Boundary Conditions for the Heisenberg Antiferromagnet

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The Heisenberg Hamiltonian

The Hamiltonian for the Heisenberg model is given by:

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

Using the definitions of the raising and lowering operators, the Hamiltonian entry simplifies to:

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

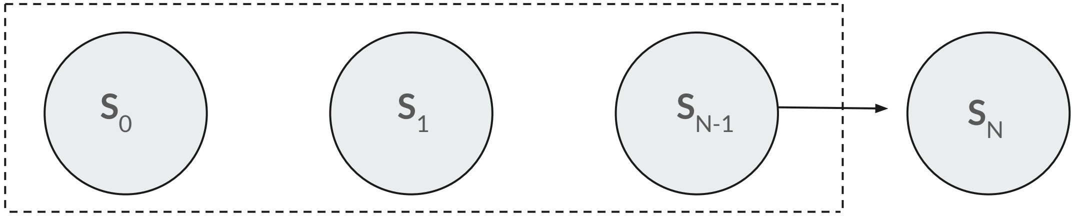
Periodic (PBC) and Antiperiodic (ABC)

Applying Periodic Boundary Conditions gets us:

$$\mathbf{S}_{N-1} \cdot \mathbf{S}_N = \mathbf{S}_{N-1} \cdot \mathbf{S}_0 = \frac{1}{2}\left(S^+_{N-1}S^-_0 + S^-_{N-1}S^+_0\right) + S^z_{N-1}S^z_0$$

Antiperiodic Boundary Conditions simply adds a minus sign:

$$\mathbf{S}_{N-1} \cdot \mathbf{S}_N = \mathbf{S}_{N-1} \cdot (-\mathbf{S}_0) = -(\mathbf{S}_{N-1} \cdot \mathbf{S}_0) = -\frac{1}{2}\left(S^+_{N-1}S^-_0 + S^-_{N-1}S^+_0\right) - S^z_{N-1}S^z_0$$



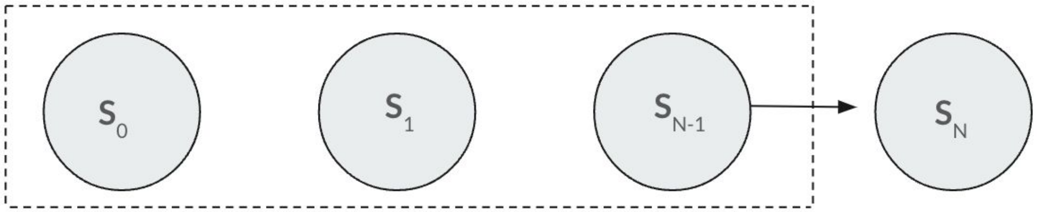
Open (OBC) and Random (RBC)

Open Boundary conditions omits boundary crossing neighbors:

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

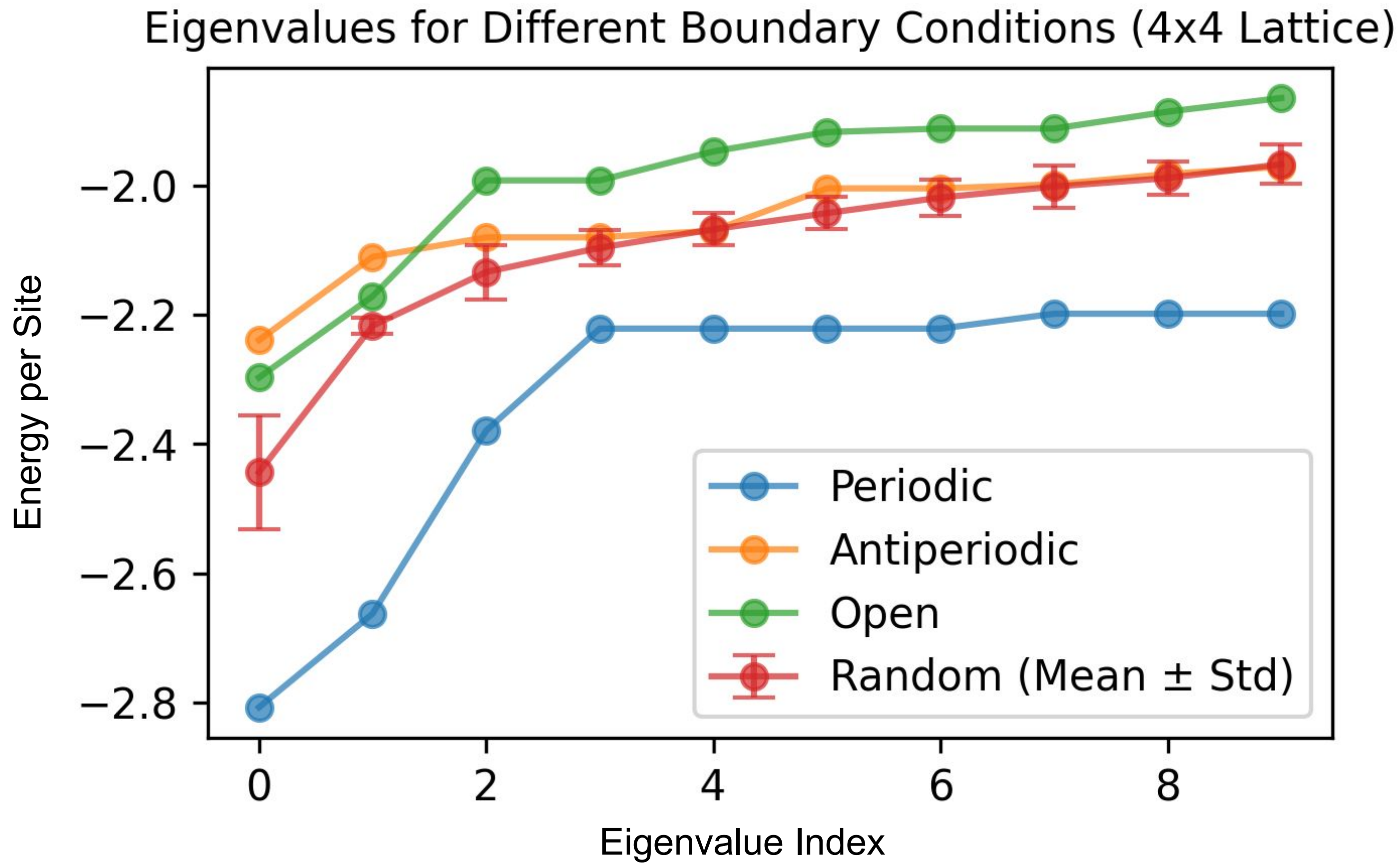
Random Boundary conditions adds a random neighbor to the boundary crossing:

$$\mathbf{S}_{N-1} \cdot \mathbf{S}_N = S^z_{N-1} S^z_{rand}$$



Details of Calculations

- Square/Rectangular Lattice Creation
- Creating/Finding Neighbor Pairs
- Hamiltonian Construction
- Finding Eigenvalues/Eigenvectors
- Spin-Spin Correlations for Ground States
- Cross-validated with NetKet (Periodic Boundary Conditions)



Eigenvalues for Different Boundary Conditions (4x4 Lattice)
Energy per Site
Eigenvalue Index
−2.0
−2.2
−2.4
−2.6
−2.8
0
2
4
6
8
Periodic
Antiperiodic
Open
Random (Mean ± Std)

Twisted (TBC)

We define Twisted Boundary conditions as:

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

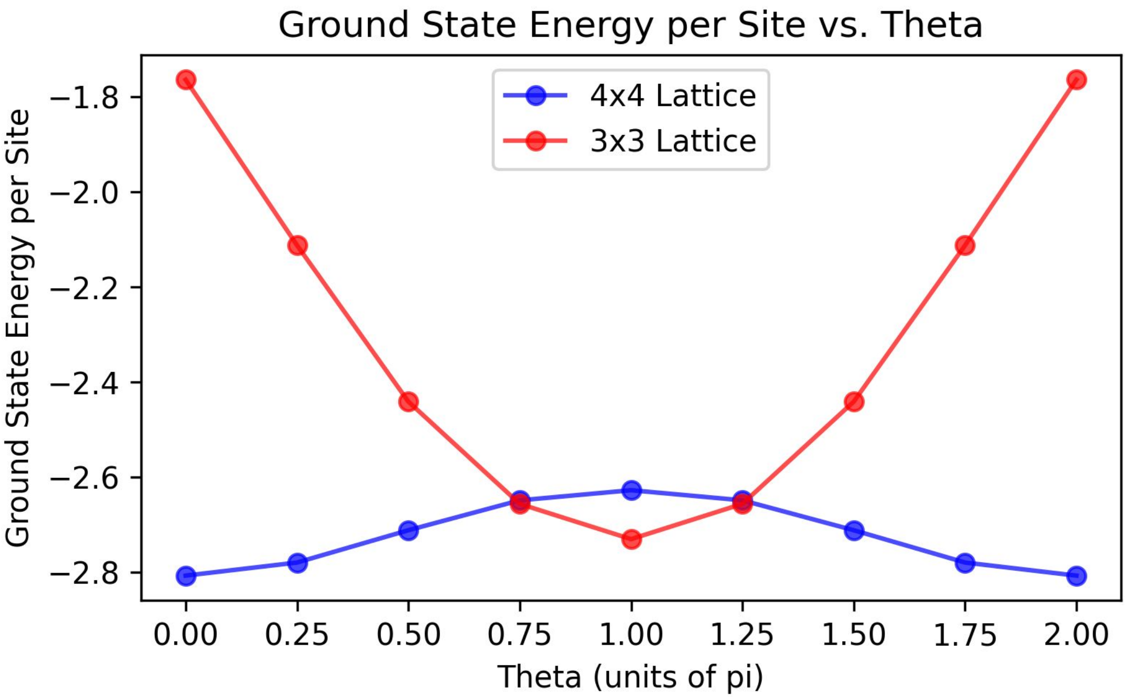
$\mathbf{t}_j$ = **Supercell lattice vector**

We can simplify this to:

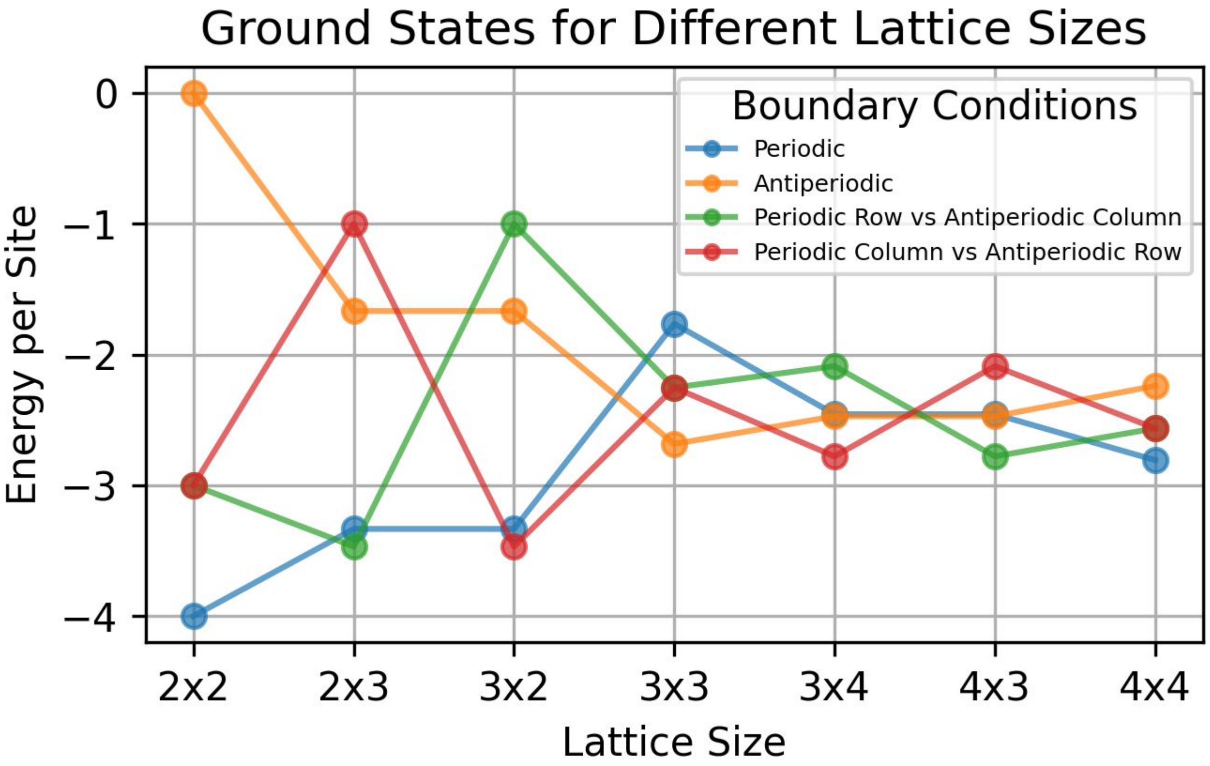
$$\mathbf{S}(\mathbf{R}_i + \mathbf{t}_j) = \begin{pmatrix} \cos(\phi_j) S_x(\mathbf{R}_i) - \sin(\phi_j) S_y(\mathbf{R}_i) \\ \sin(\phi_j) S_x(\mathbf{R}_i) + \cos(\phi_j) S_y(\mathbf{R}_i) \\ S_z(\mathbf{R}_i) \end{pmatrix}.$$

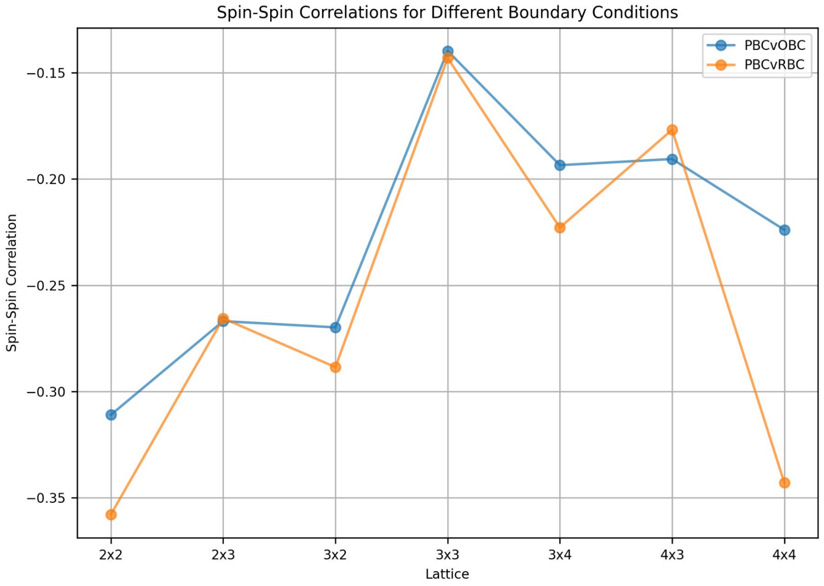
Making the Hamiltonian entry:

$$\frac{1}{2}\left(e^{-i\phi}(S_{N-1}^{+} S_0^{-}) + e^{i\phi}(S_{N-1}^{-} S_0^{+})\right) + S_{N-1}^{z} S_0^{z}$$

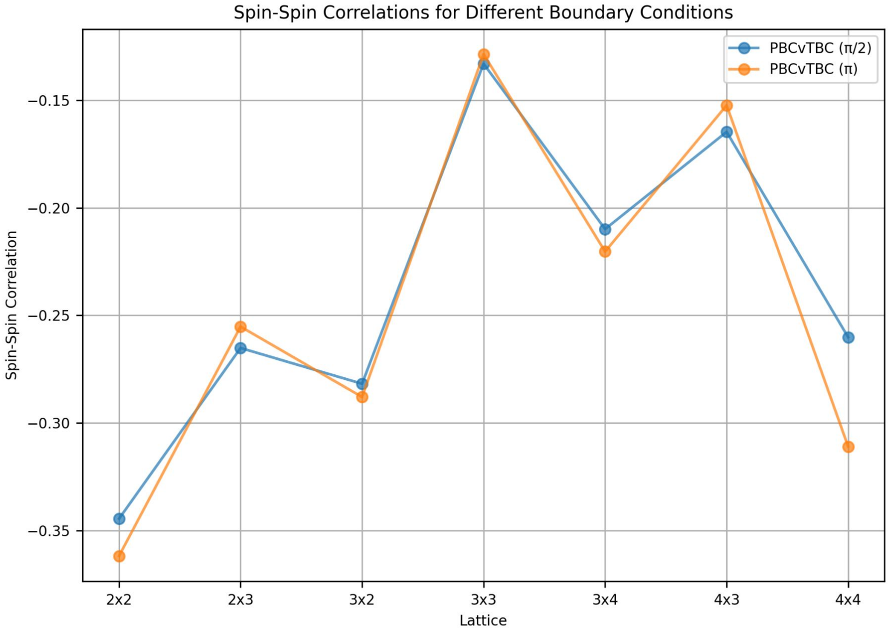

Ground State Energy per Site vs. Theta
4x4 Lattice
3x3 Lattice
Ground State Energy per Site
−1.8
−2.0
−2.2
−2.4
−2.6
−2.8
0.00
0.25
0.50
0.75
1.00
1.25
1.50
1.75
2.00
Theta (units of pi)

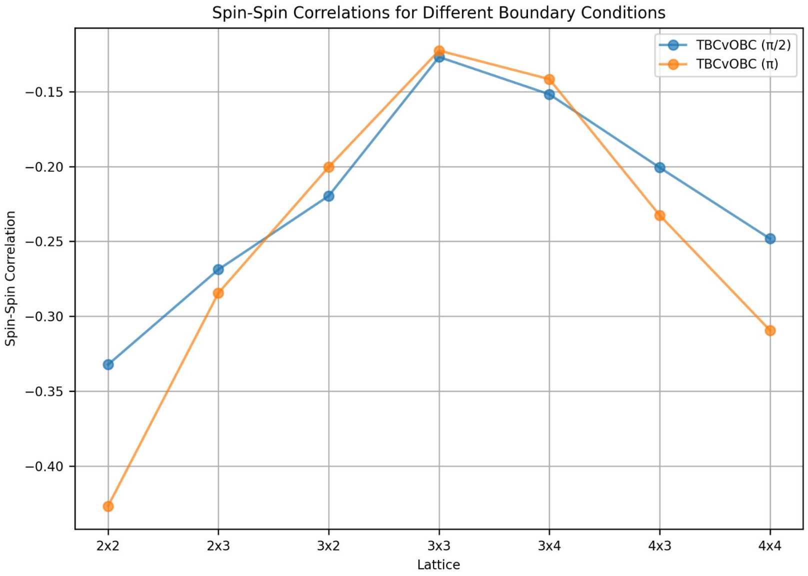
Mixing Boundary Conditions



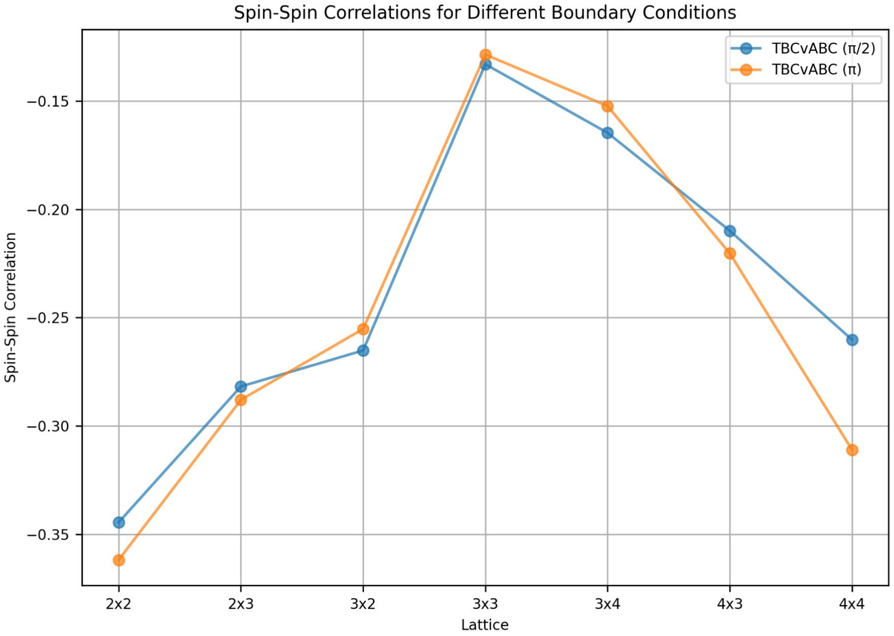


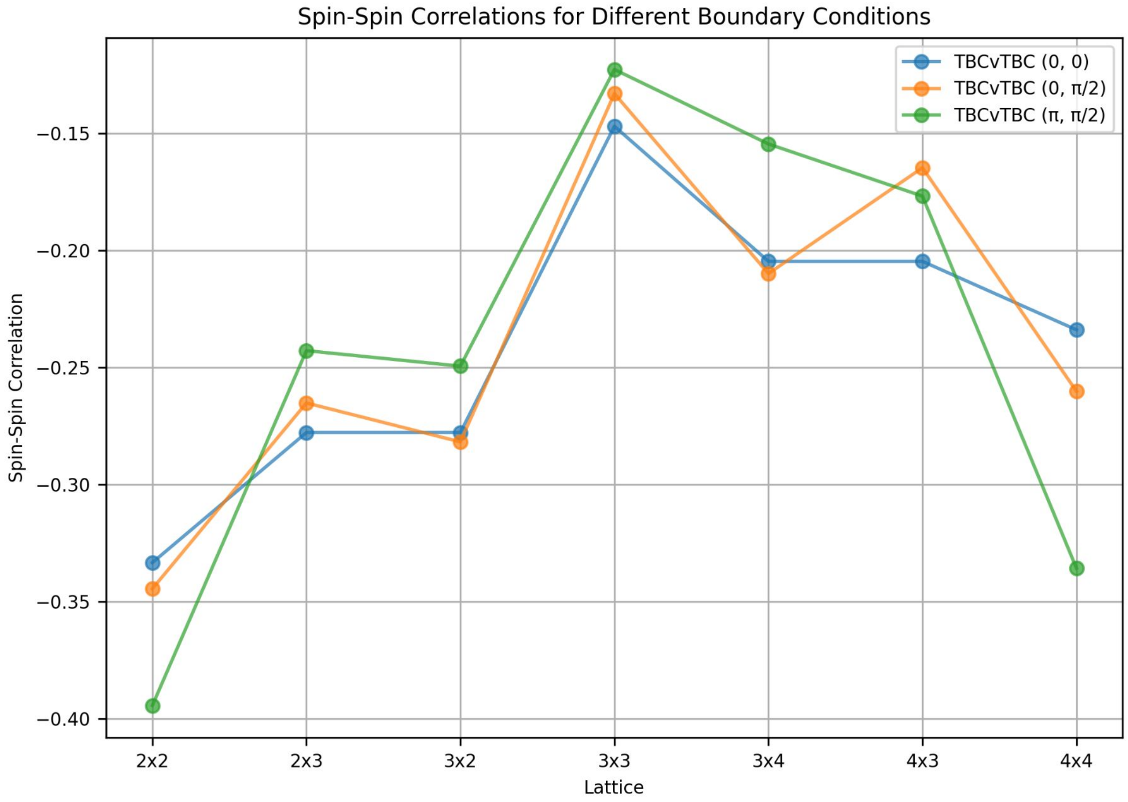
PBC = Periodic Boundary Conditions
OBC = Open Boundary Conditions
TBC = Twisted Boundary Conditions (with angle)





TBC = Twisted Boundary Conditions (with angle)
OBC = Open Boundary Conditions
ABC = Antiperiodic Boundary Conditions





TBC = Twisted Boundary Conditions (with angles)
TBC(0, 0) = Periodic Boundary Conditions