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SPIN WAVE THEORY STUDIES OF FRUSTRATED HEISENBERG MODEL

Thesis submitted to the
International School for Advanced Studies
– Condensed Matter Sector–
for the degree of

Magister of Philosophiæ

CANDIDATE
Qingfeng ZHONG

SUPERVISOR
Dr. Sandro SORELLA

OCTOBER 1992

SISSA - SCUOLA
INTERNAZIONALE
SUPERIORE
STUDI AVANZATI
TRIESTE
Strada Costiera 11

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Contents

1 Introduction

The discovery of copper-oxide superconductors with critical temperatures as high as 120K[15] raised hopes that one day we may be able to manufacture materials that superconduct at room temperature. This discovery also raised doubts about the common belief that, due to the nature of the phonon-mediated electron-electron interaction[16], there are upper bounds on the critical temperatures much lower than those achieved with the copper oxide. In addition, the lack of a significant isotope effect with substitution of the oxygen sites seems to rule out the possibility that the phonon Debye frequency is the characteristic energy scale entering in the fundamental equations. Because of a number of peculiar properties of these materials, there is a growing suspicion that a different mechanism may be responsible for their superconductivity. Their phase diagram is rich because the superconducting phase occurs near a metal-insulator transition, an antiferromagnetic as well as a structural instability, and this fact has generated many ideas and proposals for new mechanisms. It is natural to imagine that such high temperatures and pairing energy scales may arise as the low-energy scales of the interacting electronic degrees of freedom in specific lattice structures of appropriate stoichiometry, where the lattice dynamics do not play the key role.

Anderson's original suggestion[17] that novel quantum spin fluctuations in the CuO_2 planes, common in all these materials, may be responsible for the superconductivity has received significant attention. Interesting magnetic properties revealed by neutron-scattering experiments provide further support for this idea. It was conjectured that such fluctuations might destroy the antiferromagnetic long-range order in the ground state, giving rise to a new state of the spin system, a quantum "spin-liquid" state[17]. The superconductivity in these materials was then conjectured to arise from the behavior of a novel quantum fluid of a highly correlated set of electronic degrees of freedom.

The Heisenberg Hamiltonian

$$H = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \tag{1}$$

is assumed to describe the antiferromagnetic undoped insulator La_2CuO_4 or the oxygen-deficient YBa_2CuO_6 or other undoped copper-oxide materials. Doping the insulator YBa_2CuO_6 to create, for example, $YBa_{2-x}Sr_xCuO_4$ introduces holes on the CuO_2 planes. Increasing the oxygen content in the YBa_2CuO_{6+x} controls the electron filling factor of the 2D CuO_2 planes in a less obvious way because of the presence of the CuO chains.

The Heisenberg Hamiltonian can be thought of as a simple and rather general model to describe the copper-oxide superexchange antiferromagnetic interaction [18] mediated by the intervening oxygen ions via virtual hopping processes involving double occupied Cu sites. The problem of quantum antiferromagnets is rather old and longstanding; however, a number of questions arose following the discovery of copper-oxide superconductors.

The doped CuO_2 planes in this rather simple formulation may be described by the t-J model where holes are introduced. But the t-J model is difficult and analytic investigations have to resort to limiting cases. Then, we studied as a first step the frustrated Heisenberg model instead of the t-J model, since we know that the ground state of frustrated Heisenberg model may be the novel quantum spin-liquid state[3][4].

The frustrated Heisenberg model is deviced to describe the competition between long-range order and the spin fluctuation.

$$H = \frac{1}{2} J_1 \sum_{R\eta_\mu} \mathbf{S}_R \cdot \mathbf{S}_{R+\eta_\mu} + \frac{1}{2} J_2 \sum_{R\delta_\mu} \mathbf{S}_R \cdot \mathbf{S}_{R+\delta_\mu} \tag{2}$$

where η_μ is the nearest neighbor vector and δ_μ is the next nearest neighbor vector and usual periodic boundary conditions are assumed.

Many questions remain still open especially in 2D and $S = \frac{1}{2}$ for this simple model. For example there is now a considerable amount of numerical work [1][2] in order to detect a first realization spin liquid state for large enough J_2. Linear spin-wave theory [3] and series expansion [4] have indeed predicted a possible transition for $J_2 > 0.38$. However on a rigorous ground very little is known.

More clear is the knowledge about the pure ($J_2 = 0$) Heisenberg model and in the follows we give a brief summary of what is known about the system.

One-dimensional antiferromagnetic spin chains described by the Hamiltonian (1) have a ground state with no long-range order. The ground-state energy of the spin-$\frac{1}{2}$ antiferromagnetic Heisenberg chains can be calculated exactly using the Bethe ansatz[19]. However, for chains of spins higher than $\frac{1}{2}$ there is no exact solution. The excitation spectrum of such spin chains may exhibit interesting properties. More specially, it follows from the Bethe ansatz that the correlation function decays following a power law, and it has been conjectured[20] that half-integer spin chains have a gapless excitation spectrum. For integer spin chains, however, there may be a finite gap, and the spin-correlation function decays exponentially with distance.

Beyond one dimension, the exact solution for the ground-state energy or wave function of the Hamiltonian on an infinite lattice is unknown. There are some rigorous proofs regarding the nature of the ground state, however. It has been shown that the ground state of the three-dimensional antiferromagnetic Heisenberg model for spin $S \geq 1$[21] and quite recently for $S = \frac{1}{2}$ is characterized[6][7][8] by antiferromagnetic long-range order. The long-range order disappears at some finite critical temperature in 3D. In two dimension, the Heisenberg model cannot exhibit long-range order for any spin at finite temperature[22]. The situation may be quite different for the ground state (T=0) of these models. It has been shown that antiferromagnetic long-range order exists in the ground state of the isotropic antiferromagnetic Heisenberg model on a square lattice[23] and on a hexagonal lattice[24] for any $S \geq 1$. So far, no rigorous proof is available for the existence or noexistence of antiferromagnetic long-range order in the ground state of the isotropic spin- $\frac{1}{2}$ antiferromagnetic Heisenberg model on a square lattice, which is the model of our interest.

Anderson[10] extended the spin-wave theory introduced by Holstein and Primakoff[25] for ferromagnets to the study of the ground state of antiferromagnets with large spin S. Following Anderson, during the same year, Kubo[26] using the Holstein-Primakoff transformation and an expansion in powers of $\frac{1}{S}$, derived Anderson's results. The foundation of spin-wave theory is the assumption that antiferromagnetic long-range order exists in the ground state and that the amplitude of zero-point motion of quantum fluctuations about the classical Néel state is small. Initially, this approach was thought to be an expansion in powers of $\frac{1}{S}$. Since the role of quantum fluctuations becomes more important for small S, it is natural to question the speed of convergence of this approach for the smallest possible spin case, the spin-$\frac{1}{2}$ antiferromagnet.

In more recent years it was argued[27] that large-amplitude quantum fluctuations in the two dimension spin-$\frac{1}{2}$ case might give rise to a new state. It was speculated that such a state might be characterized by short-range order, in which a "spin liquid" could be formed; this state would be a superposition of states in which the spins are locally bonded to one another, forming a resonating valence bond state.

Nowadays extensive numerical and experimental results have lead to the conclusion that the 2D Heisenberg model displays long range antiferromagnetic order and that there is no evidence of any exotic behavior in the unfrustrated model.

Spin wave theory, which originally was presented as an approximate technique, is used extensively even in 2D Heisenberg model. The goal of the present thesis is to extend the spin wave theory to a frustrated system on a finite size lattice and try to see whether the spin liquid state is a physically acceptable state of nature.

In the section II, we will introduce the spin-wave theory in the infinite lattice. In section III, we will present a method for a systematic spin-wave expansion of the $J_1 - J_2$ Hamiltonian on a finite size. And finally in section IV, we will discuses the anisotropic Heisenberg model and see how long-range order can be destroyed without frustration.

2 The Spin-Wave Theory

Here we give some of the preliminaries and we define the problem to be studied. We consider an $L \times L$ square lattice of lattice spacing a and $N = L^2$ sites. The degrees of freedom are vector spin operators $\mathbf{S_r}$ attached to the site at $\mathbf{r}$ and obey the usual commutation relations

$$[S_r^\alpha, S_{r'}^\beta] = iS_r^\gamma \delta_{r,r'} \tag{3}$$

where the superscripts α, β, and γ stand for the x, y, and z components or any cyclic permutation of them. We consider periodic boundary conditions. (Notice that in our units $\hbar = 1$ and the lattice spacing $a = 1$.)

We wish to find the eigenstates and eigenvalues of Heisenberg Hamiltonian. Let $|S_r^z\rangle$ denote the eigenstates of the operator S_r^z with eigenvalue S_r^z. The Hilbert space in which the Hamiltonian operates is spanned by the basis

$$|\{S_r^z\}\rangle \equiv \prod_r |S_r^z\rangle \tag{4}$$

Since the Hamiltonian commutes with the operators of the total spin and the z component of the total spin, namely,

$$\begin{aligned} S^2_{tot} &\equiv |\sum_r S_r|^2 \\ S^z_{tot} &\equiv \sum_r S^z_r \end{aligned} \tag{5}$$

we may choose to work in a subspace with well-defined eigenvalues of S_{tot} and S^z_{tot}. Specially, Marshall[5] proved that the ground state of the antiferromagnetic Heisenberg model on a bipartite lattice is characterized by $S_{tot} = 0$.

In order to define the ground-state staggered magnetization, we add a field h to the Hamiltonian, which couples to the spins of the two sublattices differently,

$$H' = H + h\sum_r(-1)^{|r|}S^z_r \tag{6}$$

where $|r| \equiv x + y$ and x,y are the two components of the vector **r**. Then, we define

$$\begin{aligned} m^\dagger_z &\equiv \frac{1}{N}\sum_r(-1)^{|r|}S^z_r \\ m^\dagger &\equiv \lim_{h\to 0}\lim_{N\to\infty}\langle 0|m^\dagger_z|0\rangle \end{aligned} \tag{7}$$

Provided that we take the thermodynamic limit before we set the external sublattice field h to zero, if the ground-state expectation value $m^\dagger$ remains finite we shall say that the ground state is characterized by antiferromagnetic long-range order.

First, we introduce the Holstein-Primakoff transformation as implemented for antiferromagnets. An equivalent representation to the spin basis is obtained by labeling the basis states by the eigenvalues of the "spin-deviation" operator

$$n_r \equiv S - S^z_r \tag{8}$$

When the site **r** is on one sublattice, say A, and

$$n_r \equiv S + S^z_r \tag{9}$$

for a site $\mathbf{r}$ on the other sublattice B. In this representation the Hilbert space is spanned by

$$|\{n_r\}\rangle \equiv \prod_r |n_r\rangle \tag{10}$$

and eigenvalues of n_r are 0, 1, ..., 2S. A general state can be expressed as

$$|\psi\rangle = \sum_{\{n_r\}} C(\{n_r\})|\{n_r\}\rangle \tag{11}$$

The operator S^z is diagonal in this representation, while $S_r^\dagger$ and S_r^- when $\mathbf{r}$ is on the A sublattice have the following properties:

$$\begin{aligned} S_r^\dagger|n_r\rangle &= \sqrt{2S\left[1-\tfrac{n_r-1}{2S}\right]n_r}|n_r-1\rangle \\ S_r^-|n_r\rangle &= \sqrt{2S(n_r+1)\left[1-\tfrac{n_r}{2S}\right]}|n_r+1\rangle \end{aligned} \tag{12}$$

When the site r is on the B sublattice, the action of the above two operators is intercharged. It is a convenient bookkeeping device to introduce the operators

$$\begin{aligned} a_r^\dagger|n_r\rangle &\equiv \sqrt{n_r+1}|n_r+1\rangle \\ a_r|n_r\rangle &\equiv \sqrt{n_r}|n_r-1\rangle \end{aligned} \tag{13}$$

and similarly when $\mathbf{r}$ is on the B sublattice. The operators $a_r^\dagger$ and a_r obey the usual commutation relations for two-component system of bosons,

$$[a_r, a_{r'}^\dagger] = \delta_{r,r'} \tag{14}$$

$$[a_r, a_{r'}] = [a_r^\dagger, a_{r'}^\dagger] = 0$$

These equations can be obtained by applying the operators to a general state and using the definitions. We find

$$\begin{aligned} S_r^\dagger &= \sqrt{2S}f_s(n_r)a_r \\ S_r^- &= \sqrt{2S}a_r^\dagger f_s(n_r) \\ S_r^z &= S-n_r \\ n_r &= a_r^\dagger a_r \\ f_s(n_r) &= \sqrt{1-\tfrac{n_r}{2S}} \end{aligned} \tag{15}$$

for **r** on the A sublattice and

$$\begin{aligned} S_r^\dagger &= \sqrt{2S} a_r^\dagger f_s(n_r) \\ S_r^- &= \sqrt{2S} f_s(n_r) a_r \\ S_r^z &= -S + n_r \\ n_r &= a_r^\dagger a_r \end{aligned} \tag{16}$$

when **r** is on the B sublattice.

In the eqn. (13) the eigenvalue n_r is free to take any value from 0 to ∞ rather than from 0 to 2S. There is no discrepancy, since the sector of states with $0 \le n_r \le 2S$ will not be connected to states with $n_r \ge 2S$ because $|n_r = 2S\rangle$ is annihilated by $S_r^-(S_r^\dagger)$ when **r** is on A(B) sublattice:

$$S_r^- |n_r = 2S\rangle = 0 \tag{17}$$

The Hamiltonian can be expressed in terms of a and $a^\dagger$, operators using the expressions for S^z, $S^\dagger$, and S_-, and therefore the spin problem is transformed to an equivalent problem of interacting bosons:

$$\begin{aligned} H &= -NdJS^2 + 2dJS\sum_r n_r \\ &+ JS \sum_{\langle r,r'\rangle} [f_S(n_r) a_r f_S(n_{r'}) a_{r'} + a_r^\dagger f_S(n_r) a_{r'}^\dagger f_S(n_{r'})] \\ &- J \sum_{\langle r,r'\rangle} n_r n_{r'} \end{aligned} \tag{18}$$

The operator $f_S(n_r)$, if we allow n_r to take values from 0 to ∞, can be expanded as

$$f_S(n_r) = 1 - \frac{n_r}{4S} - \frac{n_r^2}{32S^2} - \cdots \tag{19}$$

We emphasize that if we truncate this expansion at any order, condition(17), which decouples the physical from the unphysical states, is no longer satisfied. If, on the other hand, we restrict ourselves in the physical subspace of 2S+1 dimensions, then this operator can be written as

$$f_S(n_r) = \sum_{m=0}^{2S} d_m(S) n_r^m \tag{20}$$

In the linear spin-wave approximation introduced by Anderson[10] for antiferromagnets, one retains in eqn. (18) terms up to quadratic in the boson operators. This means that $f_S(n_r)$ is approximated by 1 and the last term of eqn. (18) is neglected, i.e.,

$$H_{lsw} = -NdJS^2 + 2dJS\sum_r n_r + JS\sum_{\langle r,r'\rangle}(a_r a_{r'} + a_r^\dagger a_{r'}^\dagger) \tag{21}$$

This Hamiltonian connects the physical states with $0 \le n_r \le 2S$ with states having $n_r \ge 2S$. If the ground state expectation value of n_r is small compared to 2S, this approximation makes sense. This condition can be checked once the spectrum of H_{lsw} is found.

A quadratic Hamiltonian such as H_{lsw} can always be diagonalized. We introduce the Fourier transforms of these operators as

$$a_k = \sqrt{\frac{1}{N}}\sum_r e^{ik\cdot r} a_r \tag{22}$$

where the vectors k correspond to the reciprocal space of the sublattice A or B. We perform a canonical transformation to new operators α_k and $\alpha_k^\dagger$, which also obey boson commutation relations,

$$a_k = cosh\theta_k\alpha_k + sinh\theta_k\alpha_{-k}^\dagger \tag{23}$$

Substituting eqn. (23) in H_{lsw}, the function θ_k is determined so that the coefficient of $\alpha_k^\dagger\alpha_k^\dagger$ is zero. We obtain

$$tanh(2\theta_k) = \gamma_k \tag{24}$$

where

$$\gamma_k \equiv \frac{1}{d}\sum_\mu cos(k\cdot e_\mu) \tag{25}$$

where e_μ is the unit vector in the μ direction, and

$$H_{lsw} = E_0^0 + \sum_k 2\omega_0(k) n_k^\alpha \tag{26}$$

where

$$
\begin{aligned}
n_k^\alpha &= \alpha_k^\dagger \alpha_k \\
E_0^0 &= -dJSN(S+\xi) \\
\xi &\equiv \tfrac{2}{N}\sum_k [1-\sqrt{1-\gamma_k^2}] \\
\omega_0(k) &= 2dJS\sqrt{1-\gamma_k^2}
\end{aligned}
\tag{27}
$$

The ground state $|\psi_0\rangle$ is defined by the conditions $\alpha_k|\psi_0\rangle = 0$ for all k in the Brillouin zone. For square lattice, $\xi = 0.158$ and the ground state energy per site in the linear spin-wave approximation is -0.658.

Keeping terms up to $\frac{1}{S}$ in the expansion[11], we find that the diagonal terms of the Hamiltonian have the form

$$
H = E_0 + \sum_k \omega(k)[2(n_k^\alpha + n_{k_1}^\alpha n_{k_2}^\alpha) - 2(1+C_{12})n_{k_1}^\alpha n_{k_2}^\alpha] + \cdots \tag{28}
$$

where

$$
\begin{aligned}
E_0 &= -dJS^2N\left[1+\tfrac{\xi}{2S}\right]^2 \\
\omega(k) &= \omega_0(k)\left[1+\tfrac{\xi}{2S}\right] \\
C_{12} &\equiv \sqrt{1-\gamma_{k_1}^2}\sqrt{1-\gamma_{k_2}^2}
\end{aligned}
\tag{29}
$$

The ground state energy per site in this approximation for the spin- $\frac{1}{2}$ model on a square lattice is $\frac{E_0}{JN} = -0.6705$. Since the energy of the Néel state is -0.5 and in the linear spin-wave approximation is -0.658, and the next correction in the $\frac{1}{S}$ expansion is small, one might conclude that there is an apparent convergence in the case of the ground state energy. It is very different, however, to justify an expansion in powers of $\frac{n_r}{2S}$ and therefore the expansion parameter for $S = \frac{1}{2}$ is really the expectation value of n_r. That is to say, the ground state is in a linear superposition of state with very small amplitude for those with large n_r. Therefore the convergence of the expansion could be explained if

$$
\epsilon \equiv \frac{1}{N}\sum_k \langle n_k\rangle \ll 1 \tag{30}
$$

We obtain

$$\epsilon = \frac{1}{2N}\sum_k \left[\frac{1}{\sqrt{1-\gamma_k^2}} - 1\right] \tag{31}$$

and, for a square lattice, $\epsilon = 0.197$, which is a rather small number.

The energy of the elementary excitations is given by $\omega(k)$ and, in the long-wavelength limit $\omega(k \to 0) = ck$. We define

$$Z_c \equiv \frac{c}{c_0} \tag{32}$$

where c_0 is the "bare" spin-wave velocity obtained in the linear spin-wave approximation, namely, $c_0 \equiv \sqrt{2}Ja$. For the antiferromagnet on a square lattice in the above approximation the ratio $Z_c = 1 + \xi = 1.158$.

The ground state expectation value of the staggered magnetization operator for $S = \frac{1}{2}$ is obtained as

$$m^\dagger = \frac{1}{2} - \epsilon \tag{33}$$

and for a square lattice $m^\dagger = 0.3034$. Hence spin-wave theory predicts an ordered ground state with finite staggered magnetization approximately 61% of its classical value. In one dimension the integral diverges logarithmically due to the long-wavelength modes. This instability can be attributed to the fact that the ground state fails to develop long-range order in one dimension. The fact that the integral diverges also means that there is no small expansion parameter, and that the perturbative expansion around an ordered state is incorrect for spin chains.

We wish to add to the Hamiltonian a term of the form $H_\perp \sum_r S_r^x$. The perpendicular susceptibility is defined as $\chi_\perp \equiv \frac{\partial M_\perp}{\partial H_\perp}$, where $\langle M_\perp \rangle$ is the ground state expectation value of $\frac{1}{N}\sum_r S_r^x$. $\chi_\perp$ describes the response to an external magnetic field in a direction perpendicular to the staggered magnetization. We define

$$Z_\chi \equiv \frac{\chi_\perp}{\chi_{\perp,0}} \tag{34}$$

where $\chi_{\perp,0} \equiv \frac{1}{4dJ}$. Including the next correction in the $\frac{1}{S}$ expansion, we obtain the value $Z_\chi = 1 - \xi - 2\epsilon = 0.448$ for an isotropic spin-$\frac{1}{2}$ square lattice antiferromagnet.

3 The Spin-Wave Theory on Finite Size

Numerical methods on spin hamiltonians are generally limited to calculation of ground state correlation functions on a given *finite* lattice. Indeed in any finite size simulation the antiferromagnetic order parameter m is extracted by a systematic finite size study on a square lattice $N = L \times L$ of the spin-spin correlation function $C(R - R') =< \mathrm{S}_R \cdot \mathrm{S}'_R >$, i.e. :

$$m = \lim_{L\to\infty} \sqrt{\frac{1}{N} \sum_R (-1)^R C(R)}$$

. Despite the accuracy between the extrapolated order parameter m and the spin-wave prediction, the validity of SWT is still questionable in principle since the agreement is based on a single (or few) extrapolated quantities. For the above reasons it is important to apply spin-wave theory directly on finite size and compare exact data obtained by Lanczos or Monte Carlo with the SWT approximation.

Several attempts to generalize SWT on finite size have recently been published[12][13]. However, as it will became clear in the following, all these approaches are based on unnecessary approximations to avoid spurious finite size divergence for the $k = 0$ and $k = Q = (\pi, \pi)$ spin-wave modes. In these approaches these divergencies are removed by imposing an "ad hoc" holonomic constraint on the sublattice magnetization: it is set to zero (as it should) on any finite size.

In the present paper we derive a systematic spin wave expansion on a finite lattice and apply it to the J_1-J_2 model. We show here that the mentioned spin-wave divergencies ("Goldstone modes") do not affect spin rotation invariant quantities and a straightforward calculation of the spin-spin correlation function $C(R - R')$

is possible up to second order in $1/S$, fully consistent with the spin-wave theory expansion.

In order to simplify the derivation, we consider first the simpler case when $J_2 = 0$ and only the leading term in S. The classical state is the antiferromagnetic (Néel) state and we can use the following Holstein-Primakoff transformation:

$$\begin{aligned} S_i^\dagger &= \sqrt{2S}(1-\tfrac{n_i}{4S})a_i & \qquad S_j^\dagger &= \sqrt{2S}a_j^\dagger(1-\tfrac{n_j}{4S}) \\ S_i^z &= S - n_i & \qquad S_j^z &= n_j - S \end{aligned} \tag{35}$$

where a and $a^\dagger$ are canonical creation and destruction bose operators , and $n_i = a_i^\dagger a_i$ is the number of bosons at the site i. The indices i, j label lattice points R_i and R_j belonging to the two magnetic sublattices. After substituting these expressions in the hamiltonian, we can use translation invariance and write the leading term of the hamiltonian in terms of

$$a_k^\dagger = \frac{1}{\sqrt{N}}\sum_R e^{-ikR}a_R^\dagger$$

$$H = S^2 E_C + SH_{SW} + O(1)$$

$$E_C = -\frac{J_1 Z}{2}N$$

is the classical energy and H_{SW} reads:

$$H_{SW} = J_1 Z\sum_k[D_k a_k^\dagger a_k + \frac{1}{2}\eta_k(a_k^\dagger a_{-k}^\dagger + a_k a_{-k})] \tag{36}$$

Here $Z = 2d$ is the number of nearest neighbours, $\eta_k = \frac{\cos k_x + \cos k_y}{2}$, and the diagonal part in this particular case is constant $D_k = 1$. The leading part of the hamiltonian is free and can be generally diagonalized by the known Bogoliubov transformation which acts independently on any k wavevector:

$$a_k = u_k\alpha_k + v_k\alpha_{-k}^\dagger$$

with

$$u_k = \sqrt{\frac{D_k + \epsilon_k}{2\epsilon_k}}$$

$$v_k = -sgn(\eta_k)\sqrt{\frac{D_k - \epsilon_k}{2\epsilon_k}}$$

$$\epsilon_k = \sqrt{D_k^2 - \eta_k^2}$$

being the spin wave energy in unit of $J_1 ZS$. However the $k = 0$ and $k = Q$ modes, important at finite size, cannot be diagonalized by this transformation since u_k and v_k are not defined in this case. We can in fact define two hermitian operators that commute with the hamiltonian

$$Q_x = a_0^\dagger + a_0$$

$$Q_y = i(a_Q^\dagger - a_Q)$$

and write the singular $k = 0, Q$ contributions in (36) in the form:

$$H_S = \frac{J_1 SZ}{2}(D_0 Q_x^2 + D_Q Q_y^2 - D_0 - D_Q).$$

The physical meaning of these two operators becomes clear if we use the Holstein-Primakoff transformation for the total spin along the x (y) axis $S_{x(y)}^{Tot} = \sum_R S_R^{x(y)}$. Then at leading order $Q_x = S_x^{Tot}/\sqrt{\frac{S}{2N}}$ and $Q_y = S_y^{Tot}/\sqrt{\frac{S}{2N}}$ and the singular part of the hamiltonian

$$H_S \propto (S_x^{Tot})^2 + (S_y^{Tot})^2$$

represents a term which clearly favours the singlet ground state, in agreement with the Lieb-Mattis theorem[14].

Since Q_x and Q_y commute with the hamiltonian, and $[Q_x, Q_y] = 0$, we can formally diagonalize the hamiltonian *in a finite size* in a basis where Q_x and Q_y have definite quantum numbers. In the chosen basis Q_x and Q_y become classical numbers ranging continuously from $-\infty$ to ∞ and the hamiltonian H_S becomes a simple classical contribution. The ground state has then $Q_x = Q_y = 0$, i.e. it is a singlet (as it should on any finite size and for any S)[14] and can be formally written as the normalizable Fock state $|0>_\alpha$ of the operators α_k a_0 and a_Q projected onto the subspace of $Q_x = Q_y = 0$:

$$|\psi_{SW}> = \int_{-\infty}^{\infty} d\alpha \int_{-\infty}^{\infty} d\beta e^{i\alpha Q_x + i\beta Q_y} |0>_\alpha \quad (37)$$

This state is the formal ground state $|\psi_G>$ of H for $S \to \infty$ and includes usual spin-wave fluctuations on the Neél state $|N>$, i.e.

$$|0>_\alpha = \left(\prod_{k \neq 0,Q} \frac{e^{\frac{1}{2}\frac{v_k}{u_k} a_k^\dagger a_{-k}^\dagger}}{u_k} \right) |N>$$

. Unfortunately ψ_{SW} after projection on $Q_x = Q_y = 0$ is eigenstate of operators with continuous spectrum and, as it is easily seen from (37), it cannot be normalized. This singular behaviour is a consequence of the large S expansion, since at any finite S the Hilbert space is finite and any operator on a finite Hilbert space has a discrete spectrum. As a consequence for infinite S a Bose condensation of the $k = 0, Q$ modes occurs since the expectation value for the average number of modes

$$\frac{< \psi_{SW} | a_k^+ a_k | \psi_{SW} >}{< \psi_{SW} | \psi_{SW} >}$$

diverges for $k = 0$ or Q.

Nevertheless a systematic finite size study of *spin-rotation invariant quantities* as for example the ground state energy and the spin-spin correlation function $C(R-R')$ is indeed possible. For example the ground state energy derived in the previous example for $J_2 = 0$ is perfectly finite and well defined on any finite lattice. In fact, having in mind that $Q_x = Q_y = 0$, we get for the contribution to the energy linear in S -the spin wave term-:

$$< H_{SW} >= E_{SW} = \sum{}' \frac{J_1 Z}{2}(\epsilon_k - D_k) \; - \frac{J_1 Z}{2}(D_0 + D_Q)$$

where $\sum{}'$ means summation over all k but $k = 0, Q$ in the Broulluin zone. Note also the non vanishing negative term coming from the careful analysis of the singular contribution H_S. This term is negligible at infinite size but is important for any accurate estimate of the energy at finite size.

Let us consider now the general case with $J_2 > 0$.

In order to get the spin-spin correlation function $C(r)$, we add the following spin-rotation and translation invariant term to the Heisenberg Hamiltonian

$$H' = \frac{1}{2} J_1 h_r \sum_{R\tau_\mu} \mathbf{S}_R \cdot \mathbf{S}_{R+\tau_\mu}$$

where the vectors τ_μ are equivalent lattice vectors in any of the possible orthogonal directions with $|\tau_\mu| = |r|$. By use of the Helmann-Feynman theorem the spin-spin correlation function is obtained by differentiating with respect to h_r the ground state energy of the hamiltonian in presence of the external perturbation:

$$C(r) = \frac{2}{ZNJ_1} \frac{d}{dh_r} E_G(h_r).$$

In the following we describe in detail the calculation of the spin-spin correlation function on opposite sublattice. For $J_2 < 0.5$ th classical Néel state is still stable and we can use eq. (1). Then the hamiltonian can be expanded as:

$$H = S^2 E_C + S H_{SW} + H_{int} \tag{38}$$

where

$$E_C = -\frac{1}{2}(1 - \alpha - h_r)) J_1 N Z$$

H_{SW} is the leading free boson term in the expansion and has the same form as in (2) with

$$D_k = 1 - \alpha(1 - \delta_k) + h_r$$

$$\eta_k \rightarrow \eta_k + h_r \tau_k$$

$$\delta_k = \cos k_x \cos k_y$$

$$\tau_k = \frac{1}{Z}\sum_{\tau_\mu} e^{ik\tau_\mu}$$

and

$$\begin{aligned} H_{int} &= -\tfrac{1}{2N}J_1 Z \sum_{k_1k_2k_3k_4} \\ &\delta(k_1-k_2+k_3-k_4)(\eta_{k_1-k_2}-\alpha\delta_{k_1-k_2}+\beta\tau_{k_1-k_2})a^\dagger_{k_1}a_{k_2}a^\dagger_{k_3}a_{k_4} \\ &-\tfrac{1}{4N}J_1 Z \sum_{k_1k_2k_3k_4}[\delta(k_1-k_2-k_3-k_4)(\eta_{k_4}+\beta\tau_{k_4})a^\dagger_{k_1}a_{k_2}a_{k_3}a_{k_4} \\ &+\delta(k_1+k_2-k_3-k_4)\alpha\delta_{k_4}a^\dagger_{k_1}a^\dagger_{k_2}a_{k_3}a_{k_4}] + h.c \end{aligned} \tag{39}$$

where $\alpha = \frac{J_2}{J_1}$.

The next leading contribution to the energy is obtained by the evaluation of

$$E_{int} = \frac{<\psi_{SW}|H_{int}|\psi_{SW}>}{<\psi_{SW}|\psi_{SW}>}$$

$$E_{int} = -\frac{1}{2}J_1 Z\frac{N}{4}(C_\eta^2 + h_r C_\tau^2 - \alpha C_\delta'^2) + H_{fs} \tag{40}$$

where

$$C_\eta = \frac{2}{N}\sum_k{}'(V_k^2 + \eta_k U_k V_k)$$

$$C_\delta' = \frac{2}{N}\sum_k{}'(1-\delta_k)V_k^2$$

and C_τ is obtained substituting the function η_k with τ_k in the expression for C_η, while H_{fs} comes out after a careful treatment of the singular modes , yielding a finite size correction to the ground state energy:

$$H_{fs} = \frac{1}{2}J_1 Z(C_\eta + h_r C_\tau)$$

Differentiating

$$E_G = S^2E_C + SE_{SW} + E_{int}$$

with respect to h_r and letting $h_r = 0$, we can get the spin-spin correlation function between two sites on different sublattices

$$\langle \mathbf{S}_0\cdot\mathbf{S}_r\rangle = -(S - \frac{1}{2}C_\tau + \frac{1}{N})^2 + \frac{1}{N^2} - \frac{1}{2}\bar{C}_\eta\frac{\partial C_\eta}{\partial h_r} \tag{41}$$

where

$$C_\tau(r) = \frac{1}{N}\sum_k{}' \left\{ \frac{(1-\alpha+\alpha\delta_k) - \eta_k e^{ikr}}{[(1-\alpha+\alpha\delta_k)^2 - \eta_k^2]^{\frac{1}{2}}} - 1 \right\}$$

$$\bar{C}_\eta = C_\eta - C'_\delta$$

and

$$\frac{\partial C_\eta}{\partial h_r} = \alpha\frac{1}{N}\sum_k{}' \frac{[e^{ikr}(1-\alpha+\alpha\delta_k) - \eta_k]\eta_k(1-\delta_k)}{[(1-\alpha+\alpha\delta_k)^2 - \eta_k^2]^{\frac{3}{2}}}.$$

Similarly, we have the spin-spin correlation function between two sites on the same sublattice

$$\langle \mathrm{S}_0\mathrm{S}_r \rangle = (S - \frac{1}{2}C'_\tau)^2 - \frac{1}{2}\bar{C}_\eta\frac{\partial C'_\eta}{\partial h_r} \tag{42}$$

where

$$C'_\tau(r) = \frac{1}{N}\sum_k{}'(1-e^{ikr}) \left\{ \frac{(1-\alpha+\alpha\delta_k)}{[(1-\alpha+\alpha\delta_k)^2 - \eta_k^2]^{\frac{1}{2}}} - 1 \right\}$$

and

$$\frac{\partial C'_\eta}{\partial h_r} = \alpha\frac{1}{N}\sum_k{}'(1-e^{ikr})\frac{(1-\delta_k)\eta_k^2}{[(1-\alpha+\alpha\delta_k)^2 - \eta_k^2]^{\frac{3}{2}}}.$$

In the previous quantities the singular contributions of the $k = 0$,$k = Q$ modes cancel out at the end of the calculation after many non trivial simplifications and E_{int} is perfectly defined and finite quantity, as well as its derivatives with respect to the field h_r.

The above equations fulfil the sum rule $N\sum C(R) = 0$ order by order in $\frac{1}{S}$, consistent with a singlet ground state[14].

Thus we have finally obtained an ordered expansion of the spin spin correlation function:

$$C(R) = (-1)^R S^2 + \alpha(R)S + \beta(R).$$

The order parameter m can then be expanded in the following way:

$$m(L) = S + \hat{\alpha} + \hat{\beta}/S$$

with $\hat{\alpha}$ and $\hat{\beta}$ simply related to the functions $\alpha(R)$ and $\beta(R)$ on finite size:

$$2\hat{\alpha} = \frac{1}{N}\sum(-1)^R\alpha(R)$$

$$2\hat{\beta} = \left(\frac{\sum(-1)^R\beta(R)}{N} - \hat{\alpha}^2\right)$$

The ground state energy per site for $h_r = 0$ is given by:

$$E = \frac{J_1}{2}\sum_{\mu}[C(\eta_\mu) + \alpha C(\delta_\mu)]$$

From the path-integral representation of the partition function of the antiferromagnetic Heisenberg mode, we can pass to the continuum limit, where the quantum-mechanical nonlinear σ model in two space and one time dimension is obtained as a field-theoretical model that describes smooth spin fluctuations.

$$Z = \int[Dn]exp\left[-\frac{\rho_s}{2}\int_0^\beta d\tau d^dr(|\nabla n|^2 + c_0^{-2}|\partial_\tau n|^2)\right] \tag{43}$$

Then, the long wavelength behavior is determined by the spin wave stiffness ρ_s and the spin wave velocity c_0.

We calculate the first order correction to the ground state energy due to the finite size effect. We get

$$\Delta E = -\frac{J_1SZ}{4\pi N^{\frac{1}{2}}}c\left[\sqrt{2(1-2\alpha)} - \frac{1-\alpha}{S\sqrt{2(1-2\alpha)}}C_\eta(\infty) + \frac{\sqrt{2}\alpha}{S\sqrt{(1-2\alpha)}}C'_\delta(\infty)\right] \tag{44}$$

where $C_\eta(\infty)$, $C'_\delta(\infty)$ is the corresponding quantities calculated on the infinite lattice and

$$c = \frac{1}{2\pi}\sum_{m\neq 0}\frac{1}{|m|^3} = 1.438.$$

As pointing out by Fisher[28] and Ziman[29], it is proportion to the spin-wave velocity,

$$\Delta E = \frac{c_0}{\sqrt{N}}c \tag{45}$$

where c_0 is the spin-wave velocity. By compares rhs. of eqn. (44) and eqn. (45), we can get spin-wave velocity quite easily.

We also calculate the first order correlation to the square magnetization due to the finite size effect. We have

$$\Delta M^2 = \left(\frac{1}{2}M(\infty) - S\right)\sqrt{\frac{2}{(1-2\alpha)}}\frac{c'}{\sqrt{N}} - \frac{1}{2}\bar{C}_\eta(\infty)\alpha\left[\frac{1}{2(1-2\alpha)}\right]^{\frac{3}{2}}\frac{c'}{\sqrt{N}} \tag{46}$$

where $\bar{C}_\eta(\infty)$, $M(\infty)$ is the corresponding quantities calculated on the infinite lattice and

$$c' = -\frac{1}{\sqrt{N}}\sum_{m\neq 0}\frac{1}{|m|} = -0.6208.$$

Following Fisher[28] and Ziman[29], it is proportional to the spin-wave stiffness,

$$\Delta M^2 = \frac{z}{4\rho_s\sqrt{N}}c' \tag{47}$$

where ρ_s is the spin stiffness. By compares eqn. (46) and eqn. (47), we can get spin stiffness quite easily.

In order to compare our spin wave calculation, we have deviced a code to exactly diagonalize the Heisenberg model on small clusters by using Lanczos method.

We show in Tab.I a comparison of spin-wave results and exact data on finite systems obtained mainly with Quantum Monte Carlo. The accuracy of the spin wave theory is confirmed even for any finite and large size. The finite size order parameter is always slightly smaller than the spin-wave prediction (with exception of the 12×12 lattice where error bars are too large). Our results give therefore a strong support to the existence of long range order in the $S = \frac{1}{2}$ Heisenberg antiferromagnet, and that the ground state can be naturally represented by the Neél state dressed by small quantum fluctuations. The order parameter is very much close to the spin-wave predictions and in close agreement with the Monte Carlo estimate.

As we turn on J_2 the spin model is strongly frustrated and we expect the spin-wave expansion to be convergent or at least accurate in the region where the order parameter is the same as in the classical case ($S \to \infty$). With this technique we can therefore detect a possible spin liquid state by looking for a breakdown of the spin-wave expansion for large J_2. We show in Fig.1 the order parameter as predicted by spin-ave theory compared with the available exact results on a 4×4 and 6×6 lattice as a function of $\frac{J_2}{J_1}$. The agreement is very good for $\frac{J_2}{J_1} < 0.2$ and in fact the second order contribution seems already enough to give an accurate answer. The infinite size prediction plotted in the same picture should therefore be quite reliable in this region.

For J_2 large enough the second order term does not improve the first order estimate and we can define a crossover value of $J = J_C$ where the second order contribution becomes a worse estimate of the order parameter compared to first order one. As shown in Fig.1 we get $J_C = 0.30$ for the 4×4 lattice and $J_C = .35$ for the 6×6 one. These results indicate that a possible breakdown of the spin-wave expansion occurs already at $J_2 \sim 0.30$. This estimate is slightly different from the linear spin-wave result (see Fig.1) where a critical value of $\frac{J_2}{J_1} = 0.38$ for $S = \frac{1}{2}$ was found when the first order contribution of the order parameter $m_1 = S + \hat{\alpha}$ vanishes. However the next leading contribution to linear spin-wave $m_2 = S + \hat{\alpha} + \frac{\beta}{S}$, that we have explicitly calculated in this work, indicates that the previous estimate is quite approximate because the higher order corrections have opposite sign and become more and more relevant close to the transition point.

In conclusion we have developed a scheme for applying a systematic spin-wave theory on a finite lattice, and we have applied it to the frustrated Heisenberg model. This technique can be applied to more general hamiltonian with or without frustration, including triangular and Kagome' lattice, anisotropic model, local defects etc.etc. where we expect even accurate results with a minor computational effort.

The advantage is that on small size one can directly check the accuracy of the results, and have reliable prediction on the infinite systems. In the $J_1 - J_2$ Heisenberg model we have found that spin-wave theory works very well for small frustration ($J_2 < 0.2$) and very accurate estimate of spin-rotation invariant quantities can be obtained with only few terms of the expansion in $\frac{1}{S}$. We finally confirm the existence of a non classical spin-liquid state for large J_2, based on an approximate estimate for the breakdown of spin-wave expansion.

4 The Anisotropic Heisenberg Model

As we mentioned in the introduction, the ground state of one dimensional Heisenberg model does not have long-range order but that of the two dimensional Heisenberg model has. We argue that when $\frac{J_y}{J_x}$ changes from 0 to 1, the ground state of the Hamiltonian

$$H = J_x \sum_{R\eta_x} \mathbf{S_R} \cdot \mathbf{S_{R+\eta x}} + J_y \sum_{R\eta_y} \mathbf{S_R} \cdot \mathbf{S_{R+\eta y}}, \tag{48}$$

will change from a one-dimensional-like to a two-dimensional-like. So we could have a phase-transition in between.

From similar calculation as in the last section, we have

$$E = C + H_{sw} + H_{int} \tag{49}$$

where

$$
\begin{aligned}
&C = -\tfrac{1}{2}(J_x + J_y)S(S+1)Nz' \\
&H_{sw} = JSz'\sum_k \sqrt{(1+\alpha)^2 + (\eta_x + \alpha\eta_y)^2} \\
&H_{int} = -\tfrac{1}{2}Jz'\tfrac{N}{4}(C_{\eta_x}^2 + \alpha C_{\eta_y}^2) + \tfrac{1}{2}Jz'(C_{\eta_x} + \alpha C_{\eta_y}) \\
&\eta_x = cos k_x \\
&\eta_y = cos k_y \\
&C_{\eta_x} = \tfrac{2}{N}\sum_k{}'(V_k^2 + \eta_x U_k V_k) \\
&C_{\eta_y} = \tfrac{2}{N}\sum_k{}'(V_k^2 + \eta_y U_k V_k) \\
&\alpha = \tfrac{J_y}{J_x}
\end{aligned}
\tag{50}
$$

We can also get the spin-spin correlation function as in the last section,

$$
\langle \mathbf{S_0} \cdot \mathbf{S}_\tau \rangle = -(S - \frac{1}{2}C_\tau)^2 + \frac{1}{N^2} - \frac{1}{4}\alpha C \frac{\partial C_{\eta_y}}{\partial \beta} \tag{51}
$$

for the opposite sublattice.

$$
\langle \mathbf{S_0} \cdot \mathbf{S}_\tau \rangle = (S - \frac{1}{2}C'_\tau)^2 - \frac{1}{4}\alpha C \frac{\partial C'_{\eta_y}}{\partial \beta} \tag{52}
$$

for the same sublattice. where

$$
\begin{aligned}
C_\tau &= \tfrac{1}{N}\sum_k{}' \left\{ \frac{(1+\alpha) - (\eta_x + \alpha\eta_y)e^{ikr}}{\sqrt{(1+\alpha)^2 - (\eta_x + \alpha\eta_y)^2}} \right\} \\
C'_\tau &= \tfrac{1}{N}\sum_k{}'(1 - e^{ikr}) \left\{ \frac{(1+\alpha)}{\sqrt{(1+\alpha)^2 - (\eta_x + \alpha\eta_y)^2}} - 1 \right\} \\
\tfrac{\partial C_{\eta_y}}{\partial \beta} &= 2\tfrac{1}{N}\sum_k{}' \frac{(\eta_x - \eta_y)[(1+\alpha)e^{ikr} - (\eta_x + \alpha\eta_y)]}{[(1+\alpha)^2 - (\eta_x + \alpha\eta_y)^2]^{\frac{3}{2}}} \\
\tfrac{\partial C'_{\eta_y}}{\partial \beta} &= 2\tfrac{1}{N}\sum_k{}' \frac{(\eta_x - \eta_y)[(1+\alpha)(1 - e^{ikr})(\eta_x + \alpha\eta_y)}{[(1+\alpha)^2 - (\eta_x + \alpha\eta_y)^2]^{\frac{3}{2}}} \\
C &= \tfrac{1}{N}\sum_k{}' \frac{(\eta_x - \eta_y)(\eta_x + \alpha\eta_y)}{\sqrt{(1+\alpha)^2 - (\eta_x + \alpha\eta_y)^2}}
\end{aligned}
\tag{53}
$$

From above expression, we can see that when $J_y = 0$, i.e. $\alpha = 0$, the last term drops out, we recover the one-dimensional results and when $J_y = J_x$, i.e. $\alpha = 1$, the last term also drops out due to the fact that $C = 0$, we, again, recover the two dimensional results.

Numerical calculation shows that there is a phase transition at $\alpha = 0.1 - 0.2$, see Figure 2 and 3.

The part of the work is still in progress.

Table Captions

Table 1: First and second order contribution in $\frac{1}{S}$ for the staggered magnetization (eq.5) (m_1 and m_2) and ground state energy per site (E_1 and E_2) for the square lattice Heisenberg antiferromagnet as a function of the lattice size $N = L \times L$ for $J_2 = 0$. The exact values are obtained by diagonalization [1] or by quantum Monte Carlo[8].

Table 2: Same as in Tab. I, for different values of J_2, and increasing sizes 4×4 (top), 6×6 (middle, data for m_{exact} taken from Ref. 2) and $\infty \times \infty$ (bottom).

Figure Captions

Fig. 1: First order $S + \hat{\alpha}$ (dashed lines) and second order (continuous lines) correction $S + \hat{\alpha} + \frac{1}{S}\hat{\beta}$ for the order parameter m plotted for $S = 1/2$ for a 4×4 (upper curves) and 6×6 lattice (lower curves). The full squares and triangles are the exact diagonalization data for the 4×4 and 6×6 respectively. The arrows indicate the value of J_2 where the second order contribution is worse than the first order estimate, suggesting a breakdown of the expansion.

Fig. 2: The energy per size of the anisotropic Heisenberg model for L=4. The dashed line and continuous line correspond to the leading and the next leading term in the expansion in $\frac{1}{S}$. The empty dots are exact energies obtained by diagonalization.

Fig. 3: The spin-spin correlation function of the anisotropic Heisenberg model for $L_x = 4$, $L_y = 6$. The dashed line and continuous line correspond to the leading and the next leading term in the expansion in $\frac{1}{S}$. The empty dots are exact energies obtained by diagonalization.

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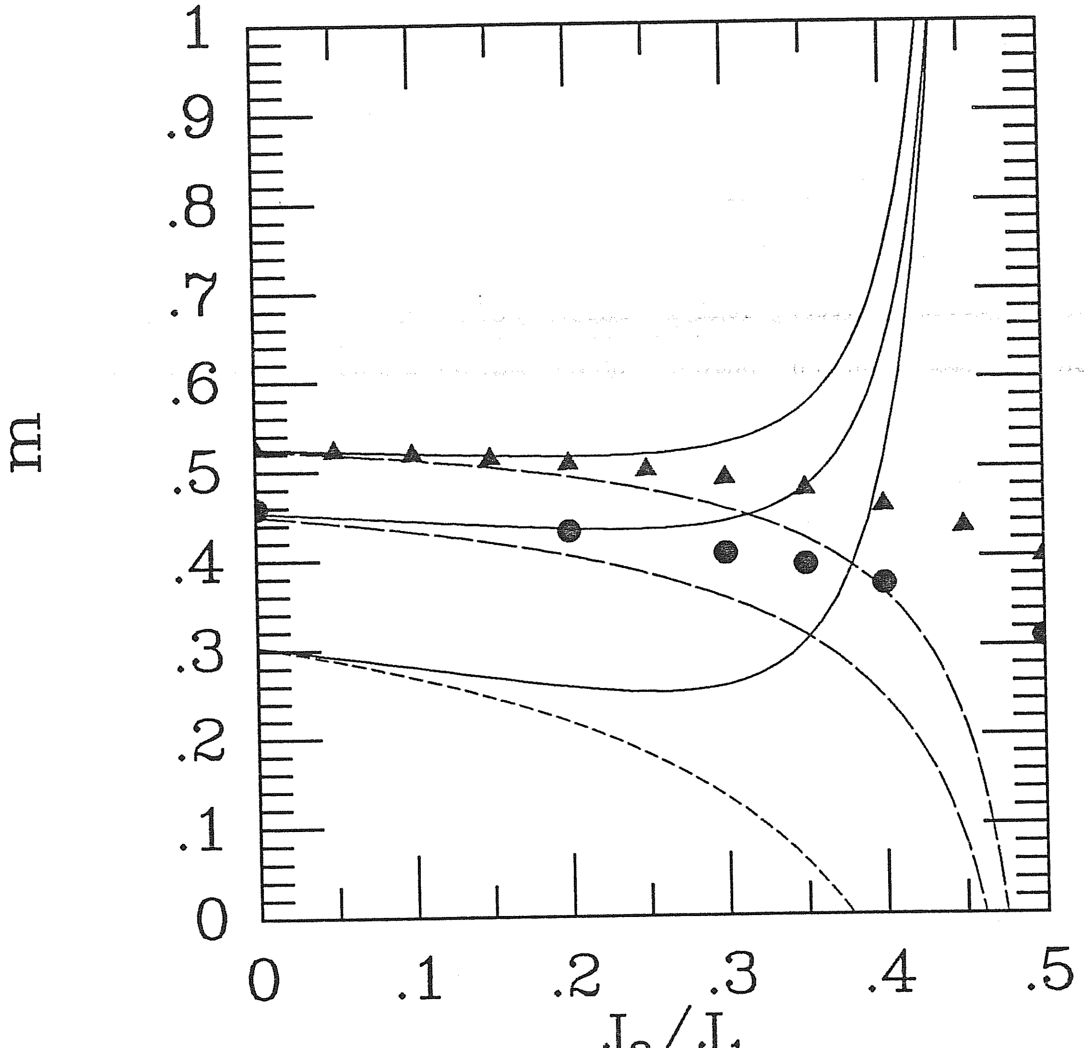
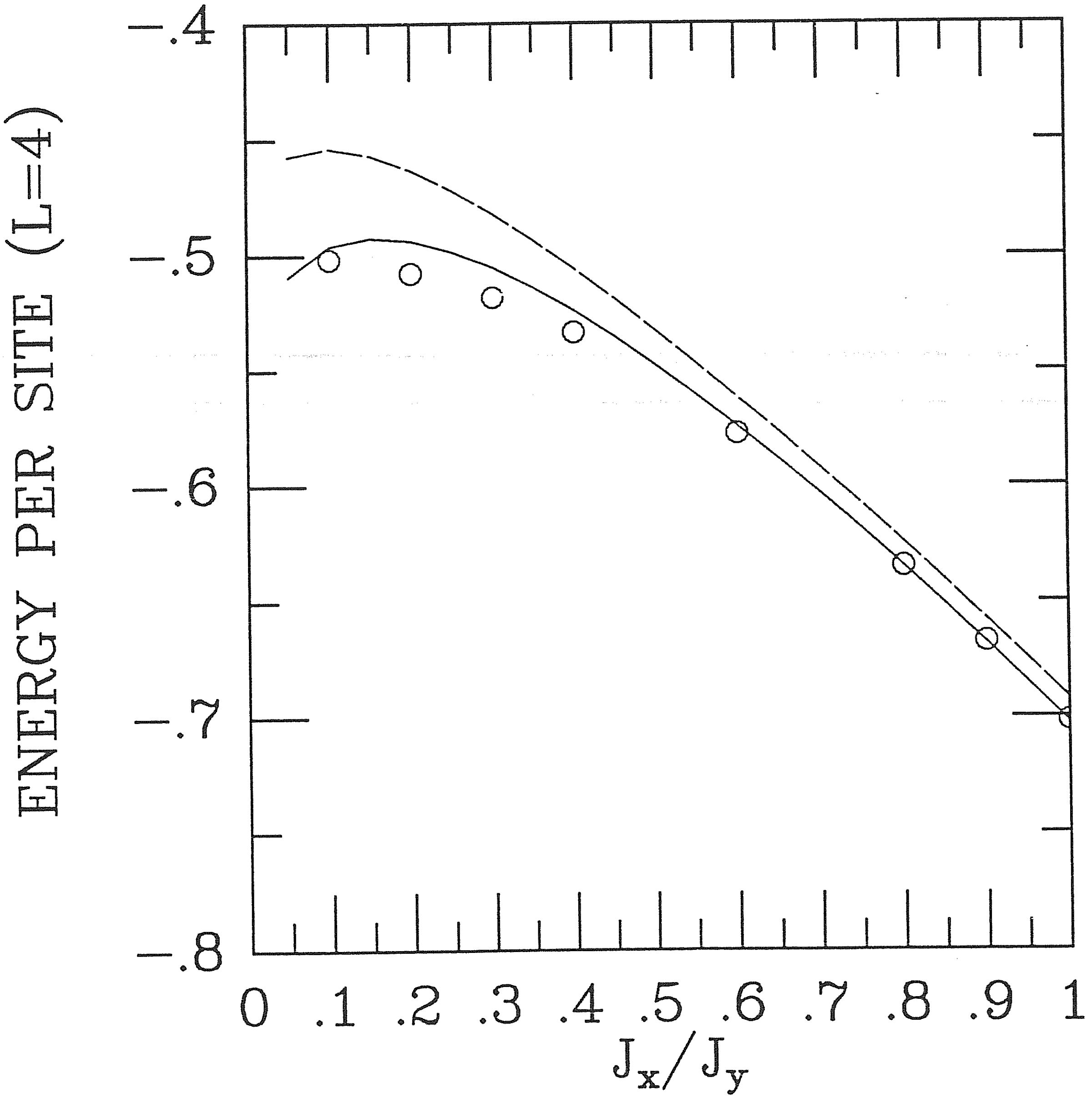
L	m_1	m_2	m_{exact}	E_1	E_2	E_{exact}
4	0.5238	0.5251	0.5259	-0.6920	-0.7026	-0.7017
6	0.4501	0.4545	0.4581	-0.6676	-0.6801	-0.6789
8	0.4133	0.4173	0.420	-0.6620	-0.6746	-0.6734
10	0.3913	0.3945	0.397	-0.6600	-0.6726	-0.6715
12	0.3766	0.3793	0.378	-0.6591	-0.6717	-0.6706
∞	0.3034	0.3034	0.3075	-0.6579	-0.6704	-0.6692

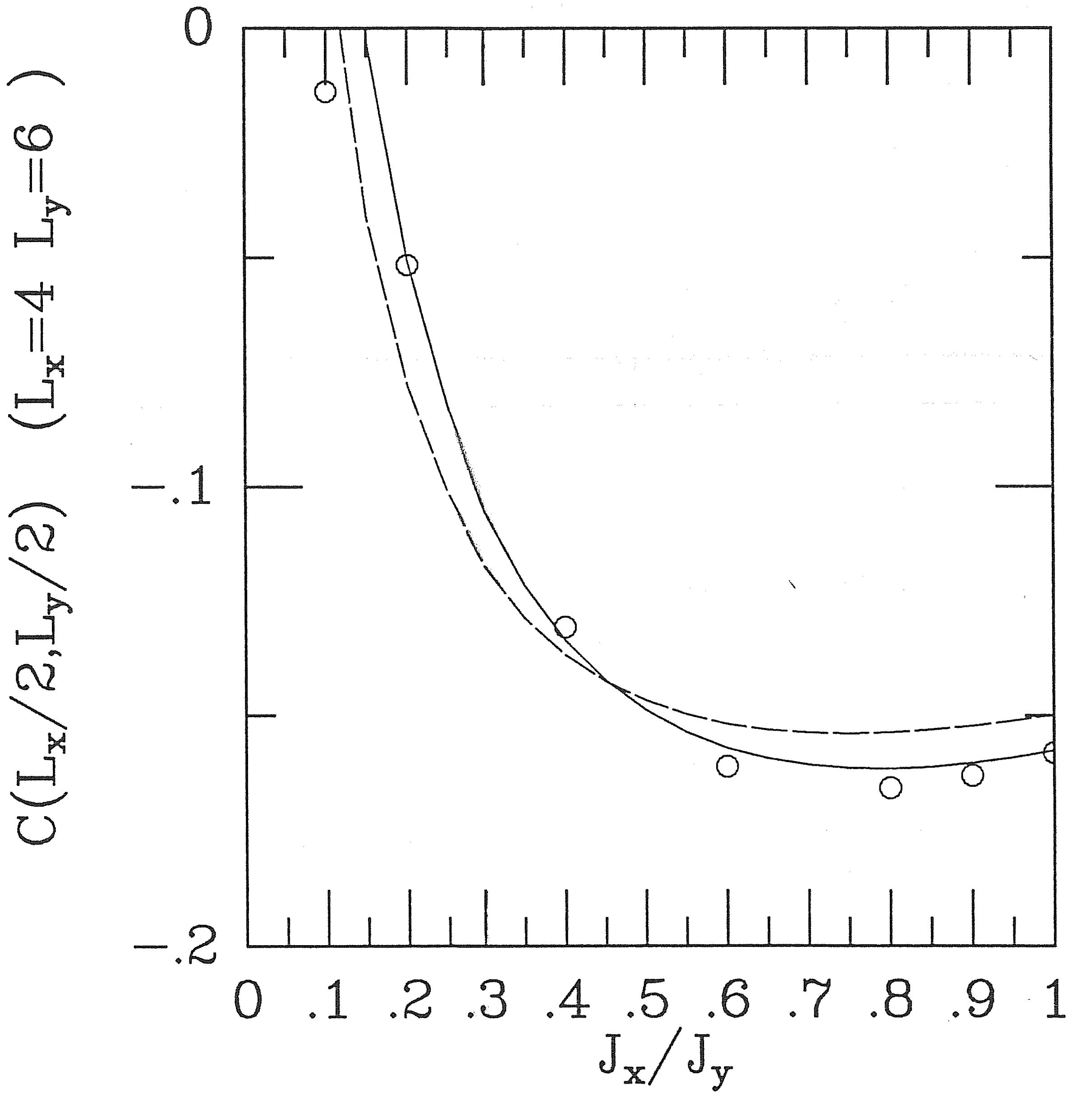
$\frac{J_2}{J_1}$	m_1	m_2	m_{exact}	E_1	E_2	E_{exact}	L
0.05	0.5184	0.5122	0.5223	-0.6711	-0.6815	-0.6806	4
0.10	0.5118	0.5193	0.5180	-0.6508	-0.6607	-0.6598	=
0.15	0.5034	0.5166	0.5129	-0.6313	-0.6402	-0.6395	=
0.20	0.4922	0.5150	0.5066	-0.6128	-0.6200	-0.6199	=
0.30	0.4553	0.5283	0.4885	-0.5801	-0.5791	-0.5830	=
0.40	0.3602	0.7357	0.4573	-0.5592	-0.5233	-0.5511	=
0.10	0.4318	0.4439	0.445	-0.6281	-0.6397		6
0.20	0.4038	0.4344	0.431	-0.5914	-0.6004		=
0.30	0.3548	0.4414	0.405	-0.5595	-0.5613		=
0.40	0.2407	0.6309	0.370	-0.5377	-0.5121		=
0.05	0.2876	0.2922		-0.6383	-0.6504		∞
0.10	0.2687	0.2804		-0.6193	-0.6308		=
0.15	0.2458	0.2685		-0.6010	-0.6114		=
0.20	0.2171	0.2576		-0.5836	-0.5924		=
0.30	0.1301	0.2580		-0.5527	-0.5541		=
0.40	-0.0606	0.5086		-0.5312	-0.5078		=



m
J_2/J_1
0
.1
.2
.3
.4
.5
.6
.7
.8
.9
1



ENERGY PER SITE (L=4)
-.4
-.5
-.6
-.7
-.8
0 .1 .2 .3 .4 .5 .6 .7 .8 .9 1
Jx/Jy



0
-.1
-.2
0 .1 .2 .3 .4 .5 .6 .7 .8 .9 1
J_x/J_y
$C(L_x/2, L_y/2)$ $(L_x=4\ L_y=6\ )$