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THE NATURE OF THE ORDERED PHASE IN THE TWO DIMENSIONAL QUANTUM XY MODEL

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The nature of the ordered phase and the phase transition in the classical XY model in two dimensions is now well understood due to the work of Kosterlitz and Thouless and others. High temperature series expansions indicate that the phase transition in the spin one half XY model in two dimemsions may be of a different nature. At T=0 the quantum nature of the s=1/2 model is manifest. The ground state supports both vortex-antivortex pairs and,more prominently, spin up - spin down pairs with $<\sigma_0^z\ \sigma_\delta^z> = -0.15$ on the square lattice. At low temperature a complete solution for the s=1/2 model on a 16 site lattice indicates that the most important excitations are states of complete symmetry formed by overturning spins. We propose that the break up of up-down spin pairs is responsible for the phase transition.

1. Introduction

The problem we would like to solve is to understand both the nature of the ordered phase in the two dimensional quantum XY model and the nature of the transition to this phase from the disordered high temperature phase. The simplest quantum mechanical many body system is probably the spin one half XY model, which is governed by the Hamiltonian

$$H = \frac{-J}{2} \sum_{\underline{r},\underline{\delta}} (\sigma_{\underline{r}}^x\ \sigma_{\underline{r}+\delta}^x + \sigma_{\underline{r}}^y\ \sigma_{\underline{r}+\delta}^y) \tag{1}$$

In (1) the σ's are Pauli matrices, $\underline{r}$ is the coordinate vector of a regular lattice site and $\underline{\delta}$ is a nearest neighbour lattice vector. The first sum extends over the N sites of the lattice and $\underline{\delta}$ extends over all nearest neighbours to the site at $\underline{r}$.

It is now well known [1] that neither the spin one half XY model nor the spin infinity or classical XY model can have a conventional second order phase transition to a state of uniform transverse magnetization.

The phase transition and the nature of the ordered phase in the spin infinity or classical XY model are now well understood due to the work of Kosterlitz and Thouless [2], Miyashita et al and others [3]. At low temperatures the ordered phase is characterized by bound vortex-antivortex pairs. At the phase transition these pairs unbind, so at high temperatures the disordered phase is characterized by isolated vortices and antivortices. This system is analogous to a plasma of ions and electrons at high temperatures which undergoes a transition to a gas phase of neutral atoms at low temperatures. The Kosterlitz-Thouless transition is a very weak transition in the sense that the correlation length, ξ, diverges as

$$\xi \sim \exp b[(T-T_C)/T_C]^{-1/2} \qquad T > T_C \tag{2}$$

and the transverse susceptibility

$$\chi \sim \xi^{2-\eta} \qquad T > T_C \tag{3}$$

where $\eta=1/4$.

This exponential behaviour has been confirmed by analysis of high temperature series for the classical XY model on the square and triangular lattices by Camp and Van Dyke and by Guttmann [4]. They found it much less plausible that thermodynamic quantities such as the transverse susceptibility have a conventional power law divergence in two dimensions than to have an exponential singularity.

For the s=1/2 XY model in two dimensions Rogiers et al [5] carried out extensive analysis on the high temperature series expansions of the transverse magnetization fluctuation, $<m_x^2>$, (essentially the susceptibility), the fourth order fluctuation in m_x, $3<m_x^2>^2-<m_x^4>$ and the second moment and the fourth moment of the transverse correlation, $<\sigma_0^x\,\sigma_r^x>$. Using the same methods of series analysis as the previous authers [4] we found for the s=1/2 model contrary results. For the thermodynamic functions of the spin one half XY model in two dimensions it is more plausible that a conventional power law singularity occurs. Specifically we estimated $K_C^T=0.76$ and $K_C^Q=1.27$ for the triangular and square lattices respectively, $\gamma=2.5\pm0.3$, $\Delta=2.8\pm0.2$ and $\nu=1.4\pm0.1$ in the usual notation.

For conventional second order phase transitions in magnetic systems universality with regard to spin magnitude, s, is supported by all the evidence. For the unconventional phase transition(s) in the two dimensional XY model the evidence from high temperature series at least does not confirm universality with respect to spin.

2. The Spin One Half XY Model at T=0

In this section we review some recent results on the nature of the ground state of the s=1/2 XY model in two dimensions, and we present some previously unpublished results. Understanding the nature of the ground state is a necessary first step in understanding the nature of the low temperature ordered phase.

For the ferromagnetic spin one half XY model on a lattice of an even number, N, of sites the ground state

(a) is non degenerate [6],

(b) belongs to the identity representation of the space group of the lattice and

(c) has $M_z = \sum_{i=1}^{N} S_i^z = 0$

To obtain further information on the ground state of the s=1/2 XY model Oitmaa and Betts [7] developed the finite lattice method in two dimensions. In this method the quantity of interest is calculated exactly on each of a series of finite lattices of N sites chosen in such a way as to be capable of tiling the infinite lattice. The values so calculated are plotted against 1/N and extrapolated to yield estimates for the infinite lattice.

We have recently calculated the ground state wave function for the 20 site cell on the square lattice. The resulting exact two spin correlations are listed in Table 1.

Table 1. Ground state correlations for the s=1/2 XY model in the 20 site cell of the square lattice.

$\underline{r}/\delta$	r/δ	$<\sigma_0^x\,\sigma_{\underline{r}}^x>$	$<\sigma_0^z\,\sigma_{\underline{r}}^z>$
(1,0)	1	0.55819	-0.17602
(1,1)	$\sqrt{2}$	0.48583	-0.02374
(2,0)	2	0.47043	-0.01903
(2,1)	$\sqrt{5}$	0.46372	-0.01853
(3,1)	$\sqrt{10}$	0.45397	-0.01387

The pattern of correlations listed in Table 1 is typical of that in all cells so far investigated. Observe the following features:

(a) the transverse correlations, $\langle\sigma_0^x\ \sigma_r^x\rangle$, are of the order of 0.5 and decrease slowly and monotonically with distance

(b) the longitudinal correlations, $\langle\sigma_0^z\ \sigma_r^z\rangle$, are all negative and also decrease monotonically with distance

(c) the nearest neighbour longitudinal correlation $\langle\sigma_0^z\ \sigma_\delta^z\rangle$, is an order of magnitude greater than further neighbour correlations

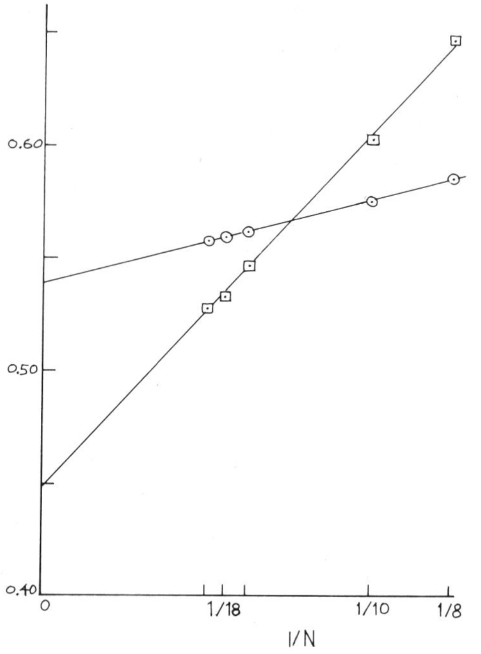

Fig. 1 Nearest neighbour correlations $\langle\sigma_0^x\ \sigma_\delta^x\rangle$ (circles) and $-3\langle\sigma_0^z\ \sigma_\delta^z\rangle$ (squares) for the s= 1/2 XY model for cells of N=8, 10, 16, 18 and 20 sites on the square lattice.

Fig. 1 shows a typical 1/N plot for the two nearest neighbour correlations. From Fig. 1 we obtain the refined estimates for the infinite square lattice, $\langle\sigma_0^x\ \sigma_\delta^x\rangle = -E_0/2NJ = 0.538\pm0.005$ and $\langle\sigma_0^z\ \sigma_\delta^z\rangle = -0.149\pm0.008$. For comparison the second order variational estimates of Suzuki and Miyashita [8] are $\langle\sigma_0^x\ \sigma_\delta^x\rangle = 0.53715$ and $\langle\sigma_0^z\ \sigma_\delta^z\rangle = -0.14286$.

Refined estimates have also been obtained for $\langle m_x^2\rangle/(g\mu_B N)^2 = 0.112\pm0.004$, the square of the transverse magnetization. Similar expressions for the two staggered magnetizations vanish, but the fluctuations in the staggered magnetizations are $\langle n_x^2\rangle/(g\mu_B)^2 N = 0.0726\pm0.0010$ and $\langle n_z^2\rangle/(g\mu_B)^2 N = 0.392\pm0.010$. In comparison Suzuki and Miyashita [8] find $\langle m_x^2\rangle/(g\mu_B N)^2 = 0.1151$, $\langle n_x^2\rangle/(g\mu_B)^2 N = 0.173$ and $\langle n_z^2\rangle/(g\mu_B)^2 N = 0.311$.

In classical models or quantum models in which the magnetization operator commutes with the Hamiltonian the susceptibility and magnetization fluctuation are equal when expressed in dimensionless units. In contrast for the s=1/2 XY model on the square lattice we find [9] for the staggered susceptibilities

$$J\chi^s_{xx}/N(g\mu_B)^2 = 0.276 = 0.38\langle n_x^2\rangle/N(g\mu_B)^2 \tag{4}$$

and

$$J\chi^s_{zz}/N(g\mu_B)^2 = 0.147 = 0.38\langle n_z^2\rangle/N(g\mu_B)^2 \tag{5}$$

More startling is the result for the uniform transverse susceptibility,

$$J\chi_{xx}/(Ng\mu_B)^2 \sim N^{0.9} \tag{6}$$

All the above results indicate that at T=0 the s=1/2 XY model is very different from the simple s=∞ XY model. Nevertheless the quantum model may also support vortices and vortex-antivortex pairs. Indeed whereas in the classical XY model vortices and vortex-antivortex pairs can occur only for T>0, as excitations, in the quantum XY models vortices and antivortices can occur due to zero point motion even at T=0. According to our definition [10] the s=1/2 XY model supports 0.025 vortices and antivortices per site on the square lattice. The number of vortex-antivortex pairs at T=0 is 0.012 per site on the square lattice, which implies that essentially all of the vortices and anti-vortices occur as "bound" pairs. Similar results hold on the triangular lattice.

There is a clear possibility that the phase transition in two dimensional quantum XY models as the temperature is raised through T_c corresponds to the unbinding of vortex-antivortex pairs, just as in the classical XY model. There is another possibility for the quantum models not open to the classical model. The phase transition may correspond to the dissolution of "bound" pairs of up and down spins. From finite lattice calculations [6,11] the number of nearest neighbour up and down spin pairs (in the z direction) is 0.15 per site in the s=1/2 XY model on each of the honeycomb, square and triangular lattices. The latter structures are thus an order of magnitude more common than the vortex-antivortex pairs and hence a priori likely to have a more important role in the phase transition.

3. The Model at Low Temperatures

Recently one of us has diagonalized completely the s=1/2 XY model Hamiltonian on each of the N=8, 10 and 16 spin cells of the square lattice [12]. This has enabled the calculation of the energy, entropy and specific heat of the model as a function of the temperature in each cell and permitted an extrapolation to the infinite lattice.

It is instructive to examine the energy level spectrum in detail in the vicinity of the ground state for the 16 spin cell. In Fig. 2 are plotted, as a function of M_z (or total z component of spin) all energy eigenvalues less than -12J. The lowest and second lowest eigenvalue for each value of M_z are also plotted. (The spectrum is of course symmetric about the M_z=0 axis)

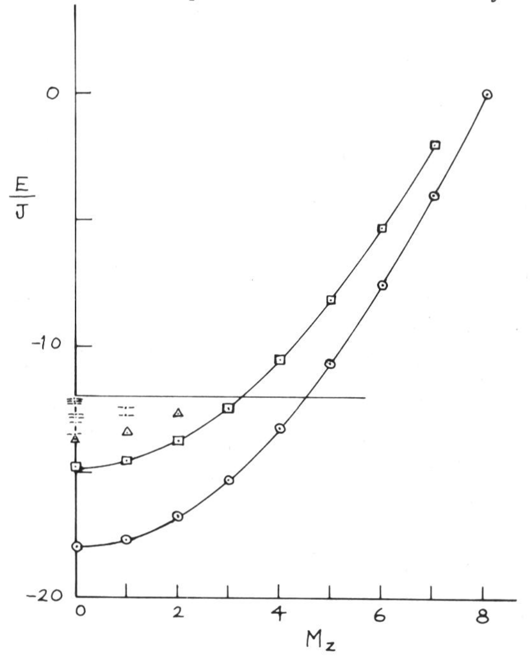

Fig. 2 Energy levels of the s=1/2 XY model on a cell of 16 sites versus longitudinal magnetization, M_z. All energies less than -12J are included. Relative ground state (circles) and first excited state (squares) are plotted for each value of M_z.

It is a consequence of the Frobenius theorem that the eigenvector of the relative ground state for each value of M_z belongs to the identity representation of the space group of the cell. In Fig. 2 these relative ground state energies have been connected by a smooth curve. This curve is very well represented by the parabola

$$E_0(M_z) = E_0(0) + 0.295JM_z^2 \tag{7}$$

The set of second lowest eigenvalues for each value of M_z are also well fitted to a parabola of slightly different curvature. The symmetry of the corresponding eigenvectors is for each value of M_z the same but different from that of the ground state.

The variational expression [8] for the relative ground state is

$$E_0(M_z) = E_0(0) + Jq/(N-1)M_z^2 \tag{8}$$

For N=16 and q=4 (8) reduces to

$$E_0(M_z) = E_0(0) + 0.267JM_z^2\ , \tag{9}$$

in remarkable agreement with the exact calcualation.

Note the N dependence of the curvature coefficient in (8). We conclude that for the very large lattice the dominant excitations at low temperature are those symmetry preserving excitations in which individual spins are turned over to increase M_z and thus to decrease $\langle\sigma_0^z\ \sigma_\delta^z\rangle$. These low lying excited states are not spin waves for they are not periodic; we might call them "spin billows".

The gap between the ground state and the lowest energy state of a different symmetry may well persist for large lattices. In other words spin waves may be unimportant at low temperatures.

We take the nature of the lowest lying excitations as further evidence in support of the picture that the phase transition corresponds to rapid breakup of spin up - spin down pairs.

4. New Series at High Temperatures

The method of high temperature series expansion has proved very successful in the investigation of conventional second order phase transitions and, as noted in Sec. 1, certain series, especially the fourth order fluctuation in the transverse magnetization, indicate a phase transition in the two dimensional s=1/2 XY model.

If our picture is correct we expect the order parameter to be

$$C = -\sum_{\underline{r},\underline{\delta}} \sigma_{\underline{r}}^z\sigma_{\underline{r}+\underline{\delta}}^z \tag{10}$$

which has the same form as the energy so might be called the "coenergy". The coenergy per site, $\langle C\rangle/N = -q/2\langle\sigma_0^z\ \sigma_\delta^z\rangle$, will remain finite but we may expect both the temperature derivative of the coenergy and the fluctuation of the coenergy, $(\langle C^2\rangle - \langle C\rangle^2)/N$, to diverge at T_C.

It is perhaps helpful to compare the high temperature series for the two nearest neighbour correlations. The first twelve terms of $\langle\sigma_0^x\ \sigma_\delta^x\rangle$ are known for several lattices [5]. For the triangular lattice

$$\begin{aligned}\langle\sigma_0^x\ \sigma_\delta^x\rangle &= 0.5K + 0.5K^2 + 0.04167K^3 - 0.625K^4 \\ &\quad -0.80139K^5 + 0.47153K^6 + \cdots\end{aligned} \tag{11}$$

We have so far derived by hand only the first few terms of the longitudinal correlation for the triangular lattice,

$$-\langle\sigma_0^z\ \sigma_\delta^z\rangle = 0.75K^2 + 0.5K^3 - 0.875K^4 - 1.675K^5 + \cdots \tag{12}$$

We observe that the longitudinal correlation is negative at high temperature as at T=0. Further, the magnitude of $\langle\sigma_0^z\ \sigma_\delta^z\rangle$ at high temperatures is an order of magnitude less than that of $\langle\sigma_0^x\ \sigma_\delta^x\rangle$, and it remains a factor of three smaller even at K=0.5, beyond which such a short series can no longer be relied upon.

Prof. E.W. Grundke and one of us (D.D.B.) are planning to generate with the aid of a computer long series for both C and the fluctuation in C.

5. Monte Carlo Method and Concluding Remarks

Suzuki et al [13] have developed a method for the Monte Carlo simulation of quantum spin systems. Their method is based on application to the Hamiltonian of the Trotter formula,

$$\exp(\beta\mathcal{H}) \equiv \exp\sum_i H_i = \lim_{n\to\infty} (\prod_i \exp H_i/n)^n \tag{13}$$

As Suzuki has shown [14] the application of (13) permits the reduction of a quantum problem in d dimensions to a classical problem in d+1 dimensions. Then it is possible to study the classical problem by Monte Carlo methods in the usual way. In practice it is necessary to use in (13) some small value of n, in which case the correspondence between the quantum and classical models is approximate. The formula (13) for finite n becomes exact at infinite temperature, so the method is seen to be an alternative to the high temperature series method.

Suzuki et al [13] have applied the above method to the spin one half Heisenberg and XY models in one dimension and to the XY model on the square lattice. They used the n=1 and n=2 approximants to (13) on lattices of n = 9×9, 15×15 and 30×30 sites respectively. They used the Monte Carlo method to compute the internal energy, specific heat and transverse susceptibility of the two dimensional XY model.

Their results for n=2 are in very good agreement with the high temperature series results down to $T\approx 1.5J/k_B$. Their susceptibility appears to diverge at $T_C\approx 1.0J/k_B$ as compared with the high temperature series divergence [5] at $T_C\approx 0.8J/k_B$. Their specific heat maximam occurs at approximately the same position as their susceptibility divergence, whereas Kelland's maximum [12] occurs at $T_C^M\approx 1.4J/k_B$. The height of the specific heat maximum of Suzuki et al [13] is $C_V^m/Nk_B = 0.9$, considerably higher than that of Kelland, who finds $C_V^m/Nk_B = 0.66$.

We believe all the above quantitative discrepancies between our results and the Monte Carlo results arise from using n=2 in the Trotter formula. Such a degree of approximation means that quantum effects are not adequately accounted for $T \lesssim 1.5J/k_B$. In particular the divergence of the susceptibility at too high a temperature could be due to Ising like effects.

In summary we have presented three types of evidence favouring a qualitative difference between the phase transitions in the classical and quantum (specifically spin one half) XY models in two dimensions:

1. Rather long high temperature series expansions for both models seem to indicate an exponential divergence of thermodynamic properties at T_C for s=∞, in conformity with the Kosterlitz-Thouless picture. On the other hand thermodynamic properties of the s=1/2 model seem to have a power law divergence.
2. The properties of the s=1/2 XY model at T=0 show very important quantum effects and are very different from those of the classical model.
3. The most important excitations of the s=∞ model at low temperatures are spin waves while for the s=1/2 model perhaps the most important excitations are symmetry preserving modes in which M_z^2 is increased from zero.

We propose that the principal mechnism responsible for the phase transition in quantum XY models in the symmetry preserving breakup of nearest neighbour pairs of up and down spins rather than the breakup of nearest neighbour pairs of vortices and antivortices as in the s=∞ model. Such a phenomenon does occur at low temperature for the s=1/2 model where spin up - spin down pairs are an order of magnitude more common than vortex-antivortex pairs.

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