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A Comparison of Methods for Simulating Quantum Dot Dynamics

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Within the field of computational quantum many-body dynamics, several approaches exist to approximating and simulating the time evolution of quantum systems with multiple particles. In this presentation, four numerical methods will be compared: the time-dependent configuration-interaction (TDCI) method, the multi-configurational time-dependent Hartree-Fock (MCTDHF) method, the time-dependent coupled-cluster (TDCC) method and time-dependent density functional theory (TDDFT). Strengths and weaknesses of these methods will be discussed, as well as possibly beneficial ways to combine them, with respect to simulation of spatially confined systems relevant to quantum chemistry, nuclear physics and quantum computing.

The TDCI, MCTDHF and TDCC methods all rely on a basis of single-particle states which has large impact on the size of the computations involved. The choice of a good basis is therefore also of relevance when discussing these methods, and in this presentation an overview of some alternatives with analytic, geometric or physical benefits will be discussed, as well as the possibility of using DFT to find a good one-body basis which sufficiently spans the many-body dynamics of a given system.

The presentation is partly based on an upcoming paper by Morten Hjorth-Jensen, Oskar Leinonen, Jonas B. Flaten and others from the University of Oslo, discussing technical aspects of and comparing various methods for simulating quantum dot systems, with simulations of several particles in a 3D harmonic oscillator as an example.

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