Ground state properties of a spin chain within Heisenberg model with a single lacking spin site

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Abstract :

The ground state and first excited state energies of an antiferromagnetic spin- $\frac{1}{2}$ chain with and without a single lacking spin site are computed using exact diagonalization method, within the Heisenberg model. In order to keep both parts of a spin chain with a lacking site connected, next nearest neighbors interactions are then introduced. Also, the Density Matrix Renormalization Group (DMRG) method is used, to investigate ground state energies of large system sizes; which permits us to inquire about the effect of large system sizes on energies. Other quantum quantities such as fidelity and correlation functions are also studied and compared in both cases.

Keywords : Heisenberg model; Next nearest neighbors interactions; Exact diagonalization; Density matrix; Spin impurity.

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