Nonlinear σ model method for the J_1-J_2 Heisenberg model

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A novel nonlinear σ model method is proposed for the two-dimensional J_1-J_2 model, which is extended to include plaquette-type distortion. The nonlinear σ model is properly derived without spoiling the original spin degrees of freedom. A disordered phase is found to continue, without quantum phase transitions, from a frustrated uniform regime to an unfrustrated distorted regime. By the continuity and Oshikawa's commensurability condition, the disordered ground states for the uniform J_1-J_2 model are plaquette states with four-fold degeneracy.

The two-dimensional (2D) J_1-J_2 model is a frustrated Heisenberg model with nearest neighbor (NN) and next nearest neighbor (NNN) antiferromagnetic exchange interactions on a square lattice. The model with spin magnitude $S = \frac{1}{2}$ is realized in mother materials of cuprate superconductors, La_2CuO_4, YBa_2CuO_6 and $Sr_2CuO_2Cl_2$ as small-J_2 systems [1, 2]. Recently found materials, Li_2VOSiO_4 and Li_2VOGeO_4, are also described by the model in the case of $J_2/J_1 \sim 1$ [3, 4]. A particular interest for the J_1-J_2 model is in a gapful disordered state, which may be formed by frustration under strong quantum fluctuations [5]. The subject has been theoretically investigated by various methods [1]: e. g. spin wave theories [6–8], nonlinear σ model (NLSM) methods [9, 10], numerical diagonalizations [11–14], quantum Monte Carlo (QMC) simulations [15–17], series expansions [18–20], and variational methods [21].

For a system only with the NN interactions (J_2=0), the ground state is believed to have an antiferromagnetic (AF) order. The NNN exchange interactions are expected to induce strong frustration to break the AF order and to form a disordered ground state around $J_2/J_1 = 0.5$. A current leading QMC calculation [15, 16] supports the disordered phase with spin-gap for $J_2/J_1 \gtrsim 0.4$. Accepting this result, the issue is the character of the ground state in the disordered phase. Candidates examined in recent several years are the uniform resonating-valence-bond (RVB) state [21], the plaquette state [16, 18], the dimer state [19–21], and a state both with dimer and plaquette structures [17]; their degeneracies are 1, 4, 4 and 8, respectively. The true ground state is still under debate. To restrict possibilities, Oshikawa's commensurability condition [22] is useful; e. g. the uniform RVB state with spin-gap is possible only if there exist gapless singlet excitations. In this Letter, we determine the true ground state as the plaquette state, assisted by the condition.

A disordered state is formed also by distortion in the exchange constants, even if there is no frustration ($J_2 = 0$). For a plaquette-type distortion, a disordered state interpreted as a 2D array of plaquette-singlets are formed [23]. Here it is a question whether the disordered state by frustration is essentially the same as that by plaquette-type distortion. If it is the same, a disordered phase continuously extends from a region of strong frustration and weak distortion to a region of weak frustration and strong distortion in a parameter space. However, if not, there exists a phase boundary between them; then the ground state of the uniform J_1-J_2 model is not plaquette-like. Hereafter we consider the J_1-J_2 model which is extended to include a plaquette-type distortion.

Among various methods to analyze spin systems, the NLSM method is effective to clarify their characters. The first successful example appeared in one-dimensional (1D) systems. A uniform spin chain with NN interactions is mapped onto an NLSM with an appropriate topological term [24]. Inhomogeneous spin chains with periodicity are treated by refined and extended NLSM methods [25, 26]. For 2D systems, an NLSM without topological term is derived for $J_2 = 0$ [27]. For $J_2 \neq 0$, Chakravarty *et al.* [9] analyzed 2D NLSM which represents the uniform J_1-J_2 model. By applying a renormalization group (RG) method to the NLSM, they constructed a standard theory for the quantum phase transition.

Despite the success, there remains ambiguity in the correspondence of a derived NLSM to the J_1-J_2 model. If one use a naive mapping in literature, a single spin variable is replaced by the sum of two new variables representing a slowly varying AF motion and a rapid fluctuation. This is not justified because the number of the degrees of freedom increases by the variable transformation. Although the mapping may give the correct NLSM phenomenologically, there is no way to confirm the correctness within the NLSM method itself. Further the increase of the degrees of freedom leaves ambiguity for the choice of the cutoff. In one dimension, the problem of the degrees of freedom has been overcome in generalized formulations [25, 26]. However there has not been proposed such a reasonable theory in two dimensions. To
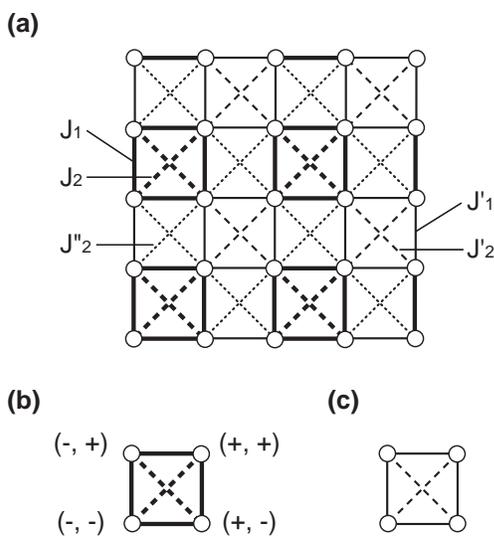
FIG. 1: (a) Lattice of the J_1-J_2 model. Lattice sites are denoted by small circles and exchange constants are by various lines between circles. (b) A plaquette consisting of four sites connected by J_1 and J_2; this is a block which is a unit in the NLSM formulation. A variable $\mathbf{n}_j$ in the pth block is relabeled as $\mathbf{n}^{\mu\nu}(p)$, where μ and ν take $+$ or $-$. The value of (μ, ν) at each site is shown. (c) Another kind of plaquette consisting of four sites connected by J_1' and J_2'.

construct a qualified 2D NLSM method is a purpose of this Letter. Using the NLSM method, to determine the character of the ground state for the 2D J_1-J_2 model is the final purpose.

The J_1-J_2 model with plaquette-type distortion is represented by the Hamiltonian:

$$H = \sum_{\langle i,j \rangle} J_{1;ij}\, \mathbf{S}_i \cdot \mathbf{S}_j + \sum_{\langle\langle i,k \rangle\rangle} J_{2;ik}\, \mathbf{S}_i \cdot \mathbf{S}_k, \qquad (1)$$

where $\mathbf{S}_i$ is the spin of magnitude S at site i. The first and the second summations are taken over NN and NNN pairs, respectively, in a square lattice. $J_{1;ij}$ takes J_1 or J_1', and $J_{2;ij}$ does J_2, J_2' or J_2'' as shown in Fig. 1(a). The system is reduced to the uniform J_1-J_2 model when $J_1 = J_1'$ and $J_2 = J_2' = J_2'' = 0$. In the limit of $J_1' = J_2' = J_2'' = 0$, the lattice is an assembly of isolated plaquettes each of which consists of four spins connected by J_1 and J_2 (Fig. 1(b)). Also, in the limit of $J_1 = J_2 = J_2'' = 0$, the lattice is an assembly of another kind of isolated plaquettes; each consists of four spins connected by J_1' and J_2' (Fig. 1(c)). Hamiltonian (1) is invariant under the simultaneous exchanges of J_1 and J_1', and of J_2 and J_2'. The symmetric case of $J_1 = J_1'$ and $J_2 = J_2'$ includes the uniform J_1-J_2 model.

We consider the quantum Hamiltonian (1) in the classical Néel ordered region. The expectation value of $\mathbf{S}_j$ for a spin coherent state at imaginary time τ is given as

$$\langle \mathbf{S}_j \rangle = (-1)^j S \mathbf{n}_j(\tau) \quad \text{with} \quad \mathbf{n}_j^2 = 1, \qquad (2)$$

where $(-1)^j$ is a symbol taking $+$ or $-$ depending on the sublattice which the jth site belongs to. The partition function is then written in a path integral formula as

$$Z = \int D[\mathbf{n}_j(\tau)] \prod_j \delta(\mathbf{n}_j^2(\tau) - 1)\, e^{-A}. \qquad (3)$$

The action A at temperature $1/\beta$ is given by

$$A = iS \sum_j (-1)^j w[\mathbf{n}_j] + \int_0^\beta d\tau H(\tau). \qquad (4)$$

The first term is the Berry phase term with the solid angle $w[\mathbf{n}_j]$ which the unit vector $\mathbf{n}_j(\tau)$ forms in period β. $H(\tau)$ in the second term is given by

$$\begin{aligned} H(\tau) = &\; \frac{1}{2}S^2 \sum_{\langle i,j \rangle} J_{1;ij}[\mathbf{n}_i(\tau) - \mathbf{n}_j(\tau)]^2 \\ &- \frac{1}{2}S^2 \sum_{\langle\langle i,k \rangle\rangle} J_{2;ik}[\mathbf{n}_i(\tau) - \mathbf{n}_k(\tau)]^2, \qquad (5) \end{aligned}$$

where the constraint $\mathbf{n}_j^2(\tau) = 1$ in the δ-function of Eq. (3) has been used. Hereafter we do not explicitly write the τ dependence of $\mathbf{n}_j(\tau)$.

We adopt a plaquette of Fig. 1(b) as a unit of transformation, and call it a *block*; we would choose another kind of plaquette in Fig. 1(c) as a block. We relabel four variables, $\mathbf{n}_j$'s, in the pth block as $\mathbf{n}^{++}(p)$, $\mathbf{n}^{+-}(p)$, $\mathbf{n}^{-+}(p)$ and $\mathbf{n}^{--}(p)$, as shown in Fig. 1(b). By analogy with the 1D case [26], we transform them as

$$\mathbf{n}^{\mu\nu}(p) = \mathbf{m}(p) + a[\mu\nu \mathbf{L}_0(p) + \mu \mathbf{L}_1(p) + \nu \mathbf{L}_2(p)]. \quad (6)$$

Here $\mathbf{L}_0(p)$, $\mathbf{L}_1(p)$ and $\mathbf{L}_2(p)$ describe small fluctuations around $\mathbf{m}(p)$. According to the variable transformation, four original constraints, $[\mathbf{n}^{\mu\nu}(p)]^2 = 1$ ($\mu, \nu = \pm$), are changed to four new constraints, $\mathbf{m}^2(p)=1$ and $\mathbf{m}(p) \cdot \mathbf{L}_q(p) = 0$ ($q = 0, 1, 2$). Thus we obtained a new set of variables, the number of which is the same as that of the original variables. This plaquette-based transformation is inevitable to keep the original degrees of freedom even in the uniform J_1-J_2 model.

In the continuum limit, the first term of the action (4) is written as $iS \sum_p \sum_{\mu,\nu} \mu\nu w[\mathbf{n}^{\mu\nu}(p)] = i(S/a) \int d\tau d^2\mathbf{r}\, \mathbf{L}_0 \cdot (\mathbf{m} \times \partial_\tau \mathbf{m})$ with lattice spacing a. For the second term of Eq. (4), we substitute Eq. (6) into Eq. (5) and taking the continuum limit. Thus, to the leading order of derivatives and fluctuations, we have the field-theoretic action

$$\begin{aligned} A = \; S^2 \int d\tau d^2\mathbf{r} \Big\{ &\frac{i}{Sa} \mathbf{L}_0 \cdot (\mathbf{m} \times \partial_\tau \mathbf{m}) \\ &+ J_0'[(\partial_x \mathbf{m})^2 + (\partial_y \mathbf{m})^2 - 2\partial_x \mathbf{m} \cdot \mathbf{L}_1 - 2\partial_y \mathbf{m} \cdot \mathbf{L}_2] \\ &+ 2(J_1 + J_1')\mathbf{L}_0^2 + (J_0 + J_0')(\mathbf{L}_1^2 + \mathbf{L}_2^2) \Big\} \qquad (7) \end{aligned}$$

with $J_0 \equiv J_1 - J_2 - J_2''$ and $J_0' \equiv J_1' - J_2' - J_2''$. This action includes all the low-energy excitations surviving

the continuum approximation, since the original degrees of freedom are not spoiled in the variable transformation (6). In Eq. (7), $\mathbf{L}_0$, $\mathbf{L}_1$ and $\mathbf{L}_2$ are massive fields [28], so that they are irrelevant to a symmetry change of the ground state.

Now we integrate out the partition function for the action (7) with respect to massive fields $\mathbf{L}_0$, $\mathbf{L}_1$ and $\mathbf{L}_2$. The resultant partition function contains the NLSM action:

$$A_{\text{eff}} = \int d\tau d^2\mathbf{r} \left\{ \frac{1}{8a^2(J_1 + J_1')}(\partial_\tau \mathbf{m})^2 \right. $$
$$\left. + S^2 \left(\frac{1}{J_0} + \frac{1}{J_0'} \right)^{-1} [(\partial_x \mathbf{m})^2 + (\partial_y \mathbf{m})^2] \right\}. \quad (8)$$

There appears no topological term even if the NNN interactions exist. The bare spin wave velocity is read as $v = 2\sqrt{2}Sa(J_1 + J_1')^{1/2}(1/J_0 + 1/J_0')^{-1/2}$. Action A_{eff} keeps the original invariance against the simultaneous exchanges of J_1 and J_1', and of J_2 and J_2', meaning that the same action is obtained if we use a plaquette in Fig. 1(c), instead of Fig. 1(b), as a block. This result reflects that the variable transformation (6) does not restrict the spin motion to form a singlet on the plaquette of Fig. 1(b).

We apply the RG analysis by Chakravarty et al. [9] to the present NLSM. We first introduce rescaled dimensionless coordinates, $x_0 = \Lambda v\tau$, $x_1 = \Lambda x$ and $x_2 = \Lambda y$, with a momentum cutoff Λ of order a^{-1}. The NLSM action (8) is then rewritten as

$$A_{\text{eff}} = \frac{1}{2g_0} \int d^3x \left(\frac{\partial \mathbf{m}}{\partial x_\mu} \right)^2 \quad (9)$$

with coupling constant $g_0 = \sqrt{2}\Lambda a S^{-1}(J_1 + J_1')^{1/2}(1/J_0 + 1/J_0')^{1/2}$. By RG equations up to one-loop approximation, the quantum phase transition from the AF ordered (Néel) state to a disordered state takes place at $g_0 = 4\pi$. Rewriting this, the phase boundary in the space of the exchange parameters is given by

$$(J_1 + J_1') \left(\frac{1}{J_0} + \frac{1}{J_0'} \right) = \frac{2}{\lambda} \quad \text{with} \quad \lambda \equiv \left(\frac{\Lambda a}{2\pi S} \right)^2. \quad (10)$$

Parameter λ represents the strength of quantum effect; $\lambda = 0$ in the classical spin limit.

To make the NLSM method complete, we determine the cutoff Λ by considering the number of degrees of freedom for the square lattice. The variable $\mathbf{m}$ is originally defined for each block of size $2a \times 2a$ (Fig. 2(b) and Eq. (6)), and is taken a continuum limit. Hence the correspondence of the momentum spaces is expressed as $(\pi/a)^2 = \pi\Lambda^2$, or the cutoff is given by $\Lambda = \sqrt{\pi}/a$. Thus Eq. (10) unambiguously determines the phase boundary between the ordered and the disordered phases.

In the uniform limit ($J_1 = J_1'$, $J_2 = J_2' = J_2''$), the system depends only on *frustration parameter* $\alpha \equiv J_2/J_1$ and Eq. (10) is reduced to $\alpha = \frac{1}{2} - \lambda$. Hence, for $S = \frac{1}{2}$ with $\Lambda = \sqrt{\pi}/a$, the critical value for α is given as
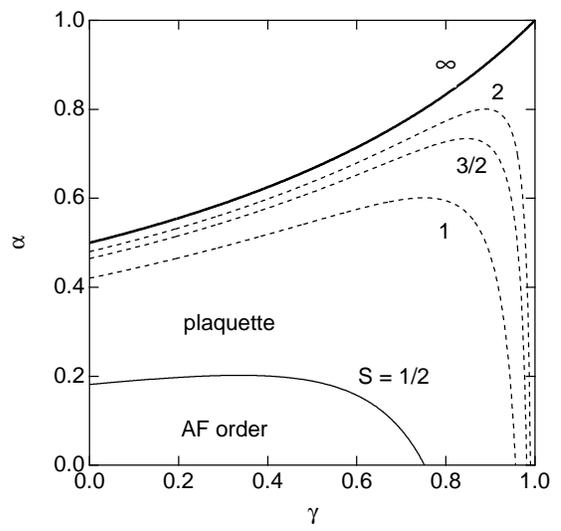

FIG. 2: Phase diagram in the space of distortion parameter γ and frustration parameter α ($=J_2/J_1$). The bold solid line for $S=\infty$ separates the classical Néel and the classical colinear phases. The region between the bold solid and the thin solid lines is the gapful plaquette phase for $S=\frac{1}{2}$. In the uniform case ($\gamma=0$), the ground states in the gapful phase are four-fold degenerate with broken translational invariance. The phase boundaries for $S = 1$, $\frac{3}{2}$ and 2 are also shown by dashed lines.

$\alpha_c \simeq 0.18$. Thus the NLSM method succeeds in producing a critical value satisfying $0 < \alpha_c < \frac{1}{2}$ without any additional assumption or interpretation. The value is smaller than ~ 0.4 estimated by the QMC simulation [15, 16]. The deviation reflects the difference between the dispersions for spin-wave excitations in the lattice and the continuum models, and may be reduced by adjusting the cutoff. Since we aim at inspecting the continuity of a phase, we do not need such a phenomenological adjustment.

In the limit of no frustration ($J_2 = J_2' = J_2'' = 0$), the plaquette distortion may cause an order-disorder transition. We denote the strength of the distortion by *distortion parameter* γ defined as $J_1' = (1-\gamma)J_1$. Then Eq. (10) produces the critical value $\gamma_c = 2 - \lambda^{-1} + \sqrt{\lambda^{-2} - 2\lambda^{-1}}$. This value decreases from 1 to 0 as λ increases from 0 to $\frac{1}{2}$.

We now examine the continuity of the ground state between both the limits above. To be concrete, we parameterize the exchange constants as $J_1' = (1 - \gamma)J_1$, $J_2' = (1 - \gamma)^2 J_2$ and $J_2'' = (1 - \gamma)J_2$ for $0 \leq \gamma < 1$. Equation (10) for the phase boundary is reduced to a simple form as $\alpha = (2 - \gamma)^{-1} - \frac{1}{2}\lambda(2 - \gamma)(1 - \gamma)^{-1}$. The phase diagram in the γ-α parameter space is shown in Fig. 2. The bold line with $S=\infty$ is the classical phase boundary between the Néel and the colinear phases [28]. The phase boundary of $S=\frac{1}{2}$ between the gapful and the gapless phases for variable $\mathbf{m}$ is the thin solid line; the state

above is gapful, while that blow is gapless corresponding to the Néel (AF) ordered state. Boundaries for other spin magnitudes S are also shown by dashed lines.

The gapful region of $\mathbf{m}$ in Fig. 2 extends continuously from the uniform limit on the α-axis ($\gamma=0$) to the limit of no frustration on the γ-axis ($\alpha=0$). Remembering that fields $\mathbf{L}_0$, $\mathbf{L}_1$ and $\mathbf{L}_2$ are gapful, there is no gapless excitation throughout the region whether it is triplet or singlet. Hence, the whole gapful region in Fig. 2 is a single disordered phase. In particular, the phase continues to the point of $(\gamma, \alpha) = (1, 0)$ [29]. Hence a disordered ground state on the α-axis finally continues to the ground state of the assembly of isolated plaquettes.

Thus there remain two possibilities for a disordered ground state of the uniform J_1-J_2 model, which is on the α-axis in the phase diagram (Fig. 2). First, the translational symmetry may be spontaneously broken; then the ground states are four-fold degenerate and one of them continues to the ground state at $(\gamma, \alpha) = (1, 0)$. Second, the symmetry may not be spontaneously broken; then the ground state is unique and is a uniform RVB state with strong fluctuations of plaquette-singlets. However, the second possibility is excluded by Oshikawa's commensurability condition [22]. Applying it to the present case, a uniform ground state with triplet excitation gap must be accompanied with other gapless excitations like singlet ones. Such gapless excitations do not exist as we have already shown. We therefore conclude that the disordered ground states for the uniform J_1-J_2 model are four-fold degenerate plaquette states with spontaneously-broken translational invariance.

In summary, we examined the disordered phase of a 2D J_1-J_2 model by a novel field-theoretic method. The method inevitably starts from a plaquette-based variable transformation not to spoil the original spin degrees of freedom, and hence becomes applicable to a system with plaquette-type distortion. Integrating the partition function with respect to massive fields, we obtained an NLSM action without topological term. Applying the RG analysis of Chakravarty et al. to the NLSM, we obtained an analytic expression for the phase boundary between the Néel phase and the disordered phase in the space of frustration and distortion parameters. The disordered phase extends continuously from the uniform limit to the limit of no frustration without any quantum phase transitions. Assisted by Oshikawa's commensurability condition, we determined the disordered ground states for the uniform J_1-J_2 model as four-fold degenerate plaquette states with spontaneously-broken translational invariance.

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[28] The present analysis is performed in the classical Néel region, $J_0 + J_0' > 0$.

[29] The NLSM method is not applicable to this point, since the continuum approximation is unsuitable to the isolated plaquettes. However the ground state is not singular at the point. In fact, the ground state is the direct product of the unique singlet ground states for the isolated plaquettes, and the excitation gap is of order J_1. As γ decreases from 1 on the γ-axis, the ground state remains nondegenerate with the plaquette symmetry at least for $J_1' \ll J_1$.