Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Symmetric tensor decomposition-configuration interaction study of BeH_2 SHUSUKE KASAMATSU, WATARU UEMURA, OSAMU SUGINO, The Institute for Solid State Physics, the University of Tokyo — The configuration interaction (CI) is a straightforward approach to describing interacting fermions. However, its application is hampered by the non-polynomially increasing computational time and memory requirements with the system size. To overcome this problem, we have been developing a variational method based on the canonical decomposition of the full-CI coefficients, which we call the symmetric tensor decomposition (STD)-CI [1]. The applicability of STD-CI was tested for simple molecular systems, but here we test it using a stringent benchmark system, i.e., the insertion of Be into H_2. The Be + H_2 system is known for strong configurational degeneracy along the insertion pathway, and has been used for assessing a method's capability to treat correlated systems. We obtained errors compared to full CI results of $\sim$10 mHartrees when using a rank 2 decomposition of the full CI coefficients. This is a huge improvement over Hartree-Fock results having errors of up to $\sim$100 mHartrees in worst cases, although not as good as, e.g., CAS-CCSD with errors less than 1 mHartree [2].

[1] Uemura and Sugino, Phys. Rev. Lett. 109, 253001 (2013).
[2] Lyakh et al., Theor. Chem. Acc. 116, 427 (2006).

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Date submitted: 10 Jan 2014 Electronic form version 1.4