Abstract Submitted
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Electronic structure calculations based on the two-body reduced density matrix, semidefinite programming, and three-index representability conditions[1] BASTIAAN J. BRAAMS, Emory Univ., Dept. of MathCS, MITUHIRO FUKUDA, Tokyo Inst. of Technology, MAHO NAKATA, Univ. of Tokyo, MICHAEL L. OVERTON, JEROME K. PERCUS, New York Univ., MAKOTO YAMASHITA, Kanagawa Univ., ZHENGJI ZHAO, LBNL — For nonrelativistic electrons in an external potential the ground state energy depends only upon the two-body reduced density matrix (2-RDM) and a lower-bound approximation may be obtained by minimizing the energy with respect to the 2-RDM subject to some representability conditions. Work going back to the 1970s and the recent work [1] showed that by imposing the well-known P, Q, and G conditions an accuracy is obtained that compares favorably to Hartree-Fock. In our work [2] we impose additional "three-index" representability conditions and demonstrate an accuracy that is fully competitive with CISD or CCSD(T) on the same model space for a variety of small molecules. The approximation has a well-defined solution - there are no local minima - and is size consistent. The poster will present further results and experience and will discuss remaining computational challenges. [1] Nakata, M. et al., J. Chem. Phys. 114 (2001) 8282–8292. [2] Zhao, Z. et al., J. Chem. Phys. 120 (2004) 2095–2104.

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