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Physica B 281&282 (2000) 819–820

PHYSICA B

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Spin correlation functions and Néel order in the 2D Heisenberg model: effects of spatial anisotropy

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Abstract

The ground-state properties of the square-lattice spin-$\frac{1}{2}$ Heisenberg antiferromagnet with spatially anisotropic couplings are investigated by Green's-function projection approaches. The staggered magnetization and the two-spin correlators are calculated; the competition between magnetic long- and short-range order is discussed in comparison with experiments on $Sr_2[Ca_2]CuO_3$. © 2000 Elsevier Science B.V. All rights reserved.

Keywords: Spatial anisotropic Heisenberg model; Magnetic short-range order; Order–disorder transition

Motivated by experiments on quasi-1D quantum spin systems, such as Sr_2CuO_3 and Ca_2CuO_3 [1], many efforts were made to clarify the dimensional crossover in the square-lattice spin-$\frac{1}{2}$ antiferromagnetic (AFM) Heisenberg model [2–5]

$$\mathscr{H} = \frac{J_x}{2}\left[\sum_{\langle i,j\rangle_x} \boldsymbol{S}_i\boldsymbol{S}_j + R\sum_{\langle i,j\rangle_y} \boldsymbol{S}_i\boldsymbol{S}_j\right]. \tag{1}$$

Here $R = J_y/J_x$ (throughout we set $J_x = 1$), and $\langle i,j\rangle_{x,y}$ denote nearest-neighbors along the x-, y-directions. In the ground state, the staggered magnetization reveals a transition from a long-range ordered (LRO) Néel state to a spin liquid with AFM short-range order (SRO) at the critical ratio R_c. Quantum Monte Carlo data provide strong evidence for $R_c = 0$ [4], which also results from RPA theories [6,7,1] and (multi-) chain mean-field approaches [4]. In previous work [5], based on a spin-rotation-invariant (SRI) Green's function theory and Lanczos diagonalizations, we found a sharp crossover in the spatial dependence of the spin correlation functions at $R_0 \simeq 0.2$.

In this paper we mainly focus on the SRO properties of the model (1) at $T = 0$ studied by a generalized RPA theory compared with the SRI theory of Ref. [5]. Both approaches are based on the projection method for two-time retarded Green's functions in calculating the dynamic spin susceptibility $\chi^{+-}(\boldsymbol{q},\omega) = -\langle\langle S^+_{\boldsymbol{q}}; S^-_{-\boldsymbol{q}}\rangle\rangle_\omega$. First, we extend the non-SRI theory of Ref. [8] to the case $R \neq 1$, hereafter referred to as Theory I. Introducing two sublattices (a, b) and taking the basis $\boldsymbol{A} = (S^{a+}_{\boldsymbol{q}}, S^{b+}_{\boldsymbol{q}})^{\mathrm{T}}$, where $S^+_{\boldsymbol{q}} = 1/\sqrt{2}(S^{a+}_{\boldsymbol{q}} + S^{b+}_{\boldsymbol{q}})$, we get

$$\chi^{+-}(\boldsymbol{q},\omega) = -\frac{M^{(1)}_{\boldsymbol{q}}}{\omega^2 - \omega^2_{\boldsymbol{q}}} \tag{2}$$

with $M^{(1)}_{\boldsymbol{q}} = -4C_{1,0}[1 - \cos q_x + R\zeta(1 - \cos q_y)]$, $\zeta = C_{0,1}/C_{1,0}$, $C_{\boldsymbol{r}} = (C^{+-}_{\boldsymbol{r}} + 2C^{zz}_{\boldsymbol{r}})/2 \equiv C_{n,m}$, $C^{+-}_{\boldsymbol{r}} = \langle S^+_{\boldsymbol{0}} S^-_{\boldsymbol{r}}\rangle = (1/N)\sum_{\boldsymbol{q}}(M^{(1)}_{\boldsymbol{q}}/2\omega_{\boldsymbol{q}})e^{i\boldsymbol{q}\boldsymbol{r}}$, and $\boldsymbol{r} = n\boldsymbol{e}_x + m\boldsymbol{e}_y$. The magnon spectrum $\bar{\omega}_{\boldsymbol{q}} = \omega_{\boldsymbol{q}}/Z^x_c$ is

$$\bar{\omega}^2_{\boldsymbol{q}} = (1 + R\zeta)^2 - (\cos q_x + R\zeta\cos q_y)^2, \tag{3}$$

where $Z^x_c = -2C_{1,0}/\langle S^{az}\rangle$. Using the identity $S^z_i = -\frac{1}{2} + S^+_i S^-_i$, the sublattice magnetization $m \equiv \langle S^{az}\rangle = -\langle S^{bz}\rangle$ is given by

$$m = \left[\frac{2(1 + R\zeta)}{N}\sum_{\boldsymbol{q}} \bar{\omega}^{-1}_{\boldsymbol{q}}\right]^{-1}. \tag{4}$$

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PII: S0921-4526(99)01064-9

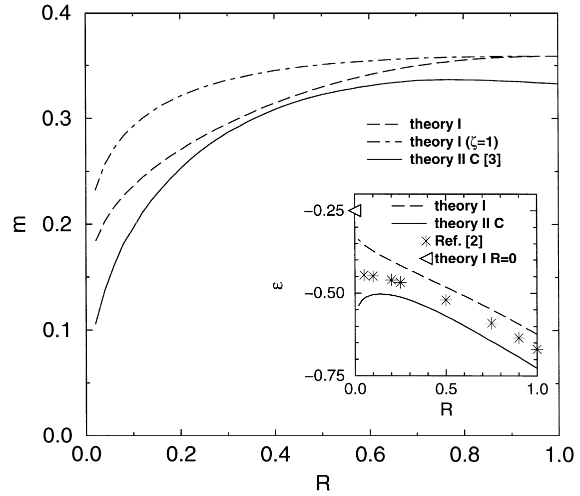

Fig. 1. R-dependence of the magnetization m and of the ground-state energy per site ε (inset).

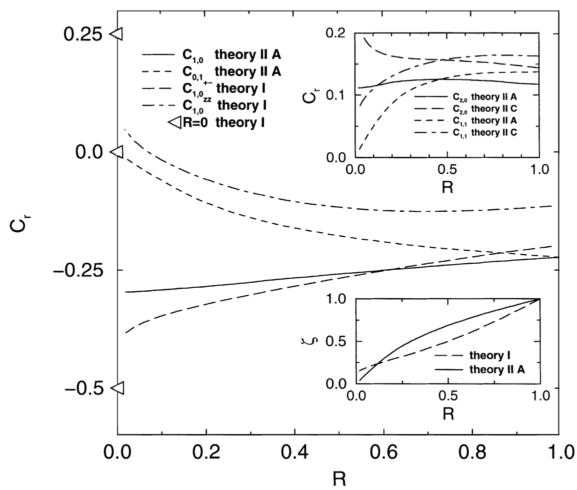

Fig. 2 . Nearest-neighbor and longer ranged (upper inset) spin correlation functions versus R. The lower inset demonstrates that there is no decoupling transition, i.e. $\zeta > 0\ \forall R$, contrary to the suggestion in Ref. [9].

The theory contains one free parameter ζ which we fix by the requirement $C^{+-}_{0,1}/C^{+-}_{1,0} \overset{(!)}{=} \zeta$. The spin-wave velocity renormalization factor Z^x_c is calculated from $Z^x_c = (1+R)[(1/N)\sum_q \bar{\omega}_q]^{-1}$. In the RPA theory of Refs. [6,7], m is given by Eqs. (4) and (3) with $\zeta \equiv 1$. For $R \ll 1$ we have $m = 0.303[1 - 0.386\ln(R\zeta)]^{-1}$ [1].

In the SRI theory [5], hereafter referred to as Theory II, the basis is chosen as $A = (S^+_q, \mathrm{i}\dot{S}^+_q)^{\mathrm{T}}$ yielding $\chi^{+-}(\boldsymbol{q}, \omega)$ and $M^{(1)}_q$ given by Eq. (2). The spectrum is calculated in the approximation $-\ddot{S}^+_q = \omega_q^2 S^+_q$, where ω_q is expressed by correlation functions and vertex parameters. Again, one parameter is free and may be determined by adjusting either the ground-state energy per site $\varepsilon(R)$ [2,3] (case A), the uniform susceptibility (case B), or $m(R)$ [4] (case C) (for details see Ref. [5]).

As seen in Fig. 1, the LRO in Theory I is reduced compared with the RPA result [6,7] due to the ratio ζ expressing the SRO anisotropy. Considering, e.g., the ordered moment in Ca_2CuO_3, where $R = 0.023$ [1], in Theory I we get $\zeta = 0.157$ and $m = 0.0956$ exceeding the experimental value [1] by a factor of about two, whereas the RPA and chain mean-field theory ($m = 0.72\sqrt{R}$ at $R \ll 1$ [4]) yield $m = 0.123$ and $m = 0.109$, respectively. Comparing $\varepsilon(R)$ (inset) with the Ising expansion data of Refs. [2,3], Theories I and II C (input $m(R)$ of Ref. [4], cf. Fig. 1) yield insufficient results at $R \lesssim 0.25$. On the other hand, in Theory II B ($R_c \simeq 0.24$ [5]), $\varepsilon(R)$ nearly agrees with the exact data at $R \lesssim 0.25$. That is, in the Green's-function theories describing LRO with $R_c = 0$, the SRO at $R \lesssim 0.25$ is reproduced inadequately.

The same qualitative behavior can be seen from C_r depicted in Fig. 2. Compared with Theory II A ($R_c \simeq 0.24$), where the correlators reasonably agree with the exact diagonalization data [5], Theory I becomes unsatisfactory at $R \lesssim 0.25$. There we have $2|C^{zz}_{1,0}| \ll |C^{+-}_{1,0}|$ and, for $R < 0.1$, $C^{zz}_{1,0} > 0$ being incompatible with the AFM SRO. Equally, the correlators $C_{1,1}$ and $C_{2,0}$ (inset) in Theory II C strongly deviate from those in Theory II A at $R \lesssim 0.25$.

To conclude, our results call for an improved theory which may describe both the LRO and SRO equally well and explain the very small moments in $Sr_2[Ca_2]CuO_3$.

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