Quantum to classical crossover in the 2D easy-plane XXZ model

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Ground-state and thermodynamical properties of the spin-1/2 two-dimensional easy-plane XXZ model are investigated by both a Green's-function approach and by Lanczos diagonalizations on lattices with up to 36 sites. We calculate the spatial and temperature dependences of various spin correlation functions, as well as the wave-vector dependence of the spin susceptibility for all anisotropy parameters Δ. In the easy–plane ferromagnetic region ($-1 < \Delta < 0$), the longitudinal correlators of spins at distance r change sign at a finite temperature $T_0(\Delta, \mathbf{r})$. This transition, observed in the 2D case for the first time, can be interpreted as a quantum to classical crossover.

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I. INTRODUCTION

The magnetic properties of low-dimensional quantum spin systems with spin anisotropy, such as the quasi-one-dimensional (1D) cuprates [1] and the quasi-2D high-T_c parent compounds [2], are of growing interest. The $S = 1/2$ XXZ model

$$\mathcal{H} = \frac{J}{2} \sum_{\langle i,j \rangle} (S_i^+ S_j^- + \Delta S_i^z S_j^z) \tag{1}$$

($\langle i, j\rangle$ denote nearest-neighbor (NN) sites; throughout we set $J = 1$) usually serves as the generic model for those systems. Recently, in the ferromagnetic (FM) region ($-1 < \Delta < 0$) of the 1D model a quantum-classical crossover in the longitudinal spin correlators was found by means of exact diagonalization (ED) [3] and a Green's-function theory [4]. For the XXZ model on a square lattice, an analytical approach to the spin susceptibility taking into account the magnetic short-range order (SRO) at arbitrary temperatures does not yet exist.

In this contribution the spin correlations in the easy-plane region $-1 < \Delta < 1$ of the 2D XXZ model are examined by both a Green's-function theory outlined in the Appendix and by exact finite-cluster diagonalizations of the model (1) on lattices with up to 36 spins using periodic boundary conditions. We mainly focus on the characteristics of a possible quantum to classical crossover in the FM regime. Moreover, for the first time, the complete wave-vector, temperature and Δ dependences of the static transverse and longitudinal spin susceptibilities are calculated.

II. GROUND-STATE PROPERTIES

In Fig. 1 our results for the magnetization $m(\Delta)$ are compared with available quantum Monte Carlo (QMC) data [5], where the ED/QMC data for the ground-state energy per site $\varepsilon(\Delta)$ (inset) is taken as input for the Green's-function approach ($C_{10}^{zz} = \frac{1}{2}\partial\varepsilon/\partial\Delta$, $C_{10}^{+-} = \varepsilon/2 - \Delta C_{10}^{zz}$).

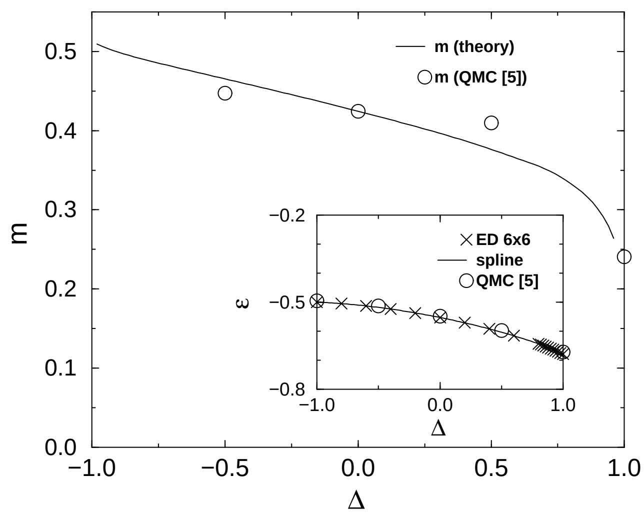

FIG. 1.: Magnetization m and ground-state energy ε of the 2D easy-plane XXZ model.

As can be seen from Fig. 2, the short-ranged correlations calculated analytically are in excellent agreement with our ED data. Let us stress that the finite-size dependence of the ED data is almost negligible by going from a 32- to a 36-site lattice. At $\Delta = 1$ the rotational symmetry $C_{\mathbf{r}}^{+-} = 2C_{\mathbf{r}}^{zz}$ is visible. At the quantum critical point $\Delta = -1$ we have $C_{\mathbf{r},\tilde{\mathcal{H}}}^{+-} = 2C_{\mathbf{r}}^{zz} = 1/6$ (cf. Eq. (14)). The non-analytical limiting behavior $\lim_{\Delta\to -1^+} C_{\mathbf{r}}^{zz} = 0$ results from both the QMC [5] and ED data (obtained in the subspace with total spin projection $S^z = 0$).

The static spin susceptibilities $\chi_{\mathbf{q}}^{\nu}(\Delta)$ are depicted in Fig. 3. In the FM region, for sufficiently low Δ values, $\chi_{\mathbf{q}}^{zz}$ shows a maximum at $\mathbf{q} = 0$ being a precursor of the FM instability (in the zz-correlators) at $\Delta = -1$. Note that $(\chi_{\mathbf{Q}}^{+-})^{-1} = 0$, reflecting the transverse long-range order (LRO) at $T = 0$, by Eq. (13) corresponds to $(\chi^{+-}_{0,\tilde{\mathcal{H}}})^{-1} = 0$. In the antiferromagnetic (AFM) region $0 < \Delta < 1$ the maximum in $\chi^{zz}_{\mathbf{q}}$ at $\mathbf{q} = \mathbf{Q}$ is indicative of the longitudinal AFM LRO at $\Delta \geq 1$.

Finally, in Fig. 4 we show the longitudinal spin-wave spectrum $\omega^{zz}_{\mathbf{q}}$ (cf. Eq. (7)). For $q \equiv |\mathbf{q}| \ll 1$ we have $\omega^{zz}_{\mathbf{q}} = c^{zz}_s q$, where the spin-wave velocity c^{zz}_s increases with Δ over the whole easy-plane region. The minimum in $\omega^{zz}_{\mathbf{q}}$ at $\mathbf{q} = \mathbf{Q}$ in the AFM region corresponds to the maximum in $\chi^{zz}_{\mathbf{q}}$ (cf. Fig. 3 a) and reflects the increase of the longitudinal AFM SRO with Δ (see also $C^{zz}_{\mathbf{r}}(\Delta)$ in Fig. 2).

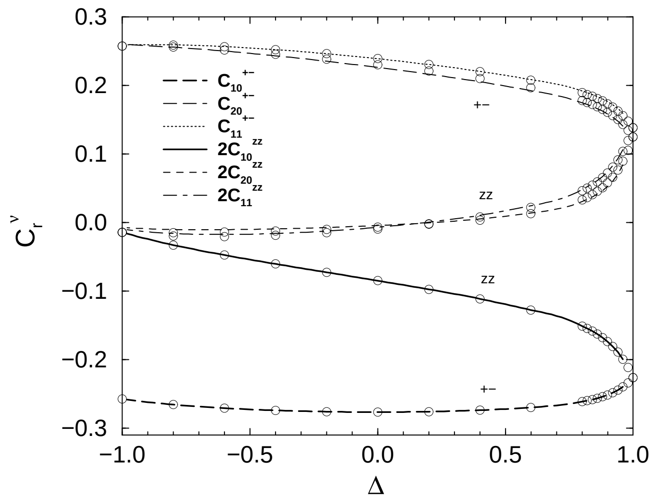

FIG. 2.: Transverse and longitudinal spin correlation functions $C^{\nu}_{\mathbf{r}}$ at $T = 0$. Symbols denote ED results obtained for a 6×6 lattice.

III. FINITE-TEMPERATURE RESULTS

The temperature dependence of the short-ranged longitudinal spin correlations is displayed in Fig. 5. Again the analytical results agree remarkably well with the ED data. In the FM region, for the first time in the 2D model, we observe the so-called "sign-changing" effect which was found numerically [3] in the 1D model and later on reproduced by our Green's-function calculations [4]. That is, at fixed separation r and with increasing temperature or at fixed temperature and with increasing r, $C^{zz}_{\mathbf{r}}$ changes sign from negative to positive values. The temperature $T_0(\Delta, \mathbf{r})$ where $C^{zz}_{\mathbf{r}}(T_0(\Delta, \mathbf{r}), \Delta) = 0$ are given in Table I. As in the 1D case, T_0 at fixed Δ decreases with increasing r. However, compared to the 1D case [4], our analytical results are in much better agreement with the ED data. The sign change of $C^{zz}_{\mathbf{r}}$ may be interpreted as a quantum to classical crossover [3] because with increasing temperature the system behaves more classically, i.e., it becomes dominated by the potential energy (negative Δ term of the Hamiltonian favoring the parallel alignment of two spins). In the AFM region we obtain the expected al-

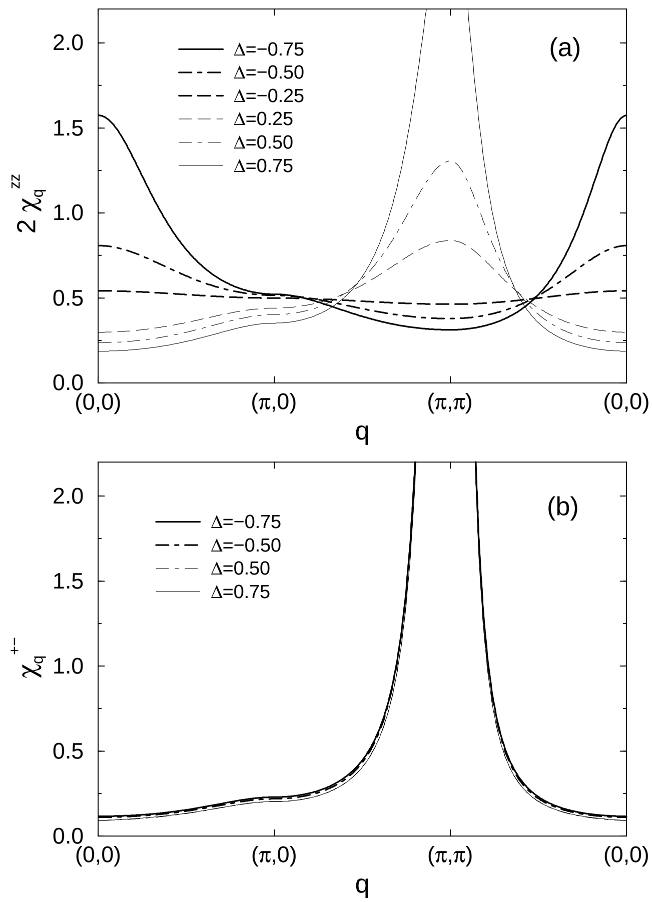

FIG. 3.: Wave-vector dependence of the longitudinal (a) and transverse (b) static susceptibilities $\chi^{\nu}_{\mathbf{q}}$ at $T = 0$.

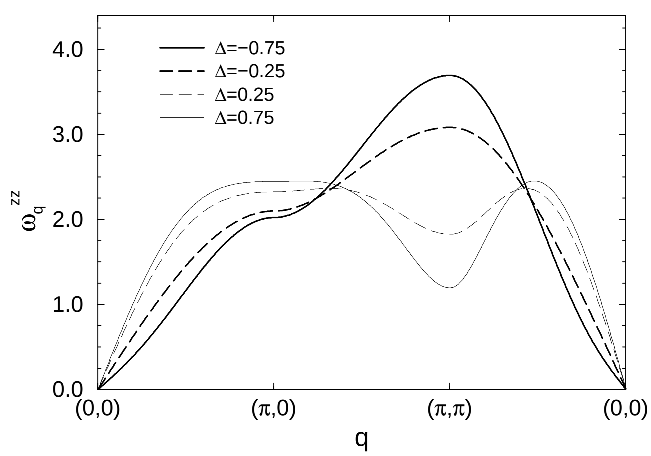

FIG. 4.: Longitudinal spin-wave dispersion $\omega^{zz}_{\mathbf{q}}$ along the major symmetry directions of the 2D Brillouin zone.

ternating signs of $C^{zz}_{\mathbf{r}}$ corresponding to the longitudinal AFM SRO.

In Fig. 6 various susceptibilities $\chi^{\nu}_{\mathbf{q}}$ at $\mathbf{q} = 0, \mathbf{Q}$ are plotted as functions of T and compared with numerical data. For $\Delta = 0.5$ the longitudinal and transverse uniform susceptibilities are in reasonable agreement with the QMC results [5] and our ED data (the up- and downturn at lower temperatures is a finite-size effect). The increase of $\chi_0^\nu(T)$, the maximum near the exchange energy ($J = 1$), and the crossover to the Curie-Weiss law are due to the decrease of AFM SRO with increasing temperature. On the other hand, the staggered susceptibility $\chi_{\mathbf{Q}}^{zz}$ is enhanced as compared with χ_0^{zz} by the longitudinal AFM SRO. In the FM region (Fig. 6 b, $\Delta = -0.5$) the maximum in χ_0^{zz}, where the analytical and numerical results yield nearly the same position, may be explained as a combined SRO and sign changing effect as discussed for the 1D model in Ref. [4]. Contrary to the AFM region, $\chi_{\mathbf{Q}}^{zz}$ is suppressed as compared with χ_0^{zz} which is caused by the FM correlations above T_0. The temperature dependence of $\chi_0^{+-} = \chi_{\mathbf{Q},\tilde{\mathcal{H}}}^{+-}$ may be explained again as a SRO effect. Here, the transverse FM SRO results in a spin stiffness against the orientation of the transverse spin components along a staggered field perpendicular to the z-direction, so that $\chi_{\mathbf{Q},\tilde{\mathcal{H}}}^{+-}$ is suppressed at low temperatures and exhibits a maximum.

TABLE I. Temperature $T_0(\Delta;\mathbf{r})$ of the sign change in the longitudinal correlation functions $C_{\mathbf{r}}^{zz}(T;\Delta)$. The corresponding results obtained from ED of a 4×4 lattice are given in parenthesis.

Δ	$T_0(\Delta;\mathbf{r})$		
	$\mathbf{r}=(1,0)$	$\mathbf{r}=(1,1)$	$\mathbf{r}=(2,0)$
-0.1	2.98 [2.540]	1.76	1.76 [1.520]
-0.3	0.96 [0.931]	0.74	0.72 [0.713]
-0.5	0.66 [0.605]	0.52 [0.527]	0.50 [0.476]
-0.7	0.46 [0.391]	0.36 [0.303]	0.34 [0.301]
-0.9	<0.2 [0.125]	<0.2 [0.106]	<0.2 [0.106]

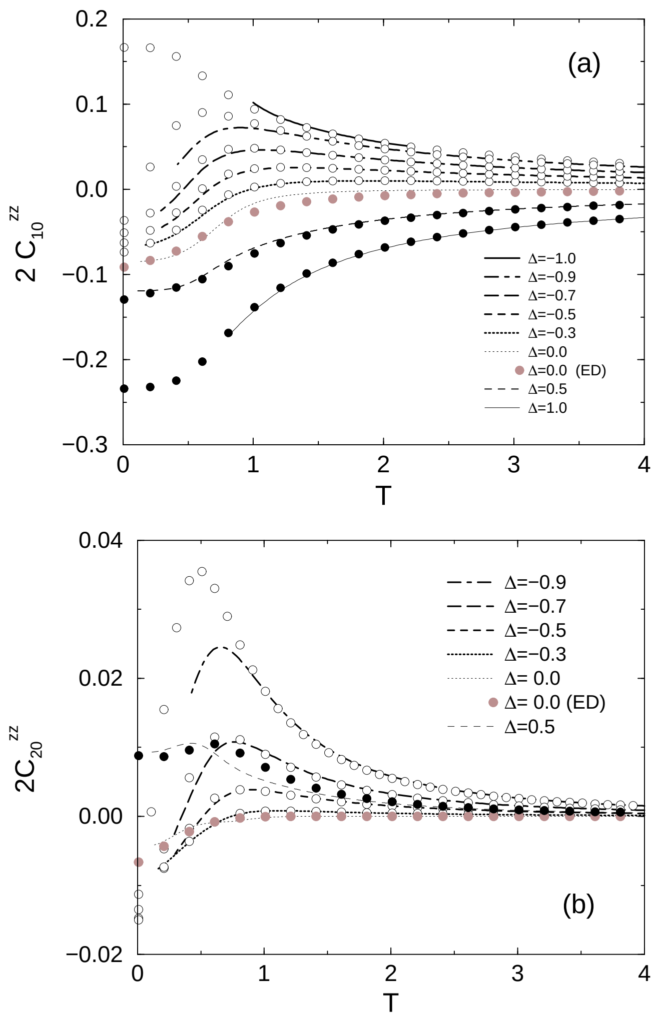

FIG. 5.: Temperature dependence of the NN (a) and next NN (b) longitudinal spin correlation functions $C_{\mathbf{r}}^{zz}$. Symbols denote ED results obtained for a 4×4 lattice.

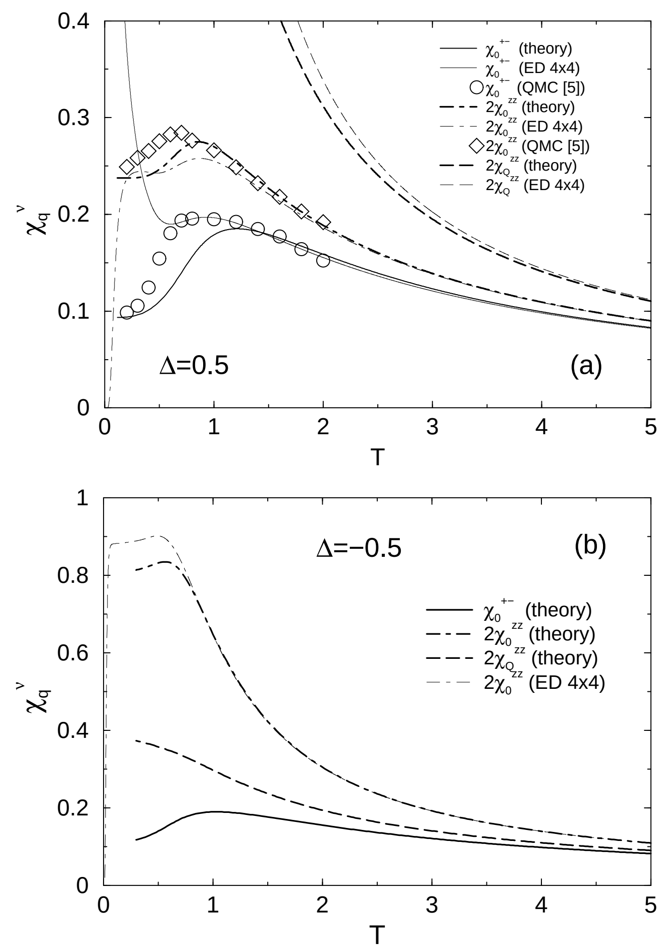

FIG. 6.: Longitudinal and transverse static spin susceptibilities $\chi_{\mathbf{q}}^\nu$ as functions of temperature T for the 2D AFM (a) and FM (b) easy-plane XXZ models.

IV. SUMMARY

To resume, we presented a Green's-function theory of magnetic LRO and SRO in the 2D easy-plane XXZ model which allows the complete calculation of all static magnetic properties in excellent agreement with numerical diagonalization data. In particular, in the FM region we found a quantum to classical crossover in the longitudinal spin correlations. We conclude that our approach is promising to be applied to other anisotropic spin models, such as the quasi-2D XXZ model for the parent compounds of high-T_c superconductors.

APPENDIX: GREEN'S-FUNCTION THEORY

The spin susceptibilities $\chi^{+-}_{\mathbf{q}}(\omega) = -\langle\langle S^+_{\mathbf{q}}; S^-_{-\mathbf{q}}\rangle\rangle_\omega$ and $\chi^{zz}_{\mathbf{q}}(\omega) = -\langle\langle S^z_{\mathbf{q}}; S^z_{-\mathbf{q}}\rangle\rangle_\omega$, expressed in terms of two-time retarded commutator Green's functions, are determined by the projection method, developed, for the XXZ chain, in Ref. [4]. Taking the two-operator basis $(S^+_{\mathbf{q}}, i\dot{S}^+_{\mathbf{q}})^T$ and $(S^z_{\mathbf{q}}, i\dot{S}^z_{\mathbf{q}})^T$ we obtain

$$\chi^\nu_{\mathbf{q}}(\omega) = -\frac{M^\nu_{\mathbf{q}}}{\omega^2 - (\omega^\nu_{\mathbf{q}})^2}\,; \quad \nu = +-,\, zz, \tag{2}$$

with

$$M^{+-}_{\mathbf{q}} = -4[C^{+-}_{10}(1-\Delta\gamma_{\mathbf{q}}) + 2C^{zz}_{10}(\Delta - \gamma_{\mathbf{q}})]\,, \tag{3}$$

$$M^{zz}_{\mathbf{q}} = -4C^{+-}_{10}(1-\gamma_{\mathbf{q}})\,, \tag{4}$$

$C^\nu_{nm} \equiv C^\nu_{\mathbf{r}}$, $C^{+-}_{\mathbf{r}} = \langle S^+_0 S^-_{\mathbf{r}}\rangle$, $C^{zz}_{\mathbf{r}} = \langle S^z_0 S^z_{\mathbf{r}}\rangle$, $\mathbf{r} = n\mathbf{e}_x + m\mathbf{e}_y$, and $\gamma_{\mathbf{q}} = (\cos q_x + \cos q_y)/2$. The spin correlators are obtained from Eq. (2) as

$$C^\nu_{\mathbf{r}} = \frac{1}{N}\sum_{\mathbf{q}} \frac{M^\nu_{\mathbf{q}}}{2\omega^\nu_{\mathbf{q}}}[1 + 2p(\omega^\nu_{\mathbf{q}})]\mathrm{e}^{i\mathbf{qr}}\,, \tag{5}$$

where $p(\omega^\nu_{\mathbf{q}}) = (\mathrm{e}^{\omega^\nu_{\mathbf{q}}/T} - 1)^{-1}$. The spectra $\omega^\nu_{\mathbf{q}}$, calculated in the approximations $-\ddot{S}^+_{\mathbf{q}} = (\omega^{+-}_{\mathbf{q}})^2 S^+_{\mathbf{q}}$ and $-\ddot{S}^z_{\mathbf{q}} = (\omega^{zz}_{\mathbf{q}})^2 S^z_{\mathbf{q}}$ introducing vertex parameters α^ν_i ($i = 1, 2$), are given by

$$\begin{aligned}(\omega^{+-}_{\mathbf{q}})^2 = {} & [(1 + 2\alpha^{+-}_2(C^{+-}_{20} + 2C^{+-}_{11})](1 - \Delta\gamma_{\mathbf{q}}) \\ & + \Delta(1 + 4\alpha^{+-}_2(C^{zz}_{20} + 2C^{zz}_{11})](\Delta - \gamma_{\mathbf{q}}) \\ & + 2\alpha^{+-}_1[C^{+-}_{10}(4\Delta\gamma^2_{\mathbf{q}} - \Delta - 3\gamma_{\mathbf{q}}) \\ & + 2C^{zz}_{10}(4\gamma^2_{\mathbf{q}} - 1 - 3\Delta\gamma_{\mathbf{q}})]\,,\end{aligned} \tag{6}$$

$$\begin{aligned}(\omega^{zz}_{\mathbf{q}})^2 = {} & 2(1-\gamma_{\mathbf{q}})[1 + 2\alpha^{zz}_2(C^{+-}_{20} + 2C^{+-}_{11}) \\ & - 2\Delta\alpha^{zz}_1 C^{+-}_{10}(1 + 4\gamma_{\mathbf{q}})]\,.\end{aligned} \tag{7}$$

In the easy-plane region $-1 < \Delta < 1$, the long-range order at $T = 0$ is reflected in our theory by $\omega^{+-}_{\mathbf{Q}} = 0$ $[\mathbf{Q} = (\pi, \pi)]$. Accordingly, the condensation part $C\mathrm{e}^{i\mathbf{Qr}}$ is separated from $C^{+-}_{\mathbf{r}}$ (cf. Eq. (5), and the magnetization m is calculated as

$$m^2 = \frac{1}{N}\sum_{\mathbf{r}} C^{+-}_{\mathbf{r}}\mathrm{e}^{-i\mathbf{Qr}} = C\,. \tag{8}$$

The parameters $\alpha^\nu_1(T)$ are determined from the sum rules $C^{+-}_{00} = 1/2$ and $C^{zz}_{00} = 1/4$. To obtain $\alpha^\nu_2(T)$ we adjust $C^\nu_{10}(T = 0)$ taken from our ED data and assume, as additional conditions for the calculation of $\chi^{zz}_{\mathbf{q}}(\omega)$ and $\chi^{+-}_{\mathbf{q}}(\omega)$, temperature independent ratios

$$R^{zz} = \frac{\alpha^{zz}_2(T) - 1}{\alpha^{zz}_1(T) - 1} \tag{9}$$

and

$$R^{+-}_{>} = \frac{\alpha^{+-}_2(T) - 1}{\alpha^{+-}_1(T) - 1} \quad \text{for} \quad \Delta > 0\,, \tag{10}$$

$$R^{+-}_{<} = \frac{\alpha^{+-}_2(T) - 1}{\alpha^{zz}_1(T) - 1} \quad \text{for} \quad \Delta < 0\,, \tag{11}$$

respectively. For the discussion it is useful to perform the unitary transformation which rotates the spins on the sublattice B around the z-axis by the angle π, $\tilde{\mathbf{S}}_i = \mathcal{U}^+\mathbf{S}_i\mathcal{U}$ with $\mathcal{U} = \prod_{l\in B} 2S^z_l$. We get $\tilde{S}^{x,y}_i = \mathrm{e}^{i\mathbf{Qr}_i}S^{x,y}_i$, $\tilde{S}^z_i = S^z_i$ and

$$\tilde{\mathcal{H}} = \frac{1}{2}\sum_{\langle i,j\rangle}(-S^+_i S^-_j + \Delta S^z_i S^z_j)\,. \tag{12}$$

Due to $\langle A\rangle_{\mathcal{H}} = \langle\tilde{A}\rangle_{\tilde{\mathcal{H}}}$ for any operator A, we obtain the relations

$$\chi^{+-}_{\mathbf{q},\mathcal{H}}(\omega) = \chi^{+-}_{\mathbf{k},\tilde{\mathcal{H}}}(\omega)\,; \quad \mathbf{k} = \mathbf{q} - \mathbf{Q}\,, \tag{13}$$

$$C^{+-}_{\mathbf{r},\mathcal{H}} = \mathrm{e}^{i\mathbf{Qr}}C^{+-}_{\mathbf{r},\tilde{\mathcal{H}}}\,, \tag{14}$$

$\chi^{zz}_{\mathbf{q},\mathcal{H}}(\omega) = \chi^{zz}_{\mathbf{q},\tilde{\mathcal{H}}}(\omega)$, and $C^{zz}_{\mathbf{r},\mathcal{H}} = C^{zz}_{\mathbf{r},\tilde{\mathcal{H}}}$. As shown in Ref. [4], the rotational symmetry at $\Delta = \pm 1$ is preserved by our theory.

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