A numerical study for two-dimensional spin 1/2 antiferromagnets: a generalization of Entanglement Perturbation Theory to two-dimensional systems

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Abstract. Two-dimensional spin 1/2 antiferromagnetic Heisenberg models are numerically studied using Entanglement Perturbation Theory, where the ground state wave function is described by a product of local matrices defined at every site, and each matrix is optimized variationally to minimize the energy. We first apply this method for the spin 1/2 antiferromagnetic Heisenberg model on the square lattices to reproduce correctly the known ground state energy and the spin structure factors. Then, we study the spin 1/2 antiferromagnetic Heisenberg model on the triangular lattice with spatially anisotropic nearest neighbor couplings, J and J', to establish the ground state phase diagram as a function of J'/J.

1. Introduction
Recently, much attention has been attracted to geometrically frustrated quantum spin systems where exotic ground states as well as nontrivial fractional excitations might appear [1]. Among them, one of the simplest systems is the spin 1/2 antiferromagnetic Heisenberg model (AFMHM) on the triangular lattice with spatially anisotropic nearest neighbor couplings J and J' (Fig. 1):

\[ H = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j + J' \sum_{\langle i,j' \rangle} \vec{S}_i \cdot \vec{S}_j, \]  \hspace{1cm} (1)

Here \( \vec{S}_i \) is the spin operator of \( |\vec{S}_i| = 1/2 \) at site \( i \), and \( \langle i,j \rangle \) (\( \langle i,j' \rangle \)) runs over a pair of nearest neighbor spins at sites \( i \) and \( j \) along the chain (between the chains) as indicated in Fig. 1. Although this model is seemingly simple, even the ground state has not been understood except for the special coupling cases of \( J'/J = 0 \) (one-dimensional limit), \( J'/J \approx 1 \) (isotropic triangular limit), and \( J'/J \gg 1 \) (isotropic square limit) [2, 3, 4]. Furthermore, this model may describe the low-energy physics of various quasi-2D triangular materials such as Cs2CuCl4 [5], \( \kappa-\text{(BEDT-TTF)}_2\text{Cu}_2\text{(CN)}_3 \) [6], and EtMe3Sb[Pd(dmit)]2 [7] for which experiments have indicate a magnetically disordered Mott insulator, i.e., a possible spin liquid state, at low temperatures. The purpose of the present study is to establish the ground state phase diagram of Eq. (1) as a function of \( J'/J \) and to understand the nature of the low-energy excitations.
The eigenfunction \( \{, \rangle \) of the corresponding Fock state in the wave function \( \{, \rangle \) refers to local states. Note that the trace of the matrix product for a given \( i \) is originally developed in one-dimensional systems [8], and recently has been applied for the 2D Hubbard model [9]. Here, we shall extend this method to 2D spin systems.

To study the ground state of Eq. (1), we use Entanglement Perturbation Theory (EPT) which is originally developed in one-dimensional systems [8], and recently has been applied for the 2D Hubbard model [9]. Here, we shall extend this method to 2D spin systems.

EPT expresses the wave function \( \{, \rangle \) by a product of local square matrices as in matrix product state [10],

\[
\{, \rangle = \sum_{\sigma_1} \sum_{\sigma_2} \cdots \sum_{\sigma_N} \text{Tr} \left[ \xi_1^{\sigma_1} \cdot \xi_2^{\sigma_2} \cdots \cdots \xi_N^{\sigma_N} \right] |\sigma_1\rangle \otimes |\sigma_2\rangle \otimes \cdots \otimes |\sigma_N\rangle,
\]

where \( \xi_i^{\sigma_i} \) is the local wave function matrix at site \( i \), and \( N \) is the number of sites. \( \sigma_i (= \uparrow, \downarrow) \) refers to local states. Note that the trace of the matrix product for a given \( \{\sigma_i\} \) is the amplitude of the corresponding Fock state in the wave function \( \{, \rangle \). The dimension \( p \) of the square matrices \( \xi_i^{\sigma_i} \) controls the accuracy of the wave function \( \{, \rangle \) when \( \{, \rangle \) is used as a variational state for \( H \), and in principle \( \{, \rangle \) with optimized \( \xi_i^{\sigma_i} \) becomes exact with \( p \rightarrow \infty \). The matrices \( \xi_i^{\sigma_i} \) are optimized to minimize the variational energy:

\[
\frac{\partial}{\partial \eta_i} \langle \psi (\eta_1, \eta_2, \cdots, \eta_N) | H | \psi (\eta_1, \eta_2, \cdots, \eta_N) \rangle \psi (\eta_1, \eta_2, \cdots, \eta_N) \rangle = 0.
\]

Here \( \eta_i \) is a vector representation of \( \xi_i^{\sigma_i} \). We then arrive at a generalized eigenvalue equation

\[
X_i (\eta_1, \cdots, \eta_{i-1}, \eta_{i+1}, \cdots, \eta_N) \eta_i = \mu Y_i (\eta_1, \cdots, \eta_{i-1}, \eta_{i+1}, \cdots, \eta_N) \eta_i \quad (i = 1, 2, \cdots, N),
\]

where \( X_i \) and \( Y_i \) are appropriate matrices depending implicitly on \( \{\eta_i\} \), and \( \mu \) is the eigenvalue. The eigenfunction \( \{\eta_i\} \) with the smallest \( \mu \) describes the optimized ground state wave function \( \{, \rangle \). The details of how to extend EPT to 2D spin systems will be discussed elsewhere [11].

3. Results

First, we study spin 1/2 AFM-HM on the square lattice with \( N = 4 \times 4 \) to check the validity of the method in 2D. As explained above, EPT is the variational method for the ground state \( \{, \rangle \), and the larger the dimension \( p \) of the matrices is, the more accurate \( \{, \rangle \) becomes. This is clearly seen in Fig. 2 where the energy expectation value is plotted as a function of \( p \). The converged ground state energy per site is \(-0.70175J\) with \( p = 31 \), which is very close to the numerically exact value \(-0.70178J\) obtained by Exact Diagonalization (ED).

Next, we calculate the spin correlation functions \( C_i (\vec{R}) = \langle \vec{S}_{R+i} \cdot \vec{S}_{R} \rangle \), and the results are compared with those obtained by ED in Table.1. The excellent agreement is observed. We have
Figure 2. The expectation value of energy for spin 1/2 AFMHM on the isotropic square lattice with $N = 4 \times 4$ as a function of the dimension $p$ of matrices $\xi_i^{\sigma}$. For comparison, the numerically exact value obtained by ED is also plotted by dashed line.

studied $C(\vec{R})$ using different lattice sizes with $N$ up to $N = 10 \times 10$, and the results will be reported elsewhere [11].

Table 1. Spin correlation functions $C(\vec{R})$ for spin 1/2 AFMHM on the isotropic square lattice with $N = 4 \times 4$. EPT results are compared with those obtained by ED. Here $\vec{R} = i_x \hat{x} + i_y \hat{y}$.

| $(i_x, i_y)$ | EPT     | ED     |
|-------------|---------|--------|
| (0,1)       | -0.35096| -0.35089|
| (1,0)       | -0.35084| -0.35089|
| (2,0)       | 0.21373 | 0.21377|
| (0,2)       | 0.21381 | 0.21377|
| (1,2)       | -0.20224| -0.20216|
| (2,1)       | -0.20216| -0.20216|
| (2,2)       | 0.17966 | 0.17963|

Encouraged by these results, we shall now study spin 1/2 AFMHM on the triangular lattice. First, we calculate the ground state energy per site $E_{GS}$ for the isotropic limit $J = J'$ with $N = 6 \times 6$, and find that $p = 44$ ($E_{GS} = -0.5450 J$) is enough to achieve the accuracy of about 2.7%, for which the numerically exact energy is $-0.5603 J$ [2]. Next, we calculate the spin structure factor $S(q) = \sum_{R} e^{-i q \cdot R} C(R) / N$ for $N = 6 \times 6$ and several values of $J'/J$. These results are shown in Fig.3. Fig.3 (b) corresponds to the isotropic limit. It is clearly seen in Fig.3 (b) that peaks appear at $q^* = (4\pi/3, 0)$ and the symmetrically equivalent $q$’s, indicating the classical Néel ordered spin structure. The calculated value of $S(q^*)$ is 0.0946 which is about 4.4% larger than the numerically exact value (0.0904) [2]. With increasing $J'/J$, we find that the spin structure factor changes abruptly at around $J'/J = 1.18$ above which $S(q)$ has peaks at $(0, \pm 2\pi\sqrt{3})$. These wave numbers correspond to the classical Néel ordered spin structure on the square lattice, namely, the one expected in $J'/J \rightarrow \infty$. Instead, with decreasing $J'/J$, we find that $S(q)$ shows several incommensurate peaks with a one-dimensional character for $J'$ smaller than about 0.8, as shown in Fig.3 (a). Since the system size studied in this paper is limited, we can not exclude, at this moment, a possibility that there exists another ordered or disordered phase [3, 4].
J′/J = 0.78 (a), J′/J = 1.00 (b), and J′/J = 1.20 (c) are used.

4. Conclusions
We have extended EPT to 2D spin systems to study the ground state properties of spin 1/2 AFMHM on the anisotropic triangular lattice. We have shown that EPT successfully reproduces the known results for spin 1/2 AFMHM on the square lattice. We then applied the method to the spatially anisotropic triangular lattice. We found that, based on our simulations for N = 6 × 6, the classical Néel order with the nearest neighbor spin angle of 120° is stable for a wide range of parameter (0.8 ≤ J′/J ≤ 1.2), and that for J′/J ≥ 1.2 the spin structure becomes collinearly Néel ordered, i.e., the one expected for J′/J → ∞. Although the evolution of the spin structure factors as a function of J′/J is clear, more systematic studies are necessary to determine the nature of various phases and the critical values of J′/J for the phase boundary. A study in this direction is now in progress [11].

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