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A novel approach to antiferromagnetism in low dimensional systems

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Abstract We develop a theory for antiferromagnetism which is asymptotically exact in the limit of high correlation. A trial ground state wave function is obtained through a bosonization of the Heisenberg Hamiltonian in the axial-anisotropy region. This state is represented as a quantum coherent state displaying long-range order. Quantities of physical interest are calculated in closed analytic form and compared with exact results or numerical simulations, showing an excellent agreement in a wide range of variation of the anisotropy parameter. We discuss the limitations of our theory near the isotropic point

1. Introduction

An insulating antiferromagnetic phase is present in the reference compounds of most copper oxides which become high temperature superconductors[1]. This fact has brought a renewed interest in the study of low dimensional antiferromagnetic systems, in part due to the belief that the mecbanism for superconductivity is of magnetic origin. As a prototype of most copper oxides, La_2CuO_4 is a likely candidate for two dimensional antiferromagnetism due to its lamellar structure'. Doping the above compound with Sr or Ba leads to superconductivity. A fundamental step for understanding the physics of these compounds, is, then, a reliable description of the highly correlated insulating phase.

The antiferromagnetic insulating regime is modeled by a half filled band Hubbard Hamiltonian which, in the highly correlated limit, is equivalent to a Heisenberg Hamiltonian for spin $s=1/2$[2]. In this sense, it is desirable to develop an

analytic theory for antiferromagnetism, even in an approximate form, for handling problems where magnetism is just one among several interactions[3]. In this paper, we would like to present one of such attempt, where an approximate analytic solution for the anisotropic Heisenberg model is proposed. Our solution is simple, can be given in closed analytic form and is asymptotically exact in the limit of high anisotropy[3]. I applies to arbitrary dimension in bipartite lattices and the accuracy of the method increases with the coordination number, i.e. with the dirnension of the systern. In this sense, the one-dimensional case is the most serious test of our theory. We will show, however, that even in this latter case, excellent agreement is found with known exact results and numerical simulations[4].

Concerning the antiferromagnetic phase of La_2CuO_4, a substantial reduction of the expected magnetic moment is observed[5]. Magnetism in this compound is ascribed to Cu^{+2} ions, and the saturated moment is estimated as being $-$ 0.4 Bohr magnetons *per* copper atom, at low temperatures, i.e. less than half the value of the free ion. A two-fold explanation of this effect can be given. It is well known that quantum fluctuations are specially important in low dimensional systems. They account for the absence of long-range order for the one-dirnensional isotropic Heisenberg chain at zero temperature. On the other hand, covalent effects may be present in copper oxides, due to the peculiar structure of Cu-O planes. In this case, part of the mornent may be of itinerant character. We will comment on this effect further, at the end of this work.

In this paper we will rnainly deal with quantum fluctuations in low dimensional systems and the departure point is the highly correlated insulating phase.

2. The trial ground state

The one-dimensional case will be worked out in some detail as an instrucive example. The following Heisenberg-Ising Hamiltonian will be studied:

$$H = J \sum_m [S_z(m)S_z(m+1) + \alpha\{S_x(m)S_z(m+1) + S_y(m)S_y(m+1)\}], \qquad (1)$$

with periodic boundary conditions. In (1), exchange constant J is positive, and $S_x(m), S_y(m)$, and $S_z(m)$ are the spin operators for s=1/2 at site m. This Hamiltonian is said to represent the so called XXZ model, with the axial-anisotropic region confined to the interval $0 < a < 1$. For the Ising limit ($a = 0$), the ground state is of Néel type and switching the transverse part of Hamiltonian (1) may be visualed as a disordering process, where pairs of neighboring spins are simultaneously flipped, the ground state being a quantum.superposition of components contained in the manifold of total $S_z = 0$. This effect has been systematically observed in numerical simulations for Heisenberg chains (see the work by Medeiros and Cabrera in this same issue) and has been the heuristic base for the construction of our approximate solution.

One has to choose one of the two possible Néel states as a reference state. Both are connected by the time inversion operator, the ground state of the infinite chain being a doublet in the anisotropic region. For our developments here, we will choose the Néel state $|N>$, where eigenvalues of $S_z(m)$ operators are $\frac{1}{2}(-1)^m$. With the usual definition of spin ladder operators, we define boson-like operators by:

$$\phi_e^+ = \sqrt{\frac{2}{N}} \left\{ \frac{1}{4}\alpha N + \sum_{m \text{ even}} S_+(m+1)S_-(m) \right\}, \tag{2a}$$

$$\phi_0^+ = \sqrt{\frac{2}{N}} \left\{ \frac{1}{4}\alpha N + \sum_{m \text{ odd}} S_+(m+1)S_-(m) \right\}, \tag{2b}$$

It is apparent that our treatment has a broken symmetry (and long-range order), since a similar construction can be realized with the other Néel state $S_z \to \frac{1}{2}(-1)^{m+1}$, interchanging the roles of operators (2a) and (2b). In the quasi-Ising limit, the ground state is close to $|N>$, and under this assumption we obtain the following algebra for the ϕ's:

$$[\phi_q, \phi_e^+] = [\phi_0, \phi_0^+] = 1, \quad [\phi_e.\phi_0] = [\phi_0, \phi_e^+] = 0, \tag{3}$$

which are boson-like commutation relations. Within the same approximation, and restricting ourselves to the manifold $S_z = 0$, the Heisenberg Hamiltonian (1) can

be written as a two-mode harmonic oscillator Hamiltonian[3] :

$$H = J(\phi_e^+ \phi_e + \phi_0^+ \phi_0) + E_g(\alpha), \tag{4}$$

where $E_g(\alpha)$ is the ground state energy (vacuum of the ϕ-bosons). In order to put forward our physical picture, we would like to represent our ground state, $|0>$ in terms of the Néel state $|N>$, which was our starting point. This can be done in closed analytic form, and after a little algebra one finds[3] :

$$|\phi>= \exp\left\{-\alpha\sqrt{\frac{N}{8}}(\phi_e^+ - \phi_e)\right\} \exp\left\{-\alpha\sqrt{\frac{N}{8}}(\phi_0^+ - \phi_0)\right\} |N>, \tag{5}$$

which can be recognized as a *quanturn mechanical coherent state*[6]. The structure of state (5) is extremely interesting: the action of ϕ-operators disorders somehow the Néel state $|N>$, and the resulting state is a quantum superposition with interference and resonating properties. However, this coherent wave packet displays long-range order, in spite of quantum fluctuations. As a net result, the magnetic moment is reduced from its saturation value, the reduction being dependent on the anisotropy parameter α. In our picture, weights for fluctuations over the Néel states increase as long as we proceed from the Ising region to the isotropic or Heisenberg point.

The advantages of our approach are several. Besides the ground state itself, closed analytic expressions can be obtained for the ground state energy, the staggered magnetization and correlation functions of any order. A theory for the excited states can also be worked out[3]. Most important is the fact that the treatment can be extended to arbitrary dimension, as long as the lattice is not frustrated for antiferromagnetic order of the Néel type[3]. The accuracy of our results increases with the coordination number and, correspondingly, with the dimension of the system. This is just a consequence of the fact that the antiferromagnetic ground state is closer to the Néel states the higher the dimensionality of the system.

3. Results

Once our trial state (5) is written out, closed analytic expressions can be obtained for the ground state energy and the staggered magnetization, calculated as the following mean values:

$$E_g = < H > = < \phi | H | 0 >, \tag{6}$$

and

$$M_s = 2| < 0 | S_z(r) | 0 > | \tag{7}$$

We quote below the closed results for the one dimensional case:

$$E_g = < H >_{1-d} = -\frac{NJ}{4}[J_0^2(2\alpha) + J_1^2(2\alpha) + 2\alpha J_1(2\alpha)], \tag{8a}$$

$$M_s = 2| < 0 | S_z(r) | 0 > |_{1-d} = J_0(2\alpha), \tag{8b}$$

and for two dimensions we get[4] :

$$E_g = < H >_{2-d} = -\frac{NJ}{2}[J_0^4(2\alpha/3) + J_0^2(2\alpha/3)J_1^2(2\alpha/3) + 2\alpha J_0^2,(2\alpha/3)J_1^2(2\alpha/3)], \tag{9a}$$

$$M_s = 2| < 0 | S_z(r) | 0 > |_{2-d} = J_0^2(2\alpha/3), \tag{9b}$$

where J_0 and J_1 are the corresponding Bessel functions of integer order. The above results are respectively shown in Fig. 1 and 2. In both cases we compare them with the linear spin-wave theory[7]. We also display available exact results for the one-dimensional case: exact values for the ground state energy of the anisotropic Hamiltonian obtained by Orbarch[8] using the Bethe *ansatz*[9] and the exact expression for the staggered magnetization obtained by Baxter[10]. For the two-dimensional case, no exact solutions are available, and we have to resort to numerical simulations. We have included in the figure extrapolated results obtained through Monte Carlo[11] and results from a Lanczos calculation for the 4 x 4 periodic finite lattice[4].

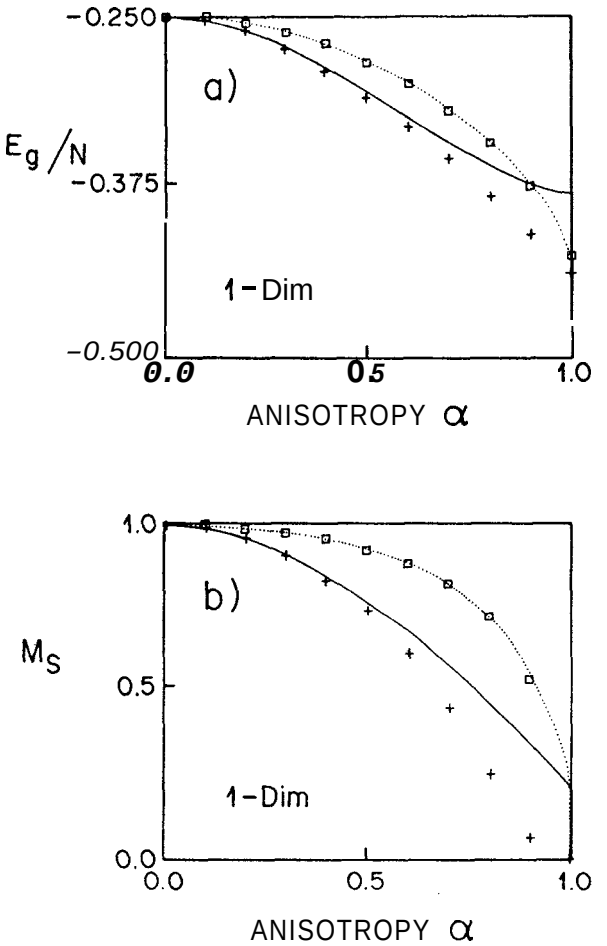

Fig. 1 - Ground state energy and the staggered magnetization for the one-dimensional case: In a) the ground state energy per spin (in units of J) is plotted as a function of anisotropy α. Our analytic result is shown by the continuous line, while exact results by Orbach[8] are shown with crosses. Squares are calculated within the linear spin-wave theory (dotted line is a guide for the eye). In b) e display the corresponding staggered magnetization, or long-range order parameter. Exact results (with crosses) are obtained from Baxter's formula[10].

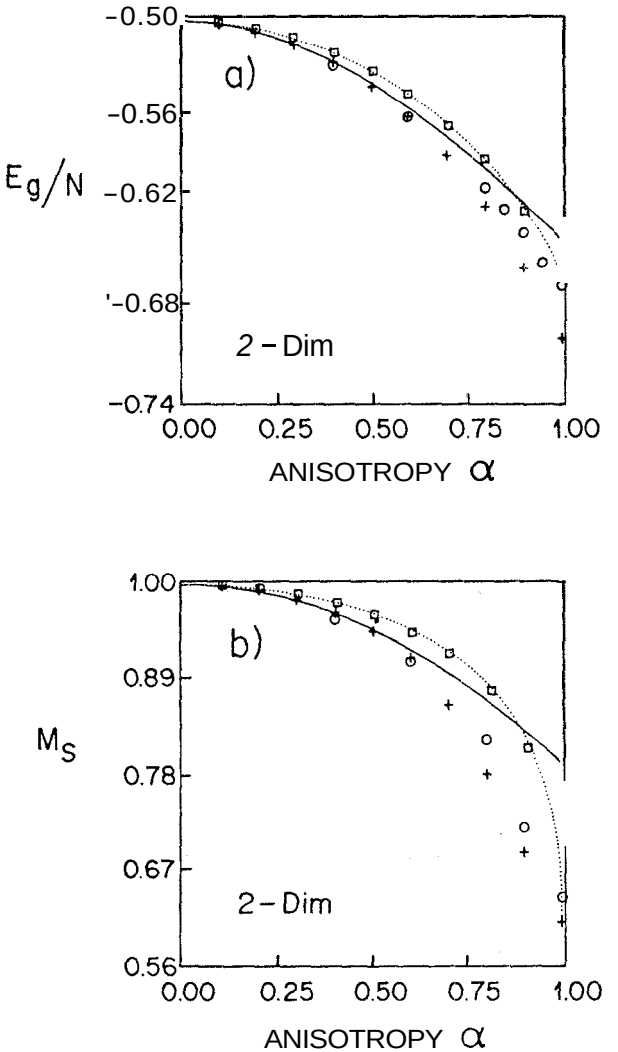

Fig. 2 - Same quantities shown in Fig. 1, now for the two-dimensional case: In a) and b), crosses display **exact numerical results using the Lanczos method for the 4 x 4 finite periodic lattice[4], and open circles show extrapolated results obtained via the Monte Carlo algorithm[11].**

A remarkable agreement with exact results or simulations is obtained in the strong anisotropy region, even for the one-dimensional case. Our solution is still a good approximation for fairly large values of the anisotropy parameter ($\alpha \sim 0.7$), in spite of the asymptotic character of our solution. This is a clear hint that the proposed structure of the ground state is essentially correct. Our constructive approach for the ground state has as a support the empirical observations made during our numerical simulations[12].

It is worth pointing out that a crossover with the linear spin wave theory occurs close to $a = 1.0$. Our localized picture and the linear spin wave approach are opposite approximations of the same phenomena. On physical grounds, we expect the localized approach to be a better description for the high anisotropic regime and a delocalization transition may occur when the anisotropy is reduced. This latter effect is related to excitations where a pair of distant spins is reversed as a direct process and not as a higher order term obtained by flipping severa1 pairs of nearest neighbors[13]. As a result, our theory overestimates long-range order at the isotropic point ($a = 1.0$), but its limitations give us the key for further improvement.

4. Conclusions

A trial approximate solution for the ground state of the anisotropic Heisenberg Hamiltonian with antiferromagnetic interactions has been put forward. Our solution is asymptotically exact, simple and can be given in closed analytic form. The physical picture that emerges from this formulation is very appealing, and derives from insights obtained in numerical simulations. Near the isotropic point, from the axial-anisotropic region, a crossover to delocalized spin excitations occurs, marking the regime where linear spin wave theory is a better approximation. Improvement of our theory may be obtained, if this latter effect is taken into account in our trial wave function. This point is currently under study[13].

As stated in the introduction, quantum fluctuations may account for the reduction of the magnetic moment of Cu^{+2} ions in copper oxide compounds. In doped samples, mobility of holes at sufficiently high concentration may blur the

antiferromagnetic order and appearance of superconductivity may imply the supression of antiferromagnetism. A different point of view can be given, if one models copper oxides compounds using an extended Hubbard model with repulsive interactions[14]. In this case, antíferromagnetism may be of itinerant nature, arising from band properties. Reduction of the magnetic moment from saturation is now ascribed to the different occupations of spin bands. Even in the insulator regime (half filled band), covalent effects induced by correlation of carriers may reduce the magnetic moment at the copper sites. We have recently found solutions of the above model, where superconductivity coexists with partial itinerant antiferromagnetism[14]. However, the latter is not a necessary condition for pairing and the superconductivity is completely suppressed when the magnetic moment saturates.

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Resumo

Desenvolvemos uma teoria do antiferromagnetismo assintóticamente exata no limite de alta correlação. Uma função de prova para o estado fundamental é obtida através de uma bosonização do Hamiltoniano de Heisenberg na região de anisotropia axial. Representamos este estado como um *estado quântico coerente* com ordem de longo alcance. As grandezas de interesse fisico são calculadas em forma analítica fechada, e comparadas com resultados exatos ou simulações numéricas, mostrando excelente acordo num extenso intervalo de variação do parâmetro de anisotropia. Discutimos as limitações da nossa teoria na vizinhança do ponto isotrópico.