Magnetic Phases of the Shastry-Sutherland Model using Projected Entangled Simplex States

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Abstract
We study the magnetic phases of the Shastry-Sutherland lattice at finite magnetic fields using the Projected Entangled Simplex States (PESS) class of tensor networks. The ground state is calculated via a projection approach by imaginary time evolution at various external fields. We study the convergence of the method and compare to results from Density Matrix Renormalization Group and Tensor Renormalization. We focus on the commensurate phases at low fields and establish the structure of the correlations at several phases.

Introduction
The Shastry-Sutherland Model (SSM) describes a two-dimensional Heisenberg antiferromagnet that captures the physical properties of real systems such as SrCu2(BO3)2. The SSM is interesting as it is known to exhibit distinct magnetic plateaus in the magnetization curve. The lattice can be thought of as an array of dimers with exchange constant $J$, interacting via weaker interdimer bonds $J'$. Figure 1a.

\[ R = J \sum_{\text{link}} S_i \cdot S_j + J' \sum_{\text{bond}} S_i \cdot S_j - h \sum_i S_i^z \]

where $h$ is the external field, and $S_i$ is the standard spin-$\frac{1}{2}$ spin operator on site $i$. The first sum is over the dimer (diagonal) bonds, while the second is over the interdimer bonds (forming a square lattice).

We use $J'/J = 0.1$, close to the physical value for SrCu2(BO3)2. At this value of $J'/J$, the zero-field ground state can be shown to simply be made up of isolated singlet states along each dimer. At higher fields, interesting patterns of $(S_z > 1)$ triplets form the magnetic plateaus.

We use the Projected Entangled Simplex States (PESS) tensor network as a variational ansatz to study the SSM. The PESS is a generalization of the Projected Entangled Pure States (PEPS) [1].

Method
PESS Representation

Figure 1: (a) The Shastry-Sutherland Model is characterized by strong ($J > J'$) dimer bonds. (b) The PESS representation of the SSM. A $4$-PESS (Figure 1, right) is used to represent the SSM. It is composed of site tensors $T_i^a$ and simple tensors $S_i$. Tensors are initialized randomly for unbiased simulations, or from a product state near a desired plateau state.

Imaginary Time Evolution

Figure 2: An iteration of imaginary time evolution step for one plaquette. (a) The site- and simple tensors are contracted, and the evolution operator is applied. The $3$-singlet bond vectors act as an approximation of the surrounding environment (only one is shown). (b) The contracted tensors is decomposed by higher order singular value decomposition (SVD) to create new tensors. The simple tensor is truncated to bond dimension $d$ and the $3$ vectors are divided out, creating new simple tensors $S_i^{(d)}$ and site tensors $T_i^{(d)}$.

We perform the ground state computation by imaginary time evolution using the simple update method. Because the Hamiltonian of adjacent plaquettes do not commute, the time evolution must be done in small time steps $\tau$ for the two plaquette sublattices $\uparrow$ and $\downarrow$.

\[ \hat{H} = \hat{H}_0 + \hat{T} \]

The first order Suzuki-Trotter decomposition of the time evolution operator is then given by

\[ e^{-i\tau \hat{H}} = e^{-i\tau \hat{H}_0} e^{-i\tau \hat{T}} \]

These terms are applied sequentially with small $\tau$. The ground state is projected out, assuming there is some finite overlap with the initial state.

\[ \langle \Psi \vert \hat{O} \vert \psi \rangle \approx \langle \Psi \vert \psi \rangle \]

Contraction of the Infinite Network

Figure 3: Transformation to a square lattice for CTMGR. Pairs of sites are contracted together, resulting in a square lattice of $1 \times 1$ state sites.

Figure 4: CTMGR seeks to compute the infinite lattice environment by a set of edge and corner tensors. (a) The tensors are contracted with their counterparts. Edge (corner) tensors are initialized by tracing over the bonds in one (two) direction(s). (b) Each site on the $1 \times 1$ array gives rise to an operator used to renormalize the tensor. (c) Each iteration extends the effective size of the environment, which is then absorbed into the environment tensor and renormalized to a boundary dimension $\chi$ using the isometries previously computed in (b).

Computation of Observables

The converged environment can be used to efficiently compute local observables.

\[ \langle \Psi \vert \hat{O} \vert \psi \rangle = \frac{\langle \Psi \vert \hat{O} \vert \psi \rangle}{\langle \Psi \vert \psi \rangle} \]

Figure 5: Computation of the expectation value of a local observable $\langle \langle \hat{O} \rangle \rangle$. A $3 \times 3$ array of tensors is used. Larger arrays can be used for higher accuracy. Correlations $\langle \langle \hat{O} \rangle \rangle$, can be computed by extending the array to include both sites $i$ and $j$.

Results

Plateau States

\[ \frac{1}{\sqrt{2}} \text{Plateau} \]

\[ \frac{1}{2} \text{Plateau} \]

Figure 6: Energy convergence as a function of bond dimension $D$. We compare the energy of the $M = 1/2$ triplets plateau state on a $1 \times 1$ unit cell with that of PEPS and DMRG. Convergence in tensor dimension $D'$ appears to be slower than that of PEPS. This is most likely because the PEPS formulation of this work contains fewer variational parameters than a PEPS of the same $D$. Instead, Convergence with boundary dimension $\chi$ for the $J'/J$ energy.

Conclusions

We have successfully computed the ground state PESS wavefunction for the SSM at various magnetization plateaus. Our results are comparable to a similar PEPS method and with a finite lattice DMRG. We plan to explore larger values of $D$.

Further investigation includes exploring more unit cell sizes and potential plateau states, such that a somewhat complete M(0) curve can be constructed. The existence of low field plateaus at various values of $J'/J$ is also of interest.

References