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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).<sup>1</sup> We use the one-dimensional Hubbard model for comparing several variations of the SPDA approach 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  $\text{Tr}({}^2D) = N(N-1)/2$ . 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  $10^{-2}$ .

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

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