Realization of a Spin Liquid in a Two Dimensional Quantum Antiferromagnet

A. Parola
Dipartimento di Fisica, Universitá di Milano, Via Celoria 16, Milano, Italy

S. Sorella and Q. F. Zhong
International School for Advanced Studies, Via Beirut 4, 34014 Trieste, Italy

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The ground state properties of the two dimensional spatially anisotropic Heisenberg model are investigated by use of field theory mappings, spin-wave expansion, and Lanczos technique. Evidence for a disorder transition induced by anisotropy at about $J_y/J_x < 0.1$ is shown. We argue that the disordered phase is gapless and its long wavelength properties can be interpreted in terms of decoupled one dimensional chains.

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The search for disordered (spin liquid) ground states in two dimensional (2D) electronic models has been pursued since the seminal work of Fazekas and Anderson [1] on quantum antiferromagnets (QAF) in frustrating lattices. This problem has been revived in the last few years due to the resonating valence bond conjecture [2], which stimulated much numerical work on the subject. Despite considerable effort, the existing evidence in favor of a spin liquid in 2D frustrated QAF is weak at best [3,4], with the single exception of the kagomé QAF where a disordered ground state is plausible [5], even if the presence of nonconventional magnetic order is still a possibility.

In this Letter, we present analytical as well as numerical evidence supporting an order-disorder transition in the square lattice $S = 1/2$ QAF driven by spatial anisotropy in the nearest neighbor coupling. This model does *not* introduce frustration and therefore presents several advantages with respect to the previously investigated systems, the most important being the absence of any plausible order parameter competing with the Néel staggered magnetization $\mathbf{m} = \sum_{\mathbf{R}} \mathbf{S}_{\mathbf{R}} \exp(\mathbf{Q}\cdot\mathbf{R})$ $[\mathbf{Q} = (\pi, \pi)]$. The model is defined by the Hamiltonian

$$H = J \sum_{\mathbf{R}} [\mathbf{S}_{\mathbf{R}} \cdot \mathbf{S}_{\mathbf{R}+\mathbf{x}} + \alpha \mathbf{S}_{\mathbf{R}} \cdot \mathbf{S}_{\mathbf{R}+\mathbf{y}}], \qquad (1)$$

where $\mathbf{S}_{\mathbf{R}}$ are spin 1/2 operators living on a square lattice, $\mathbf{x}$ and $\mathbf{y}$ are unit vectors, $J > 0$, and $\alpha \leq 1$. The isotropic limit ($\alpha = 1$) has been extensively studied by exact diagonalizations [6] and quantum Monte Carlo [7,8] with the resulting evidence of a finite staggered magnetization in the thermodynamic limit [8] $m \sim 0.3075$, quite close to the spin-wave theory (SWT) estimate $m = 0.3034$ [9]. Physically, the strongly anisotropic model (1) describes a system of weakly coupled AF chains whose study has attracted considerable interest among theoreticians and experimentalists in view of the possibility to observe the peculiar features of one dimensional physics [10].

The presence of an order-disorder transition in model (1) has been conjectured by several authors [11,12] and can be motivated by the standard mapping of the 2D quantum model (1) into the (2+1) dimensional $O(3)$ nonlinear sigma model (NLσM) defined by the action

$$S = \tfrac{1}{2} \int dx\, dy\, dt\, [\Upsilon_x (\partial_x \mathbf{n})^2 + \Upsilon_y (\partial_y \mathbf{n})^2 + \chi_0 (\partial_t \mathbf{n})^2], \qquad (2)$$

where $\mathbf{n}$ is a unit vector. The lowest order estimates of the parameters give $\Upsilon_x = J/4$, $\Upsilon_y = \alpha J/4$, $\chi_0^{-1} = 4a^2 J(1+\alpha)$ where a is the lattice spacing. Two limits of the action (2) can be easily analyzed: The isotropic model is known to be ordered for the physically relevant parameters [13], while the $\alpha \to 0$ limit of the action (2) correctly describes a stack of uncoupled (1+1) dimensional models which are disordered at any finite "temperature" $g = (\Upsilon_x \chi_0 a^2)^{-1/2}$ owing to the Mermin Wagner theorem. Most interestingly, the order-disorder transition occurs at a *finite* value of the spatial anisotropy and belongs to the universality class of the classical three dimensional Heisenberg model.

Similar conclusions can be drawn directly from SWT on the quantum Hamiltonian (1). In fact, the $1/S$ expansion of the staggered magnetization can be straightforwardly generalized to anisotropic models and predicts a breakdown of Néel order at about $\alpha_c \sim 0.03$ (0.07) at first (second) order in $1/2S$. The *increase* of the critical anisotropy parameter α_c in going from first to second order gives confidence about the actual occurrence of the transition, which is in fact enhanced by quantum fluctuations. Therefore, on the basis of the field theory mapping and SWT, we expect that by lowering the anisotropy parameter α a disordered phase sets in within a finite interval $\alpha_c > \alpha > 0$. This prediction should be qualitatively correct because field theory methods are known to reproduce the physics of QAF both in the isotropic two dimensional limit [13] and in the one dimensional ($\alpha = 0$) case, provided the topological term is included in (2) [14].

In order to test the theoretical predictions on the model (1) and to determine the properties of the two dimensional spin liquid state, we have performed Lanczos diag-

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onalizations on several lattices up to 32 sites. A proper finite size scaling of small lattice results is obviously important in order to provide a correct interpretation of the diagonalization data. Fortunately, much work has been recently devoted to this subject [15,16] showing that, in the ordered phase, the renormalization group flow drives the model towards weak coupling, making SWT asymptotically exact at long wavelengths. As a consequence, SWT is able to describe the leading size corrections in finite lattices and therefore represents a powerful method for analyzing small size data, particularly in nonfrustrated models. SWT, generalized to finite systems [17], compares quite favorably to numerical results in bipartite lattices. The good agreement also persists for the anisotropic model (1), as shown in Fig. 1 where a finite size estimate of the order parameter is plotted as a function of the anisotropy α. The breakdown of SWT at $\alpha < 0.1$ again suggests that a qualitative change in the ground state properties is occurring in this regime.

Further numerical evidence of the phase transition can be obtained by the structure of the energy spectrum as a function of the total uniform magnetization. According to a recent analysis [3] the presence of Néel long range order in the thermodynamic limit reflects in the structure of the energy spectrum in finite size systems. In fact, if long range antiferromagnetic order is present in the system, the dependence of the energy $E(S)$ on the total spin S must follow the approximate relation

$$E(S) \sim E(0) + S(S+1)/(2I_N) \qquad (3)$$

up to a maximum value $S_{\max}$ of the order of the square root of the number of sites N. Equation (3) approximately reproduces the energy spectrum of a spin-S rigid rotator with a momentum of inertia per site I_N/N corresponding to the uniform susceptibility χ of the model. Notice that this criterion correctly reproduces the absence of antiferromagnetic long range order in one dimension where the energy spectrum scales as [14] $E(S) \sim E(0) + S^2/2\chi_{1D}L$. The relation (3) is in fact quite well verified both for the isotropic system and for the anisotropic ones up to $\alpha \sim 0.1$ where significant discrepancies appear [see Fig. 2(a)]. The strong deviations from Eq. (3) which develop in the numerical data can be related to the asymptotic decoupling of the chains in the square lattice, leading to an approximate *linear* dependence $E(S) \sim E(0) + S/2\chi_{1D}L$ where L is the number of sites along each (weakly coupled) chain. In fact, in the limit $\alpha = 0$, the lowest energy at fixed total spin S is obtained by setting $S = 1$ on each chain, at least up to $S \sim$ (number of chains). This anomaly does not seem to scale to zero in the thermodynamic limit but instead persists in all the lattices we have analyzed. From our finite size data an accurate estimate of the uniform susceptibility can be extracted by a quadratic fit of the energy spectrum $E(S)$ at small but finite (uniform) magnetization S/N. The results can then be extrapolated to infinite volume by use of a finite size scaling of the form [8] $\chi^{-1} = \chi_\infty^{-1} + AN^{-1/2} + B/N$ which is known to work both in the isotropic limit and in one dimension (extreme anisotropy). The extrapolation, shown in Fig. 2(b) for several values of the anisotropy parameter, is in fact in good agreement with the known values at $\alpha = 0$ and $\alpha = 1$ (also shown in the figure) and predicts a smooth, featureless susceptibility in the whole anisotropy range. This result indicates that the system remains gapless across the phase transition and suggests that the nature of the disordered phase of this model might be more exotic than the expected nondegenerate

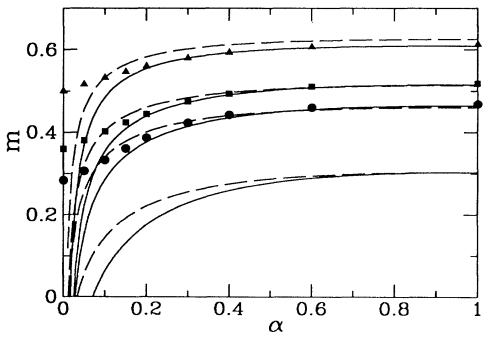

FIG. 1. Order parameter $m = \sqrt{S(\pi,\pi)/V}$ for different lattice sites compared with the first (dashed lines) and second order (continuous lines) SWT results. The Lanczos data are obtained on tilted lattices $L\sqrt{2} \times L\sqrt{2}$ with $L = 2$ (triangles), $L = 3$ (squares), and $L = 4$ (circles). The lowest curves refer to the infinite size SWT results.

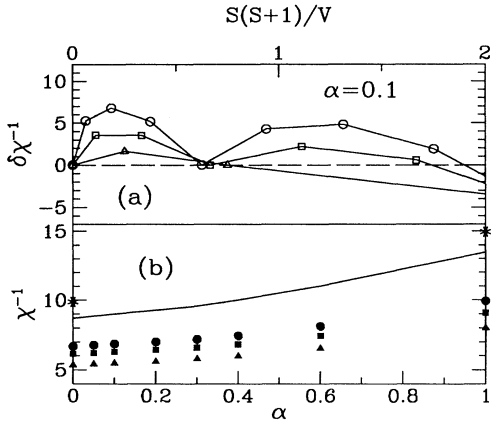

FIG. 2. (a) Rigid rotator anomaly $\delta\chi^{-1} = V(E(S) - E(0))/S(S+1) - 1/(2\chi_L)$ estimated in finite sizes for 8 (triangles), 18 (squares), and 32 (circles) lattice sites. The continuous lines are guides to the eye; the dashed line represents the ideal behavior in a quantum antiferromagnet. (b) Finite size scaling of the inverse susceptibility. The finite size data (notation as in Fig. 1) extrapolated (see text) to infinite size (continuous lines). The stars are the exact values in the isotropic and one dimensional case.

singlet, in agreement with a conjecture put forward by Haldane [14].

However, the possibility of a gapless phase contrasts with the commonly accepted phase diagram of the model (1) defined on two chains [18,19], where a gap $\Delta(\alpha)$ is believed to open at every finite value of the anisotropy parameter α. The disordered phase in the two chain model is in fact continuously connected with the $\alpha \to \infty$ limit where the gap is interpreted as the effect of the finite size of the lattice along the y direction. The same result actually holds for every *even* number of chains while an *odd* chain model remains gapless all the way to the $\alpha \to \infty$ limit. Therefore it is not too surprising that the Hamiltonian (1) on square clusters preserves the peculiarities of the odd chain sequence and does not open a gap at any α. In finite clusters, however, a gap is always present and we must investigate whether it disappears in the thermodynamic limit. We have analyzed the finite size scaling of the gap in the case of two chains ($L \times 2$), three chains ($L \times 3$) with antiperiodic boundary conditions along the y direction, and for square clusters. For any α the lowest excited state is always a triplet but its size dependence is quite different in the three cases. In order to see whether a gap is present in the strong anisotropic region we assumed that, for $\alpha \to 0$ and $L \to \infty$, the gap $\Delta(L, \alpha)$ can be expressed in a scaling form, as usual near a critical point,

$$\Delta(L, \alpha) = \Delta(L, 0)\, F[\alpha L\, (\log\, L)^{1/2}], \qquad (4)$$

where the one dimensional gap $\Delta(L, 0)$ is known to scale as $1/L$. The specific form (4) has been chosen in order to match with first order perturbation theory in α and does not depend on the number of chains of our lattice. However, the scaling function $F(x)$ behaves quite differently in the three geometries, as can be seen in Fig. 3. The correctness of our scaling form (4) can be inferred by the collapse of the finite size numerical data on a smooth curve in all cases, provided α is sufficiently small. Finite size effects reflect in the nonuniversal departure of the numerical data from the universal curve $F(x)$. The thermodynamic limit at fixed (small) α corresponds to the large x region of the scaling curve which is not directly accessible from finite size data and should be extrapolated from the numerical results of Fig. 3. In the two chain model $F(x)$ clearly goes through a minimum and then grows, suggesting a linear asymptotic behavior at large x which implies a finite gap of order $J\alpha$ at small α, in agreement with field theoretical analysis [18]. The comparison between the three chains, where a gapless phase is expected, and the square clusters shows a strong resemblance between the two cases: The scaling function is always monotonic supporting the absence of a gap.

In order to understand how a disordered gapless phase may appear in 2D it is useful to consider other physical quantities like the spin-wave velocity and the momentum dependence of the magnetic structure factor. Again, SWT provides a valuable help in the interpretation of the

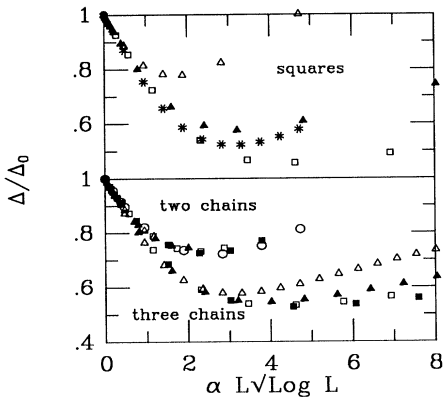

FIG. 3. Diagonalization data of the gap scaling function [see Eq. (4)] for the two chain model, three chains, and square clusters. For the two and three chains, open triangles refer to $L = 4$, full triangles $L = 6$, open squares $L = 8$, full squares $L = 10$, and open circles $L = 12$. For the square clusters open triangles correspond to 8 sites, full triangles to 18 sites, open squares to 32 sites, and stars to the 4×4 cluster.

numerical results. The spin velocity is almost constant at all anisotropies ranging between the one dimensional value $c_x = \pi/2$ and the isotropic limit [8] $c_x \sim 1.56$ which are both reproduced within 10% by second order SWT generalized to anisotropic models. A surprising result of SWT is the enhancement of the anisotropy in the spin velocity ratio induced by quantum fluctuations:

$$\left(\frac{c_y}{c_x}\right)^2 = \alpha Z(\alpha), \quad Z(\alpha) = 1 - \frac{1}{2S} C(\alpha), \qquad (5)$$

$$C(\alpha) = \frac{1}{N} {\sum_k}' \frac{(\cos k_x - \cos k_y)(\cos k_x + \alpha \cos k_y)}{\sqrt{(1+\alpha)^2 - (\cos k_x + \alpha \cos k_y)^2}}.$$

In fact, while at lowest order the spin velocity ratio coincides with the anisotropy parameter, the one loop calculation always reduces the $Z(\alpha)$ factor. Obviously, the correction $C(\alpha)$ vanishes at the isotropic point $\alpha = 1$ but diverges logarithmically in the $\alpha \to 0$ limit. Therefore, SWT suggests the occurrence of a decoupling transition at a finite value of α signaled by $Z(\alpha_c) = 0$. The same anisotropy renormalization factor $Z(\alpha)$ governs the long wavelength behavior of the physical correlation functions. In particular, the magnetic structure factor behaves as

$$S(k_x, k_y) \propto \sqrt{k_x^2 + \alpha Z(\alpha) k_y^2}. \qquad (6)$$

In order to verify these predictions we tested Eq. (6) against Lanczos diagonalizations in the 32 site lattice. The results are shown in Fig. 4 together with the zero and one-loop SWT results for the spin velocity ratio in the thermodynamic limit. The numerical data are in good agreement with the spin-wave results in the 32 site lattice, and show an even larger effect. Therefore we are led to conclude that at long wavelengths a decoupling

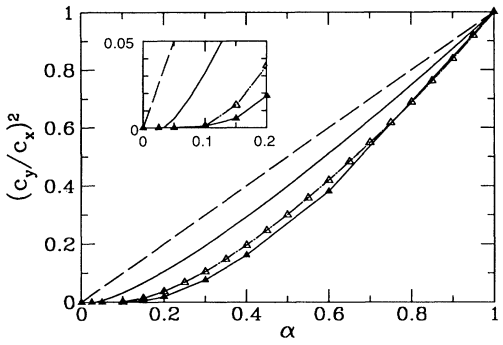

FIG. 4. Square of the spin velocity ratio vs anisotropy. The dashed line is the leading SWT result; the continuous line includes the one loop correction in the thermodynamic limit. Finite size estimates on a 32 site lattice for $\alpha Z(\alpha)$ are obtained by exact diagonalization (full triangles) and second order finite size SWT [17] (open triangles).

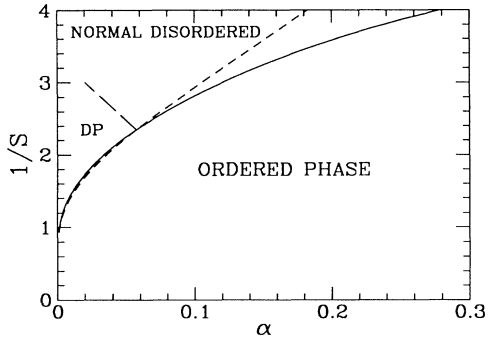

FIG. 5. Phase diagram of the spatially anisotropic Heisenberg model obtained via one-loop SWT. The order parameter vanishes along the continuous line and the spin-wave velocity ratio along the dashed line. The long dashed line indicates a crossover transition between a decoupled phase (DP) and a normal disordered phase with a finite spin velocity ratio.

transition may actually occur in strongly anisotropic spin models. The phase diagram of the anisotropic model (1) suggested by SWT is depicted in Fig. 5 for generic spin-S systems. The transition line where the staggered magnetization vanishes has been calculated at the lowest order spin-wave level together with the locus $Z(\alpha) = 0$ where we expect a "decoupling transition." At the same order in $1/S$ we have found that these two lines approximately coincide up to a critical value of $1/S$ beyond which the system disorders without decoupling. For large values of S, the transition is characterized by the vanishing of both the staggered magnetization and the spin velocity ratio leading to a picture of basically uncoupled chains (i.e., with a finite correlation length in the y direction) with interesting experimental consequences about the possibility to observe 1D behavior in real systems. In the upper part of the phase diagram, the first instability ($m = 0$) drives the system towards a strong coupling disordered phase. In this region, the further decoupling instability predicted by SWT cannot be justified any more.

We believe that this zero temperature phase diagram is qualitatively correct although higher order terms in the SWT expansion (available only for the magnetization) may quantitatively change the phase transition line. In order to fully characterize the disordered phase, topological defects must be taken into account leading to a possible difference between integer and half-integer spin systems [14].

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