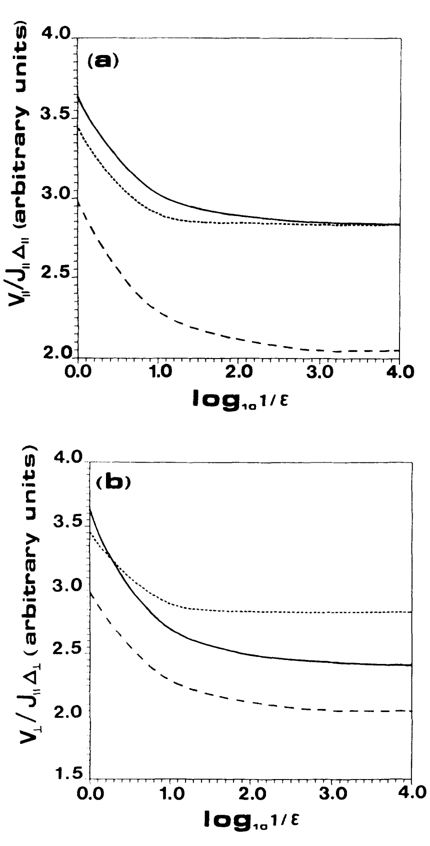

FIG. 4. (a) $v_\parallel / J_\parallel \Delta_\parallel$ and (b) $v_\perp / J_\parallel \Delta_\perp \sqrt{\epsilon}$ vs $\log_{10} 1/\epsilon$ at $T=0$ for the three approximations (conventions are as in Fig. 1).

spectrum in the presence of thermal fluctuations. This feature might effectively be avoided by spin excitations which are sustained *over a finite region* of the system and have a finite lifetime.[9] A full theory for these excitations in two dimensions remains to be developed.

Finally, Fig. 6 shows the absolute value of the two characteristic first-nearest-neighbor instantaneous correlators of the MRPA, $|F_{\parallel}|$ and $|F_{\perp}|$, vs ϵ at zero temperature as well as the behavior of $|F_{\parallel}|$ and $|F_{\perp}|$ vs T for two characteristic values of ϵ. Notice once more that the value $\epsilon \approx 10^{-3}$ determines the crossover from three to two dimensions, consistent with what has already been found for $\langle S_A^z \rangle$ and v. It is interesting to remark that $F_{\parallel}$ *is a slowly varying function of T, reaching a finite value at* T_N. (We expect this behavior to hold for the other approximations as well.) It is thus evident that $F_{\parallel}$ will extrapolate continuously above T_N, persisting to be finite in the paramagnetic phase. The short-range correlators F will presumably be relevant to describe the localized excitations mentioned above. Notice also from Fig. 6 that $|F_{\parallel}|$ *gets enhanced while approaching the two-dimensional limit,* thereby suggesting that the physical relevance of the localized excitations increases in two dimensions,[9] in agreement with experimental observations.[1] [Worth noticing, in particular, is the remarkable resemblance between the top part of Fig. 2 from Ref. 1 with the behavior of $|F_{\parallel}|$ vs T given in our Fig. 6(c).]

In this context, it is relevant to mention that measurements aiming at the determination of the instantaneous first-nearest-neighbor correlator via magneto-optical effects have already been performed on $GdAlO_3$ doped

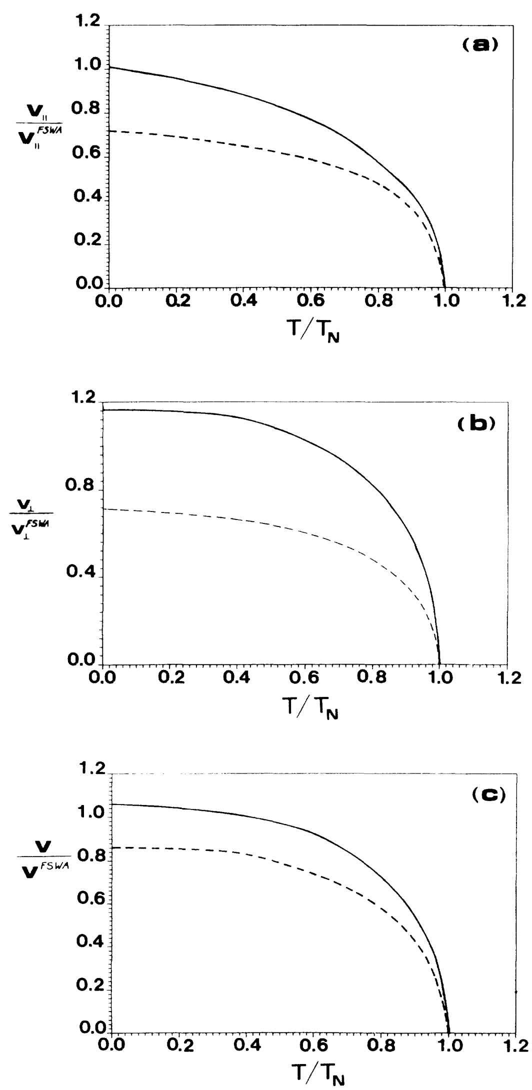

FIG. 5. (a) $v_{\parallel}/v_{\parallel}^{\mathrm{FSWA}}$ for $\epsilon=10^{-3}$, (b) $v_{\perp}/v_{\perp}^{\mathrm{FSWA}}$ for $\epsilon=10^{-3}$, and (c) v/v^{FSWA} for $\epsilon=1$, vs T/T_N: solid line (MRPA) and broken line (RPA).

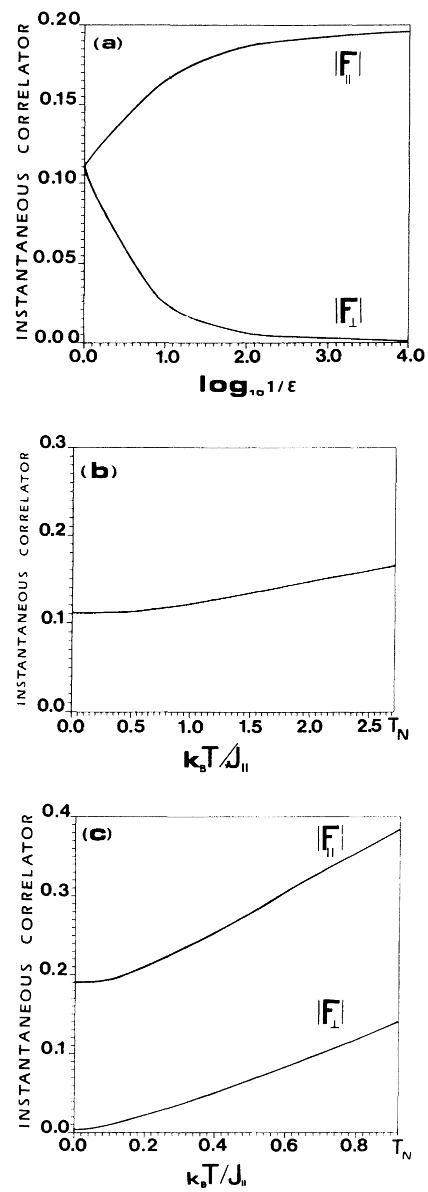

FIG. 6. First-nearest-neighbor instantaneous spin correlators within the MRPA: (a) $|F_{\parallel}|$ and $|F_{\perp}|$ vs $\log_{10}1/\epsilon$ at $T=0$; (b) $|F_{\parallel}|=|F_{\perp}|=|F|$ vs $k_BT/J_{\parallel}$ for $\epsilon=1$; (c) $|F_{\parallel}|$ and $|F_{\perp}|$ vs $k_BT/J_{\parallel}$ for $\epsilon=10^{-3}$.

with Cr^{3+},[10] a system which corresponds to the isotropic three-dimensional case ($\epsilon=1$). These measurements provide us with a value for the parameter p defined by

$$p \equiv \frac{\langle (\mathbf{S}_i - \langle \mathbf{S}_i \rangle)\cdot(\mathbf{S}_j - \langle \mathbf{S}_j \rangle)\rangle}{\langle (\mathbf{S}_i - \langle \mathbf{S}_i \rangle)^2 \rangle} \cong \frac{F}{3/4 - \langle S_A^z \rangle^2} , \quad (3.1)$$

where (i,j) are first-nearest neighbors and the last approximate equality holds within the MRPA by disregarding terms of order F^2.[15] It is evident that $-1 < p < 0$ corresponds to the antiferromagnetic situation. The data are taken just above the Néel temperature ($T_N = 3.89$ K) and give $p = -0.22 \pm 0.03$. We find $F = -\frac{1}{6}$ at T_N, yielding $p = -\frac{2}{9}$ (within an estimated 15% error) which is undoubtedly in very good agreement with the experimental value. It is also worthwhile to stress that the fitting to the data, which has led to the above experimental value, was performed by assuming p independent of temperature from about $T_N/3$ up to T_N. We find that this assumption is approximately compatible with the MRPA results, which give $p \cong -0.2$ at $T=0$.

IV. CONCLUDING REMARKS

Our original motivation to undertake the present study of the magnetic properties of an anisotropic antiferromagnet has been to determine whether they can be characterized by a well-defined crossover region when the anisotropy parameter $\epsilon = J_\perp / J_\parallel$ varies form 1 to 0. We have succeeded in finding that all relevant physical quantities (except, of course, the Néel temperature) cross over for all practical purposes to their two-dimensional values when $\epsilon \approx 10^{-3}$, in all three different theoretical decoupling procedures we have adopted.

The behavior of T_N vs ϵ in the whole range $0 \le \epsilon \le 1$ has been established by the parametrization (2.22). In this respect, a warning should be made about the determination of the anisotropy ratio ϵ from the values of T_N and $J_\parallel$, owing to the $\ln\epsilon$ dependence therein.

As already mentioned, we find an ambiguity in determining the appropriate value of ϵ when considering several physical properties, depending on the chosen approximation. We find, for instance, the same value of T_N in the FSWA or the MRPA, on the one hand, and in the RPA, on the other hand, for values of ϵ which differ by up to 10^2 (cf. Fig. 1). Moreover, we may notice from Fig. 2 that the sublattice magnetic moment $2\langle S_A^z \rangle$ converges to its two-dimensional value for $\epsilon \approx 10^{-3}$ in both the RPA and the MRPA, while that same value of $2\langle S_A^z \rangle$ is obtained in the FSWA for $\epsilon \approx 10^{-1}$.

It should be further mentioned that for $\epsilon \ll 1$ the Néel temperature could be stabilized by other effects not considered in the present treatment, such as the occurrence of an anisotropy of the effective exchange integral in spin space and/or the presence of long-range dipolar interactions. Both effects yield a finite T_N when $\epsilon=0$ without violating the thermodynamic behavior.

We have also compared the behavior of the local magnetic moment and of the spin-wave spectrum as functions of ϵ and T for the three decoupling procedures we have adopted, and found significant differences whose consideration should be relevant for a detailed fitting to experiments.

We emphasize, finally, that our calculation is valid for $T \le T_N$ since a long-range symmetry breaking has been assumed throughout. By this very assumption we have unavoidably left out other (paramagnonlike) excitations which extrapolate smoothly across T_N since they extend over a finite length scale and are thus not affected by the disappearance of long-range order. A few experiments already point unambiguously in this direction.[9] Our finding of a smooth variation with temperature of the first-nearest-neighbor instantaneous spin correlator that reaches its maximum value at T_N seems also to reinforce the relevance of the localized excitations at least close to T_N. Furthermore, the sizable enhancement of the above correlator which we have found by approaching the two-dimensional limit is an additional clue in favor of the increased weight from localized excitations in layered structures.

APPENDIX; INTEGRAL EQUATIONS FOR CALLEN MODIFIED RPA

We begin by showing that the quantities $F_\parallel^{(2)}$ and $F_\perp^{(2)}$ introduced in Eqs. (2.28) and (2.29) of the text vanish when the lattice has an inversion symmetry. Although the proof can be carried out for arbitrary ϵ, we sketch it only for the two extreme cases, namely, the isotropic three-dimensional case ($\epsilon=1$) and the purely two-dimensional case ($\epsilon=0$).

If one retains also the purely imaginary $F^{(2)}$, the equation of motion for $\chi^{+-}(\mathbf{q},\mathbf{q}',\Omega_\lambda)$ becomes

$$\{-i\Omega_\lambda - 2F^{(2)}[\omega_0 - \omega_1(\mathbf{q})]\}\chi^{+-}(\mathbf{q},\mathbf{q}';\Omega_\lambda) + (1-2F^{(1)})[\omega_0 - \omega_1(\mathbf{q})]\chi^{+-}(\mathbf{q}+\mathbf{Q},\mathbf{q}';\Omega_\lambda) = 2\langle S_A^z \rangle \delta(\mathbf{q}+\mathbf{Q}-\mathbf{q}') \quad (A1)$$

in the place of the isotropic limit of Eq. (2.30) of the text for either $\epsilon=1$ or 0. Equation (A1) can be solved in the usual way, to get

$$\chi^{+-}(\mathbf{q},\mathbf{q}';\Omega_\lambda) = -2\langle S_A^z \rangle \frac{\{i\Omega_\lambda + 2F^{(2)}[\omega_0 + \omega_1(\mathbf{q})]\}\delta(\mathbf{q}+\mathbf{Q}-\mathbf{q}') + (1-2F^{(1)})[\omega_0 - \omega_1(\mathbf{q})]\delta(\mathbf{q}-\mathbf{q}')}{(i\Omega_\lambda + 2F^{(2)}\omega_0)^2 - \{[2F^{(2)}\omega_1(\mathbf{q})]^2 + (1-2F^{(1)})^2[\omega_0^2 - \omega_1(\mathbf{q})^2]\}} . \quad (A2)$$

From this expression one can calculate the instantaneous correlator $\langle S_i^+ S_j^- \rangle$ for *any* pair (i,j), not necessarily first-nearest neighbors. One obtains

$$\langle S_i^+ S_j^- \rangle = \frac{1}{\beta}\sum_{\lambda} e^{-i\Omega_\lambda \delta} \frac{1}{N}\sum_{\mathbf{q},\mathbf{q}'} e^{i\mathbf{q}\cdot\mathbf{R}_i} \chi^{+-}(\mathbf{q},\mathbf{q}';\Omega_\lambda) e^{-i\mathbf{q}'\cdot\mathbf{R}_j}$$

$$= -2\langle S_A^z \rangle \frac{1}{N}\sum_{\mathbf{q}} e^{i\mathbf{q}\cdot(\mathbf{R}_i-\mathbf{R}_j)} \left[\frac{(1-2F^{(1)})[\omega_0-\omega_1(\mathbf{q})]+2\omega_1(\mathbf{q})F^{(2)}e^{-i\mathbf{Q}\cdot\mathbf{R}_j}}{2\tilde{\Omega}'(\mathbf{q})} \times \{ b[2\omega_0 F^{(2)}-\tilde{\Omega}'(\mathbf{q})] - b[2\omega_0 F^{(2)}+\tilde{\Omega}'(\mathbf{q})] \} + \tfrac{1}{2} e^{-i\mathbf{Q}\cdot\mathbf{R}_j} \{ b[2\omega_0 F^{(2)}-\tilde{\Omega}'(\mathbf{q})] + b[2\omega_0 F^{(2)}+\tilde{\Omega}'(\mathbf{q})] \} \right], \tag{A3}$$

where

$$\tilde{\Omega}'(\mathbf{q}) = \sqrt{[2F^{(2)}\omega_1(\mathbf{q})]^2 + (1-2F^{(1)})^2[\omega_0^2-\omega_1(\mathbf{q})^2]} \tag{A4}$$

is a modified spin-wave spectrum and

$$b(\zeta) = \frac{1}{e^{\beta\zeta}-1} \tag{A5}$$

is the Bose factor with complex argument ζ. In particular, when $i=j$ the right-hand side of Eq. (A3) must yield a real quantity. This can only occur when $F^{(2)}=0$.

Equation (A3) can also be used to determine $F^{(1)}(=F)$ self-consistently, by choosing (i,j) to be first-nearest neighbors. One obtains

$$F = -2\langle S_A^z \rangle \frac{1}{N}\sum_{\mathbf{q}}{}' \left[\frac{1}{\sqrt{1-\gamma(\mathbf{q})^2}} - \sqrt{1-\gamma(\mathbf{q})^2} \right] \times \coth\left[\frac{\beta}{2}\tilde{\Omega}(\mathbf{q}) \right], \tag{A6}$$

where $\tilde{\Omega}(\mathbf{q})$ is obtained by setting $F^{(2)}=0$ in Eq. (A4). When $\epsilon=1$ or 0 the zero-temperature value of F can be readily calculated in terms of standard Watson integrals J_D and I_D of the spin-wave theory:[11]

$$F = \frac{-(J_D-I_D)}{2J_D} = \begin{cases} -0.1094 & (\epsilon=1), \\ -0.1978 & (\epsilon=0) \end{cases}. \tag{A7}$$

A close system of equations results at finite temperature by expressing $\langle S_A^z \rangle$ in terms of $\langle S_A^+ S_A^- \rangle$ calculated with Eq. (A3) via the identity (2.15). One gets

$$\langle S_A^z \rangle = \frac{1/2}{1+2\tilde{\psi}}, \tag{A8}$$

where $\tilde{\psi}$ is obtained from ψ given by Eq. (2.17) of the text by replacing $\Omega(\mathbf{q})$ with the modified spin-wave sperctrum $\tilde{\Omega}(\mathbf{q})$ in the argument of the hyperbolic cotangent. For this reason, the MRPA and RPA values of $\langle S_A^z \rangle$ coincide in the zero-temperature limit as the renormalization factor $(1-2F)$ of the spin-wave spectrum drops out.

More generally, in the anisotropic case $(0<\epsilon<1)$ one obtains two distinct self-consistent integral equations for $F_\parallel$ and $F_\perp$ at any temperature below T_N:

$$F_\parallel = -2\langle S_A^z \rangle \frac{1}{N}\sum_{\mathbf{q}}{}' \gamma_\parallel(\mathbf{q}) \frac{\tilde{\omega}(\mathbf{q})}{\tilde{\Omega}(\mathbf{q})} \coth\left[\frac{\beta}{2}\tilde{\Omega}(\mathbf{q}) \right], \tag{A9}$$

$$F_\perp = -2\langle S_A^z \rangle \frac{1}{N}\sum_{\mathbf{q}}{}' \gamma_\perp(\mathbf{q}) \frac{\tilde{\omega}(\mathbf{q})}{\tilde{\Omega}(\mathbf{q})} \coth\left[\frac{\beta}{2}\tilde{\Omega}(\mathbf{q}) \right], \tag{A10}$$

where $\tilde{\Omega}(\mathbf{q})$ is now given by Eq. (2.33) of the text and

$$\tilde{\omega}(\mathbf{q}) \equiv \omega_1(\mathbf{q}) - \Gamma(\mathbf{q}) = 2\langle S_A^z \rangle [J_\parallel z_\parallel (1-2F_\parallel)\gamma_\parallel(\mathbf{q}) + J_\perp z_\perp (1-2F_\perp)\gamma_\perp(\mathbf{q})] \tag{A11}$$

[cf. Eqs. (2.10) and (2.31) of the text]. The equation for $\langle S_A^z \rangle$ is finally obtained in the anisotropy case from Eq. (A8) by considering the appropriate replacements $\omega_0 \to \tilde{\omega}(\mathbf{q}=0)$ and $\Omega(\mathbf{q}) \to \tilde{\Omega}(\mathbf{q})$ in the integral ψ given by Eq. (2.17) of the text.

Near the critical temperature, the quantities to be determined self-consistently are $F_\parallel$, $F_\perp$, and T_N itself. In particular, in the isotropic case $(\epsilon=1)F$ can be expressed near T_N in terms of the integral W_ϵ defined by Eq. (2.20) of the text as follows:

$$F = \frac{1-W_{\epsilon=1}}{2W_{\epsilon=1}}. \tag{A12}$$

This yields

$$\left[\frac{1}{\beta_c J z}\right]_{\text{MRPA}} = (1-2F)\left[\frac{1}{\beta_c J z}\right]_{\text{RPA}} = \left[2-\frac{1}{W_{\epsilon=1}}\right]\left[\frac{1}{\beta_c J z}\right]_{\text{RPA}}, \tag{A13}$$

where $\beta_c = (k_B T_N)^{-1}$, resulting in an increase of T_N from the RPA to the MRPA by factor 2 at most.[15]

[1]G. Shirane *et al.* Phys. Rev. Lett. **59**, 1613 (1987).
[2]K. B. Lyons *et al.*, Phsy. Rev. B **37**, 2353 (1988).
[3]J. M. Tranquada *et al.*, Phys. Rev. B **38**, 2477 (1988).
[4]G. Aeppli *et al.*, Phys. Rev. Lett. **62**, 2052 (1989).
[5]A. Singh *et al.*, Phys. Rev. Lett. **64**, 2571 (1990).
[6]See e.g., G. Rickayzen, *Green's Functions and Condensed Matter* (Academic, London, 1980), Chapter 10, and references therein.
[7]H. B. Callen, Phys. Rev. **130**, 890B (1963)); see also A. Czachor and A. Holas, Phys. Rev. B **41**, 4674 (1990).
[8]E. Manousakis, Rev. Mod. Phys. **63**, 1 (1991).
[9]Dynamic probing of the magnetic excitations in La_2CuO_4 (Refs. 2 and 4) results in a temperature independence of their spectra even above T_N. Although these excitations have commonly been interpreted in the framework of the conventional free-spin-wave theory, one should keep in mind that this theory does not admit any temperature variation of the magnon energies simply because it is valid, by definition, only in the $T \rightarrow 0$ limit. One should also keep in mind that these experiments probe a finite length scale; the magnetic excitations, therefore, cannot be plainly identified with antiferromagnetic magnons but rather with *some sort of more localized excitations* that may as well coexist with long-range magnons for $T < T_N$. In this context, we recall that the first-nearest-neighbor instantaneous spin correlator F turns out in our calculation to vary slowly with T, reaching a finite value at T_N from below. We believe that the measured spectra of Refs. 2 and 4 can be related to the dynamic fluctuations of F which extend over a finite length. Consideration of this problem, however, is beyond the scope of the present paper.
[10]M. Matsuoka *et al.*, Phys. Rev. Lett. **50**, 204 (1983); J. S. Helman *et al.*, Phys. Rev. B **44**, 6878 (1991). .
[11]P. W. Anderson, Phys. Rev. **86**, 694 (1952).
[12]It is known, however, that the reduction of $\langle S_i^z \rangle$ form its nominal saturated value $\pm 1/2$ due to the quantum and thermal fluctuations cannot be obtained consistently within the FSWA from the correlation function (2.3). A different procedure is then required within the FSWA to evaluate $\langle S_i^z \rangle$ and the extrapolated Néel temperature (cf. Ref. 11).
[13]F. J. Dyson, Phys. Rev. **102**, 1217 (1956); **102**, 1230 (1956).
[14]R. A. Tahir-Kheli and D. Ter Haar, Phys. Rev. **127**, 88 (1962); **127**, 95 (1962).
[15]The decoupling of higher-order correlators among transverse spin operators, which is required by the MRPA, introduces an error which is *quadratic* in the first-nearest-neighbor instantaneous correlator $\langle S_i^+ S_j^- \rangle$. It can be shown, in fact, that the decoupling leads to violation of the identity $S_i^+ S_i^- + S_i^- S_i^+ = 1$ for spin-$\frac{1}{2}$ operators by terms of second order in $\langle S_i^+ S_j^- \rangle$. Corrections of physical quantities should thus be considered within the MRPA only up to *linear* order in $\langle S_i^+ S_j^- \rangle$.
[16]The coupling between transverse and longitudinal fluctuations introduced by the MRPA is in line with the general principle of "conservation of the modulus" enunciated by A. Z. Patashinskii and V. L. Pokrovskii, Zh. Eksp. Teor. Fiz. **64**, 1445 (1973) [Sov. Phys. JEPT **37**, 733 (1973)].