Analytical solution of extended Hubbard models on small clusters (I): Electronic structure for the triangle, square, and tetrahedron

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The Hubbard model extended by either nearest-neighbour Coulomb correlation and/or nearest neighbour Heisenberg exchange is solved analytically for a triangle, square, and tetrahedron. All eigenvalues and eigenvectors are given as functions of the model parameters in a closed form. The groundstate crossings and degeneracies are discussed both for the canonical and grand-canonical energy levels. A multitude of ground-state level crossings is found in dependence of the three interaction constants. For the grand canonical spectra several degeneracies of levels with different occupation numbers give rise to steps higher than one in \( N(\mu, T = 0, \hbar) \). Furthermore, it is shown that the various degeneracies of the grand-canonical energy levels are partially lifted by an antiferromagnetic exchange interaction, whereas a moderate ferromagnetic exchange modifies only slightly the results of the pure Hubbard model. A repulsive nn Coulomb correlation lifts these degeneracies completely. Also application of small magnetic fields leads to drastic changes of the ground state level structure in the vicinity of the degeneration points.