Simulation of quantum dynamics and transport using multiconfiguration time-dependent Hartree methods

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The accurate theoretical treatment and simulation of quantum dynamical processes in many-body systems is a central issue in chemical dynamics and condensed matter physics. In this talk, the multilayer multiconfiguration time-dependent Hartree (ML-MCTDH) method [1] is discussed as an example of an approach that allows an accurate description of quantum dynamics and transport in systems with many degrees of freedom. The ML-MCTDH method is a variational basis-set approach, which uses a multiconfiguration expansion of the wavefunction employing a multilayer representation and time-dependent basis functions. It extends the original MCTDH method [2] to significantly larger and more complex systems. Employing the second quantization representation of Fock space, the ML-MCTDH method has recently been extended to allow the treatment of indistinguishable particles [3,4]. The performance of the ML-MCTDH method is illustrated by several application to models of charge and energy transport in molecular systems in the condensed phase [4,5,6,7].

[1] H. Wang and M. Thoss, J. Chem. Phys. **119**, 1289 (2003).
[2] H.-D. Meyer, U. Manthe, and L.S. Cederbaum, Chem. Phys. Lett. **165** , 73 (1990); H.-D. Meyer, F. Gatti, and G.A. Worth (Eds.), Multidimensional Quantum Dynamics: MCTDH Theory and Applications, Wiley-VCH, Weilheim, 2009.
[3] H. Wang and M. Thoss, J. Chem. Phys. **131**, 024114 (2009).
[4] H. Wang, I. Pshenichnyuk, R. Härtle, M. Thoss, J. Chem. Phys. **135**, 244506 (2011).
[5] I. Craig, M. Thoss, and H. Wang, J. Chem. Phys. **127**, 133503 (2007).
[6] K.A. Velizhanin, H. Wang, and M. Thoss, Chem. Phys. Lett. **460**, 325 (2008).
[7] J. Li, I. Kondov, H. Wang, and M. Thoss, J. Phys. Chem. C **114**, 18481 (2010).