Theory of magnetic order in the three-dimensional spatially anisotropic Heisenberg model

L. Siurakshina* and D. Ihle
Institut für Theoretische Physik, Universität Leipzig, D-04109 Leipzig, Germany

R. Hayn
Institut für Theoretische Physik, Technische Universität Dresden, D-01062 Dresden, Germany

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A spin-rotation-invariant Green's-function theory of long- and short-range order (SRO) in the $S=1/2$ antiferromagnetic Heisenberg model with spatially anisotropic couplings on a simple cubic lattice is presented. The staggered magnetization, the two-spin correlation functions, the correlation lengths, and the static spin susceptibility are calculated self-consistently over the whole temperature region, where the effects of spatial anisotropy are explored. As compared with previous spin-wave approaches, the Néel temperature is reduced by the improved description of SRO. The maximum in the temperature dependence of the uniform static susceptibility is shifted with anisotropy, and is ascribed to the decrease of SRO with increasing temperature. Comparing the theory with experimental data for the magnetization and correlation length of La_2CuO_4, a good agreement in the temperature dependences is obtained.

I. INTRODUCTION

The magnetic properties of spatially anisotropic antiferromagnetic (AFM) quantum spin systems, such as the quasi-two-dimensional (2D) parent compounds of high-T_c superconductors [e.g., La_2CuO_4 and $Ca(Sr)CuO_2$],[1] and the quasi-1D cuprates Sr_2CuO_3, Ca_2CuO_3,[2,3] and $SrCuO_2$,[4] are of current interest. The main problem is the influence of spatial anisotropy on the staggered magnetization m and the Néel temperature T_N in the 3D spin-$\frac{1}{2}$ AFM Heisenberg model

$$H=J_x\left[\sum_{\langle ij\rangle_x}\mathbf{S}_i\mathbf{S}_j+R_y\sum_{\langle ij\rangle_y}\mathbf{S}_i\mathbf{S}_j+R_z\sum_{\langle ij\rangle_z}\mathbf{S}_i\mathbf{S}_j\right]. \qquad (1)$$

Here $R_y=J_y/J_x$, $R_z=J_z/J_x$ (throughout we set $J_x=1$), and $\langle ij\rangle_{x,y,z}$ denote nearest-neighbor (NN) bonds along the x, y, or z directions of a simple cubic lattice. For real systems, we consider $0\leqslant R_z\ll R_y\leqslant 1$.

In the paramagnetic phase, there exists a pronounced AFM short-range order (SRO) which is reflected by a maximum in the temperature dependence of the magnetic susceptibility at T_{max}, where $0.64<T_{max}<1.2$.[5] However, random phase approximation (RPA) spin-wave theories[6,7] and mean-field theories using auxiliary-field representations (Schwinger-boson,[8,9] Holstein-Primakoff,[10,11] Dyson-Maleev,[10,12] and boson-fermion representations[13]) which were developed for the quasi-2D model with $R_y=1$, are valid only at sufficiently low temperatures. In those theories, the temperature-dependent SRO is not adequately taken into account; in particular, the maximum in the magnetic susceptibility cannot be reproduced. In the chain mean-field approaches,[14] recently improved by spin-fluctuation corrections[15] which lower m and T_N, an asymmetry between intrachain and interchain correlations is introduced. As shown in Ref. 3 on the basis of a detailed estimate of the exchange integrals for the quasi-1D cuprates using a first-principles calculation (Sr_2CuO_3: $R_y\simeq 0.004$; Ca_2CuO_3: $R_y\simeq 0.02$), all previous approaches overestimate both m and T_N. This deficiency is calling for a theory that provides an improved description of SRO over the whole temperature region. In Ref. 16, a spin-rotation-invariant Green's-function theory for the 2D isotropic Heisenberg and t-J models was developed, which yields a good description of spin-correlation functions of arbitrary range and at arbitrary temperatures. Moreover, the susceptibility maximum was obtained in good agreement with quantum Monte Carlo calculations. Applying this approach to the 2D anisotropic Heisenberg model,[17] the short-ranged spin correlations at $T=0$ are well reproduced as compared with exact diagonalization (ED) data. Accordingly, we also expect such a theory to describe the SRO properties quite well in the 3D model [Eq. (1)].

In this paper we extend the Green's-function approach of Refs. 16 and 17, and present a theory of AFM long-range order (LRO) and SRO for the 3D anisotropic Heisenberg model (1) (Sec. II). Thereby, the correlations along all spatial directions are described on the same footing. In Sec. III the ground state is investigated, where the magnetization and short-ranged spin correlation functions are calculated. In Sec. IV we present our finite-temperature results on the R_z dependence of T_N and $m(T)$, and of the AFM correlation lengths. Moreover, the effects of an arbitrary spatial anisotropy on the temperature dependence of the uniform static spin susceptibility, especially on T_{max}, are investigated. The results are compared with experiments on La_2CuO_4 (magnetization, correlation length, and magnetic susceptibility). A summary of our work can be found in Sec. V.

II. DYNAMIC SPIN SUSCEPTIBILITY

To determine the dynamic spin susceptibility $\chi^{+-}(\mathbf{q},\omega)=-\langle\langle S^+_{\mathbf{q}};S^-_{-\mathbf{q}}\rangle\rangle_\omega$ by the projection method outlined in Ref. 16, we choose the two-operator basis $\mathbf{A}=(S^+_{\mathbf{q}},i\dot{S}^+_{\mathbf{q}})^T$ and consider the two-time retarded matrix Green's function in a

generalized mean-field approximation, $\langle\langle \mathbf{A};\mathbf{A}^+\rangle\rangle_\omega = [\omega - \mathbf{M}'\mathbf{M}^{-1}]^{-1}\mathbf{M}$ with $\mathbf{M}=\langle[\mathbf{A},\mathbf{A}^+]\rangle$ and $\mathbf{M}'=\langle[i\dot{\mathbf{A}},\mathbf{A}^+]\rangle$, using Zubarev's notation.[18] We obtain

$$\chi^{+-}(\mathbf{q},\omega) = -\frac{M_{\mathbf{q}}^{(1)}}{\omega^2-\omega_{\mathbf{q}}^2}. \tag{2}$$

The spectral moment $M_{\mathbf{q}}^{(1)}=\langle[i\dot{S}_{\mathbf{q}}^+, S_{-\mathbf{q}}^-]\rangle$ is given by

$$M_{\mathbf{q}}^{(1)} = -4C_{1,0,0}(1-\cos q_x) - 4R_yC_{0,1,0}(1-\cos q_y) - 4R_zC_{0,0,1}(1-\cos q_z). \tag{3}$$

The two-spin correlation functions $C_{\mathbf{r}}=\langle S_0^+ S_{\mathbf{r}}^-\rangle \equiv C_{n,m,l}$, with $\mathbf{r}=n\mathbf{e}_x+m\mathbf{e}_y+l\mathbf{e}_z$, are calculated from

$$C_{\mathbf{r}} = \frac{1}{N}\sum_{\mathbf{q}} C_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}}, \quad C_{\mathbf{q}} = \frac{M_{\mathbf{q}}^{(1)}}{2\omega_{\mathbf{q}}}[1+2n(\omega_{\mathbf{q}})], \tag{4}$$

where $n(\omega_{\mathbf{q}})=(e^{\omega_{\mathbf{q}}/T}-1)^{-1}$. The NN correlation functions are directly related to the internal energy per site by $\epsilon = \frac{3}{2}(C_{1,0,0}+R_yC_{0,1,0}+R_zC_{0,0,1})$.

To obtain the spectrum in the approximation $-\ddot{S}_{\mathbf{q}}^+ = \omega_{\mathbf{q}}^2 S_{\mathbf{q}}^+$, we take the site representation and decouple the products of three spin operators in $-\ddot{S}_i^+$ along NN sequences, introducing vertex parameters in the spirit of the scheme proposed by Shimahara and Takada[19] and extending the decoupling given in Ref. 17:

$$S_i^+S_j^+S_l^- = \alpha_1^{x,y,z}\langle S_j^+S_l^-\rangle S_i^+ + \alpha_2\langle S_i^+S_l^-\rangle S_j^+ . \tag{5}$$

Here α_1^x, α_1^y, and α_1^z are attached to NN correlation functions along the x, y, and z directions, respectively, and α_2 is associated with the longer ranged correlation functions. We obtain

$$\begin{aligned}\omega_{\mathbf{q}}^2 = {} & 1+R_y^2+R_z^2-\cos q_x - R_y^2\cos q_y - R_z^2\cos q_z + 2\alpha_1^xC_{1,0,0}\cos(2q_x) - 2\alpha_2C_{2,0,0}\cos q_x + 2R_y^2[\alpha_1^yC_{0,1,0}\cos(2q_y) \\ & - \alpha_2C_{0,2,0}\cos q_y] + 2R_z^2(\alpha_1^zC_{0,0,1}\cos(2q_z) - \alpha_2C_{0,0,2}\cos q_z) - 2\alpha_1^xC_{1,0,0}\cos q_x + 2\alpha_2C_{2,0,0} - 2R_y^2(\alpha_1^yC_{0,1,0}\cos q_y \\ & - \alpha_2C_{0,2,0}) - 2R_z^2(\alpha_1^zC_{0,0,1}\cos q_z - \alpha_2C_{0,0,2}) + 4R_y[(\alpha_1^xC_{1,0,0}+\alpha_1^yC_{0,1,0})\cos q_x\cos q_y - \alpha_2C_{1,1,0}(\cos q_x+\cos q_y)] \\ & + 4R_z[(\alpha_1^xC_{1,0,0}+\alpha_1^zC_{0,0,1})\cos q_x\cos q_z - \alpha_2C_{1,0,1}(\cos q_x+\cos q_z)] + 4R_yR_z[(\alpha_1^yC_{0,1,0}+\alpha_1^zC_{0,0,1})\cos q_y\cos q_z \\ & - \alpha_2C_{0,1,1}(\cos q_y+\cos q_z)] - 4R_y(\alpha_1^xC_{1,0,0}\cos q_y + \alpha_1^yC_{0,1,0}\cos q_x - 2\alpha_2C_{1,1,0}) - 4R_z(\alpha_1^xC_{1,0,0}\cos q_z \\ & + \alpha_1^zC_{0,0,1}\cos q_x - 2\alpha_2C_{1,0,1}) - 4R_yR_z(\alpha_1^yC_{0,1,0}\cos q_z + \alpha_1^zC_{0,0,1}\cos q_y - 2\alpha_2C_{0,1,1}).\end{aligned} \tag{6}$$

We have checked that our scheme preserves the rotational symmetry in spin space. That is, the calculation of the longitudinal susceptibility using, instead of $\mathbf{A}=(S_{\mathbf{q}}^+, i\dot{S}_{\mathbf{q}}^+)^T$, the basis $\tilde{\mathbf{A}}=(S_{\mathbf{q}}^z, i\dot{S}_{\mathbf{q}}^z)^T$ yields $\chi^{zz}(\mathbf{q},\omega)\equiv\chi(\mathbf{q},\omega) = \frac{1}{2}\chi^{+-}(\mathbf{q},\omega)$. For $|\mathbf{q}|\ll 1$, we have

$$\omega_{\mathbf{q}}^2 = c_x^2q_x^2 + c_y^2q_y^2 + c_z^2q_z^2, \tag{7}$$

with the squared spin-wave velocities

$$c_x^2 = \frac{1}{2} - 3\alpha_1^xC_{1,0,0} + \alpha_2C_{2,0,0} - 2R_y(\alpha_1^xC_{1,0,0} - \alpha_2C_{1,1,0}) - 2R_z(\alpha_1^xC_{1,0,0} - \alpha_2C_{1,0,1}), \tag{8}$$

$$c_y^2 = R_y^2\left(\frac{1}{2} - 3\alpha_1^yC_{0,1,0} + \alpha_2C_{0,2,0}\right) - 2R_y(\alpha_1^yC_{0,1,0} - \alpha_2C_{1,1,0}) - 2R_yR_z(\alpha_1^yC_{0,1,0} - \alpha_2C_{0,1,1}), \tag{9}$$

and

$$c_z^2 = R_z^2\left(\frac{1}{2} - 3\alpha_1^zC_{0,0,1} + \alpha_2C_{0,0,2}\right) - 2R_z(\alpha_1^zC_{0,0,1} - \alpha_2C_{1,0,1}) - 2R_yR_z(\alpha_1^zC_{0,0,1} - \alpha_2C_{0,1,1}). \tag{10}$$

Considering the uniform static spin susceptibility $\chi = \lim_{\mathbf{q}\to 0} M_{\mathbf{q}}^{(1)}/(2\omega_{\mathbf{q}}^2)$, the ratio of the anisotropic functions $M_{\mathbf{q}}^{(1)}$ and $\omega_{\mathbf{q}}^2$ must be isotropic in the limit $\mathbf{q}\to 0$. That is, the conditions

$$(c_y/c_x)^2 = R_yC_{0,1,0}/C_{1,0,0} \tag{11}$$

and

$$(c_z/c_x)^2 = R_zC_{0,0,1}/C_{1,0,0} \tag{12}$$

have to be fulfilled.

The critical behavior of model (1) is reflected in our theory by the closure of the spectrum gap at $\mathbf{Q}=(\pi,\pi,\pi)$ as T approaches T_N from above, so that $\lim_{T\to T_N}\chi^{-1}(\mathbf{Q})=0$. At $T\leqslant T_N$ we have $\omega_{\mathbf{Q}}=0$, and, separating the condensation, part C,

$$C_{\mathbf{r}} = \frac{1}{N}\sum_{\mathbf{q}(\neq\mathbf{Q})} C_{\mathbf{q}}e^{i\mathbf{q}\cdot\mathbf{r}} + Ce^{i\mathbf{Q}\cdot\mathbf{r}}, \tag{13}$$

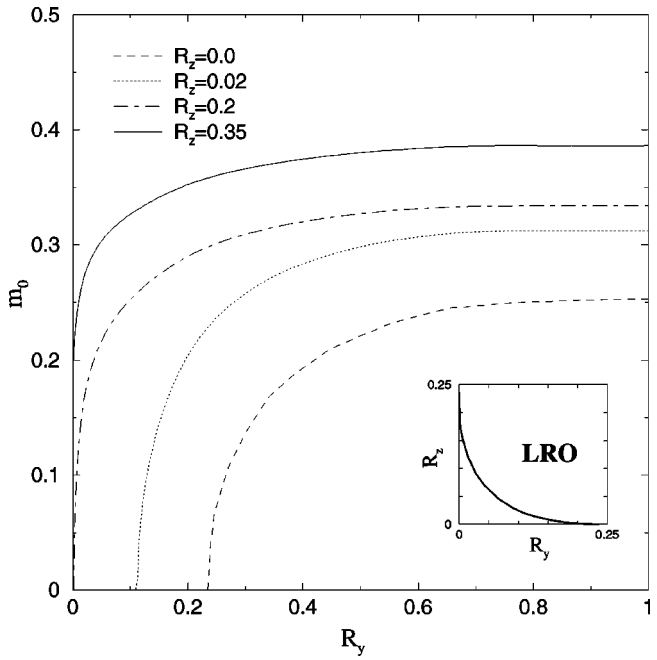

FIG. 1. Staggered magnetization at $T=0$ as a function of spatial anisotropy. The inset shows the stability region of Néel order.

where C results from Eq. (13) with $\mathbf{r}=\mathbf{0}$ employing the sum rule $C_{0,0,0}=\frac{1}{2}$. Then the staggered magnetization m is calculated as

$$m^2=\frac{1}{N}\sum_{\mathbf{r}}\langle \mathbf{S}_0\mathbf{S}_{\mathbf{r}}\rangle e^{-i\mathbf{Q}\cdot\mathbf{r}}=\frac{3}{2}C. \tag{14}$$

The theory has 14 quantities to be determined self-consistently (nine correlation functions in $\omega_{\mathbf{q}}^2$, m, and four vertex parameters) and 13 self-consistency equations [ten Eqs. (13) including $C_{0,0,0}=\frac{1}{2}$, the LRO condition $\omega_{\mathbf{Q}}=0$, and Eqs. (11) and (12)]. If there is no LRO, we have $\omega_{\mathbf{Q}}>0$, and the number of quantities and equations is reduced by one. As an additional condition for determining the free α parameter at $T=0$, we adjust the ground-state energy per site which we compose approximately as $\epsilon(R_y,R_z)=\epsilon(R_y,0)+\epsilon(0,R_z)-\epsilon(0,0)$, where $\epsilon(R_y,0)$ [and $\epsilon(0,R_z)$] is taken from the Ising-expansion results by Affleck *et al.* for the 2D spatially anisotropic Heisenberg model,[20] and $\epsilon(0,0)=-0.4431$ is the Bethe-ansatz value. This approximation is suggested to be good at least for $R_z\ll R_y$ (or $R_y\ll R_z$). To obtain an additional condition at finite temperatures, where ϵ data are not available and all vertex parameters are temperature dependent, following Refs. 19 and 16 we assume the ratio

$$r_\alpha(T)\equiv\frac{\alpha_2(T)-1}{\alpha_1^x(T)-1}=r_\alpha(0) \tag{15}$$

as temperature independent.

III. GROUND-STATE PROPERTIES

In Fig. 1 our results for the zero-temperature staggered magnetization $m_0\equiv m(T=0)$ as a function of R_y and R_z are shown. They indicate an order-disorder transition at the phase boundary $R_{z,c}(R_y)$ or $R_{y,c}(R_z)$ (cf. inset). For $R_z=0$ we obtain the critical ratio $R_{y,c}(0)\simeq 0.24$, which was already found in Ref. 17. In that paper the suppression of LRO below the finite value of $R_{y,c}$ was interpreted, in combination with ED data, as an indication of a rather sharp crossover in the spatial dependence of the spin-correlation functions in the LRO phase at the coupling ratio $R_{y,0}\simeq 0.2$. The finite value of $R_{y,c}$, however, seems to be due to the approximations in our theory, since there are strong indications for $R_{y,c}=0$ (see Ref. 14). Accordingly, we cannot explain the tiny magnetic moments of Sr_2CuO_3 and Ca_2CuO_3,[2] since, for $R_y\ll 1$,[3] we have $m=0$. This result is just opposite to the overestimation of m by all previous spin-wave theories. As seen in the phase diagram (inset of Fig. 1), the inclusion of the interplane coupling R_z stabilizes the LRO, where this effect is quite considerable even at very small values of R_z.

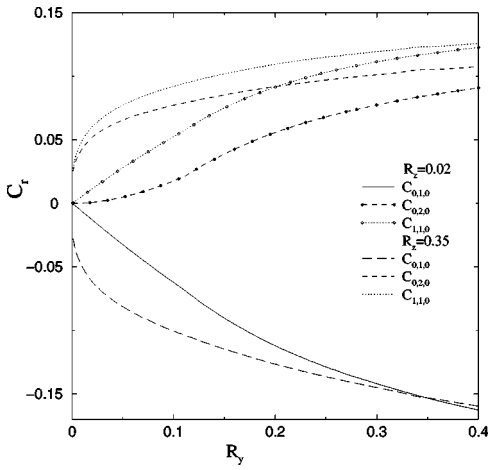

FIG. 2. Spin correlation functions at $T=0$ for different spatial anisotropies.

Figure 2 exhibits some short-ranged spin-correlation functions at $T=0$. For $R_z=0$, in Ref. 17 the correlators $C_{1,0,0}$, $C_{0,1,0}$, and $C_{1,1,0}$ as functions of R_y were found to agree well with the ED data. For $R_z=0.02$ (cf. Fig. 2) our results deviate only slightly from those at $R_z=0$. The sign changes and magnitudes of $C_{\mathbf{r}}$ reflect the AFM SRO. In the limit $R_y\to 0$ the correlations between the x-z planes vanish. At $R_z>R_{z,c}(0)\simeq 0.24$ the LRO enhances the inter-x-z plane correlators and results in their sharp drop toward their limiting value $Ce^{i\mathbf{Q}\cdot\mathbf{r}}$ as $R_y\to 0$. This is visible in the data for $R_z=0.35$ in Fig. 2.

IV. FINITE-TEMPERATURE RESULTS

At nonzero temperatures we have solved the self-consistency equations (13), supplemented by conditions (11), (12), and (15), to obtain the magnetization $m(T)$, the Néel temperature [$m(T_N)=0$], the static spin susceptibility, and the anisotropic correlation lengths.

In Fig. 3 the Néel temperature is plotted as a function of R_z. For $R_z=0$ we obtain $T_N=0$ (see Ref. 16), in agreement with the Mermin-Wagner theorem. The increase of T_N with R_z is governed by the intra-x-y plane anisotropy. At a fixed value of R_z, the decrease of T_N with decreasing R_y is in accordance with the reduced zero-temperature magnetization (cf. Fig. 1). Comparing our results for $R_y=1$ with previous

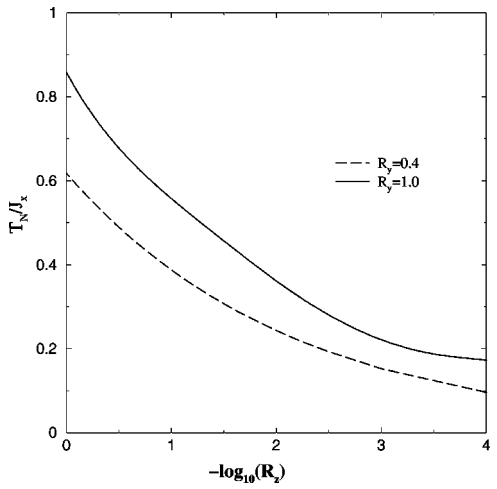

FIG. 3. Néel temperature as a function of $R_z = J_z/J_x$.

RPA and mean-field approaches (see Table I), we ascribe the reduction of T_N as compared with Refs. 6,8, and 12 to the improved description of SRO. That is, the LRO is suppressed in favor of a paramagnetic phase with pronounced AFM SRO. If R_z is fit to the Néel temperatures of real systems, the strong overestimation of T_N by previous theories results in very small values of the interplane coupling. In our approach the resulting R_z values turn out to be higher. Considering La_2CuO_4 with $T_N = 325$ K,[9,21] and putting $J = 130$ meV ($J \equiv J_x = J_y$) or $J = 117$ meV,[16] we obtain $R_z \simeq 10^{-3}$ or $R_z \simeq 1.6\times 10^{-3}$, respectively, in contrast to $R_z < 10^{-4}$ according to Refs. 6 and 12. For $Ca_{0.85}Sr_{0.15}CuO_2$ ($T_N = 540$ K and $J = 125$ meV),[22] we obtain $R_z \simeq 1.2\times 10^{-2}$ as compared with $R_z \simeq 2.5\times 10^{-2}$ obtained from a fit of the low-temperature magnetization data.[22]

Figure 4 shows the temperature dependence of the staggered magnetization at $R_y = 1$ (for the zero-temperature values, compare with Fig. 1). The shape of the normalized curve m/m_0 versus T/T_N (see the inset) depends on the single parameter R_z, and is similar to that found in previous spin-wave theories.[6–8,10] At low enough temperatures the system exhibits 3D behavior, so that the decrease of m follows a T^2 law. This was also observed by NMR experiments on La_2CuO_4 (Ref. 11) ($T_N = 312$ K), yielding $m/m_0 = 1 - a(T/T_N)^2$ with $a = 0.67$ for $T \lesssim 100$ K. The NMR data is indicated in the inset of Fig. 4 (marked by a bold curve), and agrees well with our theory for $R_z = 10^{-3}$ (as estimated above). For temperatures close to T_N our numerical results for $m(T)$ are described by the law $m(T) \propto (1 - T/T_N)^{1/2}$. The square-root temperature behavior agrees with the findings of Refs. 7,8, and 10, and with the neutron scattering data on La_2CuO_4,[9] but contradicts the result of Ref. 13 ($m \propto 1 - T/T_N$).

TABLE I. Néel temperature T_N/J_x at $R_y = 1$ compared with other approaches.

$-\log_{10}(R_z)$	Fig. 3	Ref. 6	Ref. 8	Ref. 12
4	0.17	0.48	0.29	0.25
3	0.22	0.65	0.38	0.34
2	0.36	0.80	0.54	0.47
1	0.56	1.15		0.68

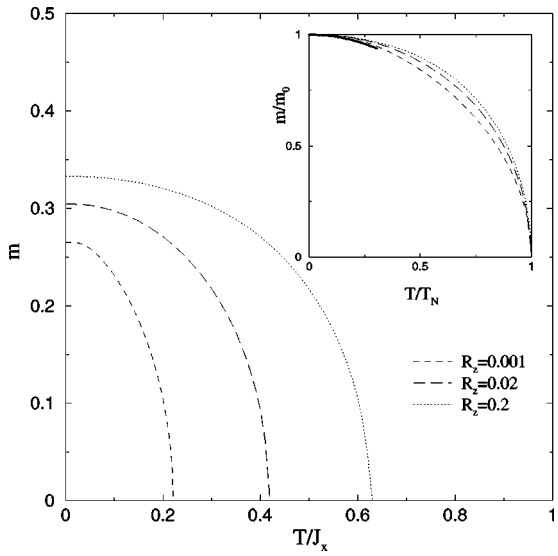

FIG. 4. Staggered magnetization vs temperature for $R_y = 1$. The inset shows the R_z dependence of the normalized curves compared with the NMR data on La_2CuO_4 (Ref. 11) (bold curve).

Considering the AFM correlation lengths above T_N and for $R_y = 1$, the expansion of $\chi(\mathbf{q})$ around $\mathbf{Q}$, $\chi(\mathbf{q}) = \chi(\mathbf{Q})[1 + \xi_{xy}^2(k_x^2 + k_y^2) + \xi_z^2 k_z^2]^{-1}$ with $\mathbf{k} = \mathbf{q} - \mathbf{Q}$, yields the intraplane correlation length

$$\xi_{xy}^2 = -\omega_{\mathbf{Q}}^{-2}\left[\frac{1}{2} + 11\alpha_1^x C_{1,0,0} + \alpha_2(C_{2,0,0} + 2C_{1,1,0}) + 2R_z(\alpha_1^x C_{1,0,0} + 2\alpha_1^z C_{0,0,1} + \alpha_2 C_{1,0,1})\right] - \frac{2C_{1,0,0}}{M_{\mathbf{Q}}^{(1)}}, \tag{16}$$

and the interplane correlation length

$$\xi_z^2 = -R_z\omega_{\mathbf{Q}}^{-2}\left[4(2\alpha_1^x C_{1,0,0} + \alpha_1^z C_{0,0,1} + \alpha_2 C_{1,0,1}) + R_z\left(\frac{1}{2} + 5\alpha_1^z C_{0,0,1} + \alpha_2 C_{0,0,2}\right)\right] - \frac{2R_z C_{0,0,1}}{M_{\mathbf{Q}}^{(1)}}. \tag{17}$$

In Fig. 5 the influence of the interplane coupling on the temperature dependence of ξ_{xy}^{-1} and ξ_z^{-1} (inset) is shown. For comparison, the intraplane correlation length at $R_z = 0$ (see also Ref. 16) is plotted, where the low-temperature expansion $\xi_{xy} = 2(2\alpha_1^x |C_{1,0,0}(0)|)^{1/2} T^{-1} \exp[2\pi\alpha_1^x m_0^2/(3T)]$ holds up to $T = 0.2$ within a deviation of about 6% from the full temperature dependence calculated by Eq. (16). For $R_z > 0$ the correlation lengths diverge at T_N, since the gap $\omega_{\mathbf{Q}}$ closes as T approaches T_N from above. In the vicinity of T_N, ξ_{xy}^{-1} and ξ_z^{-1} behave as $T - T_N$ also found by previous mean-field approaches.[12,13]

Let us compare our results for the intraplane correlation length with the neutron-scattering data on La_2CuO_4 (Ref. 21) in the range 340 K $\leqslant T \leqslant$ 820 K shown in Fig. 6. Taking J as obtained previously[16] from a least-squares fit of ξ_{xy} in the 2D model ($a = 3.79$ Å), $J = 117$ meV, for $T > 500$ K and

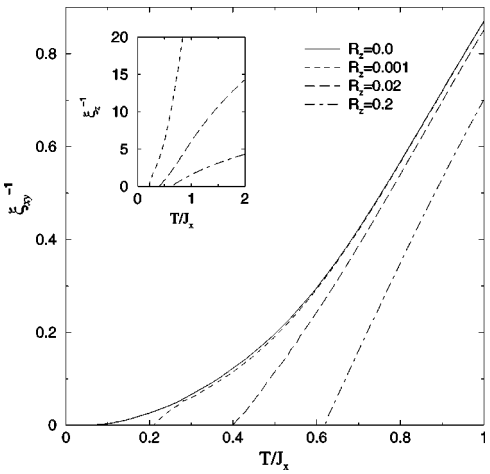

FIG. 5. Inverse antiferromagnetic correlation lengths within (ξ_{xy}^{-1}) and between the x-y planes (ξ_z^{-1}, see inset) for $R_y=1$.

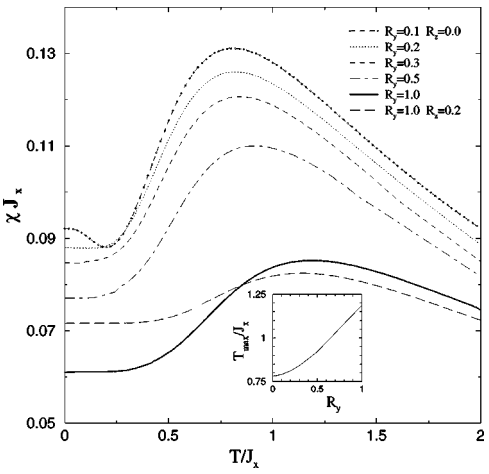

FIG. 7. Uniform static spin susceptibility vs T. The inset exhibits the position T_{max} of the maximum in $\chi(T)$ vs R_y.

$R_z \lesssim 3.5\times10^{-3}$ we obtain a good quantitative agreement with experiments. In Ref. 16 the deviation of the theory for $R_z=0$ and $T<500$ K from the experimental data was ascribed to the appearance of the preexponential factor T^{-1} in the low-temperature expansion of ξ_{xy} which is an artifact of our mean-field approach. However, this deviation may be reduced by the inclusion of the interplane coupling, since $\xi_{xy}^{-1}(T_N)=0$. For $T_N=325$ K,[21] we obtain $R_z\simeq1.6\times10^{-3}$ (see above, Fig. 3), and the theoretical ξ_{xy}^{-1} curve lies between the $R_z=0$ result and the experiments. The discrepancy between the theoretical and experimental low-temperature correlation lengths may be further reduced by the choice of higher R_z values. Taking, for example, $R_z=3.4\times10^{-3}$, we obtain a very good quantitative agreement (cf. Fig. 6) down to 360 K; however, the Néel temperature turns out to be somewhat higher ($T_N=353$ K).

Finally, we consider the uniform static spin susceptibility $\chi(T)=\lim_{\mathbf{q}\to0}\chi(\mathbf{q})$. In Fig. 7 the anisotropy effects on the temperature dependence are demonstrated. For $R_z=0$ and a strong intraplane anisotropy ($R_y<0.2$) the minimum of $\chi(T)$ at a finite temperature, being an artifact of our approach, may signal the crossover in the spatial dependence of the spin-correlation functions at $R_{y,0}\simeq0.2$, as discussed in Sec. III. Note that such a minimum in the 1D model ($R_y=0$) was also found in Ref. 23. At $R_y>0.2$, the increase of χ with temperature, the maximum at T_{max} near the exchange energy $J_x=1$ (see the inset), and the crossover to the high-temperature Curie-Weiss behavior are due to the decrease of AFM SRO with increasing temperature (cf. Ref. 16). Let us point out that the susceptibility maximum is totally missed in RPA theories.[7] With increasing R_y, we obtain an increase of T_{max} which agrees with a general tendency found in various spin−1/2 Heisenberg models, and analyzed in Ref. 5. For comparison, the exact values at $R_y=0$ and 1 are given by $T_{max}=0.64$ (Ref. 24) and $T_{max}=0.94$,[25] respectively. Since our theory allows the calculation of T_{max} at any spatial anisotropy, it may provide a reliable interpretation of experimental data on low-dimensional spin systems. Considering the maximum spin susceptibility $\chi_{max}=\chi(T_{max})$, our results again are in accordance with the general behavior:[5] χ_{max} increases with decreasing T_{max}, i.e., with decreasing R_y. Concerning the influence of the interplane coupling, the enhancement of the low-temperature susceptibility by R_z may be explained by the weakening of the SRO effect in higher dimensions. As seen from Figs. 7 and 3, the uniform susceptibility reveals no peak at the Néel temperature, contrary to the RPA result of Ref. 7. Concerning the maximum in $\chi(T)$ of La_2CuO_4, we obtain $T_{max}=1.19J=1615$ K (cf. Fig. 7, $J=117$ meV). This value roughly agrees with the estimate given by Johnston,[26] $T_{max}=1460$ K, by means of a scaling analysis of the susceptibility data below 800 K.

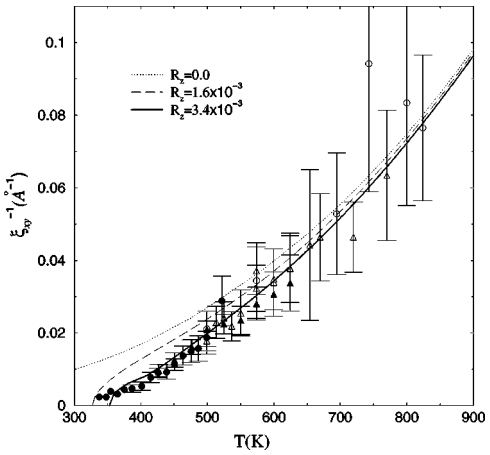

FIG. 6. Inverse antiferromagnetic intraplane correlation length in La_2CuO_4 obtained by the neutron-scattering experiments of Ref. 21 and from the theory ($R_y=1$) for different R_z values.

V. SUMMARY

In this paper we have extended the spin-rotation-invariant Green's-function theory of magnetic LRO and SRO in 2D Heisenberg models[16,17] to a 3D Heisenberg antiferromagnet with arbitrary spatial anisotropy. Our theory provides a satisfactory interpolation between the low- and high-temperature behavior, where the temperature-dependent SRO, described in terms of two-spin correlation functions, is adequately taken into account. The main results are summarized as follows.

(i) The incorporation of SRO results in a strong suppres-

sion of Néel order with increasing anisotropy and in a reduced Néel temperature as compared with previous spin-wave approaches.

(ii) The temperature dependence of the uniform static spin susceptibility reveals a maximum in the short-range-ordered paramagnetic phase and a crossover to the Curie-Weiss law. The position of the maximum is influenced by the spatial anisotropy.

(iii) Comparing the theory with experiments on the magnetization and correlation length of La_2CuO_4, a good quantitative agreement is found.

From the results of our theory we conclude that the application of this approach to extended Heisenberg models (anisotropy in spin space, frustration) may be promising to describe the SRO effects on the unconventional magnetic properties of real low-dimensional spin systems.

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*Permanent address: Laboratory of Computing Techniques and Automatization, Joint Institute for Nuclear Research, 141980 Dubna, Russia.

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