ON THE PURE STATE V-REPRESENTABILITY OF DENSITY MATRIX EMBEDDING THEORY—AN AUGMENTED LAGRANGIAN APPROACH [1]

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Density matrix embedding theory (DMET) is a quantum embedding theory designed to treat strong correlation effects in large quantum systems while maintaining reasonable computation costs. The idea behind DMET is that in complex systems the region of interest often forms merely one (small) part of a much larger system. It is therefore natural to think about numerically treating the system with two different approaches—a high-level calculation on the active region of interest, and a low-level calculation on its environment—and then 'glue' the obtained results together.

A key step in the DMET formalism is the matching of density matrix blocks obtained from the high-level and low-level theories; the ability to achieve exact matching is an important issue in the DMET procedure since its inception as, in practical calculations, this is sometimes not achievable. In such a case, the global band gap of the low-level theory vanishes, and this can require additional numerical considerations in order to obtain accurate results. We find that both the violation of the exact matching condition and the vanishing low-level gap are related to 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 where the orbitals are obtained from an auxiliary low-level system. A potential remedy is to relax the NI-PS-V assumption in DMET and allow for pure states following *arbitrary* occupation profiles. This seems to be a daunting problem as the number of distinct occupation profiles is combinatorially large. We propose to use an augmented Lagrangian method, coupled with a projected gradient descent method to solve this modified constrained optimization problem. The inclusion of this optimization over all possible occupation profiles into the self-consistent DMET workflow is christened alm-DMET. The alm-DMET method relaxes the NI-PS-V assumption, which allows the pure state to follow any occupation profile—possibly violating the Aufbau principle—while yielding an idempotent low-level density matrix. Numerical evidence shows that this relaxation of the Aufbau principle indeed allows the alm-DMET method to yield exact matching, which improves the numerical accuracy compared to conventional self-consistent DMET methods.

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).

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