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Targeting individual excited states in DMRG. JONATHAN DORANDO, JOHANNES HACHMANN, GARNET KIN-LIC CHAN, Cornell University — The low-lying excited states of π-conjugated molecules are important for the development of novel devices such as lasers, light-emitting diodes, photovoltaic cells, and field-effect transistors [1,2]. The *ab-intio* Density Matrix Renormalization Group (DMRG) provides a powerful way to explore the electronic structure of quasi-one-dimensional systems such as conjugated organic oligomers. However, DMRG is limited to targeting only low-lying excited states through state-averaged DMRG (SDMRG). There are several drawbacks; state-averaging degrades the accuracy of the excited states and is limited to at most a few of the low-lying states [3]. In this study, we present a new method for targeting higher individual excited states. Due to progress in the field of numerical analysis presented by Van Der Horst and others [4], we are able to target individual excited states of the Hamiltonian. This is accomplished by modifying the Jacobi-Davidson algorithm via a "Harmonic Ritz" procedure. We will present studies of oligoacenes and polyenes that compare the accuracy of SDMRG and Harmonic Davidson DMRG. [1] Burroughes, et al. , Nature 347, 539 (1990). [2] Shirota, J. Mater. Chem. 10, 1, (2000). [3] Ramasesha, Pati, Krishnamurthy, Shuai, Bredas, Phys. Rev. B. 54, 7598, (1997). [4] Bai, Demmel, Dongarra, Ruhe, Van Der Horst, Templates for the Solution of Algebraic Eigenvalue Problems, SIAM, 2000.

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