Computational Methods for Time Dependent Quantum Mechanics

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The numerical solution of the multi-dimensional, time-dependent Schroedinger requires the choice of a spatial representation for the wavefunction as well as a method to propagate the wavefunction from some inital time t_0 to a later time $t_0 + \delta t$.

We describe and compare a number of methods designed for the efficient evolution of an initial quantum wavepacket in both linear and non-linear potentials. The spatial part of the Hamiltonian has been discretized using either finite difference, spectral or hybrid approaches. The time propagation is accomplished using either the Lanczos/Arnoldi method, the real space product formula or the time dependent discrete variable method (TDDVR). We have examined 3, 5 and 7 point finite difference (FD) schemes, the standard Discrete Variable Method (DVR) and a new Finite Element Discrete Variable Method (FEDVR) in which a DVR is applied in a piecewise fashion to the spatial Hamililtonian. While the FD methods are simple and result in very sparse representations, we have found that they often require a substantial number of mesh points for high accuracy. As expected, the accuracy of FD discretization increases from 3, to 5, to 7 points, for most problems. The DVR approach, like most spectral methods, produces accurate results for considerably smaller grids (basis sets), but produces a denser representation of the Hamiltonian operator. The FEDVR has the advantage of spectral accuracy and high sparsity and appears to be a very effective and efficient approach to the spatial discretization process.

The Lanczos/Arnoldi and real space product formula are explicit propagation techniques

which rely on matrix vector multiplication to propagate the wavefunction from one time-step to the next. Clearly, any approach which can exploit the sparsity of the spatial representation in perfoming this operation has great advantages. This may be simply accomplished by storing only the non-zero matrix elements and their indices. In the TDDVR method, time and space are discretized using the DVR approach and this results in an implict scheme for propagating the wavefunction from one time-step to the next. While the method is unconditionally stable, it is necessary to solve a set of complex, linear algebraic equations at each propagation step whose dimension is equal to the PRODUCT of the number of spatial points times the number of time points used in that time interval. If the linear algebraic equations are solved by direct LU decomposition, a sparse spatial representation offers no advantages. However, iterative methods for the solution of these equations also rely on matrix vector multiplication and sparsity can be effectively used to reduce computational effort.

All of these techniques have been examined for computational scaling, accuracy and use on distributed memory clusters.

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