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Pair State Analysis of the Hubbard Hamiltonian in One-Dimension WILLIAM HODGE, N. A. W. HOLZWARTH, W. C. KERR, Wake Forest University — Recently, there has been renewed interest in using a variational determination of the two-particle reduced density matrix ${}^2D$ to find the ground state energy of an N-electron system. This interest can be partly attributed to progress in solving this constrained optimization problem using semidefinite programming algorithms (SDPA).[1] We use the one-dimensional Hubbard model for comparing several variations of the SPDA appproach with the exact results, considering either even or odd numbers N of electrons, either periodic or fixed boundary conditions, and various values of the Coulomb energy parameter U/t. It is convenient to use the two-electron eigenstates of the pair Hubbard Hamiltonian as a basis for representing the ${}^2D$ matrix using the normalization $\mathrm{Tr}({}^2D) = N(N-1)/2$. For example, for $N = 4$ at half filling, using all of the two-particle constraints along with the appropriate physical constraints, we find the SDPA ground state energies to differ from the exact ones by less than $4 \times 10^{-4}t$. In addition, the diagonal elements of ${}^2D$ generally differ from the exact ones on the order of 10^{-2}.

[1]Nakata, Nakatsuji, and co-workers, J. Chem. Phys. **114**, 8282 (2001), Hammond and Mazziotti, Phys. Rev. A **73**, 062505 (2006).

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