Carey M. Rosenthal
Associate Professor, Theoretical Chemistry, Tel: 215-895-2641, Fax: 215-895-1265, E-mail: rr35@drexel.edu. B.S Cornell University, Ph.D. 1969, Harvard University.

Current Research: My research interest have been most recently been concerned with optimum control theory. This is basically a search problem based on the time dependent Schroedinger equation for systems composed of atoms and molecules. How can a time dependent field be constructed which directs these systems toward a desired target. Experimentally it has been found that the search for such fields is remarkably successful. In the experimental arena the electric fields are adjusted via a learning algorithm and after roughly 1000 or so iterations it has been found that yields of the desired target state have reached optimum or near optimum values. Why is this so? From a theoretical point of view, we need to solve the time dependent Schroedinger equation with the field term regarded as an adjustable parameters or set of parameters. We then look for maxima in one of 3 quantities:

(a) transition probabilities at some final time T
(b) match to a desired target evolution operator at some final time T
(c) maximum in the expectation value of some observable at T

Earlier studies have shown that the landscape for these searches is not at all what one might have expected. There are only global maxima and minima that are encountered in the search. There are no suboptimal maxima or minima. This leads to an enormous simplification in the search problem and also partially explains why the experimental results have been so easy to obtain. Suboptimal solutions which would lead to trapping are simply not there.

Most recently we have been looking at the last of the problems listed above. Mathematically it is necessary is to look at Trace (rho.O), where O is the operator corresponding to the desired observable and rho is the density matrix of the system, thought of as a function of time. It has been found that the computational effort scales with the dimension of the system in a very desirable fashion. After a short rise, that effort scales almost logarithmically or even better shows no rise with the size of the system, provided rho or O has degeneracy. This is almost always the case for thermally realistic density matrices. Practically all of the states remain unpopulated.

In addition work has begun on the problem of tracking. This is important from the point of view of designing quantum devices or machines. From a mathematical point of view some very interesting features have been observed. Numerical singularities are encountered for some paths but not others.

Recent publications:

1. Quantum Optimally Controlled Transition Landscapes, HA Rabitz, MM Hsieh, CM Rosenthal, Science 2004
2. Landscape for optimal control of quantum mechanical unitary transformations, H Tabitz, M Hsieh, C Rosenthal, Phys. Rev. A, 2005
3. Optimal control landscapes for quantum observables, H Rabitz, M Hsieh, C Rosenthal, J. Chem. Phys, 2006