LATTICE, TIME-DEPENDENT SCHRÖDINGER EQUATION TREATMENT OF ATOMIC COLLISIONS

D. R. Schultz, M. R. Strayer, J. C. Wells[1]

Through an ongoing program of investigation, we are developing and applying a multi-dimensional lattice approach for solving the time-dependent Schrödinger equation (LTDSE) to study fundamental atomic collision processes. The objective of the work is to provide a new, more widely applicable and accurate tool aimed at better understanding the dynamics of quantum mechanical few-body problems.

From a theoretical point of view, to achieve such an advance hinges on several simplifying characteristics of atomic problems. That is, for many situations, the atomic system is described completely by a differential equation of rather simple mathematical structure (the Schrödinger equation), the interaction is simple in form (the Coulomb potential), and the well-developed techniques of eigensolution via basis function expansion and perturbation theory are generally applicable. However, for dynamic problems such as atomic collisions or interactions of atoms with strong time-varying electromagnetic fields, such a high precision description of observables has not often been achieved in calculations. The necessity to account for or thoroughly describe the possibly multi-electron, multi-center electronic continuum, the need to represent processes driven through channels involving states on more than one center, or involving the interaction among electrons, are examples of inherent complexities that limit the accuracy of calculations. Therefore, to treat ion–atom collisions, a wide range of theoretical approaches has been devised and applied which are approximate solutions of the Schrödinger equation applicable in various regimes.

Thus, our goal has been to develop an approach which can overcome many of the difficulties associated with these methods by solving the time-dependent Schrödinger equation as directly as possible on a numerical lattice, taking advantage of modern techniques of computational science. Past studies have settled controversies surrounding the low-energy behavior of the antiproton-hydrogen ionization problem[2,3] and have shown how the LTDSE method could be used to bridge the regimes of applicability of standard approaches for computing excitation in antiproton-He^+ collisions.[4] Encouraged by these first successes, we have treated in a more comprehensive study excitation of hydrogen by proton impact and compared our results with the best available theoretical and experimental data, again demonstrating the utility of the LTDSE approach.

Owing to the general character of Cartesian coordinates and the flexibility of the high-order interpolation schemes employed, application to other atomic problems such as collisions in strong electromagnetic fields, extension to lower energies by coupling a nuclear Schrödinger equation to the electronic motion, and treatment of the continuum electron production hold significant promise for this type of approach.

---

[1]ORNL Center for Computational Sciences.

[2]D. R. Schultz, P. S. Krstić, C. O. Reinhold, and J. C. Wells, *Phys. Rev. Lett.* **76**, 2882

(1996).
[3]J. C. Wells, D. R. Schultz, P. Gavras, and M. S. Pindzola, *Phys. Rev.* A **54**, 593 (1996).
[4]D. R. Schultz, J. C. Wells, P. S. Krstić, and C. O. Reinhold, *Phys. Rev.* A **56**, 3710 (1997).

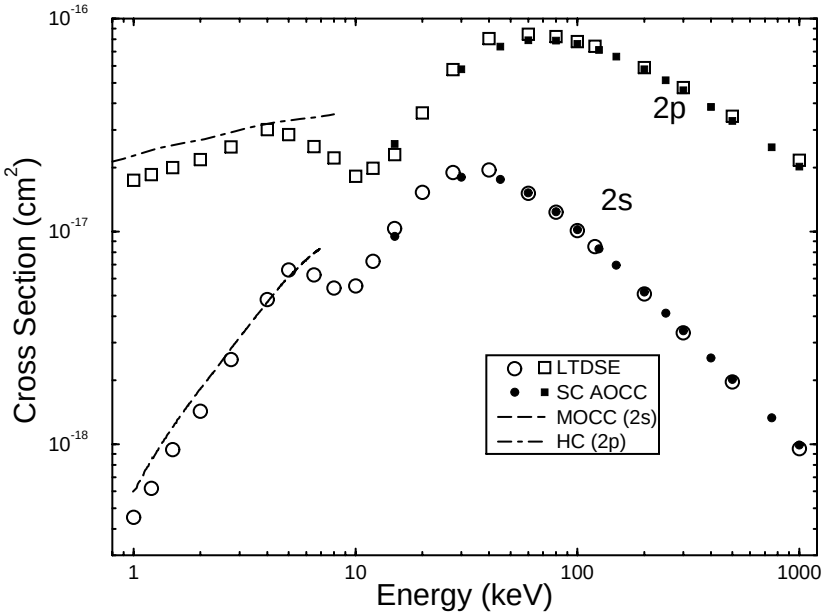

Figure 1: Comparison of new LTDSE calculations of excitation of atomic hydrogen to the 2s and 2p levels by proton impact as a function of collision energy with the best existing theoretical approaches applicable at low and high energy.