THE UNIVERSITY OF CHICAGO | **THE COMMITTEE ON COMPUTATIONAL AND APPLIED MATHEMATICS**

COLLOQUIUM

FABIAN FAULSTICH

Department of Mathematics
University of California, Berkeley

On the pure state v-representability of Density Matrix Embedding Theory

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Jones 303, 5747 S. Ellis Ave. Chicago, IL 60637

ABSTRACT

The density matrix embedding theory (DMET) algorithm is a novel and particularly promising embedding approach to the fermionic many-body problem. The central idea behind quantum embedding approaches is that, in complex systems, the region of interest often forms merely one 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 'joining' or 'matching' the obtained results. In DMET, the matching is achieved through the density matrix blocks obtained from high-level and low-level theories. Although exact matching is formally necessary, it is sometimes not achievable in practical calculations. In such a case, the global band gap of the low-level theory vanishes, and this can require additional numerical considerations. 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 noninteracting pure-state v-representable (NI-PS-V), which assumes that the low-level density matrix is constructed following the Aufbau principle. To relax the NI-PS-V condition, we develop an augmented Lagrangian method to match the density matrix blocks without referring to the Aufbau principle. Numerical results for the 2D Hubbard and hydrogen model systems indicate that, in some challenging scenarios, the relaxation of the Aufbau principle directly leads to exact matching of the density matrix blocks, which also yields improved accuracy.

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