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LARGE N EXPANSION FOR FRUSTRATED AND DOPED QUANTUM ANTIFERROMAGNETS

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ABSTRACT

A large N expansion technique, based on symplectic ($Sp(N)$) symmetry, for frustrated magnetic systems is studied. The phase diagram of a square lattice, spin S, quantum antiferromagnet with first, second and third neighbor antiferromagnetic coupling (the J_1-J_2-J_3 model) is determined in the large-N limit and consequences of fluctuations at finite N for the quantum disordered phases are discussed. In addition to phases with long range magnetic order, two classes of disordered phases are found: *(i)* states similar to those in unfrustrated systems with commensurate, collinear spin correlations, confinement of spinons, and spin-Peierls or valence-bond-solid order controlled by the value of $2S$ (mod 4) or $2S$ (mod 2) ; *(ii)* states with incommensurate, coplanar spin correlations, and unconfined bosonic spin-1/2 spinon excitations. The occurrence of "order from disorder" at large S is discussed. Neither chirally ordered nor spin nematic states are found. Initial results on superconductivity in the $t - J$ model at $N = \infty$ and zero temperature are also presented.

1. INTRODUCTION

Spurred by the discovery of high temperature superconductivity [1], the last few years have seen intense activity in the subject of two-dimensional quantum antiferromagnets. In particular, much attention has been focussed upon understanding the structure of quantum disordered phases of such antiferromagnets [2] and their possible relationship to high temperature superconductivity [3]. Large N expansions [4] on unfrustrated antiferromagnets found columnar spin-Peierls order in the disordered state for half-integer spins [5, 6, 7]. "Chiral" [8] and "spin-nematic" [9] states are among the new structures that have been proposed as ground states of frustrated quantum antiferromagnets.

This paper presents details of a new systematic analytic technique for frustrated and doped antiferromagnets (AFMs) which has been proposed recently [10]. The method relies on a large N expansion based upon models with symplectic symmetry ($Sp(N)$). The method is applied in this paper to two models:
(i) A square lattice AFM with first, second and third neighbor antiferromagnetic coupling - the J_1-J_2-J_3 model. This model has been studied elsewhere by numerical [11, 12], series-expansion [13], and mean-field [14] methods; we will compare our results with these studies later. A particular strength of our approach is that it makes the connection between the structure of the known classically ordered phases and the quantum disordered phases especially clear. It will also clarify the appearance of "order-from-disorder" [15] from quantum fluctuations for models which are classically disordered. We will find new quantum disordered phases which have unconfined bosonic spin-1/2 spinon excitations.
(ii) The square lattice $t - J$ model. We will present initial results in the mean field $N = \infty$ limit at $T = 0$. We find superconducting ground states similar in structure to those of Ref [16].

We begin by motivating the use of a symplectic large N expansion for frustrated AFMs. Previous large N methods have been based on the $SU(N)$ generalization of the $SU(2)$ AFM [4, 6, 7] and have been restricted to unfrustrated AFMs with a two sublattice structure (labeled A,B) for reasons we now explore. "Spins" are placed on sublattice A forming an irreducible representation of $SU(N)$ while those on B form the conjugate representation. Thus *e.g.* totally symmetric representations on sublattice A can be can be formed [4] by placing n_b bosons created by $b_{i\alpha}^\dagger$ where $\alpha = 1 \ldots N$ and $i \in A$; the b^α bosons transform under the fundamental representation of $SU(N)$. The conjugate representation is placed on sublattice

B by n_b bosons created by $\bar{b}_j^{\dagger\alpha}$ for $j \in B$; the $\bar{b}_\alpha$ bosons transform under the representation conjugate to the fundamental. The use of conjugate representations ensures a natural pairing between directions in spin space on the two sublattices. The only possible coupling between sites on opposite sublattices which is invariant under $SU(N)$ and bilinear in the spin operators is

$$-\,(b_{i\alpha}^{\dagger}\bar{b}_j^{\dagger\alpha})(b_i^{\beta}\bar{b}_{j\beta}) \tag{1.1}$$

(For $SU(2)$ this reduces to the usual $S_i \cdot S_j$ plus a constant). In the classical limit ($n_b \to \infty$) this coupling will induce a Néel ground state

$$\prod_{i\in A}\left(b_{i1}^{\dagger}\right)^{n_b}\prod_{j\in B}\left(\bar{b}_j^{1\dagger}\right)^{n_b}|0\rangle. \tag{1.2}$$

In a system with strong quantum fluctuations, this coupling tries to maximize the number of valence bonds

$$\left(b_{i\alpha}^{\dagger}\bar{b}_j^{\dagger\alpha}\right)|0\rangle \tag{1.3}$$

between pairs of sites on opposite sublattices. The only bilinear coupling between sites on the same sublattice is the 'ferromagnetic' coupling

$$-\,(b_{i\alpha}^{\dagger}b_{i'}^{\alpha})(b_{i'\beta}^{\dagger}b_i^{\beta}) \tag{1.4}$$

which demands that the spins on sites i and i' point in the same direction. Reversing the sign of this term will favor states in which the spins point in *any two* unequal directions; this is quite different from the antiferromagnetic coupling which explicitly pairs directions in spin space. Interactions between sites on the same and opposite lattices are thus inequivalent and there is no natural way of introducing a democratic antiferromagnetic coupling between any two sites. Only for $SU(2)$ do the ferromagnetic and antiferromagnetic couplings above become equivalent.

A proper description of a frustrated AFM therefore requires that all the spins transform under the same representation of a group, and that two spins can combine to form a singlet. For $SU(2)$ we can write $\bar{b}_{j\alpha} \equiv \varepsilon_{\alpha\beta}b_j^{\beta}$ ($\varepsilon^{\sigma\sigma'} = -\varepsilon^{\sigma'\sigma}$ and $\varepsilon^{\uparrow\downarrow} = 1$); the boson annihilation operators on all the sites now have an upper index. Singlet bonds $\varepsilon^{\sigma\sigma'}b_{i\sigma}^{\dagger}b_{j\sigma'}^{\dagger}$ can now be formed between any two sites. This structure has a natural generalization to the symplectic groups $Sp(N)$ for all N. These are the groups of $2N \times 2N$ unitary matrices U such that

$$U^T \mathcal{J} U = \mathcal{J} \tag{1.5}$$

where

$$\mathcal{J}_{\alpha\beta} = \mathcal{J}^{\alpha\beta} = \begin{pmatrix} & 1 & & & & \\ -1 & & & & & \\ & & & 1 & & \\ & & -1 & & & \\ & & & & \ddots & \\ & & & & & \ddots \end{pmatrix} \tag{1.6}$$

is the generalization of the ε tensor (note $Sp(1) \cong SU(2)$). This tensor can be used to raise or lower indices on other tensors; all representations are therefore self-conjugate. "Spins" can be created on each site by n_b bosons $b_{i\alpha}^\dagger$ where $\alpha = 1 \ldots 2N$. The b_i^α bosons transform as the fundamental representation of $Sp(N)$; the "spins" on the lattice therefore belong to the symmetric product of n_b fundamentals, which is also an irreducible representation. Valence bonds

$$\mathcal{J}^{\alpha\beta} b_{i\alpha}^\dagger b_{j\alpha}^\dagger \tag{1.7}$$

can be formed between any two sites; this operator is a singlet under $Sp(N)$ because of (1.5). An antiferromagnetic coupling should maximize the number of such bonds between two sites; we will therefore consider models described by the following Hamiltonian

$$H_{AF} = -\sum_{i>j} \frac{J_{ij}}{N} \left(\mathcal{J}^{\alpha\beta} b_{i\alpha}^\dagger b_{j,\beta}^\dagger \right) \left(\mathcal{J}_{\gamma\delta} b_i^\gamma b_j^\delta \right) \tag{1.8}$$

where i, j run over the sites of an arbitrary lattice, and J_{ij} are antiferromagnetic exchange constants. We recall the constraint

$$b_{i\alpha}^\dagger b_i^\alpha = n_b \tag{1.9}$$

which must be imposed at every site. For the group $Sp(1)$ this generates states with spin $S = n_b/2$ at every site.

We now summarize the results obtained in our study of H_{AF} for the model with nearest (J_1), second (J_2) and third (J_3) neighbor interactions on the square lattice. The large N limit was taken with the ratio n_b/N fixed; the results depend strongly on the value of n_b/N. The phases found (Figs 1-4) can be separated into two distinct types:

1. Commensurate, collinear phases

These are closely related to those found in unfrustrated $SU(N)$ AFMs [6, 7]. For large values of n_b/N these states have magnetic long range order (LRO) with the spins polarized parallel or anti-parallel to each other. Upon reducing n_b/N a transition eventually occurs to a corresponding short range ordered (SRO) phase, with a finite spin-correlation length. All the SRO phases are described at long distances and long times by the following effective action when the correlation length is not too small:

$$S_{eff} = \int d^2r \int_0^{c\beta} d\tilde{\tau} \left\{ \frac{1}{g} \left[|(\partial_\mu - iA_\mu)z^\alpha|^2 + \frac{\Delta^2}{c^2}|z^\alpha|^2 \right] \right\} + \cdots , \qquad (1.10)$$

where τ is the Matsubara time, c is the spin-wave velocity, $\tilde{\tau} = c\tau$, and μ runs over $x, y, \tilde{\tau}$. Spatial anisotropy can be also be present but has been neglected for simplicity. The action describes a complex field z^α which transforms under the fundamental of $Sp(N)$ and has a $U(1)$ charge +1; this field is related to the lattice boson b^α, although the form of the relationship varies in different phases. The $U(1)$ gauge field A_μ is related to the phases of certain link-variables, and the gauge symmetry is compact. In the SRO phase, the mass Δ is finite and is proportional to the inverse spin-correlation length. The compact $U(1)$ gauge field leads to confinement of the z quanta and Berry phases of its instantons (monopoles) [5] induce spin-Peierls order for special values of n_b [7]. The LRO phase is reached when Δ vanishes and z quanta condense in the $\mathbf{k}_0 = 0$ state [17]. To characterize the LRO phases by a gauge-invariant order parameter, we consider the expectation value of the 'spin' operators $s_a = \left\langle z^*_\alpha S^a_{\alpha\beta} z^\beta \right\rangle$ (S_a is a generator of $Sp(N)$) across the transition. In the SRO phase these vanish as a result of $Sp(N)$ invariance. In the LRO phase, the order parameter manifold, $M_{\rm coll}$ will be given by $Sp(N)$ modulo the subgroup which leave the s_a invariant. Any orientation of the z condensate can be rotated by $Sp(N)$ transformations such that $\langle z^\alpha \rangle = \bar{z}\delta^{\alpha 1}$. Now the s_a are invariant under the group $Sp(N-1)$ acting on components $\alpha > 2$. An additional factor of $U(1)$ is obtained from the symmetry associated with rotations about the 'z' axis in the $\alpha = 1, 2$ subspace under which $z^1 \to z^1 e^{i\phi}$ and $z^2 \to z^2 e^{-i\phi}$. We have therefore

$$M_{\rm coll} = \frac{Sp(N)}{U(1) \times Sp(N-1)} \qquad (1.11)$$

in direct analogy with $U(N)/(U(1) \times U(N-1)) \cong CP^{N-1}$ for the $SU(N)$ models [6, 18]; for $N = 1$ we recover CP^1 (the unit sphere, S^2). The transition from LRO to SRO is expected to be described by a non-linear sigma ($NL\sigma$) model on $M_{\rm coll}$. We note that $\pi_2(M_{\rm coll}) = Z$, the group of integers, so that topologically stable point defects in spacetime (hedgehogs) exist for all N when the spatial dimension $d = 2$, while $\pi_1 = 0$ so there are no line defects.

2. Incommensurate phases

Frustration induces phases with LRO and SRO in incommensurate helical spin configurations. All of the phases found favor planar arrangement of spins and there is no "chiral" order. In regions not too far from a commensurate phase these states are described at long distances and long times by the following effective action:

$$S_{eff} = \int d^2r \int_0^{c\beta} d\tilde{\tau} \left\{ \frac{1}{g} \left[|(\partial_\mu - iA_\mu)z^\alpha|^2 + \frac{\Delta^2}{c^2}|z^\alpha|^2 \right] + \vec{\Phi} \cdot \left(\mathcal{J}_{\alpha\beta} z^\alpha \vec{\nabla} z^\beta \right) + \text{c.c.} + V(\vec{\Phi}) \right\} + \ldots \qquad (1.12)$$

The new feature is the presence of a charge -2 two-component scalar $\vec{\Phi} = (\Phi_x, \Phi_y)$ related to lattice link fields which induce incommensurate order. The coupling between the z and $\vec{\Phi}$ is the simplest one consistent with global $Sp(N)$ symmetry and is $U(1)$ gauge invariant due to the antisymmetry of $\mathcal{J}$ (a coupling with no gradients of the form $\vec{\Phi}\mathcal{J}_{\alpha\beta}z^\alpha z^\beta$ vanishes identically). The potential $V(\vec{\Phi})$ is induced by short wavelength fluctuations; in the incommensurate phases $V(\vec{\Phi})$ will have minima at a non-zero value of $\vec{\Phi}$ leading to a Higgs phase with $\langle \vec{\Phi} \rangle \neq 0$. All of phases found in this paper have at least two gauge inequivalent minima related to each other by a square lattice symmetry; this leads to a two-fold degeneracy which can only be lifted by explicitly breaking the square lattice symmetry in H_{AF}. The minima are also such that $\langle \Phi_x \rangle$ and $\langle \Phi_y \rangle$ can simultaneously be made real in a suitable gauge. In such a gauge we see from Eqn (1.12) that the minima of the dispersion of the z^α quanta are at wavevectors $\mathbf{k}_0 = \pm g(\langle \Phi_x \rangle, \langle \Phi_y \rangle)/2$. For finite Δ this leads to incommensurate SRO. The z^α quanta have unit charge and will therefore be unconfined [19] in this Higgs phase: these SRO phases therefore possess unconfined bosonic spinons which transform under the fundamental of $Sp(N)$ [20] for all values of the on-site 'spin' n_b. In models which have the two-fold degeneracy lifted by small explicit symmetry breaking terms in H_{AF} these results appear to contradict the 'fractional quantization principle' of Laughlin [21]. As $\Delta \to 0$, the z quanta will condense at $\mathbf{k}_0$ leading to incommensurate LRO. The order-parameter manifold is now

$$M_{\text{noncoll}} = \frac{Sp(N)}{Z_2 \times Sp(N-1)} \qquad (1.13)$$

because the $U(1)$ invariance about the 'z' axis has now been reduced to Z_2 as the spins are no longer collinear. This generalizes the result for $N = 1$, $SO(3) \cong SU(2)/Z_2$ pointed out previously [22, 23]. For M_{noncoll}, $\pi_2 = 0$ but $\pi_1 = Z_2$, so there are line defects in spacetime (vortex worldlines) for $d = 2$ in this case. Instantons and vortices are suppressed in the Higgs phase, so their Berry phases are not expected to lead to spin-Peierls order. However the Berry phases could induce additional intermediate phases between the Higgs and confinement phases: this will be briefly discussed later.

The symplectic groups also have interesting applications to doped AFMs as described *e.g.* by a $t - J$ model. In such a model, the hopping term transfers spin from site to site and so resembles the ferromagnetic coupling (1.4). Thus in $SU(N)$ models with conjugate representations on neighboring sites there is no simple $SU(N)$-invariant hopping term for $N > 2$; if instead one choses all sites with the same representation, hopping can be included but not antiferromagnetic exchange. Our symplectic approach allows inclusion of both exchange and hopping for all N. In particular, using fermions with $Sp(N)$ indices for spins and bosons for holes, the large N limit justifies the decoupling of Ref [16] and produces superconductivity; phase separation into an insulating AFM and hole-rich superconductor is also present. Details of this analysis at $N = \infty$ and zero temperature are presented in Section 4.

The outline of the rest of this paper is as follows. In Section 2 we introduce the general formalism of the $Sp(N)$ large N limit for frustrated AFMs. Section 3 presents detailed results on the J_1-J_2-J_3 model. Finally Section 4 discusses initial results on the t-J model.

2. FRUSTRATED ANTIFERROMAGNETS

We begin by setting up the general framework for the large-N expansion of antiferromagnets with Hamiltonian H_{AF} (Eqn (1.8)). The large-N limit is taken with n_b/N fixed to an arbitrary value. Depending upon the values of the J_{ij} and of n_b/N, the ground state of H_{AF} may either break global $Sp(N)$ symmetry and possess magnetic long-range-order (LRO) or be $Sp(N)$ invariant with only short-range magnetic order (SRO). The structure of the large-N limit is very similar to the $SU(N)$ case, and has been discussed extensively before [4, 7] for the SRO states. We will therefore present details mainly in the LRO phases. The large N limit for these states is most conveniently taken by adapting the method of Brezin and Zinn-Justin [24]. We begin by introducing the parametrization

$$b_i^{m\sigma} \equiv \begin{pmatrix} \sqrt{N} x_i^{\sigma} \\ \tilde{b}_i^{\tilde{m}\sigma} \end{pmatrix} \tag{2.1}$$

We have introduced a natural double-index notation $\alpha \equiv (m, \sigma)$ with $m = 1 \ldots N$ and $\sigma = \uparrow, \downarrow$. The index $\tilde{m} = 2, \ldots N$. The x^σ field has been introduced to allow for a non-zero condensate $\langle b_i^{m\sigma} \rangle = \sqrt{N} \delta_1^m x_i^\sigma$; we will only consider models in which the condensate in the LRO phase can be transformed by a uniform global $Sp(N)$ rotation into this form. We insert (2.1) into H_{AF}, decouple the quartic terms by Hubbard-Stratanovich fields Q_{ij}, and enforce the constraints by the Largrange multipliers λ_i. This yields

$$H_{MF} = \sum_{i>j} \left(N J_{ij} |Q_{ij}|^2 - J_{ij} Q_{ij} \varepsilon_{\sigma\sigma'} \left(N x_i^\sigma x_j^{\sigma'} + \sum_{\tilde{m}} \tilde{b}_i^{\tilde{m}\sigma} \tilde{b}_j^{\tilde{m}\sigma'} \right) + \text{H. c.} \right) + \sum_i \lambda_i \left(N |x_i^\sigma|^2 + \sum_{\tilde{m}} \tilde{b}_{i,\tilde{m}\sigma}^\dagger \tilde{b}_i^{\tilde{m}\sigma} - n_b \right) \tag{2.2}$$

The large N limit is obtained by integrating over the $2(N-1)$ $\tilde{b}$ fields. The resulting effective action, expressed in terms of the Q_{ij}, λ_i and x_i^σ fields, will have a prefactor of N (and some terms of order 1 which are sub-dominant) and is therefore well approximated by its saddle-point value. The Q, λ, x fields are expected to be time-independent at the saddle-point and this is implicitly assumed in the following. The functional integral over the $\tilde{b}$ requires knowledge of the eigenmodes of H_{MF}. This can be done along standard lines: we first solve the eigenvalue equation

$$\begin{aligned} \lambda_i U_{i\mu} - \sum_j J_{ij} Q_{ij}^* V_{j\mu} &= \omega_\mu U_{i\mu} \\ \sum_i J_{ij} Q_{ij} U_{i\mu} - \lambda_j V_{j\mu} &= \omega_\mu V_{j\mu} \end{aligned} \tag{2.3}$$

for the N_s (= number of sites in the system) positive eigenvalues ω_μ and the corresponding eigenvectors $(U_{i\mu}, V_{j\mu})$. The bosonic eigenoperators $\gamma_\mu^{\tilde{m}\sigma}$

$$\gamma_\mu^{\tilde{m}\sigma} = \sum_i \left(U_{i\mu}^* \tilde{b}_i^{\tilde{m}\sigma} - \delta^{\tilde{m}\tilde{m}'} \varepsilon^{\sigma\sigma'} V_{i\mu}^* \tilde{b}_{i\tilde{m}'\sigma'}^\dagger \right) \tag{2.4}$$

will diagonalize H_{MF}. The inverse relation is

$$\tilde{b}_i^{\tilde{m}\sigma} = \sum_\mu \left(U_{i\mu} \gamma_\mu^{\tilde{m}\sigma} - \delta^{\tilde{m}\tilde{m}'} \varepsilon^{\sigma\sigma'} V_{i\mu}^* \gamma_{\mu\tilde{m}'\sigma'}^\dagger \right) \tag{2.5}$$

Consistency of these relations imposes certain orthogonality requirements on (U, V). It can be shown using Eqn (2.3) that these can always be satisfied. Finally the ground state energy, E_{MF} of H_{MF} is shown to be

$$\frac{E_{MF}}{N} = \sum_{i>j} \left(J_{ij} |Q_{ij}|^2 - J_{ij} Q_{ij} \varepsilon_{\sigma\sigma'} x_i^\sigma x_j^{\sigma'} + \text{H. c.} \right) - \sum_i \lambda_i \left(1 + \frac{n_b}{N} - |x_i^\sigma|^2 \right) + \sum_\mu \omega_\mu \tag{2.6}$$

We note that the ω_μ also depend upon Q, λ. Finding the ground state of H_{AF} in the large N limit is now reduced to the problem of minimizing E_{MF} with respect to the independent variables Q_{ij}, x_i^σ with the λ_i chosen such that the constraints

$$\frac{\partial E_{MF}}{\partial \lambda_i} = 0 \tag{2.7}$$

are always satisfied. It is instructive to examine the equations obtained by demanding stationarity of E_{MF} w.r.t x_i^σ:

$$\sum_j \varepsilon_{\sigma\sigma'} J_{ij} Q_{ij} x_j^{\sigma'} + \lambda_i x_{i\sigma}^* = 0 \tag{2.8}$$

This equation has two possible solutions: *(i)* $x_i^\sigma = 0$: this gives the SRO phases *(ii)* $x_i^\sigma \neq 0$: comparing Eqn (2.8) with Eqn (2.3) we see that this condition is equivalent to demanding that Eqn (2.3) possess at least one zero eigenvalue. For finite n_b, this will only occur in the limit $N_s \to \infty$, and implies the existence of gapless excitations. These are the Goldstone modes associated with the $Sp(N)$ symmetry breaking.

We now examine the large n_b/N limit of H_{MF}; it is easy to show that $Q_{ij} \sim \lambda_i \sim n_b/N$ while $x_i^\sigma \sim \sqrt{n_b/N}$. From Eqn (2.6) we observe that the sum over ω_μ can be neglected and for large n_b/N, E_{MF} reduces to

$$\frac{E_{MF}^c}{N} = \sum_{i>j} \left(J_{ij} |Q_{ij}|^2 - J_{ij} Q_{ij} \varepsilon_{\sigma\sigma'} x_i^\sigma x_j^{\sigma'} + \text{H. c.} \right) - \sum_i \lambda_i \left(\frac{n_b}{N} - |x_i^\sigma|^2 \right) \tag{2.9}$$

The minimization of E_{MF}^c w.r.t. Q_{ij} can now be easily carried out and the problem reduces to that of finding the classical ground state of H_{AF}. Thus the large n_b/N limit of the present large N equations is equivalent to the classical limit which involves $n_b \to \infty$ at fixed N. The fact that these two limits commute gives us further confidence on the usefulness of the present large N procedure.

Finally we indicate how this formalism can be used to evaluate the spin-stiffness of the LRO phases in the large N limit. One takes values of x_i^σ which minimize E_{MF} and performs a slowly varying rotation:

$$x_i^\sigma \to \left(\exp\left(i \frac{\vec{n} \cdot \vec{\tau}}{2} \vec{k} \cdot \vec{R}_i \right) \right)_{\sigma\sigma'} x_i^{\sigma'} \tag{2.10}$$

where $\vec{n}$ is the direction in spin-space about which the rotation has been performed, $\vec{\tau}$ are the Pauli matrices, and $\vec{k}$ is a small wavevector. We insert this value of x_i^σ in E_{MF}, reminimize w.r.t. the Q_{ij} while maintaining the constraints and determine the change in energy ΔE_{MF} for small $\vec{k}$. We expect in general

$$\Delta E_{MF} = \frac{N_s}{2} \rho_{\alpha\beta}(\vec{n}) k_\alpha k_\beta + \cdots \tag{2.11}$$

The co-efficient ρ is the spin-stiffness tensor of the LRO phase about the direction $\vec{n}$.

3. THE $\mathbf{J_1}$-$\mathbf{J_2}$-$\mathbf{J_3}$ MODEL

We now apply the formalism developed in the previous section to a frustrated antiferromagnet on the square lattice with first (J_1), second (J_2) and third (J_3) neighbor interactions. This model has been examined by numerical [11, 12], series [13] and mean-field [14] methods in the literature; their results will be compared with ours in section 3.D. We begin by presenting the results of the $N = \infty$ mean field theory (section 3.A). The effective actions controlling the long-wavelength, long-time fluctuations at finite N will be considered in section 3.B. Berry phases and the spin-Peierls order they induce will be disussed in section 3.C.

3.A Mean Field Theory

The energy E_{MF} for this model was minimized over all fields Q_{ij} and λ_i which were periodic with a $\sqrt{2} \times \sqrt{2}$ unit cell. All of the global minima found in fact turned out to have a periodicity with one site per unit cell: we will therefore restrict our analysis to this simpler limit. In addition, full wavevector-dependent stability matrices involving quadratic fluctuations of E_{MF} on the manifold specified by Eqn (2.7) were evaluated at representative points, and all eigenvalues found to be positive. This gives us reasonable confidence that the states described below are in fact the global minima of E_{MF}.

With one site per unit cell, the link variational parameters are the nearest neighbor fields $Q_{1,x}, Q_{1,y}$, the diagonal 2nd neighbor fields $Q_{2,y+x}, Q_{2,y-x}$ and the 3rd neighbor fields $Q_{3,x}, Q_{3,y}$. The bosonic eigenmodes can be calculated exactly and we find the eigenenergies:

$$\omega_{\mathbf{k}} = \left(\lambda^2 - 4|A_{\mathbf{k}}|^2\right)^{1/2}$$

$$A_{\mathbf{k}} = J_1\left(Q_{1,x}\sin k_x + Q_{1,y}\sin k_y\right) + J_2\left(Q_{2,y+x}\sin(k_y + k_x) + Q_{2,y-x}\sin(k_y - k_x)\right) + J_3\left(Q_{3,x}\sin(2k_x) + Q_{3,y}\sin(2k_y)\right) \qquad (3.1)$$

The wavevector $\mathbf{k}$ extends over the first Brillouin zone of the square lattice.

Our results for $J_3 = 0$ are summarized in Fig. 1. We begin by discussing the structure of the ground state at $N = \infty$. We find 3 distinct types of phases:

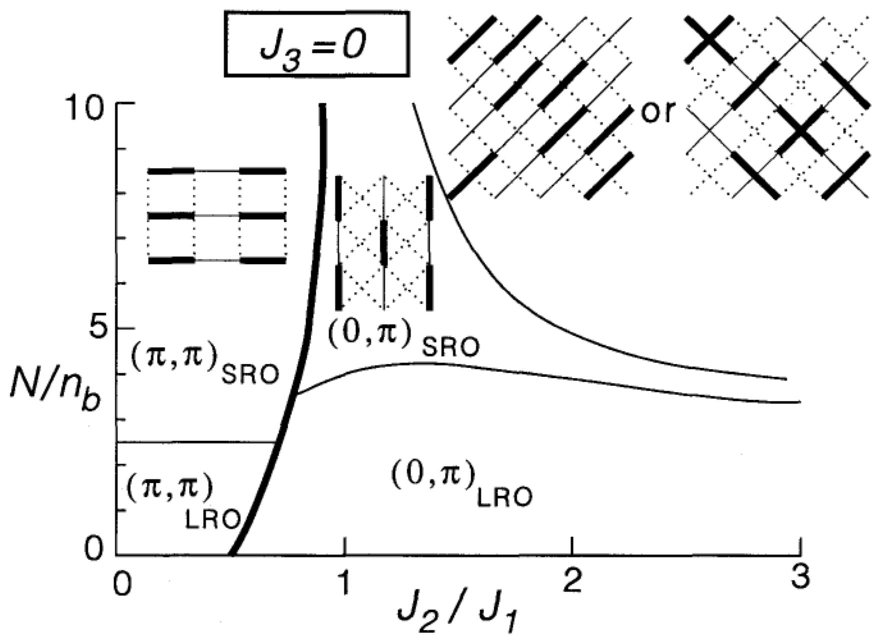

Fig 1. Ground states of H for $J_3 = 0$ as a function of J_2/J_1 and N/n_b ($n_b = 2S$ for $Sp(1) \cong SU(2)$). Thick (thin) lines denote first (second) order transitions at $N = \infty$. Phases are identified by the wavevectors at which they have magnetic long-range-order (LRO) or short-range-order (SRO). The links with $Q_p \neq 0$ in each SRO phase are shown. The large N/n_b, large J_2/J_1 phase has the two sublattices decoupled at $N = \infty$; each sublattice has Néel-type SRO. Spin-Peierls order at finite N for odd n_b is illustrated by the thick, thin and dotted lines. The (π,π)-SRO and the "decoupled" states have line-type (Ref. 7) spin-Peierls order for $n_b = 2 \pmod 4$ and are VBS for $n_b = 0 \pmod 4$. The $(0,\pi)$-SRO state is a VBS for all even n_b.

3.A.1 (π, π)

These states have $Q_{1,x} = Q_{1,y} \neq 0$, $Q_{2,y+x} = Q_{2,y-x} = Q_{3,x} = Q_{3,y} = 0$ and are the analogs of the states found in $SU(N)$ systems. Inserting these values into Eqn (3.1) we see that $\omega_{\mathbf{k}}$ has its minima at $\pm(\pi/2, \pi/2)$: this implies that the spin-spin correlation function, which involves the product of two bosonic pair correlation functions [4], will have a peak at (π, π). We have a state with $x_i^\sigma \neq 0$ (LRO) for $N/n_b < 2.5$ and the corresponding SRO state for $N/n_b > 2.5$. The boundary between LRO and SRO is independent of J_2/J_1, but this is surely an artifact of the large N limit. Finite N fluctuations should be stronger as J_2/J_1 increases, causing the boundary to bend a little downwards to the right. While properties of these states can be calculated numerically for all values of J_2/J_1 and N/n_b, we tabulate a few analytic results for the LRO phase in an expansion in powers of N/n_b. The ground state energy is

$$E_{MF} = -NN_s \left(\frac{n_b}{N}\right)^2 \left[2J_1 + 4(1 - I_1)J_1 \left(\frac{N}{n_b}\right) + \cdots\right] \tag{3.2}$$

where $I_1 = 0.84205$ is obtained from an integral over the Brillouin zone. The spin-stiffness for spin rotations about an axis perpendicular to the Néel axis is found to be

$$\rho_{\alpha\beta} = \delta_{\alpha\beta} N \left(\frac{n_b}{N}\right)^2 \frac{1}{2} \left[J_1 - 2J_2 + [4J_2(I_2 - 1) - J_1(I_1 + I_2 - 2)] \left(\frac{N}{n_b}\right) + \cdots\right] \tag{3.3}$$

with $I_2 = 1.39320$.

3.A.2 $(\pi, 0)$ or $(0, \pi)$

The $(0, \pi)$ states have $Q_{1,x} = 0$, $Q_{1,y} \neq 0$, $Q_{2,y+x} = Q_{2,y-x} \neq 0$, and $Q_{3,x} = Q_{3,y} = 0$ and occur with LRO and SRO. The degenerate $(\pi, 0)$ state is obtained with the mapping $x \leftrightarrow y$. For $J_2/J_1 > 1/2$, the classical limit, has independent Néel order on each of the A and B sublattices; quantum fluctuations, which are automatically included in the present approach, cause the Néel order parameters to align ("order from disorder") leading to the LRO states. To understand the nature of the transition between LRO at (π, π) to LRO at $(\pi, 0)$ or $(0, \pi)$ we need the energy and stiffness of the latter states for small N/n_b. We find

$$E_{MF} = -NN_s \left(\frac{n_b}{N}\right)^2 \left[J_1 + 2J_2 + (2J_1 + 4J_2 - 4J_1 I_3) \left(\frac{N}{n_b}\right) + \cdots\right] \tag{3.4}$$

where I_3 is a Brillouin zone integral whose value depends upon J_2/J_1; we will only need its value at $J_2/J_1 = 0.5$: $I_3 = 0.88241$. The stiffness of the $(0, \pi)$ state is soft at small n_b/N for wavevectors in the x-direction:

$$\rho_{xx} = N\left(\frac{n_b}{N}\right)^2 \frac{1}{2}\left[2J_2 - J_1 + 2\left[J_2(2 + I_5 - 2I_4) + J_1(I_4 - 1)\right]\left(\frac{N}{n_b}\right) + \cdots\right] \quad (3.5)$$

where I_4, I_5 are Brillouin zone integrals dependent upon J_2/J_1. Again we will only need their values at $J_2/J_1 = 0.5$ which are $I_4 = 1.28576$ and $I_5 = 0.32767$. Comparing Eqns (3.2) and (3.4) we see that the energies of the (π,π)-LRO and $(0,\pi)$-LRO states become equal at

$$J_2 = J_1\left[\frac{1}{2} + 0.08072\left(\frac{N}{n_b}\right) + \cdots\right] \quad (3.6)$$

At this value of J_2/J_1 the stiffness of the (π,π) state is found to be

$$\rho_{\alpha\beta}(\pi,\pi) = 0.1949N\left(\frac{n_b}{N}\right)\delta_{\alpha\beta} + \cdots \quad (3.7)$$

while the stiffness of the $(0,\pi)$ state is

$$\rho_{xx}(0,\pi) = 0.2446N\left(\frac{n_b}{N}\right) + \cdots \quad (3.8)$$

Thus both stiffnesses are positive and indicate that the transition between the states is first order. Note that in both stiffnesses the leading $N(n_b/N)^2$ term is absent; these stiffnesses thus vanish classically and have appeared directly as a result of quantum fluctuations—another example of "order from disorder". These results contradict arguments in Ref. [25] that another 'spin liquid' phase exists at arbitrarily small N/n_b near $J_2/J_1 = 0.5$. While we agree that quantum fluctuations are very important in a 'fan' emanating from $J_2/J_1 = 0.5$, $N/n_b = 0$, we have found that these fluctuations just reinforce the classical order. At larger values of N/n_b we have a continuous (at $N = \infty$) transition to the $(0,\pi)$-SRO or $(\pi,0)$-SRO state. The transition between this state and (π,π)-SRO remains first-order.

3.A.3 "Decoupled"

For J_2/J_1 and N/n_b both large, we have a "decoupled" state with $Q_{2,y+x} = Q_{2,y-x} \neq 0$ and $Q_1 = Q_3 = 0$. In this case Q_p is non-zero only for sites on the same sublattice. The two sublattices have Néel type SRO which will be coupled by finite N fluctuations. The $N = \infty$ state does not break any lattice symmetry.

We now turn to $J_3 \neq 0$ (Figs 2-4), where we find a new class of phases:

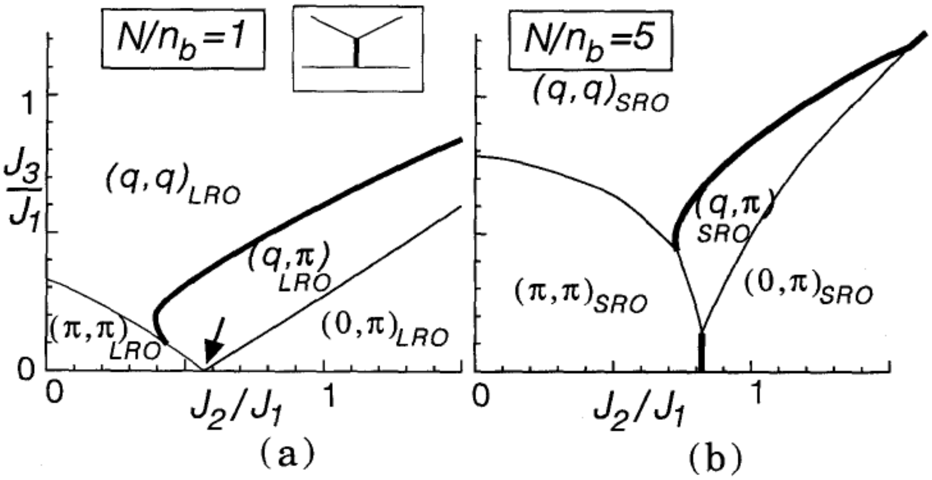

Fig 2. As in Fig 1 but as a function of J_2/J_1 and J_3/J_1 for (a) $N/n_b = 1$ and (b) $N/n_b = 5$. The inset in (a) shows the region at the tip of the arrow magnified by 20: a direct first-order transition from (π,π)-LRO to $(0,\pi)$-LRO occurs up to $J_3/J_1 = 0.005$.

3.A.4 Incommensurate phases

It is known that for finite J_3, the classical magnet has phases with incommensurate helical (coplanar) order [13]. Our phase diagram for a small value of N/n_b ($N/n_b = 1$, Fig 2a) is similar to the classical one. All of the LRO phases undergo continuous transitions to SRO with the same spatial distribution of the Q_p and the accompanying broken rotational symmetry of the lattice. These SRO phases are shown in Fig 2b. The two new classes of phases which did not appear at $J_3 = 0$ are: (i) $\pm(q,\pi)$ phases with $Q_{1,x} \neq Q_{1,y} \neq 0$, $Q_{2,x+y} = Q_{2,y-x} \neq 0$, $Q_{3,x} \neq 0$ and $Q_{3,y} = 0$; the degenerate $\pm(\pi,q)$ helix is obtained by the mapping $x \leftrightarrow y$. (ii) $\pm(q,q)$ phases with $Q_{1,x} = Q_{1,y} \neq 0$, $Q_{2,x+y} \neq 0$, $Q_{2,y-x} = 0$, $Q_{3,x} = Q_{3,y} \neq 0$; this is degenerate with $(q,-q)$ phases[26]. The wavevector q varies smoothly from 0 to π and is determined by doubling the wavevector at which $\omega_{\mathbf{k}}$ has a minimum; it is continuous across second-order phase boundaries (Fig 2a). In contrast to the classical limit [13], for N/n_b finite it requires a finite J_3 to induce helical order; the first order transition from (π,π) to $(\pi,0)$ order persists for small J_3 as shown in the inset of Fig 2a. This suggests that quantum fluctuations induce an effective ferromagnetic J_3 in the model with bare $J_3 = 0$; a finite bare antiferromagnetic J_3 is required to compensate for this.

The broken discrete symmetries in states with SRO at $(0,\pi)$ and (q,π) are identical: both are two-fold degenerate due to a breaking of the $x \leftrightarrow y$ symmetry. The states are only distinguished by a non-zero value of Q_3 in the (q,π) phase and the accompanying incommensurate correlations in the spin-spin correlation functions. However Q_3 is gauge-dependent and so somewhat unphysical as an order parameter. In the absence of any further fluctuation-driven lattice symmetry breaking (see below), the transition between SRO at $(0,\pi)$ and (q,π) is an example of a *disorder line* [27]; these are lines at which incommensurate correlations first turn on.

Fig 3 shows the transition from LRO to SRO as a function of N/n_b for $J_3 = 0.35J_1$. Similar transitions also appear in Fig 4 which has $J_3 = J_2/2$. There are several notable features of these two phase diagrams:

(i) An intermediate state in which $Sp(N)$ symmetry is only partially restored (spin-nematic [9]) does not appear in the large N limit. We expect the transition from (q,q)-LRO to (q,q)-SRO to be described by a $NL\sigma$ model on the manifold M_{noncoll}. A $d = 1+\epsilon$ expansion of a similar $NL\sigma$ model [28] for $N = 1$ has been recently carried out and does not show any tendency towards such ordering.

(ii)The Q_p variables can all be chosen real in all the phases, indicating the absence

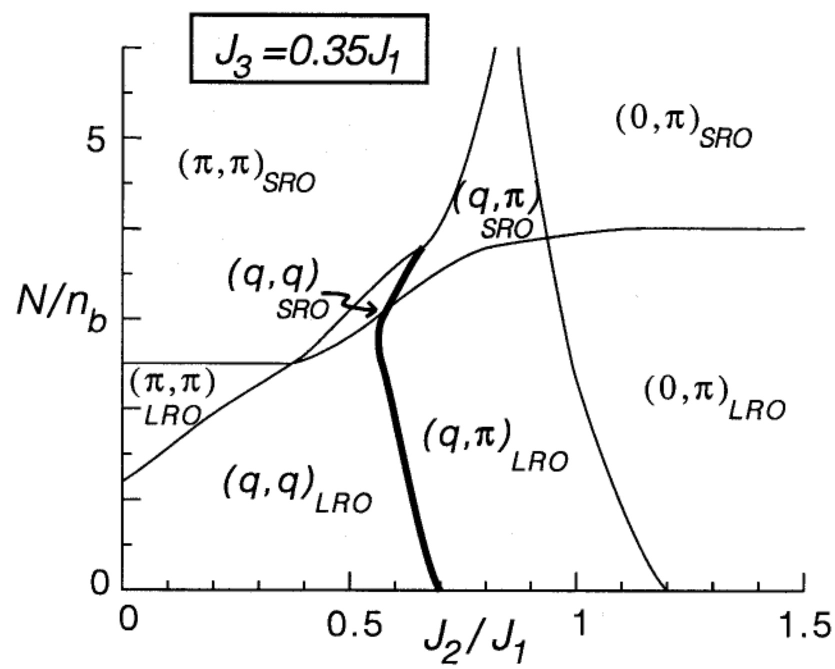

Fig 3. As in Fig. 1 but for $J_3/J_1 = 0.35$.

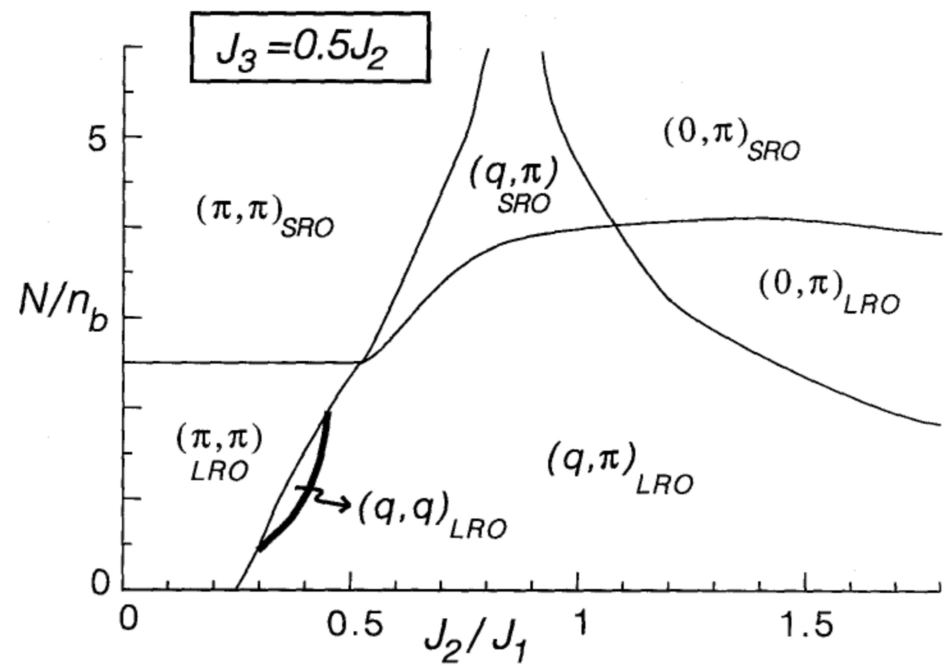

Fig 4. As in Fig. 1 but for $J_3/J_2 = 0.5$.

of "chiral" [8] order.

(*iii*) The commensurate states squeeze out the incommensurate phases as N/n_b increases in both phase diagrams. We expect that this suppression of incommensurate order by quantum fluctuations is a general feature of frustrated AFMs.

3.B Fluctuations - Long Wavelength Effective Actions

This section will examine the form of the effective action controlling the long-wavelength fluctuations of the b^α quanta and the link fields Q_p. We will focus mainly on the SRO phases in the region close to the transition to the LRO phases.

We begin by examining the (π,π)-SRO phase; this phase has already been examined in considerable detail in Ref [7] for the $SU(N)$ AFM; here we adapt the results to the $Sp(N)$ AFM. As noted above, this phase has the mean field values $Q_{1,x} = Q_{1,y} = \bar{Q}_1$, and $\omega_{\mathbf{k}}$ has minima at $\pm\vec{G}$, with $\vec{G} = (\pi/2, \pi/2)$. Close to the LRO phases, fluctuations of the b^α will be strong at $\pm\vec{G}$. We therefore parametrize

$$b_i^\alpha = \varphi_+^\alpha(\vec{r}_i)e^{i\vec{G}\cdot\vec{r}_i} + \varphi_-^\alpha(\vec{r}_i)e^{-i\vec{G}\cdot\vec{r}_i} \tag{3.9}$$

where $\varphi_\pm$ are assumed to have slow spatial variations. The most important component of the fluctuations of the Q_{ij} are those of their phases. In particular, as noted in Ref [7], the mean-field theory has an unbroken gauge symmetry; the transformation

$$b_i^\alpha \to b_i^\alpha e^{i\gamma_i\theta} \tag{3.10}$$

where $\gamma_i = 1(-1)$ for $r_{ix} + r_{iy}$ even (odd), leaves all $\langle Q_{ij}\rangle$ invariant. A staggered component of the phases of the Q_{ij} acts as the vector potential associated with this gauge symmetry. We therefore write

$$Q_{i,i+\hat{x}} = \bar{Q}_1 \exp\left(i\gamma_i A_x(\vec{r}_i + \hat{x}/2)\right) \tag{3.11}$$

where again A_x is slowly varying; a similar equation holds for A_y. The time-component of the gauge-field is the fluctuation in the Lagrange multiplier:

$$\lambda_i = \bar{\lambda} + i\gamma_i A_\tau(\vec{r}_i) \tag{3.12}$$

We now insert the ansatzes (3.9), (3.11) and (3.12) into the Lagrangian $\mathcal{L}$ associated with H_{AF} and perform a gradient expansion on all the terms. The final result is most compactly expressed in terms of the fields

$$\begin{aligned} \psi_1^\alpha &= (\varphi_+^\alpha + \varphi_-^\alpha)/\sqrt{2} \\ \psi_{2\alpha} &= -i\mathcal{J}_{\alpha\beta}(\varphi_+^\beta - \varphi_-^\beta)/\sqrt{2} \end{aligned} \tag{3.13}$$

and has the form

$$\mathcal{L} = \int \frac{d^2r}{a^2} \left[\psi_{1\alpha}^* \left(\frac{d}{d\tau} + iA_\tau \right) \psi_1^\alpha + \psi_2^{\alpha *} \left(\frac{d}{d\tau} - iA_\tau \right) \psi_{2\alpha} + \bar{\lambda} \left(|\psi_1^\alpha|^2 + |\psi_{2\alpha}|^2 \right) - 4J_1 \bar{Q}_1 \left(\psi_1^\alpha \psi_{2\alpha} + \psi_{1\alpha}^* \psi_2^{\alpha *} \right) + J_1 \bar{Q}_1 a^2 \left[\left(\vec{\nabla} + i\vec{A} \right) \psi_1^\alpha \left(\vec{\nabla} - i\vec{A} \right) \psi_{2\alpha} + \left(\vec{\nabla} - i\vec{A} \right) \psi_{1\alpha}^* \left(\vec{\nabla} + i\vec{A} \right) \psi_2^{\alpha *} \right] \right] \quad (3.14)$$

We now introduce the fields

$$z^\alpha = (\psi_1^\alpha + \psi_2^{\alpha *})/\sqrt{2}$$
$$\pi^\alpha = (\psi_1^\alpha - \psi_2^{\alpha *})/\sqrt{2}.$$

From Eqn (3.14), it is clear that the the π fields turn out to have mass $\bar{\lambda} + 4J_1\bar{Q}_1$, while the z fields have a mass $\bar{\lambda} - 4J_1\bar{Q}_1$ which vanishes at the transition to the LRO phase. The π fields can therefore be safely integrated out, and $\mathcal{L}$ yields the following effective action, valid at distances much larger than the lattice spacing:

$$S_{eff} = \int \frac{d^2r}{\sqrt{8}a} \int_0^{c\beta} d\tilde{\tau} \left\{ |(\partial_\mu - iA_\mu) z^\alpha|^2 + \frac{\Delta^2}{c^2} |z^\alpha|^2 \right\}, \quad (3.15)$$

Here $c = \sqrt{8} J_1 \bar{Q}_1 a$ is the spin-wave velocity, $\Delta = (\lambda^2 - 16 J_1^2 \bar{Q}_1^2)^{1/2}$ is the gap towards spinon excitations, and $A_{\tilde{\tau}} = A_\tau / c$; this action is of the form (1.10) quoted in the introduction. Thus, in its final form, the long-wavelength theory consists of a massive z^α scalar (spinon) coupled to a compact $U(1)$ gauge field.

We now examine the changes in the above actions as one moves from the (π,π)-SRO phase into the (q,q)-SRO phase (Fig 2b) (a very similar analysis can be performed at the boundary between the (π,π)-SRO and the (π,q)- SRO phases). This transition is characterized by a continuous turning on of non-zero values of $Q_{i,i+\hat{y}+\hat{x}}$, $Q_{i,i+2\hat{x}}$ and $Q_{i,i+2\hat{y}}$. It is easy to see from Eqn (3.10) that these fields transform as scalars of charge $2\gamma_i$ under gauge transformation associated with A_μ. Performing a gradient expansion upon the bosonic fields coupled to these scalars we find that the Lagrangian $\mathcal{L}$ of the (π,π)-SRO phase gets modified to

$$\mathcal{L} \to \mathcal{L} + \int \frac{d^2r}{a} \left(\vec{\Phi}_A \cdot \left(\mathcal{J}_{\alpha\beta} \psi_1^\alpha \vec{\nabla} \psi_1^\beta \right) + \vec{\Phi}_B \cdot \left(\mathcal{J}^{\alpha\beta} \psi_{2\alpha} \vec{\nabla} \psi_{2\beta} \right) + \text{c.c.} \right) \quad (3.16)$$

where $\vec{\Phi}_{A,B} \equiv (J_3 Q_{3,x} + J_2 Q_{2,y+x}, J_3 Q_{3,y} + J_2 Q_{2,y+x})$ with the sites on the ends of the link variables on sublattices A, B. Finally, as before, we transform to the z, π variables, integrate out the π fluctuations and obtain

$$S_{eff} = \int \frac{d^2r}{\sqrt{8}a} \int_0^{c\beta} d\tilde{\tau} \left\{ |(\partial_\mu - iA_\mu) z^\alpha|^2 + \frac{\Delta^2}{c^2} |z^\alpha|^2 + \vec{\Phi} \cdot \left(\mathcal{J}_{\alpha\beta} z^\alpha \vec{\nabla} z^\beta \right) + \text{c.c.} + V(\Phi) \right\} \quad (3.17)$$

Here $\vec{\Phi} = (\vec{\Phi}_A + \vec{\Phi}^*_B)/(2J_1\bar{Q}_1 a)$ is a scalar of charge -2; terms higher order in $\vec{\Phi}$ have been dropped. We have also added a phenomenological potential $V(\Phi)$ which is generated by short wavelength fluctuations of the b^α quanta. This action is of the general form (1.12), and as noted earlier, is the simplest one consistent with the requirements of $U(1)$-gauge and global $Sp(N)$ invariance. In a phase with $\langle\vec{\Phi}\rangle \neq 0$ and real, we see from Eqn (3.17) that the minimum of the dispersion of the z^α quanta is at a wavevector $\mathbf{k}_0 = (\langle\Phi_x\rangle, \langle\Phi_y\rangle)/2$: this will lead to incommensurate order. The action (3.17) thus demonstrates clearly the intimate connection between the Higgs phenomenon and the appearance of incommensurate correlations.

We now turn to the $(0,\pi)$-SRO phase; we will find that its properties are quite similar to the (π,π)-SRO phase. We recall that this phase has the mean-field values $Q_{2,y+x} = Q_{2,y-x} = \bar{Q}_2$, $Q_{1,y} = \bar{Q}_1$ and $Q_{1,x} = 0$. The excitation energies $\omega_{\mathbf{k}}$ now have minima at $\pm\vec{G}$ with $\vec{G} = (0,\pi/2)$. We therefore parametrize the b^α fields as in Eqn (3.9), but using the new value of $\vec{G}$. This phase also has an unbroken $U(1)$ gauge symmetry; the main difference is in the staggering pattern of the charges of the b^α quanta. With the choice of the constants $\gamma_i = 1(-1)$ for r_{iy} even (odd) in Eqn (3.10) it is easily verified that all mean-field expectations $\langle Q_{ij}\rangle$ remain invariant. The phases of the link fields are parametrized as in Eqn (3.11) in terms of a vector potential A but with the new γ_i; the diagonal link fields have the parametrization

$$Q_{i,i+\hat{y}+\hat{x}} = \bar{Q}_2 \exp\left[i\gamma_i\left(A_y(\vec{r}_i + \hat{y}/2 + \hat{x}/2) + A_x(\vec{r}_i + \hat{y}/2 + \hat{x}/2)\right)\right] \qquad (3.18)$$

and similarly for $Q_{i,i+\hat{y}-\hat{x}}$. The remaining analysis is essentially identical to that for the (π,π)-SRO phase and we obtain the same final effective action S_{eff} (Eqn (3.15)) with an additional spatial anisotropy. The connection between the z^α quanta and the lattice bosons and between A_μ and the phases of the link fields are now of course different.

The transition from $(0,\pi)$-SRO to (q,π)-SRO follows the treatment above of the transition from (π,π)-SRO to (q,q)-SRO; the final action for the incommensurate phase has the same form as Eqn (3.17).

3.C Berry Phases

For the unfrustrated $SU(N)$ magnets, Berry phases associated with instanton tunneling events had particularly strong consequences in the SRO phase [5, 7]. Very similar effects occur in the commensurate SRO phases of the J_1-J_2-J_3 model. We consider the various phases in turn:

3.C.1 (π, π)

This phase is essentially identical to the $SU(N)$ case [7]. The instantons have Berry phases $n_b \zeta_s \pi/2$ where $\zeta_s = 0, 1, 2, 3$ on dual lattice points with (even,even), (even,odd), (odd,odd), (odd, ,even) co- ordinates. Condensation of the instantons leads to spin-Peierls order of column (shown in Fig. 1) or line type (not shown) for $n_b = 1, 3 \pmod 4$ and 2 respectively, or a featureless VBS state [29] for $n_b = 0 \pmod 4$, throughout the (π, π) SRO phase. The b^α quanta are confined by the compact $U(1)$ gauge force, with a confinement length scale determined by the instanton density [30].

3.C.2 "Decoupled"

We can apply the analysis of subsection 3.C.1 to each sublattice separately, giving *e.g.* for $n_b = 1 \pmod 4$ the type of spin-Peierls correlations shown in Fig. 1. There is a total of $4 \times 4 = 16$ states for this case but coupling between the sublattices will reduce this to 8 states, all of one of the two types shown. The state with the 'dimers' parallel to one another has more possibilities for resonance using the J_1 bonds and is likely to be the ground state. For $n_b = 2 \pmod 4$, there will be $2 \times 2/2 = 2$ states, and for $n_b = 0 \pmod 4$, just one.

3.C.3 $(0, \pi)$

As in the other collinear phases, this state possesses instantons which are the remnants of hedgehogs in the LRO phase. A natural location for these instantons is at the center of the horizontal links which have $Q_{1,x} = 0$; the spins at the ends of these links are ferromagnetically aligned and are most susceptible to large deformations. The Berry phase for a configuration of well separated instanton charges m_s at co-ordinates $\mathbf{R}_s$ can be calculated as before [7, 5] and we find

$$S_B = i n_b \sum_s \sum_i [m_s \gamma_i \theta_s(\mathbf{r}_i)] \tag{3.19}$$

where $\theta_s(\mathbf{r}_i)$ is an angle which winds by 2π as $\mathbf{r}_i$ moves around $\mathbf{R}_s$, the sum over i extends over all the sites of the lattice and γ_i is the staggering associated with the $(0, \pi)$ phase *i.e.* $\gamma_i = 1(-1)$ for r_{iy} even (odd). The sum over i can be evaluated in a manner similar to Ref [5]. Consider first an isolated instanton of unit charge at $\mathbf{R}_s$; rewrite the summation in (3.19) as one over vertical links of the square lattice:

$$S_B = i n_b \sum_i \frac{\gamma_i}{2} [\theta_s(\mathbf{r}_i) - \theta_s(\mathbf{r}_{i+\hat{y}})] \tag{3.20}$$

The symmetry of the mean-field $(0,\pi)$ state with one instanton now requires that the contribution of the links be odd under reflection across the horizontal line running through $\mathbf{R}_s$. The majority of the links will cancel against their reflection partners, the only exceptions being the links which intersect the cut in the angle field $\theta_s(\mathbf{r}_i)$; these will yield an additional contribution of $i\pi n_b$. We expect that these symmetry considerations will also be valid for a configuration of well separated instantons. Combining the contributions of all the instantons we obtain finally

$$S_B = i\pi n_b \sum_s m_s [R_{sx}] \tag{3.21}$$

where $[R_{sx}]$ is the integer part of R_x. In the SRO phase the instantons interact with a Coulombic $1/R$ potential; the instanton plasma can therefore be mapped onto a dual sine-Gordon model [7] in which the instanton Berry phases appear as frustrating phase-shifts in the arguments of the cosine term [7]. This model can be analyzed in a manner which closely parallels Ref [7]. The Berry phases lead to condensation of the instanton charges and to spin-Peierls order of the type shown in Fig. 1 for n_b odd, and a VBS state for n_b even. Combined with the choice $(0,\pi)$ or $(\pi,0)$ this gives degeneracies $2,4,2,4$ for $n_b = 0,1,2,3 \pmod 4$.

3.C.4 Incommensurate Phases

As the action (3.17) makes clear, these phases require an additional charge -2 field $\vec{\Phi}$ for their description. In the SRO phases, the z^α quanta can be integrated out and we are left with a lattice gauge theory of a compact $U(1)$ gauge field and a charge -2 scalar. The scalar fields can form vortices with flux quantum π: instantons can change this flux by 2π, so only a Z_2 quantum number is topologically stable [31], in agreement with the analysis of the LRO phase. If the vortices proliferate it will be necessary to consider Berry phases associated with them and the instantons to understand the SRO phase. The following phases can occur in such a lattice gauge theory [19]:

(*i*) A Higgs phase in which the vortices and instantons are suppressed; Berry phase effects are therefore unimportant and this phase will be insensitive to the precise value of n_b. The b^α quanta carry charge 1 and are unconfined [19]: these are spinons transforming under the fundamental of $Sp(N)$. No such excitations were found in the commensurate phases. Gauge excitations have a gap controlled by the magnitude of the Higgs field $\langle\vec{\Phi}\rangle$. The incommensuration is also controlled by $\langle\vec{\Phi}\rangle$, as has been noted earlier. There is no breaking of lattice symmetries beyond those found at $N=\infty$. However with periodic boundary conditions the ground

state has an additional factor of 4 degeneracy for all n_b: the additional states are obtained by changing the sign of all Q_p fields cut by a loop wrapped around the system [31]. This phase is expected to survive in our phase diagram at finite N.
(*ii*) A confinement phase with proliferation of vortices and instantons, confinement of spinons, and a gap towards gauge excitations controlled by the instanton density [30]. A plausible scenario is that this phase in fact coincides with the (π,π)-SRO phase and possesses spin-Peierls order driven by the Berry phases of instantons.
(*iii*) Additional intermediate phases driven by the Berry phases of the instantons and vortices—this possibility is under investigation.

3.D Comparison With Numerical And Series Results

Many numerical [11] and series analyses [13] have appeared on the model with $J_3 = 0$ for the spin-1/2 $SU(2)$ model *i.e.* $N = 1$, $n_b = 1$ in the notation of this paper. They find (π,π)-LRO at small J_2/J_1, $(\pi,0)$-LRO at large J_2/J_1 and an intermediate SRO phase around $J_2/J_1 = 1/2$. This is in agreement (see Fig 1) with our prediction in section 3.A.1 that the phase boundary between (π,π)-LRO and (π,π)- SRO bends downwards at finite N with increasing J_2/J_1. Analyses of this intermediate phase at J_2/J_1 [11, 13] shows clear evidence of columnar spin-Peierls ordering [7], also in agreement with the results of Ref [7] and section 3.C.1. An additional intermediate phase with $(0,\pi)$-SRO has not been ruled out.

It would clearly be interesting to find the new incommensurate SRO phases with unconfined spinons of this paper in numerical work on models with $N = 1$, $n_b = 1$. Our results suggest that such phases will only occur in models with a finite J_3. A numerical analysis of the J_1-J_2-J_3 model along the line $J_3 = 0.5J_2$ has recently been performed [12]. For comparison, we display the large N results for these models in Fig 4. As in Fig 4, these investigators [12] find correlations at (π,π) at small J_2/J_1 and at $(0,\pi)$ at large J_2/J_1. Their results at intermediate J_2/J_1 are inconclusive but suggestive of a (π,q) phase. A systematic analysis to resolve this issue and to distinguish SRO from LRO would be useful.

4. THE t-J MODEL

This section will extend our results to a limited class of doped AFMs. These are described by the t-J models in which electrons hop with matrix element t, have a nearest-neighbor antiferromagnetic exchange J, and have restrictions on their occupation number at each site due to the strong Coulomb interactions. Ideally one would like to dope AFMs which have spins in the representations examined above, *i.e.* transforming under the symmetric product of n_b fundamentals of $Sp(N)$, and take the large N limit with n_b/N constant. Parameters can then be chosen to obtain the experimentally observed [2] Néel LRO state in the undoped limit. These models require the introduction of bosons b^α carrying $Sp(N)$ spin, and spinless fermions to represent the holes [26]. The Pauli exclusion principle now restricts the density of fermions to be order 1 and it appears that a simple large-N limit does not exist.

We examine here the doping of AFMs which have spins transforming under the antisymmetric product of m fundamentals of $Sp(N)$ (this representation is *not* irreducible); the large N limit will be taken with m/N constant. Such spins are most conveniently described by introducing fermions f^α transforming under the fundamental of $Sp(N)$. The holes are now represented by spinless bosons b. The physical 'electron' is therefore

$$c_i^\alpha = f_i^\alpha b_i^\dagger \tag{4.1}$$

The local constraint of the t-J model is

$$f_{i\alpha}^\dagger f_i^\alpha + b_i^\dagger b_i = m \tag{4.2}$$

for every site i. We will focus exclusively on the case in which the states are half filled at zero doping: $m = N$. This approach is an adaptation of the large N limits of Ref [32, 33] for $SU(N)$ t-J models. Unlike the $SU(N)$ case, the states on each site do not form an irreducible representation of $Sp(N)$ at zero doping. Two fermions can combine to form on-site singlets $\mathcal{J}^{\alpha\beta} f_{i\alpha}^\dagger f_{i\beta}^\dagger$. There is, however, no energy gained out of forming such states; they in fact reduce the ability of the site to form energetically favorable singlet bonds with other sites.

For undoped AFMs with exchange interactions of the type (1.8), the large N limit can be taken following the $SU(N)$ case. For weak frustration [34] the ground states are fully dimerized into pairs of sites forming singlet bonds. (Note that the bosonic large N theories of Section 3 also give only dimerized ground states in the limit of large N/n_b for n_b odd: see Figs 1,3,4.) Néel -type states which are important for $N = 1$ are not found. However at large dopings, the present large-N offers a natural way of describing metallic states with a Fermi surface satisfying Luttinger's theorem, the existence of which appears to be suggested by some experiments on the high-T_c materials [35]. Thus the following calculation, while probably not experimentally relevant at small doping, might capture the correct physics at moderate and large dopings.

We will consider the following Hamiltonian

$$H_{tJ} = -\frac{t}{N}\sum_{<ij>} b_i f^\dagger_{i\alpha} f^\alpha_j b^\dagger_j - \frac{J}{N}\sum_{<ij>}\left(\mathcal{J}^{\alpha\beta} f^\dagger_{i\alpha} f^\dagger_{j\beta}\right)\left(\mathcal{J}_{\gamma\delta} f^\delta_j f^\gamma_i\right) + \sum_i \lambda_i\left(f^\dagger_{i\alpha} f^\alpha_i + b^\dagger_i b_i - N\right) + \mu\sum_i\left(b^\dagger_i b_i - N\delta\right) \quad (4.3)$$

The last two terms enforce the local constraint (4.2) and fix the average hole density at $N\delta$. Here we will focus exclusively on the $N=\infty$ limit at zero temperature. This requires a complete condensation of the b bosons $\langle b_i\rangle = \sqrt{N}\bar{b}_i$ and introduction of the link-field

$$\Delta_{ij} = \frac{1}{N}\left\langle \mathcal{J}^{\alpha\beta} f^\dagger_{i\alpha} f^\dagger_{j\beta}\right\rangle \quad (4.4)$$

which performs the Hubbard-Stratanovich decomposition of the exchange interaction. We note that this decoupling is very similar to that performed in Refs [16]; in the present calculation however it is uniquely enforced by the large N limit. As in Ref [16], at $T=0$, our solutions have $\bar{b}_i \neq 0$ (for $\delta \neq 0$) and $\Delta_{ij} \neq 0$ which describe a superconducting state. We have examined mean-field equations numerically with two sites per unit cell (with both the 2×1 and $\sqrt{2}\times\sqrt{2}$ unit cells) and determined the global ground states over this manifold. The results are summarized in Fig 5. A large part of the phase diagram in fact turns out to have a unit cell of just one site. In this case $\bar{b}_i = \sqrt{\delta}$, $\Delta_{i,i+\hat{x}} \equiv \Delta_x$, $\Delta_{i,i+\hat{y}} \equiv \Delta_y$ and the quasi-particle energy spectrum $\epsilon_{\mathbf{k}}$ is

$$\epsilon_{\mathbf{k}} = \left[\left(\lambda - 2t\delta\left(\cos k_x + \cos k_y\right)\right)^2 + 4J^2\left|\Delta_x \cos k_x + \Delta_y \cos k_y\right|^2\right]^{1/2} \quad (4.5)$$

We find 4 different types of superconducting states which are described below. With the exception of the first phase which has coexisting spin-Peierls order, all phases are combination of extended s (s^*) and d wave pairing with no on-site pairing.

(i) Coexistence of spin-Peierls order and superconductivity: This phase occurs for small t or small δ and has a 2×1 unit cell with the spatial distribution of the Δ_{ij} shown in Fig 5. All three $\Delta_1, \Delta_2, \Delta_3$ cannot be made real in any gauge so this phase also breaks time-reversal invariance. At $t=0$ and δ arbitrary, or $\delta = 0$ and t arbitrary, we have $\Delta_1 \neq 0$, $\Delta_2 = \Delta_3 = 0$: the system is now a fully dimerized insulator. The quasi-particle spectrum is found to have a gap over the

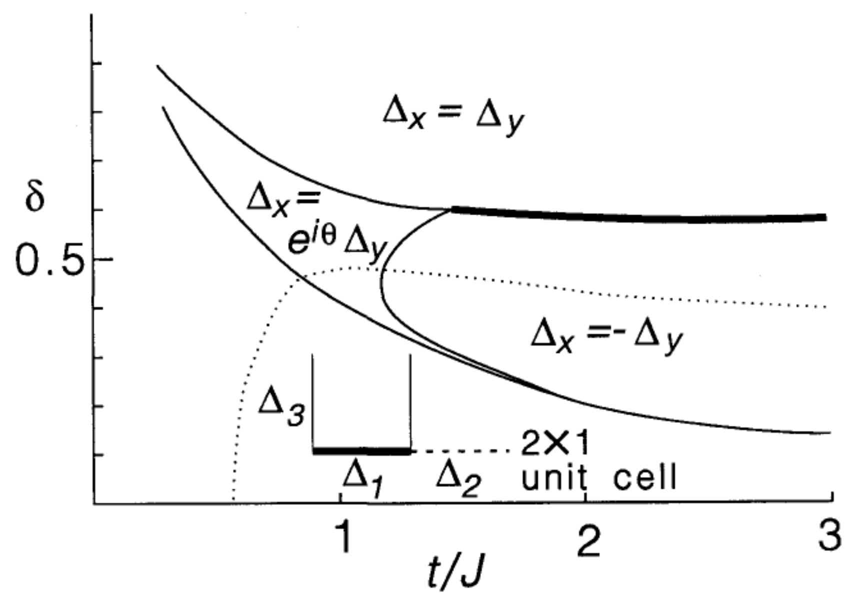

Fig 5. Ground state of the $t - J$ model H_{tJ} at $N = \infty$ as a function of t/J and the hole concentration δ. All phases, except the lines $t = 0$ and $\delta = 0$, are superconducting. The region below the dotted line is susceptible to separation into an insulating antiferromagnet with $\delta = 0$ and a hole-rich phase with δ on the dotted line. The boundary towards phase separation approaches $\delta = 0$ as $t/J \to \infty$.

entire Brillouin zone. This is the only phase which has a unit cell larger than one site.

(*ii*) $s^* + id$-wave superconductor: Occurs around $t/J \approx 1$ and $\delta \approx 0.5$ and has $\Delta_x = e^{i\theta}\Delta_y$ where the phase θ varies smoothly with t/J and δ. Such a state has been considered previously by Kotliar [36]. The quasi-particle spectrum is fully gapped and time-reversal symmetry is broken.

(*iii*) d-wave superconductor: This phase occurs for moderate and large t/J at small δ and has $\Delta_x = -\Delta_y$ and has been considered previously by Kotliar and Liu [37]. The quasi-particle gap vanishes at 4 isolated points $(\pm k^0, \pm k^0)$ in the Brilluoin zone.

(*iv*) s^*-wave superconductor: Finally for large δ we obtain an extended s-wave solution with no on-site pairing which has $\Delta_x = \Delta_y$. There is again a fully gapped excitation spectrum; for large $t\delta/J$, the gap vanishes as $t\delta \exp(-ct\delta/J)$ where c is a constant of order unity.

Finally we address the issue of the stability of the phases discussed above towards phase separation. A realistic model of the high-T_c materials should also include the long-range Coulomb interactions between the electrons and between the rare-earth ions and the electrons. These interactions will reduce any tendency towards phase separation. It is nevertheless interesting to examine this issue for H_{tJ} alone. The results of a Maxwell construction on the energy-versus-doping curve are shown in Fig 5. The region below the dotted line is susceptible to separation into an insulating antiferromagnet with $\delta = 0$ and a hole-rich phase with δ on the dotted line. The boundary towards phase separation approaches $\delta = 0$ as $t/J \to \infty$, in agreement with Ref [38]. However at small values of t/J, in particular at $t = 0$, we find no phase separation, unlike Emery *et. al.* [38]. The absence of phase separation at $t = 0$ in the present calculation is due to the extra stability acquired at large N by fully dimerized solutions with every site less than half-filled.

5. CONCLUSIONS

This paper has presented details on the application of a new large N expansion based on the symplectic groups $Sp(N)$ which was introduced recently [10]. These groups naturally generalize to all values of N the physics of $SU(2) \cong Sp(1)$ antiferromagnetism: the pairing of spins with opposite directions in spin space. They lead to a particularly appealing treatment of frustrated antiferromagnets with all antiferromagnetic exchange interactions treated democratically. The large N limit was taken by placing spins on each site which transform as n_b symmetric products on the fundamental of $Sp(N)$, and fixing n_b/N at an arbitrary value ($n_b = 2S$ for $SU(2)$). For large n_b/N the ground states become identical to the classical solutions and possess magnetic long range order (LRO). Upon reducing n_b/N all the LRO states under continuous transition to short range ordered (SRO) states whose properties are closely connected to the LRO states. In particular for the square lattice model with first, second, and third neighbor interactions (Figs 1-4) we found two distinct classes of states:

(i) LRO states with commensurate, collinear order led at smaller values of n_b/N to SRO states with a gap to all excitations, spinons confined by a compact $U(1)$ gauge force, and spin-Peierls or valence-bond-solid order controlled by the value of n_b (mod 4) .

(ii) LRO states with incommensurate, coplanar order led at smaller values of n_b/N to SRO states with a gap to all excitations and unconfined spinons and no spin-Peierls order. A charge -2 scalar in a Higgs phase was responsible for liberating the spinons [19]. These incommensurate SRO states appear to contradict the 'fractional quantization principle' of Laughlin [21]. This principle asserts that spin-1/2 excitations of a non-degenerate 'spin-liquid' ground state must interact with a gauge force which endows them with fractional statistics. The SRO states found in this paper have a two-fold degeneracy but this can easily be lifted by adding small explicit symmetry breaking terms to H_{AF} (this can be done for the (q,π)-SRO phase by modifying J_3 on just the x-directed links, and for the (q,q)-SRO phase by changing J_2 on the links in the $(1,1)$ direction). The modified model now has a non-degenerate ground state, no gapless excitations, and unconfined spin-1/2 spinon excitations with bosonic statistics, contradicting Ref [21].

Additional intermediate phases between the Higgs and confinement SRO phases are possible and are presently under investigation. No chirally ordered [8] or spin-nematic [9] states were found.

An initial discussion of the application of the symplectic groups to doped antiferromagnets was also presented. In this case they allow a natural implementation of both antiferromagnetic exchange and hole hopping terms, and emphasize the natural connection between antiferromagnetism and singlet superconductive pairing [3]. In particular a study of the $T = 0$, $N = \infty$ limit of a $t - J$ model with spins represented by fermions and holes by spinless bosons yields superconducting ground states (Fig 5) in much the same manner as Ref [16]. Extension of these results to finite temperature and finite N is clearly of great interest and is currently in progress.

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REFERENCES

[1] J.G. Bednorz and K.A. Muller, Z. Phys. **B64**, 188 (1986); M.K. Wu *et. al.*, Phys. Rev. Lett. **58**, 908 (1987).

[2] S. Chakravarty, B.I. Halperin, and D.R. Nelson, Phys. Rev. Lett. **60**, 1057 (1988), Phys. Rev. B **39**, 2344 (1989).

[3] P.W. Anderson, Science **235**, 1196 (1987); S. Liang, B. Doucot, and P.W. Anderson, Phys. Rev. Lett. **61**, 365 (1988).

[4] D.P. Arovas and A. Auerbach, Phys. Rev. B **38**, 316 (1988); Phys. Rev. Lett. **61**, 617 (1988).

[5] F.D.M. Haldane, Phys. Rev. Lett. **61**, 1029 (1988)

[6] N. Read and S. Sachdev, Nucl. Phys. B**316**, 609 (1989).

[7] N. Read and S. Sachdev, Phys. Rev. Lett. **62**, 1694 (1989); Phys. Rev. B (in press).

[8] V. Kalmeyer and R.B. Laughlin, Phys. Rev. Lett. **59**, 2095 (1987). X.-G. Wen, F. Wilczek and A. Zee, Phys. Rev. B **39**, 11413 (1989).

[9] P. Chandra, P. Coleman, and A.I. Larkin, Phys. Rev. Lett. **64**, 88 (1990); preprint; P. Chandra and P. Coleman, Int. J. Mod. Phys. B **3**, 1729 (1989).

[10] N. Read and S. Sachdev, preprint.

[11] E. Dagotto and A. Moreo, Phys. Rev. Lett. **63** 2148 (1989); R.R.P. Singh and R. Narayan, Phys. Rev. Lett. **65**, 1072 (1990).

[12] A. Moreo, E. Dagotto, T. Jolicoeur, and J. Riera, "Incommensurate correlations in the $t-J$ and frustrated spin-1/2 Heisenberg models", Santa Barbara preprint.

[13] M.P. Gelfand, R.R.P. Singh, and D.A. Huse, Phys. Rev. B **40**, 10801 (1989); M.P. Gelfand, preprint.

[14] S. Sachdev and R.N. Bhatt, Phys. Rev. B , **41**, 4502 (1990).

[15] C. Henley, Phys. Rev. Lett. **62**, 2056 (1989).

[16] G. Baskaran, Z. Zou, and P.W. Anderson, Sol. State Comm. **63**, 973 (1987); A.E. Ruckenstein, P.J. Hirschfeld, and J. Appel, Phys. Rev. B **36**, 857 (1987).

[17] D. Yoshioka, J. Phys. Soc. Jpn, **58**, 3733 (1989).

[18] I. Affleck, Nucl. Phys. **B257**, 397 (1985); Nucl. Phys. **B265**, 409 (1985).

[19] See *e.g.* E. Fradkin and S.H. Shenker, Phys. Rev. **D19**, 3682 (1979).

[20] Unconfined spin-1/2 spinons are also predicted to appear in unfrustrated systems in $d = 3$; A. Kol and N. Read, unpublished.

[21] R.B. Laughlin, Science **242**, 525 (1988).

[22] B.I. Halperin and W.M. Saslow, Phys. Rev. B **16**, 2154 (1977).

[23] T. Dombre and N. Read, Phys. Rev. B **39**, 6797 (1989).

[24] E. Brezin and J. Zinn-Justin, Phys. Rev. B **14**, 3110 (1976).

[25] P. Chandra and B. Doucot, Phys. Rev. B **38**, 9335 (1988).

[26] Similar incommensurate states with valence bonds connecting sites on the same sublattice are also found in a study of doped systems; B.I. Shraiman and E.D. Siggia, Phys. Rev. Lett. **62**, 1564 (1989); C. Jayaprakash, H.R. Krishnamurthy and S. Sarkar, Phys. Rev. B **40**, 2610 (1989); C.L.Kane *et al*, *ibid* **41**,2653 (1990); B. Chakraborty *et al*, Phys. Rev. B (in press).

[27] J. Stephenson, Can. J. Phys. **48**, 2118, 1724 (1970).

[28] P. Azaria, B. Delamotte, and T. Jolicoeur, Phys. Rev. Lett. **64**, 3175 (1990).

[29] I. Affleck, T. Kennedy, E.H. Lieb, and H. Tasaki, Phys. Rev. Lett. **59**, 799 (1987); Commun. Math. Phys. **115**, 477 (1988).

[30] A.M. Polyakov, Nucl. Phys. B **120**, 429 (1977).

[31] N. Read and B. Chakraborty, Phys. Rev. B **40**, 7133 (1989).

[32] I. Affleck and J.B. Marston, Phys. Rev. **B37**, 3774 (1988).

[33] M. Grilli and B.G. Kotliar, Phys. Rev. Lett. **64**, 1170 (1990)

[34] D. Rokhsar, Phys. Rev. B **42**, 2526 (1990) has shown that a large class of frustrated AFMs dimerize in the fermionic large-N limit for $SU(N)$. It is likely that a similar result holds for the fermionic large-N limit of $Sp(N)$.

[35] C. G. Olson *et. al.*, Science **245**, 731 (1989).

[36] B.G. Kotliar, Phys. Rev. B , **37**, 3664 (1988).

[37] B.G. Kotliar and J. Liu Phys. Rev. B , **38**, 5142 (1988).

[38] V.J. Emery, S.A. Kivelson, and H.Q. Lin, Phys. Rev. Lett. **64**, 475 (1990).