Magnetic order in the quasi-two-dimensional easy-plane XXZ model

D. Ihle
Institut für Theoretische Physik, Universität Leipzig, D-04109 Leipzig, Germany

C. Schindelin
COI GmbH, Erlanger Straße 62, D-91074 Herzogenaurach

H. Fehske
Physikalisches Institut, Universität Bayreuth, D-95440 Bayreuth, Germany

(April 22, 2022)

PACS numbers: 75.10.-b, 75.10.Jm, 75.40.-s

1. INTRODUCTION

To understand the unconventional behavior of high-\(T_c\) superconductors, which is mainly ascribed to a strong antiferromagnetic (AFM) short-range order (SRO), the magnetic properties of the quasi-two-dimensional (2D) parent compounds were probed preferably by neutron scattering and NMR experiments, e.g., on La\(_2\)CuO\(_4\) \cite{1–4}, Ca\(_{0.85}\)Sr\(_{0.15}\)CuO\(_2\) \cite{5}, YBa\(_2\)Cu\(_3\)O\(_{6+x}\) \((x < 0.4)\) \cite{6} and L\(_2\)CuO\(_4\) \((L=Nd, Pr)\) \cite{7}. In particular, the staggered magnetization \cite{1–3,5,6} and the AFM long-range order (LRO) in the magnetic properties of the pseudocubic lattice, respectively, were considered \cite{1–7} and treated by linear spin-wave theories for related spin models \cite{for refs. [9] and [13], respectively.}

Within this theory we examine the combined effects of spatial and spin anisotropy on the AFM long-range order (LRO) at \(T = 0\) (Sec. II), the Néel transition temperature, and on the AFM correlation length (Sec. III). In Sec. IV we compare our results with experiments. For La\(_2\)CuO\(_4\), Sr\(_2\)Cu\(_2\)O\(_4\)Cl\(_2\), and Ca\(_{0.85}\)Sr\(_{0.15}\)CuO\(_2\) our theory predicts, in addition to the usual Néel transition, a further transition far below room temperature, where the spin correlators between the \(z\)-components start to develop AFM LRO.

II. GROUND-STATE LONG-RANGE ORDER

Analyzing the magnetic LRO described by the staggered magnetizations \(m^{\nu} [\nu = \pm, z, z z; \text{cf. Eq. (11)}]\) at \(T = 0\) as functions of \(R_z\) and \(\Delta\), we obtain transverse
LRO in the whole parameter region considered and two solutions differing in the existence of longitudinal LRO. That is, we obtain a phase with \( m^z = 0 \) (phase I) and a phase with \( m^z \neq 0 \) (phase II), where in both phases we have \( m^+ \neq 0 \). The stabilization of longitudinal LRO in the easy-plane region by the interplane coupling may be due to the reduction of quantum spin fluctuations in higher dimensions.

In Fig. 1 the \( R_z - \Delta \) phase diagram is shown, where for \( R_z \neq 0 \) the transition across the phase boundary denoted respectively by \( R_{z,c}(\Delta) \) and \( \Delta_c(R_z) \) is found to be of second order (cf. inset). Let us consider the phase transition in the vicinity of the critical point \( (\Delta, R_z) = (1, 0) \) in more detail. In our approach the solution for \( m^z \) turns out to depend sensitively on the input data for \( \partial \epsilon(\Delta, 1)/\partial \Delta \equiv \epsilon' \) used to determine the vertex parameter \( \alpha_z^2 \), where \( \epsilon(\Delta, 1) \) denotes the ground-state energy of the 2D XXZ model (see Appendix). Taking for \( \epsilon(\Delta, 1) \) the exact diagonalization (ED) data on lattices with up to 36 sites (without finite-size scaling) from Ref. [13], we obtain \( \lim_{R_z \to 0} \Delta_c(R_z) \equiv \Delta_0 = 0.958 \). On the other hand, taking the Monte Carlo (MC) data from Ref. [14], which have to be interpolated between the few available points \( \Delta = 0, \pm 0.5, \pm 1 \), we get \( \lim_{\Delta \to 1} R_{z,c}(\Delta) = R_{z,0} = 4.08 \times 10^{-2} \). However, as is well known, at \( R_z = 0 \) there is no longitudinal LRO for \( 0 < \Delta < 1 \) which means that we must have \( \Delta_0 = 1 \). Moreover, we expect the interplane coupling to be a relevant perturbation with respect to the stabilization of LRO analogous to the situation in the 2D spatially anisotropic Heisenberg model [11,15], where LRO at a finite arbitrary small interchain coupling was found [15]. Therefore, we make the reasonable assumption \( R_{z,0} = 0 \). To fulfill the requirements \( \Delta_0 = 1 \) and \( R_{z,0} = 0 \) simultaneously, so that the phase boundary touches the critical point \( (\Delta, R_z) = (1, 0) \), as input for \( \epsilon' \) we use a linear combination of the ED [13] and Monte Carlo data [14], \( \epsilon' = x\epsilon'_{\text{ED}} + (1 - x)\epsilon'_{\text{MC}} \). We find that the above requirements may be fulfilled, if \( x \) is chosen as \( x \approx 0.44 \).

In the limit \( \Delta = 1 \) we have rotational symmetry \( (C_2^z = C_4^z/2) \), so that \( \sqrt{2m^z(R_z)} = m^z(R_z) \equiv \sqrt{2/5m(R_z)} \) with \( m \) defined as in Refs. [9–11]. In this limit, our result for \( m^z(R_z) \) agrees with that of Ref. [9]. As can be seen in the inset, the effects of spin anisotropy on the longitudinal and transverse LRO are opposite: We have \( \partial m^z/\partial \Delta > 0 \), whereas \( \partial m^+ /\partial \Delta < 0 \) which agrees, at \( R_z = 0 \), with the Monte Carlo data [14] and the results of Ref. [13].

### III. FINITE-TEMPERATURE PROPERTIES

Considering the AFM LRO in the phases I and II \( [m^+(T = 0) \neq 0] \) at \( R_z > R_{z,c} \) at nonzero temperatures, the solution of the self-consistency equations (5), supplemented by the conditions for the vertex parameters [cf. Eqs. (12) and (15) to (17)], results in two second-order phase transitions at \( T^+_N(R_z, \Delta) \) and \( T^z_N(R_z, \Delta) \) \( [m^+(T^+_N) = 0] \) with \( T^+_N > T^z_N \) and \( T^z_N(R_{z,c}) = 0 \). Figure 2 shows the Néel temperatures as functions of \( R_z \), i.e., the \( T - R_z \) phase diagram for different spin anisotropies. For \( R_z = 0 \) we obtain \( T^+_N = 0 \), in agreement with the Mermin-Wagner theorem. At \( \Delta = 1 \) we

![FIG. 1:](image1.png)

**FIG. 1:** \( R_z - \Delta \) phase diagram and transverse and longitudinal zero-temperature magnetizations (inset) in the quasi-2D easy-plane XXZ model.

![FIG. 2:](image2.png)

**FIG. 2:** \( T - R_z \) phase diagram in the quasi-2D easy-plane XXZ model. Below the Néel temperature \( T^z_N \) the phase with longitudinal long-range order becomes stable. The curves below the solid line belong to \( T^z_N \).
have $T_N^{-+} = T_N^{++} \equiv T_N$. As compared with the results of Ref. [9], our values for $T_N$ are somewhat higher (by about 9%) due to numerical uncertainties. On the other hand, in comparison with previous RPA and mean-field approaches (cf. Ref. [9]) our Néel temperatures are reduced by the improved description of SRO. For example, the $T_N$ values found by the Schwinger-boson approach of Ref. [16] exceed our results by a factor of about 1.7 on the average.

Concerning the influence of spin anisotropy on the Néel transitions, we obtain $\partial T_N^{++}/\partial \Delta < 0$ and $\partial T_N^{++}/\partial \Delta > 0$, corresponding to the $\Delta$ dependence of $m''$ (cf. inset of Fig. 1). The dependence on $\Delta$ of $T_N^{-+}$ is in qualitative agreement with the behavior found in previous approaches [1,2]. There, $T_N$ (being identified with $T_N^{-+}$) is given as $T_N/J = -2\pi M_0 \{\alpha_{\text{eff}}/[\pi^2 M_0 \ln(4\alpha_{\text{eff}}/\pi)]\}^{-1}$ (Ref. [1]) with $M_0 = 0.3, \alpha_{\text{eff}} = 4\alpha_{\text{xy}} + 2R_z$, and $\alpha_{\text{xy}} = 1 - \Delta$ or as $T_N/J = -4\pi \rho_S (\ln \alpha_{\text{eff}})^{-1}$ (Ref. [2]), where $\rho_S$ is the spin stiffness. However, in contrast to those mean-field (Schwinger boson) results, in our theory the combined influence of spatial and spin anisotropy on $T_N^{-+}$ cannot be expressed in terms of a single effective parameter. Considering the variations $\delta R_z$ and $\delta \alpha_{\text{xy}}$ under the condition $\delta T_N^{-+} = 0$ we get $\text{sgn}(\delta \alpha_{\text{xy}}) = -\text{sgn}(\delta R_z)$. Whereas the $T_N$ formulas quoted above yield $\delta \alpha_{\text{xy}} = -\delta R_z/2$ for all $R_z$, from Fig. 2 we obtain a $R_z$ dependent relation between $\delta \alpha_{\text{xy}}$ and $\delta R_z$.

In Fig. 3, our numerical results for the temperature dependence of the magnetization $m''$ are depicted. They may be described by a $T^2$ decrease at low enough temperatures (3D behavior) and by $m''(T) \propto (1 - T/T_N^0)^{1/2}$ for temperatures close to $T_N^0$, as was also found in the $\Delta = 1$ limit [9]. The influence of spatial and spin anisotropy on $m''(T)$ is analogous to that on $m''(T = 0)$ shown in the inset of Fig. 1.

In the inset of Fig. 3 the inverse AFM intraplane correlation lengths above $T_N^0$ are plotted, where the effects of the interplane coupling and spin anisotropy are visible. In the vicinity of $T_N^{-+}$ the temperature dependence of $(\xi_{xy}^{zz})^{-1}$ changes from an exponential law in the 2D case ($T_N^{-+} = 0$) to a linear behavior for $R_z > 0$. Equally, $(\xi_{xy}^{zz})^{-1}$ near $T_N^{++}$ behaves as $T - T_N^{++}$. According to the influence of spin anisotropy on $T_N^0$ we get $\partial \xi_{xy}^{zz}/\partial \Delta > 0$ and $\partial \xi_{xy}^{zz}/\partial \Delta < 0$. The behavior of $\xi_{xy}^{-+}$ qualitatively agrees with the anisotropy dependence of the mean-field expression for $\xi$ (being identified with $\xi_{xy}^{-+}$) given in Ref. [2], $\xi = \xi_0 \{1 - \alpha_{\text{eff}} \xi_0^2\}^{-1/2}$, where $\xi_0$ denotes the correlation length for $R_z = 0$ and $\Delta = 1$.

Finally let us consider the heuristic relation between $T_N^{-+}$ and the transverse 2D correlation length at $T_N^{-+}$ which is often used in describing the experimental data [17] and is given by $Q(R_z, \Delta) = 0.25$ with $Q(R_z, \Delta) = R_z(T_N^{-+})^{-1}[m''(T = 0, R_z = 0, \Delta)]^2$. By our results, $Q(R_z, \Delta)$ in the experimentally relevant region (cf. Sec. IV) $2 \times 10^{-4} \leq R_z \leq 2 \times 10^{-2}$ and at $\Delta = 1(0.8)$ is found to vary between 0.21 (0.31) and 0.095 (0.23). That is, the heuristic estimate is roughly confirmed by our theory.

### IV. COMPARISON WITH EXPERIMENTS

Let us first compare our results for the transverse intraplane correlation length $\xi_{xy}^{-+}$ with the neutron-scattering data on La$_2$CuO$_4$ (Ref. [4]) in the range $340 \text{ K} \leq T \leq 820 \text{ K}$ plotted in Fig. 4. Based on the 2D Heisenberg model ($\Delta = 1$), in Ref. [18] the exchange energy $J$ was determined by a least-squares fit ($a = 3.79$ Å), where for our choice of the vertex parameters the realistic value $J = 117$ meV was found. Here, we fix this value and consider the effects of spatial and spin anisotropy on $\xi_{xy}^{-+}(T)$. The deviation of the theory for $R_z = 0$ and $T < 550 \text{ K}$ from the experimental data may be reduced by the inclusion of the interplane coupling, since $\xi_{xy}^{-+}(T_N) = 0$. For $\Delta = 1$ and $T_N = 325 \text{ K}$ [1,4] we obtain $R_z = 1.2 \times 10^{-3}$, and the theoretical low-temperature $\xi_{xy}^{-+}$ curve lies only somewhat above the experiments (cf. Fig. 4). Taking into account the spin anisotropy $\alpha_{xy} = 1.5 \times 10^{-4}$ [2] or $\alpha_{xy} = 5.7 \times 10^{-4}$ [4], for $T_N^{-+} = 325 \text{ K}$ we get $R_z = 3.0 \times 10^{-4}$. For those parameters we obtain an excellent agreement between theory and experiment over the whole temperature region. Note that the theoretical curves for $\alpha_{xy} = 2 \times 10^{-4}$ (cf. Fig. 4) and $\alpha_{xy} = 2 \times 10^{-3}$ agree within the accuracy of drawing.

![Fig. 3: Staggered magnetizations versus temperature. The inset shows the inverse intraplane correlation lengths above the corresponding Néel temperatures.](image-url)
Concerning our prediction of phase II with longitudinal LRO in La$_2$CuO$_4$, for $\alpha_{xy} = 1.5 \times 10^{-4}$ ($5.7 \times 10^{-4}$) we obtain the longitudinal zero-temperature magnetic moment $\mu^{zz} \equiv 2\mu_B m^{zz} = 6.6 \times 10^{-2}\mu_B$ ($6.1 \times 10^{-2}\mu_B$) as compared with the transverse moment $\mu^{+\pm} \equiv 2\mu_B m^{+\pm} = 0.55\mu_B$. For the Néel temperature we find $T_N^{zz} = 2.6 \times 10^{-2} J$ ($2.4 \times 10^{-2} J$) equally to $T_N^{\pm\pm} = 35$ K (33 K) [$J = 117$ meV]. With regard to the experimental verification of the two phases, the magnitude of the longitudinal moment ($\mu^{zz} \gtrsim 0.1\mu^{++}$) may be large enough to allow a separation between $\mu^{zz}$ and $\mu^{++}$ by polarized neutron-scattering studies on single crystals of La$_2$CuO$_4$ [19].

Next we consider the compound Sr$_2$CuO$_2$Cl$_2$ which is the best experimental realization of an $S = 1/2$ 2D Heisenberg antiferromagnet, where $J = 125 \pm 6$ meV, $\alpha_{xy} = 1.4 \times 10^{-4}$, and $T_N^{++} = 256.5$ K [20]. Keeping $T_N^{++}$ and $\alpha_{xy}$ fixed (we take $\alpha_{xy} = 2 \times 10^{-4}$, as for La$_2$CuO$_4$) and choosing $J = 125$ meV, 120 meV, and 110 meV, we obtain the interplane coupling $R_z = 2.0 \times 10^{-5}$, 4.0 $\times 10^{-5}$, and 1.0 $\times 10^{-4}$, respectively. On the average we have $R_z \simeq 5 \times 10^{-5} \ll \alpha_{xy}$ in qualitative agreement with the estimate given in Ref. [20]. In Fig. 5 our results for the transverse intraplane correlation length ($a = 3.967$ Å), where $(\xi_{xy}^{++})^{-1} \propto T - T_N^{++}$ near the transition to phase I, are compared with the neutron-scattering data [20]. For $J = 125$ meV we obtain a very good agreement between theory and experiment at low enough temperatures ($T \lesssim 400$ K), whereas for $J = 110$ meV the agreement is good at higher temperatures.

The data on the predicted phase II in Sr$_2$CuO$_2$Cl$_2$ calculated for $J = 125$ meV, 120 meV, and 110 meV are obtained as $\mu^{zz} / \mu_B = 2.8 \times 10^{-2}$, 3.9 $\times 10^{-2}$, and 5.5 $\times 10^{-2}$ (for comparison, $\mu^{++} / \mu_B = 0.54$) and as $T_N^{zz} = 7$ K, 12 K, and 18 K, respectively. As in La$_2$CuO$_4$, the magnitude of the longitudinal moment ($\mu^{zz} \simeq 4 \times 10^{-2}\mu_B \simeq 0.08\mu^{++}$) may be large enough to be detected by polarized neutron-scattering experiments on Sr$_2$CuO$_2$Cl$_2$ single crystals.

![FIG. 5.: Inverse antiferromagnetic transverse intraplane correlation length in Sr$_2$CuO$_2$Cl$_2$ obtained by the neutron-scattering experiments of Ref. [20] (symbols) and from the theory for different exchange energies $J$.](image)

![FIG. 4.: Inverse antiferromagnetic transverse intraplane correlation length in La$_2$CuO$_4$ obtained by the neutron-scattering experiments of Ref. [4] (symbols) and from the theory for different spatial and spin anisotropies.](image)
V. SUMMARY

In this paper we presented a Green’s-function theory for the quasi-2D easy-plane XXZ model allowing the calculation of all static magnetic properties at arbitrary temperatures, where we focused on the effects of spatial and spin anisotropy on the AFM LRO and the correlation length. As a qualitatively new result, for appropriate model parameters we obtained two phase transitions, where the paramagnetic phase with pronounced AFM SRO becomes unstable against a phase with transverse LRO only and, at a lower temperature, a phase with both transverse and longitudinal LRO. Comparing the theory with neutron-scattering experiments on the correlation length of La$_2$CuO$_4$, an excellent agreement is found.

Furthermore, the second Néel transition (to the phase with longitudinal LRO) in La$_2$CuO$_4$, Sr$_2$CuO$_2$Cl$_2$, and Ca$_{0.85}$Sr$_{0.15}$CuO$_2$ is predicted to occur at about 30 K, 10 K, and 190 K, respectively. Our goal is to stimulate a wider discussion and new experiments in this direction.

Acknowledgments. The authors are greatly indebted to B. Keimer and R. Hayn for stimulating discussions.

APPENDIX: THEORY OF SPIN SUSCEPTIBILITY

The spin susceptibilities $\chi^+ (q)$, $\chi^z (q)$, where $\chi^+ (q)$ denotes the two-time retarded commutator Green’s function, are determined by the projection method taking, as for the XXZ chain [12], the basis $\{ iS^+_0, iS^+_q \}$ and $\{ iS^z_q \}$, respectively. We obtain

$$\chi^+ (q) = - \frac{\langle [iS^+_0, iS^-_q] \rangle}{\omega^2 - (\omega_q)^2}; \quad \nu = +, - , z,$$

with the first spectral moments $M^{\nu} = \langle [iS^\nu_0, \sigma^-_q] \rangle$ and $M^{zz} = \langle [iS^z_0, S^z_q] \rangle$ given by the exact expressions

$$M^{\nu} = - 4[C^{\nu}_{q,0,1} (1 - \Delta \gamma_q) + 2C^{\nu}_{q,0,0} (\Delta - \gamma_q)]$$

$$M^{zz} = - 4C^{zz}_{q,0,1} (1 - \Delta \cos q_z) + 2C^{zz}_{q,0,0} (\Delta - \cos q_z)$$

$$C^{\nu}_{q,0,1} = \langle [S^\nu_0, S^+_{q,1}] \rangle, \quad C^{zz}_{q,0,1} = \langle [S^z_0, S^+_{q,1}] \rangle, \quad r = n \mathbf{e}_x + m \mathbf{e}_y + l \mathbf{e}_z, \quad \gamma_q = (\cos q_x + \cos q_y)/2.$$

The spin correlators are calculated as

$$C^\nu_r = \frac{1}{N} \sum_q \frac{M^{\nu}_q}{2 \omega^2_q} [1 + 2p(\omega^\nu_r)] e^{iqr},$$

where $p(\omega^\nu_r) = (e^{\omega^\nu_r/T} - 1)^{-1}$. The NN correlation functions are related to the internal energy per site $\varepsilon = 2[C^{zz}_{q,0,1} + \Delta C^{zz}_{q,0,0}] + R_z(C^{zz}_{q,0,1} + \Delta C^{zz}_{q,0,0}).$

The spectra $\omega^\nu_r$ are calculated in the approximations $\tilde{S}_i = (\omega^\nu_i)^2 S^\nu_0$ and $\tilde{S}_q = (\omega^\nu_q)^2 S^\nu_q$, where products of spin operators in $S^\nu_i$ and $S^\nu_i$ along NN sequences $\langle i, j, l \rangle$ are decoupled. Introducing vertex parameters in the spirit of the scheme by Shimahara and Takada [21] and extending the decouplings given in Refs. [11,9,12], we have

$$S^+_i S^+_j S^+_l = \alpha_{1r,1z}^+ (S^+_i S^+_j) S^+_l + \alpha_{2r}^+ (S^+_i S^+_j) S^+_l,$$

$$S^z_i S^+_j S^+_l = \alpha_{1z,1z}^z (S^+_i S^+_j) S^+_l,$$

$$S^z_i S^+_j S^+_l = \alpha_{z}^z (S^+_i S^+_j) S^+_l.$$

Here, $\alpha_{1r,1z}^+ \tau_\nu$ and $\alpha_{1z,1z}^z \tau_\nu$ are attached to NN correlations in the $xy$-plane and along the $z$ direction, respectively, and $\alpha_{z}^z$ is associated with longer ranged correlation functions. We obtain

$$\langle \omega^\nu_q \rangle^2 = \left[ 1 + 2\alpha_{1z}^+ (C^{zz}_{0,1,0} + 2C^{zz}_{1,1,0}) \right] (1 - \Delta \gamma_q)$$

$$+ \Delta [1 + 4\alpha_{1z}^+ (C^{zz}_{0,0,0} + 2C^{zz}_{1,1,0})] (\Delta - \gamma_q)$$

$$+ 2\alpha_{1z}^+ C^{zz}_{1,0,0} (\Delta - \gamma_q - \cos q_z)$$

$$+ 4\alpha_{1z}^+ C^{zz}_{0,0,1} (\Delta - \cos q_z)$$

$$2\alpha_{1z}^+ C^{zz}_{1,0,0} (1 - \Delta \gamma_q - \Delta \cos q_z)$$

$$+ 2\alpha_{1z}^+ C^{zz}_{0,0,1} (\Delta - \cos q_z - \Delta)$$

$$+ 2\alpha_{1z}^+ C^{zz}_{1,0,0} (\Delta - \gamma_q - \Delta)$$

$$+ 4\alpha_{1z}^+ C^{zz}_{1,0,0} (\Delta - \cos q_z)$$

$$+ 4\alpha_{1z}^+ C^{zz}_{0,0,1} (\Delta - \cos q_z)$$

$$+ 4\alpha_{1z}^+ C^{zz}_{0,0,1} (\Delta - \cos q_z)$$

$$+ 4\alpha_{1z}^+ C^{zz}_{0,0,1} (\Delta - \cos q_z)$$

Note that in the special cases $R_z = 0$ and $\Delta = 1$ the spectra reduce to the expressions given in Refs. [13] and [9], respectively.
The LRO in the correlators $C_{rr}^\nu$ is reflected in our theory by the closure of the spectrum gap at $Q = (\pi, \pi, \pi)$ as $T$ approaches $T_K^\nu$ from above, so that $\lim_{T \to T_K^\nu} (\chi_Q^\nu)^{-1} = 0$ and $\omega_Q^\nu = 0$ at $T \leq T_K^\nu$. Separating the condensation part $C_{rr}^\nu e^{-iQr}$ from $C_{rr}^\nu$ [cf. Eq. (5)], the magnetization $m^\nu$ is calculated as
\[(m^\nu)^2 = \frac{1}{N} \sum_r C_{rr}^\nu e^{-iQr} = C^\nu. \tag{11}\]

Considering the uniform static longitudinal susceptibility $\chi_{zz}^\nu = \lim_{q \to 0} M_q^{zz}/(\omega_q^zz)^2$, the ratio of the anisotropic functions $M_{zz}^q$ and $(\omega_q^zz)^2 = c_{zz}^2 (q_{\perp}^2 + q_{\parallel}^2) + c_{zz}^2 q_{\parallel}^2$ must be isotropic in the limit $q \to 0$. This yields the condition
\[(c_{zz}/c_{xy})^2 = R_z C_{zz}^{t+, 0,0}/C_{zz}^{t+, 0,0} \tag{12}\]
with the squared spin-wave velocities
\[c_{zz}^2 = \frac{1}{2} + \alpha_{zz}^2 (2C_{2,0,0}^{t+, 1,0} + 2C_{2,1,0}^{t+, 1,0}) - 5$$\Delta \alpha_{zz}^2 C_{1,0,0}^{t+, 1,0}
+ 2R_z (\alpha_{zz}^2 C_{1,0,0}^{t+, 1,0} - \Delta \alpha_{zz}^2 C_{1,0,0}^{t+, 1,0}), \tag{13}\]
\[c_{xy}^2 = R_z (\frac{1}{2} + 2\alpha_{xy}^2 C_{1,0,0}^{t+, 0,0} - 3\Delta \alpha_{xy}^2 C_{0,0,1}^{t+, 0,0})
+ 4R_z (\alpha_{xy}^2 C_{1,0,0}^{t+, 1,0} - \Delta \alpha_{xy}^2 C_{1,0,0}^{t+, 1,0}). \tag{14}\]

Concerning the vertex parameters in our self-consistency scheme, three parameters are fixed by the sum rules $C_{zz}^{t+, 0,0} = 1/2$, $C_{zz}^{t+, 0,0} = 1/4$, and by Eq. (12) for all $T$. To determine the free parameters taken as $\alpha_{zz}^2$ and $\alpha_{xy}^2$, we need additional conditions. Let us consider the ground-state energy per site which we compose approximately, following Ref. [9], as $\epsilon(\Delta, R_z) = \epsilon(\Delta, R_z) + \epsilon(\Delta, 1) - \epsilon(\Delta, 0)$. Here, $\epsilon(\Delta, R_z)$ denotes the ground-state energy of the 2D spatially anisotropic XXZ model [Eq. (1) without sum in $y$ direction], where the values in the 1D ($R_z = 0$) and 2D cases ($R_z = 1$) are taken from Ref. [22] and the exact data of Refs. [13,14], respectively. Since $\epsilon(\Delta, R_z)$ is known for $R_z = 0$, 1 and $\Delta = 1$ (taken from the Ising-expansion results by Affleck et al. [23]), we approximate $\epsilon(\Delta, R_z)$ by the linear interpolation $\epsilon(\Delta, R_z) = \epsilon(\Delta, 0) + [\epsilon(\Delta, 1) - \epsilon(\Delta, 0)]|e(1, 0) - e(1, 1)|$. At $T = 0$, we adjust $\alpha_{zz}^2$ to $\epsilon(\Delta, R_z)$ and $\alpha_{xy}^2$ to $\partial \epsilon/\partial \Delta = 2C_{zz}^{t+, 1,0} + R_z C_{0,0,1}^{t+, 1,0}$. To formulate conditions for $\alpha_{zz}^2$ and $\alpha_{xy}^2$ also at finite temperatures, we follow the reasonings of Refs. [21,10,12]. That means, we conjecture that the “vertex corrections” $\alpha_{zz}^2(T) - 1$ and $\alpha_{xy}^2(T) - 1$ have similar temperature dependences and vanish in the high-$T$ limit. Correspondingly, as the simplest interpolation between high temperatures and $T = 0$ we assume the ratio of two vertex corrections as temperature independent and fixed by the ground-state value, i.e.,
\[\frac{\alpha_{zz}^2(T) - 1}{\alpha_{zz}^2(T) - 1} = \text{const.} \tag{15}\]
\[\frac{\alpha_{xy}^2(T) - 1}{\alpha_{xy}^2(T) - 1} = \text{const.} \tag{16}\]

To determine $\alpha_{zz}^2(T)$, as compared with $\alpha_{zz}^2(T)$ fixed by the “isotropy condition” (12) resulting from $\chi_{zz}^\nu$, we first note that an analogous condition cannot be derived from $\chi_{zz}^\nu = \lim_{q \to 0} M_q^{zz}/(\omega_q^zz)^2$, since both $M_q^{zz}$ and $\omega_q^zz$ have non-zero $q \to 0$ limits [cf. Eqs. (3) and (9)]. Therefore, for $\alpha_{zz}^2(T)$ we make the plausible ansatz assuming the ratio $\alpha_{zz}^2(T)/\alpha_{zz}^2(T)$ as $\nu$ independent, i.e.,
\[\frac{\alpha_{zz}^2(T)}{\alpha_{zz}^2(T)} = \frac{\alpha_{zz}^2(T)}{\alpha_{zz}^2(T)} \tag{17}\]

From the solution of the self-consistency equations the AFM correlation lengths above $T_K^\nu$ may be evaluated. They are obtained by the expansion of $\chi_{zz}^\nu$ around $Q$, $\chi_{zz}^\nu = \chi_{zz}^\nu(1 + (\xi_{zz}^\nu)^2(k_{\perp}^2 + k_{\parallel}^2) + (\xi_{zz}^\nu)q_{\parallel}^2)^{-1}$ with $k = q - Q$. The squared intraplane correlation lengths are given by
\[(\xi_{zz}^\nu)^2 = (\omega_q^zz)^2 - (\omega_q^zz)^2 \tag{18}\]
\[\times \left[ \frac{\Delta}{2} + \Delta \alpha_{zz}^2 \left( 2C_{2,0,0}^{t+, 1,0} + 2C_{2,1,0}^{t+, 1,0} + 2C_{1,1,0}^{t+, 1,0} \right) 
+ \alpha_{zz}^2 \left( (4\Delta + \frac{\Delta}{2})C_{1,1,0}^{t+, 1,0} + (8 + 3\Delta)C_{1,0,0}^{t+, 1,0} \right) 
+ R_z (\alpha_{zz}^2 (C_{1,0,0}^{t+, 1,0} + 2C_{1,0,0}^{t+, 0,0}) + \alpha_{zz}^2 (C_{0,0,0}^{t+, 1,0} + 2C_{0,0,0}^{t+, 0,0})) 
+ \Delta (C_{1,0,0}^{t+, 0,0} + 2C_{1,0,0}^{t+, 0,0})/M_q^{zz}, \right] \tag{19}\]
[7] M. Matsuda, K. Yamada, K. Kakurai, H. Kadowaki, T. R. Thurston, Y. Endoh, Y. Hidaka, R. J. Birgeneau, M. A. Kastner, P. M. Gehring, A. H. Moudden, and G. Shirane, Phys. Rev. B 42, 10098 (1990).
[8] V. Yu. Irkhin, A. A. Katanin, and M. I. Katsnelson, Phys. Rev. B 60, 1082 (1999).
[9] L. Siurakshina, D. Ihle, and R. Hayn, Phys. Rev. B 61, 14601 (2000).
[10] S. Winterfeldt and D. Ihle, Phys. Rev. B 56, 5535 (1997); ibid 59, 6010 (1999).
[11] D. Ihle, C. Schindelin, A. Weiße, and H. Fehske, Phys. Rev. B 60, 9240 (1999).
[12] C. Schindelin, H. Fehske, H. Büttner, and D. Ihle, Phys. Rev. B 62, 12141 (2000).
[13] H. Fehske, C. Schindelin, A. Weiße, H. Büttner, and D. Ihle, Brazil. Jour. Phys. 30, 720 (2000).
[14] Y. Okabe and M. Kikuchi, J. Phys. Soc. Jpn. 57, 4351 (1988).
[15] A. W. Sandvik, Phys. Rev. Lett. 83, 3069 (1999).
[16] P. Kopietz, Phys. Rev. Lett. 68, 3480 (1992).
[17] S. Chakravarty, B. I. Halperin, and D. R. Nelson, Phys. Rev. Lett. 60, 1057 (1988); Phys. Rev. B 39, 2344 (1989).
[18] S. Winterfeldt and D. Ihle, Phys. Rev. B 58, 9402 (1998).
[19] B. Keimer, private communication.
[20] M. Greven, R. J. Birgeneau, Y. Endoh, M. A. Kastner, M. Matsuda, and G. Shirane, Z. Phys. B 96, 465 (1995); M. Greven, R. J. Birgeneau, Y. Endoh, M. A. Kastner, B. Keimer, M. Matsuda, G. Shirane, and T. R. Thurston, Phys. Rev. Lett. 72, 1096 (1994).
[21] H. Shimahara and S. Takada, J. Phys. Soc. Jpn. 60, 2394 (1991); ibid 61, 989 (1992).
[22] C. N. Yang and C. P. Yang, Phys. Rev. 150, 321 (1966); ibid 327 (1966).
[23] I. Affleck, M. P. Gelfand, and R. R. P. Singh, J. Phys. A 27, 7313 (1994).