ON THE PURE STATE V-REPRESENTABILITY OF DENSITY MATRIX EMBEDDING THEORY—PRACTICAL SIMULATIONS [1]

FABIAN M. FAULSTICH *, RAEHYUN KIM *, ZHI-HAO CUI †, ZAIWEN WEN ‡, GARNET KIN-LIC CHAN †, AND LIN LIN *§

Density matrix embedding theory (DMET) formally requires the matching of density matrix blocks obtained from high-level and low-level theories. Since the birth of DMET in 2012, proposed by Garnet K.-L. Chan and coworkers, said matching is built on the assumption that the high-level density matrix blocks are non-interacting pure-state v-representable (NI-PS-V), which assumes that the low-level density matrix is constructed following the Aufbau principle. We carefully examine this assumption, identify potential failure modes, and propose a remedy.

We present numerical evidence showing that the NI-PS-V assumption is violated in certain common scenarios, which leads to gapless low-level Hamiltonians and high-level 1-RDM blocks that *cannot* be exactly matched. Comparing to DFT calculations, where the violation of the NI-PS-V is rather an exception, our simulations suggest that this violation can appear more frequently in DMET. The alm-DMET circumvents the NI-PS-V condition in its entirety by allowing the pure state to follow any occupation profile. We present numerical results of the alm-DMET method for three prototypical systems which we identify as displaying violations of the NI-PS-V: a hole-doped 2D Hubbard model, a linear H_{36} system, and an H_6 model. In each case, relaxing the Aufbau principle allows the alm-DMET method to satisfy the matching condition exactly and we find that this improves the numerical accuracy of the embedding.

REFERENCES

[1] F. M. Faulstich, R. Kim, Z.-H. Cui, Z. Wen, G. K. Chan, and L. Lin, *On the pure state v-representability of density matrix embedding theory*, arXiv:2110.09558, (2021).

*Department of Mathematics, University of California, Berkeley, California 94720, United States

†Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, California 91125, United States

‡Beijing International Center for Mathematical Research, BICMR, Peking University, Beijing, China

§Computational Research Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, United States