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Exploiting Low Separation Rank Structures in Many-Body Methods SCOTT THORNTON, Stony Brook University — With the rapid advancement of high-performance computing capabilities, electronic structure calculations of large, complex, realistic molecules are now feasible with Hartree-Fock (HF) and density functional theory (DFT). However, due to their inherent inability to capture the necessary electron correlation effects, it is sometimes necessary to go beyond the single-particle picture of HF and DFT. One technique for going beyond DFT is that of the GW method. The GW method includes screening effects at the random phase approximation (RPA) level. The implementation of the GW method can be cumbersome due to the fact that all of the functions involved are six dimensional. One approach to numerical computing in higher dimensional spaces is to discover and exploit low separation rank structure in physical quantities. We will discuss techniques that advance beyond those currently discussed in the literature seeking a unified framework that provides rigorous error control and greater computational efficiencies.

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