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Pair State Analysis of the Hubbard Hamiltonian in One-Dimension W. B. HODGE, N. A. W. HOLZWARTH, W. C. KERR, Wake Forest University — Using two-electron states as the basis, we have analyzed the one-dimensional Hubbard Hamiltonian (HH) with periodic boundary conditions for many-electron systems. The N-electron energy eigenvalues are simply the sum of the pair energies (eigenvalues of the two-particle reduced HH) weighted by two-particle density matrix elements. We are investigating the possibility that this approach will lead to a useful approximation scheme. For many weakly correlated systems, the pair-energy sum can be truncated and still the ground state energy can be obtained with reasonable accuracy. For example, in the case of six sites at half-filling (with U/t = 1) we need only include 12 of the 45 triplet pair states and 6 of the 21 singlet pair states, and still the ground state energy can be found with only 6% error. A comparison between the exact and approximate results for this system and several others are presented.

William Hodge
Wake Forest University

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