Boundary Conditions for the Heisenberg Antiferromagnet Lattice Model

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This project aims to better understand the effects of different boundary conditions on the Heisenberg antiferromagnet model. This model aims to use a computationally feasible lattice to simulate the much more complicated lattice structure of larger systems. Gaining a better understanding of these boundary conditions is important because they help us approximate the results of these larger systems. This is because they, aside from open boundary conditions, consider each site to have four neighbors and thus four separate interactions. We explored how periodic, antiperiodic, twisted, open, and random boundary conditions affect the eigenvalues and spin-spin correlations of our system. By computationally constructing and diagonalizing the Hamiltonian to find the energies of the system, we were able to simulate these boundary conditions to observe it's effects on different square and rectangular lattices. We then generated plots and compared the results of simulating different Hamiltonian's to better understand how these boundary conditions changed the resultant energies. As expected, our results show that different boundary conditions give different energies and spin-spin correlations for the Heisenberg antiferromagnet. We noticed that for any singular lattice, we were also capable of simulating one boundary condition across periodic neighbors in the same row and a different boundary condition across periodic neighbors in the same column. We found that simulating two different boundary conditions in two different directions on the same rectangular lattice could, in some cases, lead us to an even lower ground state energy than using any one boundary condition yielded. These findings provide a better understanding of how we can use different boundary conditions to approximate infinite-sized systems, aiding any future computational research on material systems.