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Workshop on Time-Dependent Quantum Molecular Dynamics

Brian Head Utah, March 13−17, 1999
Organizers: Gregory A. Voth and Jack Simons

During the period March 13−17, 1999, the Henry Eyring Center for Theoretical Chemistry organized and hosted a workshop on time-dependent quantum molecular dynamics in Brian Head, Utah. The workshop was financially co-sponsored by the Henry Eyring Center, the Office of Naval Research, the IBM Corporation, the University of Florida Quantum Theory Project, and the University of Utah Center for High Performance Computing. The goal of the workshop was to bring together leading researchers from the theoretical chemistry community in the general area of quantum molecular dynamics. The underlying concept behind the meeting, however, was the notion that the solution of the time-dependent Schrödinger equation, in a variety of different contexts, is likely to become one of the central efforts in theoretical chemistry in the 21st century. It was felt by the two workshop organizers, Jack Simons and myself, that a "critical mass" of researchers and ideas is now in place in order for this effort to progress forward in full force. In addition, there seems to be no doubt that the effort to deal with quantum dynamics through both accurate and efficient theoretical and numerical methods is timely in light of the demands of the larger chemistry community. One needs only to explore the rapidly growing experimental literature in the areas of charge migration (e.g., electron and proton transfer), vibrational dynamics and energy relaxation, nonadiabatic transitions, chemical reaction dynamics, and surface and bulk diffusion, to name a few. These fundamental processes occur not only in the traditional areas of chemistry, but they are also increasingly being revealed as important in biological, atmospheric, and materials science research. A common underlying theme in all of these important research areas is the need to solve the time-dependent Schrödinger equation, or at least a requirement to extract some degree of useful information from it.

During the latter half of this century, a primary concern of many theoretical chemists has been the solution of the *time-independent* Schrödinger equation for electrons in atoms and molecules, i.e., quantum chemistry. While much remains to be done on that very important problem, one can confidently assert that much has already been accomplished over 50 or more years of research. Evidence for this assertion may be found from many sources, and the recent Nobel Prize to John Pople and Walter Kohn is but one example. The *time-dependent* Schrödinger equation, however, has yielded significantly less progress to researchers (though no doubt there *has* been significant progress). In no small part, this lack of progress is because of the vast diversity of contexts in which the equation is found. To put it more technically, the potential energy functions which serve as input into the equation vary widely from system to system. Usually, they are the result of the application of the Born−Oppenheimer approximation and, as such, have few general principles which govern their final form and behavior. It is an inescapable fact that in most important cases the potential energy function is highly nonlinear and many-dimensional. The normal mode (harmonic) approximation for which exact solutions exist was found many years ago to be severely limited in real applications. It is also well known that a frontal numerical assault on the quantum dynamics problem runs into complications extremely rapidly as the dimensionality of the system increases. In fact, the numerical effort becomes "exponentially complex." Therefore, the need for insightful, accurate, and efficient approximation schemes becomes very great, perhaps like few other problems in the field of theoretical chemistry.

In this special issue of *The Journal of Physical Chemistry*, one will find contributions submitted by many of the invited workshop participants, as well as from others who attended the meeting. Taken as a whole, the various methods and problems described herein provide an overview of the state-of-the-art in the very challenging and rapidly evolving field of time-dependent quantum molecular dynamics.

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