Real-space renormalization group study of the anisotropic antiferromagnetic Heisenberg model of spin $S = 1$ on a honeycomb lattice.

A.S. Boyarchenkov, A.S. Ovchinnikov*, I.G. Bostrem, N.V. Baranov

Department of Physics, Ural State University, 620083, Ekaterinburg, Russia

Y. Hosokoshi

Osaka Prefecture University, Osaka 599-8531, Japan

K. Inoue

Department of Chemistry, Hiroshima University, Hiroshima 739-8526, Japan

(Dated: 3 декабря 2018 г.)

The real-space RG approach is applied to study critical temperatures of system consisting of interacting spin chains of spin $S = 1$ with an inner antiferromagnetic exchange which form a honeycomb crystal lattice. Using anisotropic Heisenberg model we calculate critical temperature as a function of anisotropic parameter and the ratio of interchain and intrachain interactions. A comparison our results with those obtained from RGRS calculations for the same model of spin-1/2 on a square lattice is given.

I. INTRODUCTION.

The study of low-dimensional magnetic systems made of spin chains attracts much attention for last decades. If the interchain coupling is less than intrachain one, at higher

temperatures these systems exhibit properties intrinsic to one-dimensional magnets. However, at lower temperatures the interchain interaction comes into play and begins to govern a magnetic behavior of the system.

In this work we apply the real space renormalization group (RSRG) procedure to the antiferromagnetic Heisenberg (AH) model of spin $S = 1$ on a honeycomb lattice made of antiferromagnetic spin $S = 1$ chains with an antiferromagnetic interchain coupling. We are interested in the critical properties of the 2D system, and explore how the interchain coupling affects the criticality of the model. Simultaneously, we elucidate an effect of an exchange anisotropy on the critical temperature and build the phase diagram of the anisotropic Heisenberg (AH) model of spin $S = 1$ on a honeycomb lattice with two kind of exchange couplings.

First of all, the interest to the problem is motivated by synthesis of a family of related organic biradicals $PNNNO$, $PIMNO$ and F_2PNNNO whose magnetic properties have been examined by susceptibility and magnetization measurements[1]. Each biradical involves two spins of $S = 1/2$, which are coupled ferromagnetically (J_F). In their turn, these spin pairs couple antiferromagnetically in the crystal. Due to the strong ferromagnetic coupling J_F, antiferromagnetic chains of $S = 1$ are seen in both $PNNNO$ and F_2PNNNO (see Fig. 2(a) Type-I in Ref.[1]). $PNNNO$ has interchain interactions in three-dimensions ($3D$), whereas F_2PNNNO has two-dimensional ($2D$) interchain interactions. $PNNNO$ is well understood by one-dimensional antiferromagnetic chain model. The compound undergoes $3D$ Néel order at $\sim$ 1 K due to the weak interchain coupling. The crystal structures of F_2PNNNO is shown in Fig.1. In the extreme limit of $J_F \to \infty$, the model becomes equivalent to the coupled antiferromagnetically (J'_{AF}) antiferromagnetic uniform chains of $S = 1$ with the intrachain exchange integral J_{AF}. F_2PNNNO with comparable values of two kinds of the

antiferromagnetic interactions J_{AF} and J'_{AF} forms a $2D$ system on a honeycomb lattice. It has been found that a magnetism of F_2PNNNO is characterized by the singlet ground state and an energy gap above the state. This finding is supported by the high-field magnetization process which shows a plateau in the magnetization curve. We have to point out once that a modelling of real spin-1/2 system by spin 1 system implies some mistake and one have to apply the results of the RSRG analysis to the real compounds with caution.

The results for the spin-1 lattice may be useful also for the theory of $S = 1$ bosons (ultracold atoms ^{23}Na) trapped in an optical lattice in the regime of one particle per site for suitable interaction between the bosons[2,3].

According to recent quantum Monte Carlo results for spin-1/2 weakly anisotropic antiferromagnets on the square lattice an ordered low-temperature phase develops for very small anisotropy of order $10^{-3} \div 10^{-2}$ (in units of exchange coupling)[4]. These results are in contradiction with the RSRG treatment for the same model predicting considerably larger value of the critical anisotropy (~ 0.2). In view of this discrepancy, the RSRG analysis for the $S > 1/2$ case is of a particular theoretical interest and besides it is instructive to compare a critical behavior of systems of integer and half-integer spins. We mention the results of investigations of ground states of spin-3/2 (spin-2) systems on the hexagonal (square) lattice by using vertex state models[5,6]. It has been shown that these systems exhibit an anisotropy-induced second order phase transition from disordered phase with exponential decay of two-spin correlations to the Neel order phase with dominant long-range correlations. The phase transition belongs to the $2D$ Ising-model universality class.

After the RSRG approach has been applied successfully to study the 2D Ising systems[7,8] a number of works have been dedicated to the investigation of phase transitions in quantum systems within the method[9,10,11]. In last decade, the RSRG methods have been performed to

calculate the phase diagram for the anisotropic antiferromagnetic Heisenberg (AAH) model of $S = 1/2$ on the square lattice[12,13]. This approach uses a hierarchical lattice to approximate the square one, and performs a partial trace over internal degrees of freedom. Recently, in order to study weakly interacting classical and quantum spin chains the linear-perturbation real-space renormalization group (LPRG) method has been suggested[14]. The LPRG uses the existence of the small parameter – the ratio of interchain to intrachain coupling. This perturbative method involves RG transformation, which for the Ising spins is the standard decimation procedure and for the quantum spins is the generalization of the Suzuki-Takano approximate decimation[15]. However, in practice, the LPRG using perturbation theory with the interchain interactions as the perturbation parameters is only reliable for small values of the ratio interchain to intrachain interaction.

We use an extension to $S = 1$ case of the quantum RSRG approach originally suggested by Mariz et al. for the $S = 1/2$ AH model[16]. An application of the renormalization group method to interacting quantum spin chains encounters standard difficulties connected with a necessity of a decomposition of the exponential operators, and additional proliferation of the new interactions due to the vector character of the spin operators.

The paper is organized as follows. In Sec. II the RSRG method is formulated for $S = 1$ and applied to the honeycomb lattice formed by interacting antiferromagnetic chains. Our results and conclusions are given in Sec. III.

II. MODEL.

We consider a system (anisotropic Heisenberg model) whose dimensionless Hamiltonian is defined by

$$-\beta H = \sum_{<i,j>} K_{ij} \left[(1-\Delta_{ij}) \left(S_i^x S_j^x + S_i^y S_j^y \right) + S_i^z S_j^z \right] \tag{1}$$

where $\beta = 1/k_B T$, $K_{ij} \equiv J_{ij}/k_B T$, J_{ij} is the exchange coupling constant, $\langle ij \rangle$ denotes first-neighboring lattice sites, Δ_{ij} is the anisotropic parameter, and S_i^α $\{\alpha = x, y, z\}$ is the spin 1 on the site i. The Hamiltonian (1) describes the Ising ($\Delta_{ij} = 1$), isotropic Heisenberg ($\Delta_{ij} = 0$) and XY-model ($\Delta_{ij} = -\infty$).

We mention briefly main operations lying in base of the approach of Ref.[16]. A parallel array of two bonds characterized respectively by (K_1, Δ_1) and (K_2, Δ_2) is equivalent to a single bond characterized by (K_p, Δ_p) given by

$$K_p = K_1 + K_2,$$

$$K_p \Delta_p = K_1 \Delta_1 + K_2 \Delta_2.$$

The extension of the approach, that is nothing but Migdal-Kadanoff procedure[17,18], to n parallel bonds is straightforward.

For a series array of two bonds characterized by (K_1, Δ_1) and (K_2, Δ_2) the procedure involves difficulties due to non-commutativity effects. Under rescaling and removal of intermediate spins (decimation), the Hamiltonian changes and is characterized by a new set of parameters that are functions of the original set. The initial Hamiltonian is given by

$$H_{123} = K_1 \left[(1-\Delta_1) \left(S_1^x S_3^x + S_1^y S_3^y \right) + S_1^z S_3^z \right] + K_2 \left[(1-\Delta_2) \left(S_3^x S_2^x + S_3^y S_2^y \right) + S_3^z S_2^z \right].$$

We have to replace this array by a single bond whose Hamiltonian is

$$H'_{12} = K_s \left[(1-\Delta_s) \left(S_1^x S_2^x + S_1^y S_2^y \right) + S_1^z S_2^z \right] + K'_0. \tag{2}$$

We impose the preservation of the partition function between terminal sites 1 and 2, i.e.

$$\exp H'_{12} = \mathrm{Tr}_3 \exp H_{132}, \tag{3}$$

where Tr_3 denotes the tracing operation over the states of the intermediate spin 3, K'_0 is an additive constant included to make Eq. (3) possible. Equation (3) establishes the relation between the set of parameters (K_1, Δ_1), (K_2, Δ_2) and the set of renormalized parameters (K_s, Δ_s, K'_0). For the anisotropic spin-1/2 Heisenberg model corresponding expressions may be found explicitly[16],[12].

In order to construct recursion relations of the RG transformation (3) for the spin-1 model we should expand both sides over an appropriate matrix basis to equate coefficients of the expansion. To avoid a proliferation problem we chose those quantities that correspond to coupling constants in the initial Hamiltonian (1).

Due to properties of Pauli matrices the matrix representation for H and $\exp H$ in the case of spin 1/2 has the same form, i.e. H and $\exp H$ have non-zero matrix elements in the same positions. For the $S = 1$ this rule does not hold that results in an essential complication of RG procedure.

Following the treatment of Ref.[16], we expand $\exp H'_{12}$ as

$$\exp H'_{12} = \sum_{n_1=0}^{\infty} \sum_{n_2=0}^{\infty} K_{n_1 n_2} A_1^{n_1} \otimes A_2^{n_2},$$

where $\otimes$ is the outer product, $A_{1,2}$ is ordinary powers of the spin operators $S_{1,2}^{x,y,z}$ and the coefficients $K_{n_1 n_2}$ depend on K_s, Δ_s and K'_0. Since, $A_{1,2}^n$ are the 3×3 matrices we expand them over the basis that consists of the polarization matrices T_q^k ($k = 0, 1, 2$ and $q = -k, -k+1, \ldots, k$) (see Appendix A)

$$A_i^n = a\,(T_i)_0^0 + \sum_{M=\pm 1,0} b^M\,(T_i)_M^1 + \sum_{M=\pm 2,\pm 1,0} c^M\,(T_i)_M^2\,,\ (i = 1, 2).$$

In their turn, the matrices T_q^k may be written through the spin operators explicitly[19]

$$T_0^0 = \frac{1}{\sqrt{3}} I,\ T_{\pm 1}^1 = \mp \frac{1}{2}\left(S_x \pm i S_y\right),\ T_0^2 = \sqrt{\frac{3}{2}}\left((S^z)^2 - \frac{2}{3} I\right),$$

$$T_{\pm 1}^2 = \mp \frac{1}{2}\left[\left(S_x S_z + S_z S_x\right) \pm i\left(S_y S_z + S_z S_y\right)\right],\ T_{\pm 2}^2 = \frac{1}{2}\left[(S^x)^2 - (S^y)^2 \pm i\left(S_x S_y + S_y S_x\right)\right].$$

The transformation $\exp(H)$ should preserve the symmetry of the Hamiltonian H. Thus, the requirement of invariance gives the most general form

$$\exp H_{12} = \alpha_1 \left((T_1)_0^0 \otimes (T_2)_0^0\right) + \alpha_2 \left((T_1)_0^1 \otimes (T_2)_0^1\right) + \alpha_3 \left((T_1)_0^2 \otimes (T_2)_0^2\right) + \beta \left((T_1)_1^1 \otimes (T_2)_{-1}^1 + (T_1)_{-1}^1 \otimes (T_2)_1^1\right)$$

$$+ \gamma \left((T_1)_2^2 \otimes (T_2)_{-2}^2 + (T_1)_{-2}^2 \otimes (T_2)_2^2\right) + \sigma \left((T_1)_1^2 \otimes (T_2)_{-1}^2 + (T_1)_{-1}^2 \otimes (T_2)_1^2\right) \qquad (4)$$

with a new set of coupling parameters α_1, α_2, α_3, β, γ, σ. For the Hamiltonian (2) the above formula gives

$$\exp H_{12} = \begin{pmatrix} A_{12} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & B_{12} & 0 & C_{12} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & D_{12} & 0 & F_{12} & 0 & G_{12} & 0 & 0 \\ 0 & C_{12} & 0 & B_{12} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & F_{12} & 0 & E_{12} & 0 & F_{12} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & B_{12} & 0 & C_{12} & 0 \\ 0 & 0 & G_{12} & 0 & F_{12} & 0 & D_{12} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & C & 0 & B_{12} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & A_{12} \end{pmatrix}, \qquad (5)$$

where the matrix elements are $A_{12} \equiv \alpha_1/3 + \alpha_2/2 + \alpha_3/6$, $B_{12} \equiv \alpha_1/3 - \alpha_3/3$, $C_{12} \equiv -\beta/2 - \sigma/2$, $D_{12} \equiv \alpha_1/3 - \alpha_2/2 + \alpha_3/6$, $E_{12} \equiv \alpha_1/3 + 2\alpha_3/3$, $F_{12} \equiv -\beta/2 + \sigma/2$, $G_{12} \equiv \gamma$.

Similarly, we obtain the closed expression for the expansion of $Tr_3 \exp H_{123}$ akin to that of $\exp H_{12}$ with the coefficients in the expansion (4) are functions of the parameters coming into H_{123} (see Appendix B for details).

To calculate the exponentials we will diagonalize numerically the 9×9 and 27×27 matrices associated with H_{12} and H_{123}. By using

$$\exp H_{12} = U_{12} \exp(H_{12}^D) U_{12}^\dagger, \ \exp H_{123} = U_{123} \exp(H_{123}^D) U_{123}^\dagger,$$

where U_{12}, U_{123} are the unitary matrices turning H_{12}, H_{123} into the diagonal forms H_{12}^D, H_{123}^D, we can find numerically $\exp H_{12}$ and $\exp H_{123}$ as functions of corresponding coupling parameters. The same matrix structure (5) of $\exp H_{12}$ and $Tr_3 \exp H_{123}$ is supported by the numerical calculation. The numerical procedure produces a set $\{\alpha_1, \alpha_2, \alpha_3, \beta, \gamma, \sigma\}$ for $\exp H_{12}$ and $\left\{\bar{\alpha}_1, \bar{\alpha}_2, \bar{\alpha}_3, \bar{\beta}, \bar{\gamma}, \bar{\sigma}\right\}$ for $\mathrm{Tr}_3 \exp H_{132}$. To obtain the required RG equations we impose

$$\alpha_1 = A_{12} + B_{12} + D_{12} = \bar{A}_{12} + \bar{B}_{12} + \bar{D}_{12} = \bar{\alpha}_1, \tag{6}$$

$$\alpha_2 = A_{12} - D_{12} = \bar{A}_{12} - \bar{D}_{12} = \bar{\alpha}_2, \tag{7}$$

$$\beta = -C_{12} - F_{12} = -\bar{C}_{12} - \bar{F}_{12} = \bar{\beta} \tag{8}$$

and

$$\alpha_3 = E_{12} - B_{12} = \bar{E}_{12} - \bar{B}_{12} = \bar{\alpha}_3, \ \ \gamma = G_{12} = \bar{G}_{12} = \bar{\gamma}, \ \ \sigma = F_{12} - C_{12} = \bar{F}_{12} - \bar{C}_{12} = \bar{\sigma}. \tag{9}$$

The number of these equations exceeds the number of interactions that enter into the Hamiltonian (2) because all possible bilinear couplings between terminal sites come into play. Thus, in order to carry out the RG decimation we retain the three equations (6,7,8) which implicitly determine K_s, Δ_s and K_0' as functions of (K_1, Δ_1), (K_2, Δ_2). This set of equations is a counterpart of RG relations for the case of $S = 1/2$ (see Eqs.(12) in Ref.[16]).

Now, we have to chose an appropriate hierarchical lattice. We take one of the simplest cells, conserving a point symmetry of the full lattice, with 6 sites and 6 bonds, depicted in Fig.2. We then impose that the correlation function between the two terminal sites 3 and 6

of the original and renormalized graphs are preserved. At the first step we apply decimation, the spins 1 and 3 (or 4 and 6) survive whereas the spins 2 and 5 are removed. At the second step the decimation procedure is repeated removing the spins 1 and 4. Finally, to obtain the renormalized parameters we apply Migdal-Kadanoff bond moving combining the "pieces" in parallel, which leads to the recursion relations

$$\begin{aligned} (K_S, \Delta_S) &= R_S\left(K_2, \Delta_2; K_1, \Delta_1\right), \\ \left(K_S^{'}, \Delta_S^{'}\right) &= R_S\left(K_S, \Delta_S; K_1, \Delta_1\right), \\ (K_p, \Delta_p) &= 2\left(K_S^{'}, \Delta_S^{'}\right). \end{aligned} \tag{10}$$

We have evaluated numerically the renormalization transformation from the original set of coupling parameters to the set of renormalized parameters. Critical points are then evaluated as non-trivial fixed points of the above relations which can be rewritten as the composite function

$$(K_p, \Delta_p) = 2R_S\left(R_S\left(K_1, \Delta_1; K_2, \Delta_2\right); K_1, \Delta_1\right). \tag{11}$$

Unlike to the case of $S = 1/2$ we can not obtain RG relations explicitly. Instead of this, we briefly outline the numerical procedure. Input fixed parameters are the ratio of interchain to intrachain coupling $C_1 = J_{AF}^{'}/J_{AF}$ and the anisotropic parameter $\Delta = \Delta_1$ and what's more $\Delta_2 = C_1\Delta$ (the feature of anisotropy is the same both for the intrachain and interchain couplings). At given starting value K_{1i} of the intrachain coupling (then the interchain coupling is $K_{2i} = C_1 K_{1i}$) we apply two successive decimation steps to produce a renormalized coupling $K_S^{'}$. During each of the step we solve Eqs.(6,7,8) using the standard routine for non-linear systems of equations[20]. Then, we double the result obtained after these transformations to get a final value K_f depending on the starting value K_{1i}. To complete we find a fixed point K_c of the equation $K_{1i} = K_f(K_{1i})$ by using bisection method.

III. RESULTS.

The critical inverse temperature $K_c = 1/T_c$ as a function of C_1 for several Δ values is presented in Fig.3. As seen, the critical temperature rapidly decreases when the interchain coupling becomes weaker. Our results for the critical temperature as a function of the anisotropy Δ are shown in Fig.4. The universality class for the whole critical curve is the same as for the Ising model. By contrast to some RSRG calculations for $S = 1/2$ the phase diagrams for ferromagnetic and antiferromagnetic models are the same: the critical temperature reaches zero at a critical value of Δ, Δ_c, which is greater than zero. The weaker interchain coupling the stronger quantum fluctuations. So, as one could expect, the Δ_c value is larger if the C_1 shifts to lower values.

For the lowest temperatures we could work we have observed no sign of the reentrant behavior found in some previous RGRS treatments. The Néel temperature behaves as

$$T_N \sim \frac{1}{\ln(\Delta - \Delta_c)}$$

near $\Delta = \Delta_c$ that agrees with the result found for the case $S = 1/2$. Our calculation can not be carried out down to $T = 0$; therefore we can not make any definite conclusions about the ground state of the model. The scaling law holds for different values of the ratio of interchain to intrachain coupling (Fig.5). In Ref.[21,22], the logarithmic dependence of T_N and T_c with respect to $\Delta - \Delta_c$ is established using scaling arguments with $\Delta_c = 0$. Recent quantum Monte Carlo results[4] for the anisotropic 2D $S = 1/2$ Heisenberg model have shown that it develops an ordered low-temperature phase even for very small anisotropies $\Delta \sim 10^{-3}, 10^{-2}$. The latter gives strong evidence of large values of a critical anisotropy is an artifact of the real-space renormalization approach.

At this point, it is worthwhile to compare our results with those from RGRS calculations

for antiferromagnetic AH model of $S = 1/2$ on a square lattice. These RSRG analysises lead to non-equivalence between the criticality of the ferromagnetic (F) and antiferromagnetic (AF) models, a reentrant behavior in the (T, Δ) diagram[12,13].

It is well known that in classical spin models, such as as the Ising or classical Heisenberg models, on bipartite lattices the critical temperature is the same for ferromagnetic exchange (Curie temperature) as for antiferromagnetic exchange (Neel temperature). This is a direct consequence of the free energy being an even function of the exchange parameter. However, for the quantum spin 1/2 Heisenberg model the Curie and Neel temperatures are unequal[23]. Recently, this question has been reinvestigated using high-temperature series expansions for the spin 1/2, 1 and 3/2 Heisenberg ferromagnet and antiferromagnet in 3-dimensions[24]. The difference between the temperatures decreases rapidly with increasing spin S. In some quantum systems, such as the quantum spin 1/2 XY and transverse Ising models, an isomorphism between the criticality of the F and AF cases is observed[25]. Critical properties of the quantum spin-1/2 2D Heisenberg model with anisotropic interaction treated by the Green's function technique yields $T_c = T_N$ for all values of the anisotropy parameter[26,27]. RSRG methods give contradictory results of the problem because of underlying approximations whose effects are hard to control in a systematic way. In Refs.[12,13] it was obtained by RG approach $T_N < T_c$ for 2D anisotropic Heisenberg limit $0 \leq \Delta < 1$ due to a special choice of the hierarchical lattice approximating a square one. The critical temperature T_c for 2D ferromagnetic spin 1/2 anisotropic Heisenberg model tends gradually to zero when decreasing the anisotropy parameter Δ, i.e. $T_c = 0$ in the isotropic Heisenberg limit $\Delta = 0$ in accordance with Mermin-Wagner theorem[28]. The results for the antiferromagnetic exchange are very similar to the $S = 1/2$ case, there is no long-range Néel order for the anisotropy parameter $\Delta < \Delta_c$. The question is not yet settled and more work is needed to put these

points on firmer grounds.

An observation of reentrance behavior for the spin 1/2 antiferromagnetic AH model on the square lattice has been reported by some authors[12,13]. This result suggests that there is an ordered phase at relatively high temperature but not at very low temperature. A full understanding of this phenomena is still lacking, but it's most likely the reentrance behavior is an artifact of the RGRS method. In Refs.[29] the authors attribute the reentrance to the effect of finite size in the renormalization and for larger clusters it should be absent.

In conclusion, the real-space renormalization group is employed to study the anisotropic Heisenberg model of spin $S = 1$ on a honeycomb lattice with two kinds of antiferromagnetic couplings. We calculate dependencies of the critical temperature on the parameters of the magnetic anisotropy, and on the ratio of interchain and intrachain exchange interactions. The entire critical line is found to belong to the universality class of the Ising model. In accordance with the early RSRG predictions for the antiferromagnetic AH model of spin $S = 1/2$ on a square lattice our calculations recover an existence of large finite critical anisotropy Δ_c that should be considered, however, as an artifact of the real-space renormalization technique.

Acknowledgments

We would like to thank Prof. M. V. Sadovskii for discussions. We acknowledges partial financial support from the grant NREC-005 of US CRDF (Civilian Research & Development Foundation).

Appendix A

The polarization matrices for the spin $S = 1$ has the explicit form

$$T_{00} = \frac{1}{3}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix},\ T_{11} = -\frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix},\ T_{1-1} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix},$$

$$T_{10} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix},\ T_{20} = \frac{1}{\sqrt{6}}\begin{pmatrix} 1 & 0 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & 1 \end{pmatrix},\ T_{21} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix},$$

$$T_{2-1} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix},\ T_{22} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},\ T_{2-2} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}.$$

Appendix B

We first take care of $H_{12}^{'}$ and express it in the basis $|M_1 M_2\rangle$. In this basis $H_{12}^{'}$ becomes

$$H_{12}^{'} = \begin{pmatrix} K_0^{'} + K_S & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & K_0^{'} & 0 & W_S & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & K_0^{'} - K_S & 0 & W_S & 0 & 0 & 0 & 0 \\ 0 & W_S & 0 & K_0^{'} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & W_S & 0 & K_0^{'} & 0 & W_S & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & K_0^{'} & 0 & W_S & 0 \\ 0 & 0 & 0 & 0 & W_S & 0 & K_0^{'} - K_S & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & W_S & 0 & K_0^{'} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & K_0^{'} + K_S \end{pmatrix}$$

where $W_S = K_S\,(1 - \Delta_S)$.

Performing the same calculation for H_{123}, now using the basis $|M_1 M_3 M_2\rangle$, we arrive at a 27×27 which has 4 independent blocks of size 9×9

$$H_{123} = \begin{pmatrix} A_1 & B_2 & 0 \\ B_1 & A_2 & B_2 \\ 0 & B_1 & A_3 \end{pmatrix},$$

where the 9×9 A_1, B_1, B_2, A_2 and A_3 are given by

$$A_1 = \begin{pmatrix} K_1 + K_2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & K_1 & 0 & W_2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & K_1 - K_2 & 0 & W_2 & 0 & 0 & 0 & 0 \\ 0 & W_2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & W_2 & 0 & 0 & 0 & W_2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & W_2 & 0 \\ 0 & 0 & 0 & 0 & W_2 & 0 & -K_1 - K_2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & W_2 & 0 & -K_1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -K_1 + K_2 \end{pmatrix},$$

$$A_2 = \begin{pmatrix} K_2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & W_2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -K_2 & 0 & W_2 & 0 & 0 & 0 & 0 \\ 0 & W_2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & W_2 & 0 & 0 & 0 & W_2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & W_2 & 0 \\ 0 & 0 & 0 & 0 & W_2 & 0 & -K_2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & W_2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & K_2 \end{pmatrix},$$

$$A_3 = \begin{pmatrix} -K_1 + K_2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -K_1 & 0 & W_2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -K_1 - K_2 & 0 & W_2 & 0 & 0 & 0 & 0 \\ 0 & W_2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & W_2 & 0 & 0 & 0 & W_2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & W_2 & 0 \\ 0 & 0 & 0 & 0 & W_2 & 0 & K_1 - K_2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & W_2 & 0 & K_1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & K_1 + K_2 \end{pmatrix},$$

$$B_2 = B_1^T = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ W_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & W_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & W_1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & W_1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & W_1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & W_1 & 0 & 0 & 0 \end{pmatrix},$$

where $W_1 = K_1\,(1 - \Delta_1)$ and $W_2 = K_2\,(1 - \Delta_2)$.

---

* Corresponding author.

[1] Y. Hosokoshi, Y. Nakazawa, K. Inoue, K. Takizawa, H. Nakano, M. Takahashi, and T. Goto, Phys. Rev. B **60**, 12924 (1999).

[2] T.L. Ho, S.K. Yip, Phys. Rev. Lett. **84**, 4031 (2000).

[3] S. Yip, J. Phys.: Condens. Matter **15**, 4583 (2003).

[4] A. Cuccoli, T. Roscilde, V. Tognetti, R. Vaia, P. Verrucchi, Phys. Rev. B **67**, 104414 (2003).

[5] H. Niggemann, A. Klumper, J. Zittartz, Z. Phys. B **104**, 103 (1997).

[6] Y. Hieida, K. Okanishi, Y. Akutsu, New J. Phys. **1**, 7 (1999).

[7] Th. Niemeijer and J.M.J. van Leeuwen, Phys. Rev. Lett. **31**, 1412 (1973).

[8] L.P.Kadanoff and A. Houghton, Phys. Rev. B **11**, 377 (1975).

[9] J. Rogiers, R. Dekeyser, Phys. Rev. B **13**, 4886 (1976).

[10] A.L. Stella and F. Toigo, Phys. Rev. B **17**, 2343 (1978).

[11] R.C. Brower, F. Kuttner, M. Nauenberg, and K. Subbarao, Phys. Rev. Lett. **38**, 1231 (1977).

[12] A.M.C. de Souza, Phys. Rev. B **48**, 3744 (1993).

[13] N.S. Branco and J.R. de Sousa, Phys. Rev. B, **62** 5742 (2000).

[14] J. Sznajd, Phys. Rev. B, **63** 184404 (2001).

[15] M. Suzuki and H. Takano, Phys. Lett. A 69, 426 (1979); H. Takano and M. Suzuki, J. Stat. Phys. 26, 635 (1981).

[16] A.M. Mariz, C. Tsallis, and A.O. Caride, J. Phys. C: Solid State Phys. **18**, 4189 (1985).

[17] A.A. Migdal, Zh. Eksper. Teoret. Fiz. **69**, 810, 1457 (1975) [Sov. Phys., JETP **42**, 413, 743 (1975)].

[18] L.P. Kadanoff, Ann. Phys. **100**, 359 (1976).

[19] D.A. Varshalovich, A.N. Moskalev, V.K. Khersonskii, *Quantum theory of angular momentum* (World Scientific, 1988).

[20] W.H. Press, B.P. Flammery, S.A. Teukolsky, W.T. Vetterling, *Numerical Recipies in C: The Art of Scientific Computing* (Cambridge University Press, 1992).

[21] H.-Q. Ding, J. Phys.: Condens. Matter **2**, 7979 (1990).

[22] S.S. Aplesnin, Phys. Solid State **207**, 491 (1998).

[23] G. S.Rushbrooke and P. J. Wood, Mol. Phys. **6**, 409 (1963).

[24] J. Oitmaa, W. Zheng, J. Phys.: Condens. Matter **16** 8653 (2004).

[25] J. R. de Souza and I.G. Araujo, J. Mag. Mag. Mat. **202**, 231 (1999).

[26] R.P. Singh, Z.C. Tao, M. Singh, Phys. Rev. B **46**, 1244 (1992).

[27] B.G. Liu, Phys. Rev. B **41**, 9563 (1990).

[28] N.D. Mermin, H.Wagner, Phys. Rev. Lett. **17**, 1133 (1966).

[29] J. R. de Souza and I.G. Araujo, Phys. Lett. A **272**, 333 (2000).

Рис. 1: The magnetic model for F_2PNNNO. (a) Uniform chains with intramolecular ferromagnetic coupling (J_F) and intrachain antiferromagnetic coupling (J_{AF}). The chains interact antiferromagnetically (J'_{AF}). (b) The extreme limit of the model when $J_F \to \infty$: antiferromagnetic honeycomb lattice with $S = 1$.

Рис. 2: Two-terminal graph used for renormalization purposes.

Рис. 4: Néel temperature T_N vs Δ phase diagram for different values of the $C_1 = J'_{AF}/J_{AF}$ ratio: 1.0 (1); 0.5 (2); 0.3 (3). The region above (below) the critical line represents disordered (ordered) phase. The dotted lines are guides-to-the-eyes.

Рис. 5: Phase diagram T_N vs Δ for small T_N near Δ_c: $C_1 = 1.0$ and $\Delta_c \simeq 0.46$ (a), $C_1 = 0.5$ and $\Delta_c \simeq 0.62$ (b), $C_1 = 0.3$ and $\Delta_c \simeq 0.76$ (c).

Рис. 3: Critical inverse temperature (K_c) vs $C_1 = J'_{AF}/J_{AF}$ found from the RG recursion relations for different anisotropy: $\Delta = 1.0$ (1), $\Delta = 0.8$ (2), $\Delta = 0.6$ (3).