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Quantum Monte Carlo study of magnetism in the Lieb Lattice

NATANAEL COSTA, TIAGO SANTOS¹, THEREZA PAIVA, RAIMUNDO DOS SANTOS, Universidade Federal do Rio de Janeiro, RICHARD SCALETTAR, UC Davis — The Hubbard model on the ‘Lieb lattice’ provides an important example of how flat band systems may lead to ferromagnetism: at half filling Lieb proved that a ferrimagnetic ground state *can* be achieved. Since a rigorous proof that long range order does indeed emerge is still lacking, here we report Determinant Quantum Monte Carlo (DQMC) simulations for this model. We found that the spin correlation between nearest neighbors are always antiferromagnetic, and that for small U ferromagnetic long range order does set in in the ground state. However, spatial spin correlations weaken as U is increased, and we established that long range order is suppressed above $U_c \approx 4.5$. We obtain the dependence of the magnetization with the on-site repulsion U , and show that it displays a maximum at $U \approx 3$. The behavior of the compressibility and of the double occupancy across this transition is also discussed.

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