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Locality of Interaction in Quantum Chemistry and some Applications

Abstract

I will review some recent results on the locality of interaction in the tight-binding model (treated as a toy-model for quantum chemistry). Specifically, I will show how one can decompose the density of states into spatially localised contributions. Some applications of this observation include: (1) equivalence of the canonical and grand-canonical ensembles for the electrons (with H Chen and J Lu); (2) construction of multi-scale methods with controlled approximation errors (with H Chen); (3) a generalisation of Brillouin-zone sampling to incommensurate layers of 2D lattices (with D Massat and M Luskin).