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A NEW APPROACH TO QUANTUM ANTIFERROMAGNETS

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Last years, motivated by a possible link with the electronic models of the new copper oxide superconductors, two-dimensional quantum antiferromagnetic models have been studied extensively by different analytical and numerical techniques [1, 2]. As a result a good understanding of the Heisenberg model with the nearest-neighbor couplings on a square lattice has been reached. Many authors have demonstrated how precise analytical estimates of the ground-state characteristics of this model even for $S = 1/2$ can be obtained by the conventional spin-wave theory (SWT). The so-called third-order SWT results for the ground-state energy [3], [4], magnetization [3], spin-wave velocity [5], spin-stiffness constant [6], and transverse susceptibility [3] coincide very well with the most precise Green-function Monte Carlo and series expansion estimates.

However, spin-wave expansions (or 1/S expansions) turned out not to be well-behaved series for other models. For example, the big $O(1/S)$ correction to the magnetization of the spin -1/2 $J_1 - J_2$ model, obtained in [7, 8, 9], discredits the predictions of the SWT for this model. A simple analysis [4] shows that in the case of the frustrated $J_1 - J_2$ model the interaction operator of the SWT contains a quadratic part, which vanishes in the limit of the Heisenberg model with the nearest-neighbor couplings ($J_2 = 0$). Moreover, it can be easily proven that just the quadratic part causes the large $O(1/S)$ correction to the magnetization of the frustrated system. Therefore it is natural to try to eliminate this essential part of the interaction. In the $J_1 - J_2$ model the quadratic term has been eliminated [10] by the procedure known as the Bogoliubov principle of excluding the dangerous diagrams [11]. Then, treating the residual spin-wave interaction as a perturbation, a very efficient scheme for the evaluation of the ground-state characteristics of this frustrated model has been constructed [10].

A quadratic term exists in the interaction operator of SWT for many antiferromagnetic models. The Bogoliubov principle can be applied in these cases as well and thus some new general approach to the ground state of the quantum antiferromagnets can be proposed. The basic steps of such a type of approach for the ordered antiferromagnets are presented in this communication. The Hamiltonians we will consider have the form

$$H = \sum_{<ij>} J_{ij} \left[S_i^z S_j^z + \alpha \left(S_i^x S_j^x + S_i^y S_j^y \right) \right] \qquad (1)$$

where the sum runs over the interacting pairs of spins on a square or cubic lattice and α is the exchange-anisotropy parameter, $0 \leq \alpha \leq 1$.

1. *Bosonic representation.* To deal with Hamiltonian (1), we use the Dyson-Maleev (DM) formalism. In the case of Neel or stripe ordering (only these situations will be considered in the present work) the system (1) can be regarded as a two-sublattice model, where A (B) sublattice contains the spins up (down). Then by standard manipulations we convert Hamiltonian (1) into the following DM Hamiltonian

$$H_{DM} = W_0 + H_0 + H_2 + H_4 \qquad (2)$$

where W_0 is a constant; H_0 is a diagonal quadratic term:

$$H_0 = \sum_k A_k (a_k^+ a_k + b_k^+ b_k); \qquad (3)$$

H_2 is a nondiagonal quadratic term:

$$H_2 = \sum_k B_k (a_k^+ b_k^+ + a_k b_k), \qquad (4)$$

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and the quartic part H_4 can be written as:

$$H_4 = \sum_{(1234)} \Delta(1-2-3+4) \left(\Gamma_1 a_1^+ a_2 b_3^+ b_4 + \Gamma_2 a_1^+ a_2 a_3 b_4 + \Gamma_3 a_1^+ b_2^+ b_3^+ b_4 \right) \qquad (5)$$

where Δ is the Kronecker symbol and the wave-vectors k_i run over the sublattice Brillouin zone.

2. *Canonical transformation.* Next we perform the $u-v$ transformation in a form, taken from the SWT , namely:

$$a_k = u_k \alpha_k - v_k \beta_k^+, \quad b_k = u_k \beta_k - v_k \alpha_k^+. \qquad (6)$$

In the SWT this transformation has been employed to diagonalize the quadratic part $H_0 + H_2$ of the Hamiltonian [see (3) and (4)]. This part is proportional to S and it dominates in the systems with large spins [$H_4 \sim O(1)$] . In quantum systems,however, an essential quadratic part is possible to appear from the H_4 term after performing the transformation (6). Indeed , replacing in Eq.(2) the bare operators a_k and b_k by the operators α_k and β_k one may obtain the Hamiltonian in a form similar to that in Eq.(2). Then we impose the basic condition of the Bogoliubov principle of excluding the dangerous diagrams:

$$\langle 0 \mid H_{DM} \mid 2 \rangle = 0, \quad \mid 2 \rangle = \alpha_k^+ \beta_k^+ \mid 0 \rangle.$$

This brings us to the following equations for u_k and v_k :

$$u_k^2 - v_k^2 = 1, \quad Q_k(u_k, v_k) = 0 \qquad (7)$$

where Q_k is the coefficient in the nondiagonal quadratic part of the transformed Hamiltonian.

Having the solution of Eq.(7) the DM Hamiltonian can be written in the form:

$$H_{DM} = W + h_0 + V \qquad (8)$$

where W is a constant;

$$h_0 = \sum_k E_k \left(\alpha_k^+ \alpha_k + \beta_k^+ \beta_k \right) \qquad (9)$$

represents an ideal gas of quasiparticles, and the interaction is expressed by the following normal-ordered operator:

$$V = \sum_{(1234)} \Delta(1+2-3-4)[\phi^{(1)} \alpha_1 \alpha_2 \beta_3 \beta_4 + \phi^{(2)} \alpha_3^+ \alpha_4^+ \beta_1^+ \beta_2^+ + \phi^{(3)} \alpha_3^+ \alpha_1 \alpha_2 \beta_4 +$$
$$+ \phi^{(4)} \alpha_4^+ \beta_1^+ \beta_2^+ \beta_3 + \phi^{(5)} \beta_2^+ \beta_3 \beta_4 \alpha_1 + \phi^{(6)} \alpha_3^+ \alpha_4^+ \beta_1^+ \alpha_2 +$$
$$+ \phi^{(7)} \beta_1^+ \beta_2^+ \beta_3 \beta_4 + \phi^{(8)} \alpha_3^+ \alpha_4^+ \alpha_1 \alpha_2 + \phi^{(9)} \alpha_4^+ \alpha_3 \beta_1^+ \beta_3]. \qquad (10)$$

3. *Self-consistent equations.* The Hamiltonian can be written in the form Eq.(8) only if a solution of the equations (7) exists. These self-consistent equations reduce to equations for a few scalar quantities. For example, in the case of the stripe order of the $J_1 - J_2$ model the relations for two scalars read:

$$a = \frac{Z_2}{Z_1}, \quad b = \frac{Z_3}{Z_1} \qquad (11)$$

where

$$Z_1 = S - R_1 + R_2, \quad Z_2 = S - R_1 + R_3, \quad Z_3 = S - R_1 + R_4.$$

The quantities R_i are defined as

$$R_1 = \frac{2}{N}\sum_k v_k^2, \quad R_2 = \frac{2}{N}\sum_k v_k^2 \cos k_x,$$

$$R_3 = \frac{2}{N}\sum_k \eta_k u_k v_k, \quad R_4 = \frac{2}{N}\sum_k u_k v_k \cos k_y,$$

$$\eta_k = \cos k_x \cos k_y, \quad u_k = \sqrt{\frac{1+\epsilon_k}{2\epsilon_k}}, \quad v_k = \mathrm{sign}(C_k)\sqrt{\frac{1-\epsilon_k}{2\epsilon_k}},$$

$$\epsilon_k = \sqrt{1 - \frac{C_k^2}{D_k^2}}, \quad C_k = b\cos k_y + 2a\nu\eta_k, \quad D_k = b - 1 + \cos k_x + 2a\nu, \quad \nu = \frac{J_2}{J_1}. \qquad (12)$$

It can be shown that the quasiparticle energy is given by the expression $E_k = 2Z_1\sqrt{D_k^2 - C_k^2}$. Therefore the parameters a and b are nothing but renormalization parameters for the spin-wave spectrum E_k. In the classical limit we have $a = 1$ and $b = 1$. These values correspond to the SWT formulas. In some cases (nearly isotropic spin chain, quasi-one-dimensional antiferromagnet) there is not a solution of the self-consistent equations. Hence, in these systems H_2 cannot be eliminated by the transformation (6). Other methods, maybe nonperturbative, or another type of transformation should be employed for investigation of H_{DM} in these cases.

The solution of the self-consistent equations can be found numerically. In a number of systems the obtained parameter values differ significantly from the SWT ones. This had to be expected because an essential part of the interaction between SWT magnons is incorporated into the zero-order Hamiltonian h_0 considered here.

4. *The zero-order theory.* The Hamiltonian H_{DM} can be treated employing perturbation theory, the residual spin-wave interaction V being the perturbation. The quadratic part h_0 [see Eq.(9)] describes a gas of noninteracting spin waves. The magnetization of such a noninteracting gas is expressed as

$$m_0 = S - R_1. \qquad (13)$$

The zero-order value of the ground-state energy E_0 is given by the constant term W in (8). For the collinear phase of the $J_1 - J_2$ model we have

$$E_0 = N\,(\,Z_1^2 - Z_3^2 - 2\nu Z_2^2).$$

It is easy to obtain formulas for the other ground-state characteristics as well.

In isotropic systems, frustrated or nonfrustrated, the description based on h_0, turns out to be equivalent to the description of ordered phases, obtained earlier by Takahashi's modified spin-wave theory (MSWT) [12, 13] and Schwinger-boson mean-field theory(SBMFT) [14, 15, 16]. The predictions of these theories are close to the most precise numerical estimates. In strongly anisotropic systems our zero-order theory yields the exact results for the energy, magnetization and susceptibility, known from the series

expansions above the Ising limit. Therefore, the Hamiltonian h_0 might be regarded as a good starting point for perturbation-type calculations.

5. *Corrections caused by the residual spin-wave interaction.* Treating the interaction term V by the second-order perturbation theory one can obtain the first nonvanishing corrections to energy, magnetization and other characteristics (there are no $O(V)$ corrections). The correction to the ground-state energy has a form:

$$\Delta E = -4\sum_{(1234)} \Delta(1+2\doteq 3-4)\,\frac{\phi^{(1)}(1234)\phi^{(2)}(3412)}{E_1+E_2+E_3+E_4}. \qquad (14)$$

The correction to the magnetization has a more complicated structure similar to that of the $O(1/S)$ correction in the nearest-neighbor Heisenberg model.

The numerical evaluation of the six-dimensional integrals involved in these formulas is by no means a simple task, especially in the case of isotropic systems. In this case the integrands have a discontinuity at the points where one or more $k_i = 0$. These singularities reflect the well-known singular behavior of the $u_k - v_k$ transformation at $k = 0$. A correct treatment of the Umklapp processes is also needed in these calculations.

The corrections ΔE and Δm have been evaluated by the method used previously in our paper[4] for the calculation of the $O(1/S^2)$ correction to the ground-state energy of the Heisenberg model. We have obtained small ΔE and Δm in the $J_1 - J_2$ [10], $J_1 - J_2 - J_3$, XXZ and spatially anisotropic models. The results for the last models will be published elsewhere. The obtained small corrections show that the effects caused by the residual spin-wave interaction in these systems can be evaluated successfully in the framework of a finite-order perturbation theory. It should be noticed that in some cases the small corrections change qualitatively the zero-order results. For example, in the second-order approximation we have found for the spin-1/2 $J_1 - J_2$ model[10] a narrow window between the Neel and collinear phases instead of the MSWT overlap.

To conclude, the basic steps of the new approach to quantum antiferromagnets have been presented. By a canonical transformation we have eliminated the quadratic part of the interaction operator. Treating the residual spin-wave interaction as a perturbation we have calculated the second-order corrections to the energy and magnetization and showed the efficiency of the proposed theory for a number of two-dimensional antiferromagnetic models. Our approach resembles the oscillator representation method developed lately by Efimov and co-workers[17] for the polaron problem, anharmonic oscillator and some field models.

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References

[1] E. Manousakis, Rev. Mod. Phys., **63**, 1 (1991).

[2] T. Barness, Int. J. Mod. Phys. C **2**, 659 (1991).

[3] C. Hamer, Z. Weihong and P. Arndt, Phys. Rev. B **46**, 6276 (1992); Z. Weihong and C. Hamer, *ibid.* **47**, 7961 (1993).

[4] I. Gochev, Phys. Rev. B **47**, 1096 (1993).

[5] C. Canali and S. Girvin, Phys. Rev. B **45**, 7127 (1992).

[6] J. Igarashi and A. Watabe, Phys. Rev. B **43**, 13456 (1991).

[7] S. Chakravarty, B. Halperin and D. Nelson, Phys. Rev. B **39**, 2344 (1989).

[8] H. Xu and C. Ting, Phys. Rev. B **42**, 6861 (1990).

[9] Q. Zhong and S. Sorella, Europhys. Lett. **21**, 355 (1992).

[10] I. Gochev, Phys. Rev. B **49**, 9594 (1994).

[11] V. Tolmachev, *Theory of Bose gas*, "Nauka" , M., (1965) (in Russian).

[12] M. Takahashi, Phys. Rev. Lett., **58**, 168 (1987).

[13] A. Barabanov and O. Starykh, Pis'ma Zh.Eksp.Teor.Fiz., **51**, 271 (1990).

[14] D. Arovas and A. Auerbach, Phys. Rev. B **38**, 316 (1988).

[15] F. Mila, D. Poilblanc and C. Bruder, Phys. Rev. B **43**, 7891 (1991).

[16] H. Ceccatto, C. Gazza and A. Trumper, Phys. Rev. B **45**, 7832 (1992).

[17] G. Efimov and G. Gandbold, Phys. Stat. Sol.(b), **168**, 165 (1991);
M. Dineykhan and G. Efimov, Preprint JINR E4-94-75, Dubna (1994).

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