Wavefunction expansions in the solid state: Reaching the thermodynamic limit

A talk by George Booth
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Quantum chemical methods based on an explicit wavefunction expansion have been shown to be highly accurate. The biggest impediment to their use in computational electronic structure in the solid state is the convergence with supercell size required to reach the thermodynamic limit and converge finite size effects. Here, we discuss a quantum embedding method, density matrix embedding theory, which aims to rigorously map the infinite bulk system onto a finite quantum impurity model through an exact decomposition of a mean-field wavefunction. Obvious similarities with DMFT will be discussed, but key differences will also be highlighted.