Boundary Conditions for the Heisenberg Antiferromagnet Lattice Model

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1 Introduction

This short writeup explains some details about our studies of different boundary conditions on the Heisenberg antiferromagnet for different square and rectangular lattices. We focus on the eigenvalues and spin-spin correlations of periodic, antiperiodic, twisted, open, and random boundary conditions. Understanding these boundary conditions is important because they help us approximate the results of much larger systems, by simulating computationally feasible lattices.

2 Heisenberg Hamiltonian

The Hamiltonian for the Heisenberg model is given by

$$\mathcal{H} = J_1 \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \tag{1}$$

where $\langle i, j \rangle$ indicates the set of distinct nearest neighbor pairs. From the definition of the spin raising and lowering operators, $S_i^{\pm} = S_i^x \pm i S_i^y$, we can rewrite the dot product of two spins:

$$\mathbf{S}_i \cdot \mathbf{S}_j = \frac{1}{2} \left(S_i^+ S_j^- + S_i^- S_j^+ \right) + S_i^z S_j^z \tag{2}$$

If we have a finite set of N spins on a line, $\{S_0, S_1, \ldots S_{N-1}\}$ and want to approximate an infinite system, there are several ways to handle the spins at the edge of our simulation cell.

2.1 Periodic Boundary Conditions

We can apply periodic boundary conditions, which gives:

$$\mathbf{S}_{N-1} \cdot \mathbf{S}_N = \mathbf{S}_{N-1} \cdot \mathbf{S}_0 = \frac{1}{2} \left(S_{N-1}^+ S_0^- + S_{N-1}^- S_0^+ \right) + S_{N-1}^z S_0^z \tag{3}$$

2.2 Antiperiodic Boundary Conditions

We can apply antiperiodic boundary conditions, which adds a negative sign across our periodic boundary conditions:

$$\mathbf{S}_{N-1} \cdot \mathbf{S}_N = \mathbf{S}_{N-1} \cdot (-\mathbf{S}_0) = -(\mathbf{S}_{N-1} \cdot \mathbf{S}_0) = -\frac{1}{2}\left(S_{N-1}^+ S_0^- + S_{N-1}^- S_0^+\right) - S_{N-1}^z S_0^z \tag{4}$$

2.3 Twisted Boundary Conditions

We can apply twisted boundary conditions, defined in Sec. 3 which gives:

$$\mathbf{S}_{N-1} \cdot \mathbf{S}_N = \mathbf{S}_{N-1} \cdot \left(e^{i\phi S_0^z} \mathbf{S}_0 e^{-i\phi S_0^z}\right) \tag{5}$$

Which can be separated into its x, y, and z components:

$$S_{N-1}^x (e^{i\phi S_z} S_0^x e^{-i\phi S_z}) + S_{N-1}^y (e^{i\phi S_z} S_0^y e^{-i\phi S_z}) + S_{N-1}^z S_0^z \tag{6}$$

Using Eq. (25), $S_x = \frac{1}{2}(S^+ + S^-)$, and $S_y = \frac{1}{2i}(S^+ - S^-)$ we get:

$$\begin{aligned}
\mathbf{S}_{N-1} \cdot \mathbf{S}_N =& S_{N-1}^x \left(\cos(\phi) S_0^x - \sin(\phi) S_0^y\right) + \\
& S_{N-1}^y \left(\sin(\phi) S_0^x + \cos(\phi) S_0^y\right) + S_{N-1}^z S_0^z \\
=& \cos(\phi)\left(S_{N-1}^x S_0^x + S_{N-1}^y S_0^y\right) + \sin(\phi)\left(S_{N-1}^y S_0^x - S_{N-1}^x S_0^y\right) + S_{N-1}^z S_0^z \\
=& \frac{1}{2}\cos(\phi)\left(S_{N-1}^+ S_0^- + S_{N-1}^- S_0^+\right) + \frac{1}{2i}\sin(\phi)\left(S_{N-1}^+ S_0^- - S_{N-1}^- S_0^+\right) + S_{N-1}^z S_0^z \\
=& \frac{1}{2}\left(e^{-i\phi}(S_{N-1}^+ S_0^-) + e^{i\phi}(S_{N-1}^- S_0^+)\right) + S_{N-1}^z S_0^z
\end{aligned}$$

2.4 Open Boundary Conditions

Open boundary conditions simply tell us that the spins at the edge of the simulation cell might be missing some neighbors compared to spins on the interior:

$$\mathbf{S}_{N-1} \cdot \mathbf{S}_N = 0 \tag{7}$$

i.e. we drop this term from $\mathcal{H}$.

2.5 Random Boundary Conditions

Random boundary conditions add fixed spins at random when crossing the boundary, while maintaining $S_{tot}^z = 0$ to the best of our ability. This results in:

$$\mathbf{S}_{N-1} \cdot \mathbf{S}_N = S_{N-1}^z S_{\text{rand}}^z \tag{8}$$

Where S_{rand}^z is randomly chosen from a lattice-perimeter-sized list of equal spin ups and downs, such that each spin is chosen only once.

3 Twisted Boundary Conditions

Fouet *et al.*[1] use the spin rotation operator to define twisted boundary conditions (TBC) as follows: [1]

$$\mathbf{S}(\mathbf{R}_i + \mathbf{t}_j) = e^{i\phi_j S_z(\mathbf{R}_i)} \mathbf{S}(\mathbf{R}_i) e^{-i\phi_j S_z(\mathbf{R}_i)}. \tag{9}$$

3.1 Spin-$\frac{1}{2}$ rotation operator

Here we expand the spin rotation operator given by the exponentiation of $\hat{S}_z$, which for a spin-1/2 system is $\hat{S}_z = \frac{1}{2}\sigma_z$.

$$e^{i\phi\sigma_z} = \sum_{n=0}^{\infty} \frac{(i\phi\sigma_z)^n}{n!} \tag{10}$$

Recognizing that $\sigma_z^2 = I$, where I is the 2×2 identity matrix:

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \sigma_z^2 = I \tag{11}$$

Separating the series into its even and odd terms:

$$e^{i\phi\sigma_z} = \sum_{n=0}^{\infty} \frac{(i\phi\sigma_z)^{2n}}{(2n)!} + \sum_{n=0}^{\infty} \frac{(i\phi\sigma_z)^{2n+1}}{(2n+1)!} \tag{12}$$

Recalling the cosine series, we can see that the first term in Eq. (12) is:

$$\sum_{n=0}^{\infty} \frac{(i\phi\sigma_z)^{2n}}{(2n)!} = \sum_{n=0}^{\infty} \frac{[(i\phi\sigma_z)^2]^n}{(2n)!} = \sum_{n=0}^{\infty} \frac{(-1)^n \phi^{2n} I}{(2n)!} \tag{13}$$

$$= I \sum_{n=0}^{\infty} \frac{(-1)^n \phi^{2n}}{(2n)!} = \cos(\phi) I \tag{14}$$

Likewise, the sine series tells us that the second term in Eq. (12) becomes:

$$\sum_{n=0}^{\infty} \frac{(i\phi\sigma_z)^{2n+1}}{(2n+1)!} = i\sigma_z \sum_{n=0}^{\infty} \frac{(-1)^n \phi^{2n+1}}{(2n+1)!} = i\sin(\phi)\sigma_z \tag{15}$$

Therefore:

$$e^{i\phi\sigma_z} = \cos(\phi) I + i\sin(\phi)\sigma_z, \tag{16}$$

so in terms of the spin-$\frac{1}{2}$ operators:

$$e^{i\phi S_z} = e^{i(\phi/2)\sigma_z} = \cos\left(\frac{\phi}{2}\right) I + 2i \sin\left(\frac{\phi}{2}\right) S_z, \tag{17}$$

[1] At the beginning of their paper they use $\mathbf{t}_j$ to represent the primitive lattice vectors, but here it seems like they must refer to the supercell lattice vectors.

3.2 Simplifying the TBC

Expanding Eq. (9) into its vector components:

$$\mathbf{S}(\mathbf{R}_i + \mathbf{t}_j) = e^{i\phi_j S_z(\mathbf{R}_i)} \mathbf{S}(\mathbf{R}_i) e^{-i\phi_j S_z(\mathbf{R}_i)} \tag{18}$$

$$= e^{i\phi_j S_z(\mathbf{R}_i)} \begin{pmatrix} S_x(\mathbf{R}_i) \\ S_y(\mathbf{R}_i) \\ S_z(\mathbf{R}_i) \end{pmatrix} e^{-i\phi_j S_z(\mathbf{R}_i)} \tag{19}$$

$$= \begin{pmatrix} e^{i\phi_j S_z(\mathbf{R}_i)}\, S_x(\mathbf{R}_i)\, e^{-i\phi_j S_z(\mathbf{R}_i)} \\ e^{i\phi_j S_z(\mathbf{R}_i)}\, S_y(\mathbf{R}_i)\, e^{-i\phi_j S_z(\mathbf{R}_i)} \\ e^{i\phi_j S_z(\mathbf{R}_i)}\, S_z(\mathbf{R}_i)\, e^{-i\phi_j S_z(\mathbf{R}_i)} \end{pmatrix} \tag{20}$$

We can simplify the S_x term using Eq. (17):

$$[2i\sin(\phi_j/2) S_z(\mathbf{R}_i) + \cos(\phi_j/2) I]\, S_x(\mathbf{R}_i)\, [-2i\sin(\phi_j/2) S_z(\mathbf{R}_i) + \cos(\phi_j/2) I] \tag{21}$$

Expanding, and dropping the common factor of $\mathbf{R}_i$ in all spin operators, we get:

$$\begin{aligned} &\cos(\phi_j/2) I S_x \cos(\phi_j/2) I - 2i\sin(\phi_j/2) S_z S_x 2i\sin(\phi_j/2) S_z \\ &- \cos(\phi_j/2) S_x 2i\sin(\phi_j/2) S_z + 2i\sin(\phi_j/2) S_z S_x \cos(\phi_j/2) \\ = &\cos^2(\phi_j/2) S_x + 4\sin^2(\phi_j/2) S_z S_x S_z \\ &+ 2i\sin(\phi_j/2)\cos(\phi_j/2)\,[S_z, S_x] \end{aligned}$$

Noting that $[S_z, S_x] = iS_y$, $S_z^2 = \frac{1}{4}I$, and $S_z S_x S_z = -\frac{1}{8}S_x$:

$$\cos^2(\phi_j/2) S_x(\mathbf{R}_i) - 2\cos(\phi_j)\sin(\phi_j) S_y(\mathbf{R}_i) - \sin^2(\phi_j) S_x(\mathbf{R}_i) \tag{22}$$

Using the double angle formulas:

$$= \cos(\phi_j) S_x(\mathbf{R}_i) - \sin(\phi_j) S_y(\mathbf{R}_i) \tag{23}$$

Doing the same process for the Sy term gives:

$$= \sin(\phi_j) S_x(\mathbf{R}_i) + \cos(\phi_j) S_y(\mathbf{R}_i) \tag{24}$$

Putting it all together Eq. (20) becomes:

$$\mathbf{S}(\mathbf{R}_i + \mathbf{t}_j) = \begin{pmatrix} \cos(\phi_j) S_x(\mathbf{R}_i) - \sin(\phi_j) S_y(\mathbf{R}_i) \\ \sin(\phi_j) S_x(\mathbf{R}_i) + \cos(\phi_j) S_y(\mathbf{R}_i) \\ S_z(\mathbf{R}_i) \end{pmatrix}. \tag{25}$$

3.3 Aside on Spin-$\frac{1}{2}$ subtleties

Equation (16) is an identity of the σ matrices, which are used to represent the spin operators for spin-$\frac{1}{2}$. However, Eq. (17) only holds for spin-$\frac{1}{2}$. To see this, consider spin-1. The possible S_z values are 1, 0, and -1, so the matrix for S_z in the basis with quantization axis along $\hat{z}$ is

$$\hat{S}_z^{(1)} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \tag{26}$$

Proving Eq. (16) made use of the identity $\sigma_z^2 = 1$, which for spin-$\frac{1}{2}$ means $S_z^2 = \frac{1}{4}I$. But clearly for spin-1, $\left(\hat{S}_z^{(1)}\right)^2$ is not proportional to the $3{\times}3$ identity matrix, so Eq. (17) need not hold for spin operators with other values of total spin.

In the same way, $\sigma_z\sigma_x\sigma_z = -\sigma_x$, so for spin-$\frac{1}{2}$ we have $S_zS_xS_z = -\frac{1}{8}S_x$. However, the latter relationship need not hold for other spins; in fact, for spin-1 $S_z^{(1)}S_x^{(1)}S_z^{(1)} = 0$!

To treat all spins on an equal footing, one needs to work only with the defining property of the spin operators, namely the commutation relations:

$$[S_x, S_y] = i\hbar S_z. \tag{27}$$

Evaluating expressions like Eq. (9) can be done using the Baker-Hausdorff lemma,

$$e^{\hat{A}}\hat{B}e^{-\hat{A}} = \hat{B} + \left[\hat{A}, \hat{B}\right] + \frac{1}{2!}\left[\hat{A}, \left[\hat{A}, \hat{B}\right]\right] + \frac{1}{3!}\left[\hat{A}, \left[\hat{A}, \left[\hat{A}, \hat{B}\right]\right]\right], \tag{28}$$

which depends only on the commutators of the operators involved, not their pairwise products. We leave it as an exercise to verify Eq. (25) using Eq. (28).

4 Conclusions and Further Understanding

In this section, we'll look more closely at the different boundary conditions through plots.

4.1 Periodic, Open, Random, and Antiperiodic Boundary Conditions

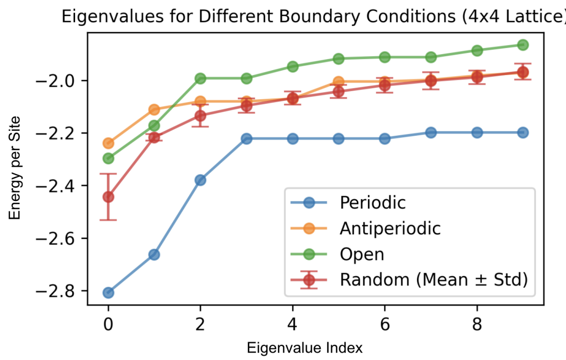

Figure 1: Lowest ten eigenvalues of varying boundary conditions on a 4x4 lattice.

By plotting the energy per site for the lowest trn eigenvalues, we can notice that periodic boundary conditions produce the lowest eigenvalues for a 4x4 lattice. When considering the antiferromagnetic state, we can notice that antiperiodic boundary conditions create the most frustrated state, leading to the highest energy per site for the ground state.

4.2 Mixing Boundary Conditions

We can consider the antiferromagnetic state even further for different lattice sizes.

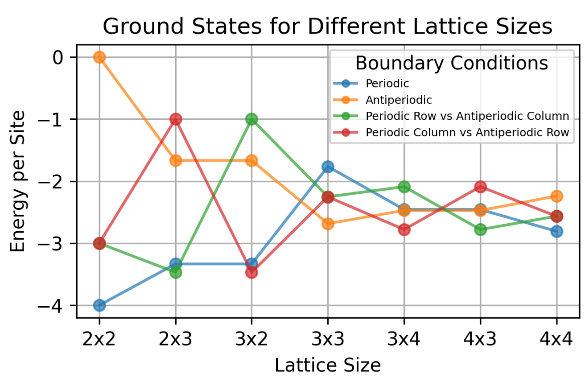

Figure 2: Comparing periodic and antiperiodic boundary conditions with mixes of periodic rows with antiperiodic columns and vice versa.

We can see from this plot that antiperiodic boundary conditions in an "odd" direction produce a neighbor that keeps the state antiferromagnetic. Likewise, periodic boundary conditions in an "even" direction also keep the state antiferromagnetic. This means that mixing boundary conditions will produce the lowest ground state for rectangular lattices, as shown above.

4.3 Twisted Boundary Conditions

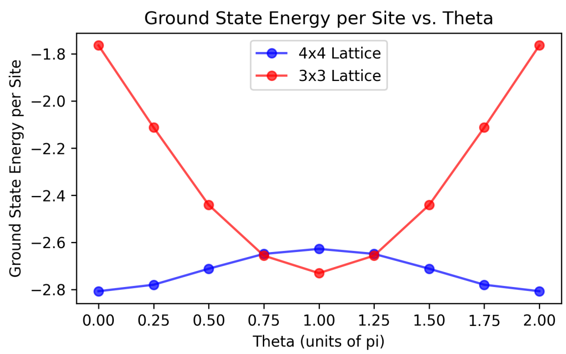

Figure 3: Ground state energy per site with twisted boundary conditions as a function of theta for a 3×3 and 4×4 lattice.

From this plot, we can see the periodicity of twisted boundary conditions as we change theta.

4.4 Spin-Spin Correlations

By continuing to mix all of these boundary conditions we can notice a key similarity:

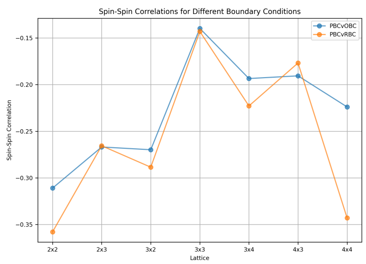

Figure 4: Spin-spin correlation comparing periodic rows and open columns (blue) with periodic rows and random columns (orange).

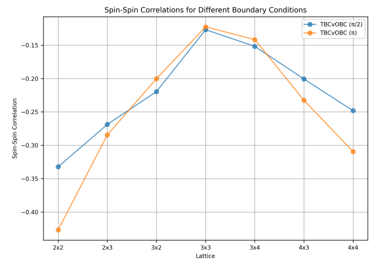

Figure 5: Spin-spin correlation comparing twisted rows with theta of $\frac{\pi}{2}$ (blue) and open columns with twisted rows with theta of π and open columns (orange).

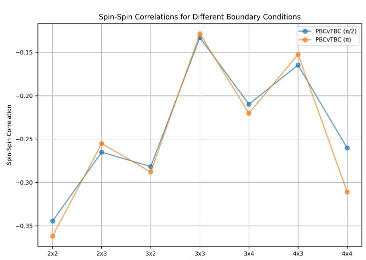

Figure 6: Spin-spin correlation comparing periodic rows and twisted columns with a theta of $\frac{\pi}{2}$ (blue) with periodic rows and twisted with a theta of π (orange).

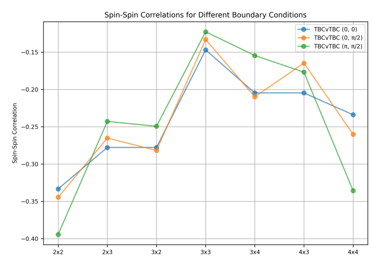

Figure 7: Spin-spin correlation comparing entirely periodic boundary conditions (blue), periodic rows and twisted columns with theta of $\frac{\pi}{2}$ (orange), and twisted rows with theta of π with twisted columns with theta of $\frac{\pi}{2}$ (green).

It seems like no matter how you mix boundary conditions, they always seem to prefer the antiferromagnetic state over the ferromagnetic one.

References

[1] JB Fouet, P Sindzingre, and C Lhuillier. An investigation of the quantum J_1-J_2-J_3 model on the honeycomb lattice. *The European Physical Journal B-*

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