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Finite Hubbard clusters with large spin polarization[1] ERIK NIELSEN, Department of Electrical Engineering, Princeton University, Princeton, NJ 08544, R.N. BHATT, Department of Electrical Engineering, Princeton University; Princeton Center for Theoretical Physics, Princeton, NJ 08544 — A generalized Hubbard model can be used to characterize hydrogenic impurities in semiconductors. It has been shown that the ground state spin of such impurity clusters is very sensitive to a cluster's electron number and geometry [1]. An understanding of how these factors affect cluster magnetization is particularly relevant in light of the current ability to position phosphorus donors with nanometer accuracy within bulk silicon [2]. We present numerical results for two-dimensional clusters showing the effect of geometry and electron-hole asymmetry present in real systems of hydrogenic donors. We also consider the robustness of high-spin cluster ground states to perturbations of site position, and discuss the general features of clusters found to possess a high-spin ground state, in particular the fully spin-polarized state.
[1] Erik Nielsen and R. N. Bhatt, Phys. Rev. B 76, 161202 (2007).
[2] J. L. O'Brien et al., Phys. Rev. B 64, 161401 (2001).

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Erik Nielsen
Department of Electrical Engineering,
Princeton University, Princeton, NJ 08544

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