Novel Local Symmetries and Chiral-Symmetry-Broken Phases in $S=\frac{1}{2}$ Triangular-Lattice Heisenberg Model

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Using a non-mean-field approach the triangular-lattice $S=\frac{1}{2}$ Heisenberg antiferromagnet with nearest- and next-nearest-neighbor couplings is shown to undergo an Ising-type phase transition into a chiral-symmetry-broken phase (Kalmeyer-Laughlin–like state) at small T. Removal of next-nearest-neighbor coupling introduces a local Z_2 symmetry, thereby suppressing any finite-T chiral order.

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The triangular-lattice Heisenberg model has played an important role in our understanding of the resonating-valence-bond (RVB) states[1-8] in Heisenberg antiferromagnets. Recent developments in the RVB theory of high-T_c superconductors[9-12] have drawn our attention to this problem again. Kalmeyer and Laughlin[13] proposed a Laughlin-like variational RVB ground state for this problem. This RVB state manifestly breaks the chiral symmetry. As pointed out recently by Wen, Wilczek, and Zee[14] (WWZ) and also by Wiegmann[15] nonzero expectation values of operators like $\mathbf{S}_i\cdot(\mathbf{S}_j\times\mathbf{S}_k)$ imply chiral-symmetry breaking. It is clear that chiral symmetry also implies the breaking of parity (P) and time reversal. WWZ also suggested using a fermionic mean-field theory[10] for an RVB state exhibiting chiral-symmetry breaking on the frustrated square lattice.

In a pioneering work, Villain[16] pointed out unexpected discrete degeneracies in classical frustrated spin systems with continuous symmetries and introduced (among many variables) pseudoscalar variables like $\mathbf{S}_i\cdot(\mathbf{S}_j\times\mathbf{S}_k)$ as leading to an Ising-like finite-T phase transition. From Villain's work and the subsequent work[17-20] by many authors, it is clear that this Ising-like phase transition is a novel "topological" phase transition. The two-spin correlation function decays exponentially even in the ordered phase. It is a phase transition from one classical spin liquid to another classical spin liquid. By classical spin liquid we mean a paramagnetic phase of classical Heisenberg spins. The only property that distinguishes the two paramagnets is the long-range order in the handedness of triplets of neighboring spins in an otherwise disordered magnet.

Kawamura and Miyashita[19] (KM) have studied the classical-spin triangular Heisenberg antiferromagnets by generalizing the works of Villain,[16] Lee *et al.*,[17] and Miyashita and Shiba.[18] KM suggest a novel SO(3) order parameter and a finite-T Kosterlitz-Thouless–type of phase transition. This transition is also between two classical spin-liquid states. The works of Lee, Joannopoulos, and Negele[6] and Imada[6] suggest that such a phase transition is absent for the $S=\frac{1}{2}$ problem. This strongly suggests that quantum fluctuations and perhaps the half-integer nature of the spins suppress the above chiral phase transition.

Using an order-parameter theory developed by me recently,[21] we study the $S=\frac{1}{2}$ triangular-lattice Heisenberg system in order to understand the nature of the low-temperature phase. We find a novel local Z_2 symmetry in the free-energy functional written in terms of a real (pseudo)scalar chiral variable. This local symmetry prevents any finite-T chiral-ordered state. However, minor modifications such as the introduction of next-nearest-neighbor coupling (αJ) converts this local Z_2 symmetry into a global one. This leads to a finite-T Ising phase transition and we locate the Ising phase boundary approximately. For α positive the chiral variables (which are defined for every elementary triangle) order ferromagnetically. In terms of symmetry this state is the same as the Kalmayer-Laughlin RVB state. For α negative the chiral variables order antiferromagnetically and hence this state, unlike the previous case, breaks translational invariance as well. Neither chiral state breaks the global spin rotation symmetry nor has Néel-type long-range order at nonzero T, and we call these chiral RVB states. Chiral RVB states are likely to have a gap for excitations, since a discrete symmetry has been broken.

We study the $S=\frac{1}{2}$ problem by a new approach using chiral order parameters. The chirality operator was introduced by WWZ[14] for the quantum $S=\frac{1}{2}$ problem,

$$\hat{\chi}_{ijk}\equiv\mathbf{S}_i\cdot(\mathbf{S}_j\times\mathbf{S}_k)\,, \tag{1}$$

where $\mathbf{S}_i$ is the spin-half operator. The above operator changes sign under odd permutations of subscripts i, j, and k and also changes sign under the time-reversal (antiunitarity) transformation. This operator measures the handedness of the three fluctuating spins (a triad) at sites i, j, and k. WWZ also found a remarkable identity

$$\hat{\chi}_{ijk}^2=-\tfrac{1}{16}(\mathbf{S}_i+\mathbf{S}_j+\mathbf{S}_k)^2+\tfrac{15}{64}\,, \tag{2}$$

which expresses a three-spin coupling in terms of two spin couplings. The above identity is valid only for $S=\frac{1}{2}$ spins. The eigenvalues of $\hat{\chi}$ are $\pm\sqrt{3}/4$ and 0.

I have used this identity to develop an order-parameter theory[21] for the two-dimensional problems. Consider the triangular-lattice Hamiltonian

$$H=J\sum_{\text{nn}}\mathbf{S}_i\cdot\mathbf{S}_j+\alpha J\sum_{\text{nnn}}\mathbf{S}_i\cdot\mathbf{S}_j\,, \tag{3}$$

where αJ is the next-nearest-neighbor (nnn) coupling and J is the nearest-neighbor (nn) coupling. We can rewrite the above as

$$H=\tfrac{1}{2}J\sum_{\langle ijk\rangle}(\mathbf{S}_i+\mathbf{S}_j+\mathbf{S}_k)^2+\alpha J\sum_{\text{nnn}}\mathbf{S}_i\cdot\mathbf{S}_j-\tfrac{9}{4}NJ\,, \tag{4}$$

where the first summation is over the shaded triangles of Fig. 1(a). The second summation over the nnn decomposes into *three independent* triangular-lattice Hamiltonians each having nearest-neighbor coupling αJ in the $\sqrt{3}\times\sqrt{3}$ sublattices. Thus the first term can be viewed as coupling the three independent spin systems.

We rewrite Eq. (4) using the WWZ identity to get

$$H=-8J\sum_{\langle ijk\rangle}\hat{\chi}^2_{ijk}+\alpha J\sum_{\text{nnn}}\mathbf{S}_i\cdot\mathbf{S}_j+\text{const}\,. \tag{5}$$

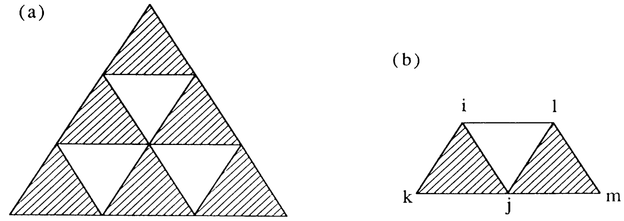

FIG. 1. (a) The shaded triangles are the ones on which $\hat{\chi}_{ijk}$ and m_{ijk} are defined. (b) Two triangles sharing a corner. The first nontrivial Ising-like coupling of chiral variables occurs between these two triangles.

Notice that the first term favors chiral fluctuations owing to the negative sign in front. Since the operators $\hat{\chi}_{ijk}$ are not independent if they share a common site, the chiral fluctuations get correlated even for $\alpha=0$. This together with the correlation arising from the nnn couplings leads to interesting chiral phases. The partition function is

$$Z(\beta)=\operatorname{Tr}e^{-\beta H}=\operatorname{Tr}\left\{T\exp\left[-\alpha J\sum_{\text{nnn}}\int_0^\beta\mathbf{S}_i\cdot\mathbf{S}_j\,d\tau\right]\exp\left[8J\sum_{\Delta}\int_0^\beta\hat{\chi}^2_{ijk}\,d\tau\right]\right\}, \tag{6}$$

where T is Feynman's time ordering which helps us to treat the operators as though they are commuting.

First, consider the case of $\alpha=0$. We linearize the exponential using the Hubbard-Stratanovic identity to get

$$Z(\beta)=\int\mathcal{D}m\operatorname{Tr}\left\{T\exp\left[16J\sum_{\Delta}\int_0^\beta\chi_{ijk}(\tau)m_{ijk}(\tau)d\tau\right]\exp\left[-8J\sum\int_0^\beta m^2_{ijk}(\tau)d\tau\right]\right\}. \tag{7}$$

The auxiliary variables $m_{ijk}(\tau)$ are real scalar variables and will be called the chiral variables. To have a consistent sign convention for the product χm in the exponential we define $m_{ijk}(\tau)$ to be a "pseudoscalar" variable:

$$m_{ijk}(\tau)=-m_{ikj}(\tau)\,. \tag{8}$$

In the functional integral the boundary condition is

$$m_{ijk}(\tau)=m_{ijk}(\tau+\beta)\,. \tag{9}$$

The effective free-energy functional is defined through the equation

$$Z(\beta)=\int\mathcal{D}m\,e^{-\beta F[m]}\,. \tag{10}$$

Expanding Eq. (7) in powers of m, taking the trace, and collecting the cumulants we get the following for $F[m]$:

$$\begin{aligned}\beta F[m]={}&8\beta J\sum\int_0^\beta m^2_{ijk}(\tau)d\tau-N\ln 2-\frac{(16J)^2}{2!}(\operatorname{Tr}\chi^2)\sum\int_0^\beta m^2_{ijk}\,d\tau\\&+\frac{(16J)^4}{4!}\operatorname{Tr}(\chi^4)\sum\int m^4_{ijk}(\tau)d\tau-\frac{(16J)^4}{(2!)^2}\sum[\operatorname{Tr}(\chi^2)]^2\int m^2_{ijk}(\tau)m^2_{jlm}(\tau')d\tau d\tau'\\&+\frac{(16J)^4}{4!}\sum\operatorname{Tr}(T\chi\chi\chi\chi)m(\tau)m(\tau_2)m(\tau_3)m(\tau_4)d\tau_1d\tau_2d\tau_3d\tau_4+\cdots\,,\end{aligned} \tag{11}$$

where the last term has a nontrivial time dependence arising from time ordering in $\operatorname{Tr}[T\chi(\tau_1)\chi(\tau_2)\times\chi(\tau_3)\chi(\tau_4)]$. This term contains only two distinct χ's and m's corresponding to two neighboring triangles that share a vertex.

The above expansion has a remarkable local Z_2 symmetry (in space) term by term:

$$m_{ijk}(\tau)\rightarrow\sigma_{ijk}m_{ijk}(\tau)\,, \tag{12}$$

where $\sigma_{ijk}=\pm 1$ and is independent of τ. This symmetry is easily shown to exist for the case $\alpha=0$ using the trace properties of χ operators on the triangular lattice.

The time dependence of the coefficients in the expansion is nonlocal in time at $T=0$. It is like a long-range interaction between chiral variables in the time direction. However, for finite T, the length of the time direction is finite and by making the static approximation we can make qualitatively exact statements for finite T. Moreover, the free-energy expansion given by Eq. (11) is a high-temperature expansion. This converges for high temperatures and there is no physical reason for it not to converge at low temperatures. We conclude from our local symmetry using the Elitzur-Wegner theorem[22] that we cannot have finite-temperature chiral-symmetry breaking at any finite temperature for the model with pure nearest-neighbor coupling. The m variable has both sign (Z_2) and magnitude fluctuations. Inspection of the above free energy shows that the probability distribution for m^2 is peaked around a nonzero value for $T < kT$. We also do not expect any finite-T transition of area- to power-law behavior of the Wegner-Wilson loop because two-dimensional Z_2 gauge theories are always confining.

A necessary but not sufficient prerequisite for spontaneous symmetry breaking is the absence of any local symmetries in the corresponding variables. We show below that this can be obtained by making the nnn coupling α nonzero. In the expansion for $F[m]$ terms which break local symmetry and retain only global symmetry start appearing. The first and important such term is

$$-\frac{(\beta 16J)^2}{2!}\sum\int a_1(\tau_1,\tau_2)m_{ijk}(\tau_1)m_{jlm}(\tau_2)d\tau_1\,d\tau_2\,, \tag{13}$$

where

$$a(\tau_1,\tau_2)=\frac{\mathrm{Tr}T\exp(-\int_0^\beta \alpha J\sum_{\mathrm{nnn}}\mathbf{S}_i\cdot\mathbf{S}_j d\tau)\chi_{ijk}(\tau_1)\chi_{jlm}(\tau_2)}{Z_\alpha}. \tag{14}$$

and $Z_\alpha=\mathrm{Tr}[\exp(-\beta\alpha J\sum_{\mathrm{nnn}}\mathbf{S}_i\cdot\mathbf{S}_j)]$. By expanding in powers of α we can see that the above is nonzero only for finite α. We find that the above is a product of two-spin correlation functions in the sublattice Hamiltonians. In the static approximation it takes a simple form,

$$a(\tau_1,\tau_2)\approx\tfrac{1}{12}(\langle\mathbf{S}_0\cdot\mathbf{S}_\Delta\rangle_\alpha)^2\equiv\tfrac{1}{12}g_1^2(\alpha,\beta)\,, \tag{15}$$

where $g_1(\alpha,\beta)$ is the nearest-neighbor spin-spin correlation function of the $\sqrt{3}\times\sqrt{3}$ Hamiltonian with coupling αJ at inverse temperature β. Thus Eq. (13) is an Ising-like ferromagnetic nearest-neighbor interaction among chiral variables,

$$-\tfrac{1}{24}(16\beta J)^2 g_1^2(\alpha)\sum m_{ijk}m_{jlm}\,, \tag{16}$$

which has only the global Z_2 symmetry. Inspection shows that other higher-order terms which also have only the global symmetry are small and the expansion is convergent at high temperatures.

We estimate the chiral transition temperature (T_c) as a function of α by the following procedure. The chiral variables m are soft variables. They have, however, a well defined root-mean-square value which is the largest at small T. This is because the free-energy functional $F[m]$ has two well defined minima for $T < J$. Hence, at low T we can approximate

$$m_{ijk}\approx m_0(\beta)\tau_{ijk},\quad m_0(\beta)=\langle m_{ijk}^2\rangle_m^{1/2}\,,$$

where the average $\langle\,\rangle_m$ stands for the functional average with the Boltzmann factor $\exp[-\beta F(m)]$ and τ_{ijk} is an Ising variable $=\pm 1$. To get a feel for $m_0(\beta)$, the largest value of $m_0(\beta)$ is the eigenvalue of the operator $\hat{\chi}_{ijk}$ which is $\sqrt{3}/4$. The least value is 0. For three coupled spins the value of $m_0(\beta)$ is

$$m_0(\beta)\approx\sqrt{3}/4(1+e^{-8\beta J})^{1/2}\,.$$

This value gets reduced for the triangular-lattice problem by a finite amount because the three spins are coupled to the rest of the system. Thus, we rewrite our Ising interaction as

$$-\tfrac{1}{24}(8\beta J)^2 g_1^2(\alpha)m_0^2(\beta)\sum\tau_{ijk}\tau_{jlm}\,.$$

From the above equation we define the effective ferromagnetic coupling between the chiral variables τ_{ijk} as

$$\tilde{J}_{\mathrm{chiral}}=\tfrac{1}{24}\beta^{-1}(16\beta J)^2 g_1^2(\alpha,\beta)m_0^2(\beta)\,.$$

The above is a good approximation for βJ not very large compared to unity. Thus we have a ferromagnetic Ising model defined on a triangular lattice with nearest-neighbor interaction as an effective chiral Hamiltonian. Using the standard result for the transition temperature of this well-known ferromagnetic Ising model we get an expression for the chiral transition temperature,

$$(1/8\ln 3)(16\beta_c J)^2 g_1^2(\alpha,\beta_c)m_0^2(\beta_c J)=1\,.$$

We have thus obtained an implicit equation for the transition temperature. It is easily checked that our analysis is valid for very large α as well. In fact, for $\alpha\gg 1$ the transition temperature saturates and is independent of α, and it is given by

$$kT_c\approx(27/8\ln 3)J\,.$$

For α positive and <1 the expression for T_c is

$$kT_c\approx\sqrt{\alpha}(3\ln 3)^{1/4}\,.$$

For α large and negative the three sublattices are ferromagnetically coupled and chiral fluctuations are reduced, leading to a large reduction in the transition temperature. Notice that in getting the above asymptotic result for the transition temperatures we have used the fact that the two-spin correlation function $g_1(\alpha,\beta_c)$ appearing in the implicit equation for T_c is bounded by a value $\frac{3}{4}$ from above. The resultant phase diagram is shown in Fig. 2.

A way to check if there is any antiferromagnetic chiral state is to find $\langle\chi_{ijk}\rangle$ for a shaded triangle ($\equiv\langle\chi_s\rangle$) and an unshaded triangle ($\equiv\langle\chi_u\rangle$). Using a different type of partitioning of the lattice I have shown that if there is a chiral-symmetry breaking, the value of the order parameter satisfies the following relation: $\langle\chi_s\rangle=\pm\langle\chi_u\rangle$ for $\alpha=\pm 1$. Thus we find that the chiral order for $\alpha>0$ is ferromagnetic. As far as symmetry is concerned it is the same as the Kalmayer-Laughlin state. For $\alpha<0$ the chiral order is antiferromagnetic. The large chiral fluctuations or the three-sublattice Néel order (if it exists) is likely to make a nonzero critical value of α necessary for chiral-symmetry breaking to occur in the ground state.

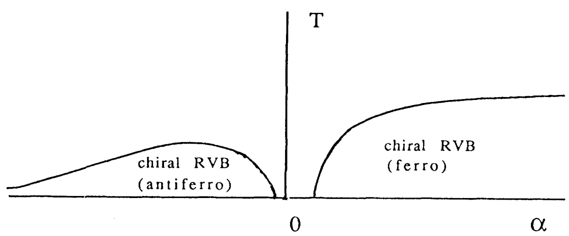

FIG. 2. Phase diagram as a function of the strength α of the next-nearest-neighbor coupling.

In a separate paper I have argued[23] that chiral fluctuations are the source of RVB state formation. The fact that the Hamiltonian, for α (the nnn coupling $=0$), becomes a simple sum $-\sum \chi_{ijk}^2$ alone suggests that the system will be dominated by chiral fluctuations at small T. Also, long-range order in $\hat{\chi}_{ijk}$ does not imply conventional spin long-range order and indeed we have a rotationally invariant phase. The neglect of time dependence in our analysis makes it difficult to make a definite statement about the nature of order in the ground state. However, it is clear that the chiral fluctuations will discourage any ordinary type of Néel long-range order among the spins. Thus I believe that the low-temperature chiral-ordered phase is a quantum paramagnet or quantum spin liquid which we call a chiral RVB state. As far as I know, the present paper is the first to show in a physically rigorous way the existence of RVB states in frustrated Heisenberg systems. The low-temperature chiral RVB state is similar to the Laughlin state in the sense that the sign of chirality is the same for any three spins forming an elementary triangle.

It will be interesting to test the Kalmayer-Laughlin wave function as a variational wave function for our problem, particularly for $\alpha > 1$. Surprisingly, numerical study of finite triangular-lattice systems with nnn coupling does not seem to exist in spite of many works[24-31] (numerical and analytical) on the corresponding problem in the square lattice. It will be interesting to check our prediction of the chiral RVB state at low T and the associated Ising phase transition. Using the formalism outlined in this paper, I have also studied[21] the frustrated square-lattice problem and found new local symmetries and novel chiral phases.

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