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“Quantum Monte Carlo approach to exact diagonalisation of electronic Hamiltonians.”

Abstract: We have developed a quantum Monte Carlo approach which can converge onto the exact ground-state of electronic (more generally fermonic) Hamiltonians represented in exponentially large Hilbert spaces. I will describe this algorithm, as well as show applications to some atomic, molecular and solid-state systems, including the 3d-atoms, and a 3-band Hubbard model of cuprates. Prospects to use this algorithm in more general contexts, including the calculation of excited states, will also be discussed.