The Abdus Salam International Centre for Theoretical Physics

School in Computational Condensed Matter Physics:
From Atomistic Simulations to Universal Model Hamiltonians

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FULL CONFIGURATION INTERACTION QUANTUM MONTE CARLO

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Abstract:

In these lectures we will introduce and cover in some detail the full CI QMC methodology for computing the exact ground state energy (within a given basis) of an electronic Hamiltonian. We will start will some necessary basic quantum chemistry background, followed by a description of the FCIQMC algorithms and how they work in practice, in particular for the calculation of the total energy. Next, we will show how the sampled FCIQMC wavefunction can be used to compute properties, in other words, expectation values of arbitrary operators (which in general do not commute with the Hamiltonian). The reduced density matrices are generic examples of such operators. Finally, in the last session, we will have the opportunity get some hands-on experience with the our code (neci) in doing practical FCIQMC calculations.