Ground-State Phase Diagrams
of the Two-Dimensional Quantum
Heisenberg Spin Glass Models*

Yoshihiko NONOMURA and Yukiyasu OZEKI
Department of Physics, Tokyo Institute of Technology,
Oh-okayama 2-12-1, Meguro-ku, Tokyo 152, Japan

Abstract

Ground-state properties of the two-dimensional $S = 1/2$ random Heisenberg models are investigated by the exact-diagonalization method. The phase diagram of the bond-random model (the $\pm J$ model) is the same as that of the corresponding Ising spin glass model, in spite of quantum fluctuation. In the site-random model, the spin glass phase exists at least in the ferro-rich case. In comparison with the corresponding Ising model, the Néel phase of this model becomes much narrower in the ferro-rich case, while it is comparable in the antiferro-rich case.

KEYWORDS: quantum spin glass, Heisenberg model, ground-state phase transition, site-random model, exact diagonalization

While various aspects of quantum effects in random spin systems have been investigated, the recent progress in the random quantum Heisenberg model, the most realistic model for spin glass materials, is restricted to studies in one dimension.[1, 2, 3] Quite recently, one of the present authors (Y. N.) investigated[4] the $S = 1/2$ asymmetric Heisenberg Mattis model in two dimensions.[5, 6] He found that its ground-state phase diagram does not change[4] from that of the corresponding Ising Mattis model,[6] in spite of quantum fluctuation. He also found that accurate calculations are possible only using quite small clusters (up to the 20-spin one) in the antiferromagnetic region.

In classical spin glass systems, unexpected behavior was reported for the site-random Ising spin glass model in two dimensions[7] by Shirakura et al.[7] They analyzed this model using Monte Carlo simulations, and found that the spin glass phase may be stable at finite temperatures. The present authors investigated[8] the ground state of the same model in detail using the numerical transfer-matrix method,[9] and found that the ferromagnetic and the Néel phase regions are wider than the expected values obtained from the corresponding $\pm J$ model. They also proposed that such structure of the phase diagram can be understood well in terms of the site-percolation picture.

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On the basis of these findings, we investigate ground-state phase diagrams of several two-dimensional $S = 1/2$ random Heisenberg models described by the following Hamiltonian,

$$\mathcal{H} = -\sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j.$$  \hfill (1)

Properties of the models depend on the choice of randomness in $J_{ij}$. We consider the conventional bond-random model (the $\pm J$ model)\cite{11} in which the distribution function of $J_{ij}$ is given by

$$P(J_{ij}; p) = p\delta(J_{ij} - 1) + (1 - p)\delta(J_{ij} + 1),$$ \hfill (2)

and the site-random model\cite{7, 8, 9} defined through

$$J_{ij} = \frac{J}{2} [\epsilon(1 - \omega_i \omega_j) + \omega_i + \omega_j],$$ \hfill (3)

where $\omega_i$ is an independent random variable with the distribution

$$P(\omega_i; c) = c\delta(\omega_i - 1) + (1 - c)\delta(\omega_i + 1).$$ \hfill (4)

The latter model is characterized by the Ising variable $\omega_i$ located at each site. This parametrization represents mixed crystals; i.e. $\omega_i = +1$ and $\omega_i = -1$ correspond to different ions. In the case $\epsilon = +1$, $J_{ij} = +J$ unless $\omega_i = -1$ and $\omega_j = -1$. We call this case “ferro-rich” (F-rich). Similarly, in the “antiferro-rich” (AF-rich) case ($\epsilon = -1$), $J_{ij} = -J$ unless $\omega_i = +1$ and $\omega_j = +1$. Note that these two cases are not equivalent in quantum spin systems.

We have two purposes in the present study. One is to clarify effects of quantum fluctuation in spin glass systems. Since quantum fluctuation plays an important role in the antiferromagnetic region, we calculate the Néel order parameter $m_{st}$ defined in

$$m_{st}^2 \equiv \frac{1}{N^2} \sum_{i,j} (-1)^{i-j} \left[ \langle \vec{S}_i \cdot \vec{S}_j \rangle \right]_r.$$ \hfill (5)

Our other purpose is to investigate the difference between bond-random systems and site-random systems. As in the Ising spin glasses, we consider the spin-glass (SG) order parameter $m_{sg}$ defined in

$$m_{sg}^2 \equiv \frac{1}{N^2} \sum_{i,j} \left[ \langle \vec{S}_i \cdot \vec{S}_j \rangle^2 \right]_r.$$ \hfill (6)

In Ising systems, the lower critical dimension $d_{lc}$ of the SG phase has been expected to be in the range $2 < d_{lc} < 3$\cite{12} in the bond-random model, while it is expected to be equal to that of the pure Ising model, $d_{lc} = 1$\cite{13} in the site-random model. In quantum Heisenberg systems, though $d_{lc}$ has been reported to be greater than three\cite{13, 14} in the bond-random model, the above argument suggests that it is equal to that in the pure quantum Heisenberg model, $d_{lc} = 2$, in the site-random model. If this is the case, the SG order of the three-dimensional site-random Heisenberg model is expected to be stable even at finite temperatures, which is consistent with experimental results.

\*If the existence of the SG order parameter at finite temperatures is established in two dimensions as pointed out by Shirakura et al.\cite{7}, $d_{lc} = 1$ is trivial. The one-dimensional nearest-neighbor spin glass model is not frustrated, and can be identified with the ferromagnetic Ising model by means of a gauge transformation.
We use the exact-diagonalization method in the present letter. Although the size of treatable clusters is quite small in this method, plausible estimation is expected in the antiferromagnetic region, as in the case of the asymmetric quantum Heisenberg Mattis model. Calculations are carried out on the 8,10,16,18,20-spin Oitmaa-Betts-type clusters. In the site-random model, we average all the configurations. In the bond-random model, we average all the bond configurations in the 8 and 10-spin clusters, and average one thousand randomly chosen samples in the 16, 18 and 20-spin clusters.

First, we show the data of the Néel order parameters. These quantities in the bond-random, the AF-rich site-random and the F-rich site-random models are plotted in Figs. 1(a), 1(b) and 1(c), respectively. They are scaled well by $N^{-1/2}$, as in the two-dimensional pure antiferromagnetic Heisenberg model ($p = 0$ or $c = 0$ case). By the least-squares fitting of the 10,16,18,20-spin data, we estimate the critical concentrations of the Néel phase as

\[ p_c = 0.11 \pm 0.01 \quad \text{(bond-random model)} , \]
\[ c_c = 0.36 \pm 0.03 \quad \text{(AF-rich site-random model)} , \]
\[ c_c = 0.13 \pm 0.02 \quad \text{(F-rich site-random model)} . \]

In the corresponding Ising spin glass models, these critical concentrations were estimated as $p_c = 0.11 \pm 0.01$, $c_c = 0.37 \pm 0.01$ and $c_c = 0.41 \pm 0.01$ respectively.

In the bond-random Ising model ($\pm J$ Ising model), the Néel phase boundary in the $p$-$T$ plane is vertical to the $p$-axis. Namely, the Néel order is not destroyed by thermal fluctuation in the low-temperature region. If the effect of quantum fluctuation is similar to that of thermal fluctuation, the equivalence of $p_c$ in the Heisenberg model and the Ising model can be understood. Numerically, the estimates of $c_c$ are also consistent with each other in the AF-rich site-random Heisenberg model and Ising model. Although verticality of the phase boundary has been shown only in the bond-random model, a similar mechanism might work for the Néel order of the AF-rich site-random model. On the other hand, the estimates of $c_c$ are quite different in the F-rich site-random model ($c_c \sim 0.13$ in the Heisenberg model, while $c_c \sim 0.41$ in the Ising model). This nontrivial quantum effect cannot be explained by the above thermal-quantum equivalence. A study of the origin of such large difference is now in progress.

Next, we show the data of the SG order parameters. These quantities are scaled by $1/N$, as pointed out in the case of the two-dimensional Heisenberg Mattis model. An example of the fitting is given in Fig. 2 for the F-rich site-random model. Similar good scaling behavior is also observed in the other models. The estimates of the SG order parameter are plotted versus $p$ or $c$ in Fig. 3. These results suggest that the SG order parameter in the site-random model is nonvanishing in the whole parameter region of the concentration $c$ in both the F-rich model and the AF-rich model. However, even in the bond-random model, the SG order parameter also seems to be nonvanishing. In the two-dimensional bond-random Ising model, this order parameter is stable only in the vicinity of $p = 0$ and $p = 1$ in the ground state. This should also be the case in the present bond-random Heisenberg model, in which the SG order is weakened more by quantum fluctuation. Thus, there still remains a finite-size effect in the present calculation, and the existence of the SG order cannot be concluded only from these results. In fact, in the AF-rich site-random model, the estimate of the SG order parameter...
decreases as $c$ increases, and becomes as small as those in the bond-random model around $c \sim 0.5$.

The estimate of the SG order parameter in the Heisenberg Mattis model[4] is also displayed in Fig. 3. The previous study of this model[4] showed that the SG order parameter is nonvanishing at all concentrations. The concentration dependence in the F-rich site-random model is similar to that in the Mattis model, except for small reduction around $c \sim 0.5$. Even in this region, the estimate of the order parameter is larger than that at $c = 0$. Thus, we can at least claim that the SG order remains nonvanishing in the F-rich site-random Heisenberg model in two dimensions.

In summary, we study ground-state phase diagrams of various $S = 1/2$ Heisenberg spin glass models in two dimensions. In the bond-random model (the ±$J$ model), the critical concentration of the Néel phase is estimated as $p_c = 0.11 \pm 0.01$, which is consistent with the corresponding Ising spin glass model. Such equivalence is expected to be related to the vertical phase boundary in the phase diagram of the bond-random Ising model. In the site-random model, the critical concentration is consistent with the Ising spin glass model in the AF-rich case ($c_c = 0.36 \pm 0.03$), while that in the F-rich case ($c_c = 0.13 \pm 0.02$) is decreased much more than that of the corresponding Ising model ($c_c \sim 0.41$). This reduction is the only clear quantum effect displayed in the present study. Moreover, the evidence for the existence of the spin glass phase is found in the two-dimensional quantum Heisenberg site-random model in the ground state, at least in the F-rich case. Studies on the mechanism of the large reduction of the Néel phase in the F-rich site-random model and structures of excitation spectra in the present models are now in progress.

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Figure Captions

Figure 1: The Néel order parameters of 8,10,16,18,20-spin clusters are plotted versus \( N^{-1/2} \) (a) in the bond-random Heisenberg model for \( p = 0.0, 0.1, 0.12, 0.15 \) (from above to below), (b) in the AF-rich site-random Heisenberg model for \( c = 0.0, 0.2, 0.3, 0.35, 0.4 \) and (c) in the F-rich site-random Heisenberg model for \( c = 0.0, 0.05, 0.1, 0.15, 0.2 \). The straight lines are drawn by the least-squares fitting of the last four data of each set.

Figure 2: The SG order parameters of 8,10,16,18,20-spin clusters are plotted versus \( 1/N \) in the F-rich site-random Heisenberg model for \( c = 0.0, 0.2, 0.4, 0.6 \) (from above to below). The straight lines are drawn by the least-squares fitting of the last four data.

Figure 3: The estimates of the SG order parameter in the thermodynamic limit in the bond-random model (solid line with crosses), the AF-rich site-random model (solid line with circles), the F-rich site-random model (solid line with diamonds) and the asymmetric Mattis model (broken line).
