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Estimates of the Ground State Eigenvalue of the Two Dimensional Spin 1/2 X-Y Model

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ABSTRACT

An estimate as well as upper and lower bounds are presented for the ground state energy density per spin of the two dimensional spin 1/2 X-Y model on a square lattice. The energy density is estimated to be $\epsilon_0 = -1.099 \pm 0.004$ and is bounded by $-1.12498 \leq \epsilon_0 \leq -1.09440$.

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I. INTRODUCTION

The X-Y model was introduced in 1956 as a limiting form of the quantum lattice fluid by Matsubara and Matsuda.[1] The one dimensional model was solved by Lieb Schultz and Mattis[2] and does not give rise to any critical behaviour. The three dimensional model, although it cannot be solved exactly, gives consistant evidence[3] for a ferromagnetic phase transition with order parameter $|\sigma_\perp|$. The two dimensional model remains enigmatic. In spite of theorems forbidding the existance of long range order at finite temperatures[4] the analysis of high temperature series expansions[3] indicate the existance of critical behaviour, on the other hand analysis by renormalization group methods[5] gives contradictory results. Stanley and Kaplan[6] have proposed an alternative kind of phase transition in which no long range order developes but the susceptability diverges below the critical temperature.

The X-Y model and other two dimensional spin systems have come to be of interest to elementary particle theorists because of the close relationship between these systems and lattice gauge theories in four dimensions.[7] The existance of a phase transition for the X-Y model would imply the possbility of a phase transition for QED at sufficiently strong coupling constant.[8]

One large impediment to a complete understanding of the X-Y model is the absence of any low temperature series expansions and a general lack of understanding of the ground state. We do not offer any solution to this dilema but rather constraints which the ground state must satisfy. The estimate and bounds to be presented may be of use in constructing global fits to the free energy together with information from high temperature series expansions and other methods.

In the second section of this paper we discuss those bounds which may be derived from analysis of finite systems. The methods are entirely standard. The upper bounds are from mean field theory and the lower bounds are from the diagonalization of finite Hamiltonians. In the third section we present an analysis of a perturbative expansion of the ground state energy from the limiting case of the pure Ising model, and demonstrate upper and lower bounds as well as a direct estimate of the energy density.

II. BOUNDS FROM FINITE SYSTEMS

The Hamiltonian we will study is

$$\begin{aligned} H &= -\frac{1}{2} J \sum_{<ij>} (\sigma_x^i \sigma_x^j + \sigma_y^i \sigma_y^j) \\ &= - J \sum_{<ij>} (\sigma_+^i \sigma_-^j + \sigma_-^i \sigma_+^j) , \end{aligned} \tag{2.1}$$

where $<ij>$ runs over all nearest neighbor pairs of a square lattice, and the σ's are the usual Pauli spin matrices. J only provides an overall scale and will always be set to one in the following. There are several ways in which information about a finite system can provide bounds on the behaviour of the infinite volume limit.

First, if $|\Phi>$ is an arbitrary normalized state then $E_\Phi = <\Phi|H|\Phi> \geq E_0$ the ground state eigenvalue of H. The mean field or Hartree approximation results if we choose $|\Phi> = \bigotimes_i |\phi_i>$ where each $|\phi>$ is an identical normalized state of a finite number, say M, of the total number of degrees of freedom of the system which we denote N. The terms in the Hamiltonian seperate into those which act only on one $|\phi>$ and those which couple two adjacent $|\phi>$'s. The resulting bound has the generic form

$$E_0 \leq \min_{|\phi>} -\frac{N}{M}\left[\sum_{<ij>}{}' <\phi|\sigma_+^i \sigma_-^j + \sigma_-^i \sigma_+^j|\phi> + \sum_{<ij>}{}'' <\phi|\sigma_+^i|\phi><\phi|\sigma_-^j|\rho> + \text{h.c.}\right] . \tag{2.2}$$

The first sum counts those bonds which lie in $|\phi>$, and the second sum those bonds from one $|\phi>$ to its closest neighbors, and to obtain the best bound one varys over all normalized states so as to minimize the energy.

If we modify the Hamiltonian of Eq. 2.1 by arbitrarily moving bounds around, then under quite general conditions the resulting Hamiltonian has a lower spectrum than the translationally invariant one from which we began. Futhermore if all of the bonds connecting blocks are moved into the interior of those blocks then the Hamiltonian is split into a sum of independent operators which may be diagonalized seperately. We consider the simplest case where H is written as a sum of rectangular blocks with periodic boundary conditions within each block.[9] The resulting bound is

$$E_0 \geq \frac{N}{m_x n_y} E_0^{(n_x, n_y)} , \tag{2.3}$$

where $E_0^{(n_x, n_y)}$ is the lowest eigenvalue of

$$H^{(n_x, n_y)} = - \sum_{<ij>}^{n_x n_y} (\sigma_+^i \sigma_-^j + \sigma_-^i \sigma_+^j) . \tag{2.4}$$

The bounds of Eqs. 2.2 and 2.3 have been computed for a variety of different blocks and in some cases for different arrangements of the blocks in the plane. The results are given in Table 1. The numbers represent the energy density per spin in the ground state. The upper bounds marked (a, b, c) refer to packing as a square array, a staggered array, and as a doubly staggered array. The best bounds we obtain are

$$-1.124797 \leq \epsilon_0 \leq -1.043751 . \tag{2.5}$$

III. BOUNDS FROM PERTURBATION THEORY

There is a simple way to split the X-Y model Hamiltonian into a free and interaction term which we can treat perturbatively. This is most natural if we write it rather as the "Z-X model" i.e.

$$\begin{aligned} H(g) &= -\frac{1}{2} \sum_{\langle ij \rangle} \left(\sigma_z^i \sigma_z^j + g\, \sigma_x^i \sigma_x^j\right) \\ &= H_0 + g V \quad . \end{aligned} \tag{3.1}$$

H_0 is trivially diagonalized, and we can take the ground state to have all spins pointing down. V is a sum of terms each of which flips two adjacent spins. When $g = 1$ we recover the X-Y model. It of course is impossible to say anything rigorous on the basis of a few terms in perturbation theory unless one knows something about the asymptotic behaviour of the series, but we believe that we can make a strong case for the validity of bounds derived from the perturbation series of Eq. 3.1. To prepare for this we must consider the one dimensional model which is exactly solvable.

The ground state energy density per spin in the one dimensional anisotropic X-Y model corresponding to the Hamiltonian of Eq. 3.1 has a series expansion[10]

$$\epsilon(g) = \sum_{k=0}^{\infty} \epsilon_k g^k$$

$$\epsilon_0 = -1/2$$

$$\epsilon_{2n} = -[(2n-3)!!/(2n)!!]^2/2 \qquad (3.2)$$

$$\epsilon_{2n+1} = 0 .$$

We note in particular that all of the terms are negative, and that the series converges for $|g| \leq 1$. When $g = 1$ the terms in the series fall off as $1/k^3$ so that $\epsilon(g)$ and $\epsilon'(g)$ exist at $g = 1$ but $\epsilon''(g)$ diverges. We may also write H in a slightly different form as

$$H = -\frac{1}{2} \sum_{<ij>} [(1-\gamma)\sigma_x^i \sigma_x^j + \gamma \sigma_y^i \sigma_y^j] , \qquad (3.3)$$

where γ measures the asymetry, and the corresponding ground state eigenvalue as

$$\epsilon(\gamma) = \frac{2}{\pi} E[4\gamma(1-\gamma)]$$

$$= \frac{2}{\pi} E(z) \equiv \epsilon(z) , \qquad (3.4)$$

where E is the complete elliptic integral of the second kind. In terms of the variable z, ϵ has the series expansion

$$\epsilon(x) = \sum_{k=0}^{\infty} \epsilon_k z^k$$
$$\epsilon_k = [(2k-1)!!/(2k)!!]^2/(2k-1) \,. \tag{3.5}$$

This time all of the terms past the first are positive and the convergence at $z=1$ is $\sim 1/k^2$. In conclusion if we only know a few terms of the series for $\epsilon(g)$ for the one dimensional model then Eq. 3.2 and 3.5 would provide upper and lower bounds on the ground state eigenvalue.

For the two dimensional case we have worked out the terms in the perturbation expansion of $\epsilon(g)$ through order g^2 which allows us to compute the series $\epsilon(z)$ through order z^7. They are

$$\epsilon(g) = -1 - g^2/12 - 37g^4/4320 - 38917g^6/15552000 - \ldots$$
$$\epsilon(z) = -2 + z/2 + 11z^2/96 + 7z^3/128 + 18323z^4/552960 + 50141z^5/2211840 + 5318430838z^6/31850496000 + 1647011113z^7/127401984000 + \ldots \tag{3.6}$$

We notice that the signs in these series are the same as in the one dimensional case. Analysis of the coefficients show that they are consistant with power behaviour. The coefficients in the series $\epsilon(g)$ fall of roughly as $1/k^3$, and for $\epsilon(z)$ roughly as $1/k^{3/2}$. They are both almost certainly convergent. If we take as bounds the series as they stand with $g = z = 1$ we obtain

$$-1.2452978 \leq \epsilon_0 \leq -1.0944005 \tag{3.7}$$

The upper bound represents a substantial improvement over the mean field result. The lower bound due to its rather slow convergence does not do too well.

From the coefficients of the two series we may also attempt to directly compute ϵ_0 by extrapolating the series. In each case the coefficients were fit to the form (quite well in fact)

$$\epsilon_n = a(n-b)^c \ , \tag{3.8}$$

with the results

$$\begin{array}{ccc} & \underline{\epsilon(g)} & \underline{\epsilon(z)} \\ a = & -0.0125 & 0.257 \\ b = & 0.109 & 0.332 \\ c = & -2.762 & -1.575 \end{array} \tag{3.9}$$

The fitted form was then used to sum the remainder of the series analytically with the results

$$\epsilon_0 = -1.09728 \text{ and } -1.10151 \ , \tag{3.10}$$

for $\epsilon(g)$ and $\epsilon(z)$ respectively in agreement with each other and consistant with the other bounds. Taking their average as our estimate and their difference as an estimate of the error in the extrapolation procedure we obtain

$$\epsilon_0 = -1.099 \pm 0.004 \ . \tag{3.11}$$

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Note Added

We have recently learned that J. Oitmaa, and D. D. Betts[11] have also investigated the problem of the ground state energy density for the X-Y model by an analysis of finite blocks of spins and obtain a result which agrees fairly closely with our result.

REFERENCES

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[2]E. H. Lieb, T. Schultz, and D. C. Mattis, Ann. Phys., 16, 407 (1961).

[3]D. D. Betts, "Phase Transitions and Critical Phenomena," Vol. 3, C. Domb and M. S. Green eds., Academic Press, London and New York, 1974, and many of the references contained therein.

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

[5]D. M. Lublin, Phys. Rev. Lett., 34, 568 (1975), J. Rogiers and R. Dekeyser, Phys. Rev., B13, 4886 (1976), D. D. Betts and M. Plischke, Canadian J. Phys., 54, 1553 (1976).

[6]H. E. Stanley and T. Kaplan, Phys. Rev. Lett., 17, 913 (1966).

[7]A. A. Migdal, "Phase Transitions in Gauge and Spin Lattice Systems," (Landau Inst. preprint), R. Balian, J. Drouffe, and C. Itzykson, Phys. Rev., D11, 395 (1975).

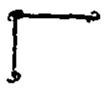
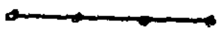
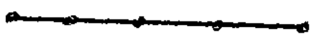
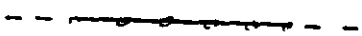
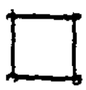
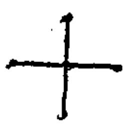
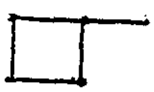
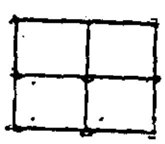
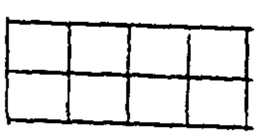
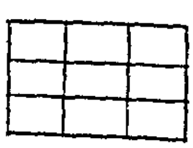
[8]K. G. Wilson, Phys. Rev., D10, 2445 (1974).

[9]The argument usually given does not strictly apply in the case of finite blocks with periodic boundary conditions, but this is easily shown to be a bound as well.

[10]See e.g. R. J. Baxter, Ann. Phys., 70, 323 (1972).

[11]D. D. Betts, private communication.

TABLE I.

Block	Lower Bound	Upper Bound
	-2	-1
	-1.6666	-1.0279(a) -1.0333(b)
	----	-1.0333
	-1.7071	-1.0314(a) -1.0312(b) -1.0312(c)
	-1.6472	----
 (∞)	-1.6366	----
	-1.4142	-1.0435
	----	-1.0335
	----	-1.0432
	-1.1496658	-1.043751
	-1.1279159	----
	-1.124927	----