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SUPERCOMPUTERS AND THE FUTURE OF COMPUTATIONAL ATOMIC SCATTERING PHYSICS

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The advent of the supercomputer has opened new vistas for the computational atomic physicist. Problems of hitherto unparalleled complexity are now being examined using these new machines, and important connections with other fields of physics are being established. This talk briefly reviews some of the most important trends in computational scattering physics and suggests some exciting possibilities for the future.

Spectacular advances in computer technology made over the past two decades are opening new vistas for science in general, and scattering physics in particular. The formation of supercomputer centers around the world has made these machines available to many scientists, and has allowed workers at widely dispersed locations to collaborate on programs and calculations based at a single remote facility. As the speed and memory of computers continues to increase, a new breed of physicist is emerging, a hybrid between the traditional analytic theorist and the experimentalist. Problems which are too complex for analytic approaches, such as those involving many coupled equations or a very large number of independent variables, can now be solved numerically. By varying the parameters of the calculation, the behavior of very complex systems can be simulated starting from only fundamental assumptions. In some cases this new type of physics is leading to a rethinking of fundamental issues in the underlying science itself.

The following paragraphs will briefly examine some of the advances in supercomputer technology which have brought about this new thinking and some of the scattering physics problems that are being approached by means of large scale calculations. I will also present some connections being forged between atomic physics and other areas such as elementary particle and solid state physics.

The rapid advance of computer capability is illustrated in Figure 1, which shows the log of the number of numerical calculations that the machine can perform per second plotted against the year in which it became available.[1] This curve demonstrates that computer speed is increasing exponentially at a rate of an order of magnitude every decade. In the early years these impressive increases were achieved by more sophisticated central processor designs and by reducing the signal transit time between components by means of more compact assembly. Recently, advanced architectures such as vector processing machines have been developed which can simultaneously process whole arrays of numbers. Another major development is the construction of massively parallel machines, which contain hundreds or thousands of independent processors connected by a common memory. Each of the individual processors solves a predetermined small part of the overall problem, with some form of integration of the results occurring later on. A challenge associated with many-processor machines, however, is the special programming which is sometimes required to make full use of the machines' capabilities. Most large physics computer codes are written in the Fortran language, essentially a single processor, sequential language. Indeed, some theoretical methods used in computational scattering physics were developed with this programming in

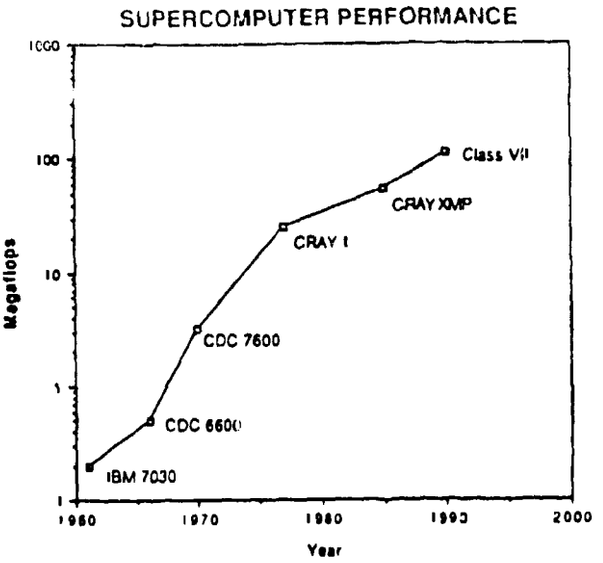

Figure 1. Supercomputer speed measured in millions of floating point (numerical) operations per second.

mind. To make full use of the capabilities of massively parallel processing machines may require not only a rewrite of the codes, but a reconsideration of the physics problem that is under study.

What all of this means to the atomic physicist can be illustrated by the example of electronic structure calculations. In 1930 it took Douglas Hartree many months of laborious hand calculations to compute the electronic structure of an atom such as rubidium. By 1960 such a calculation could be performed overnight on a digital computer, although considerable effort was required to master the primitive programming languages available at that time. By 1970 Hartree-Fock structure calculations were routine, and standard programs were available. Today, using a Cray computer or its equivilant, the atomic structure of rubidium can be computed in about one second.

It is important to note, however, that even these prodigious advances in computational power are themselves inadequate for a brute force attack on any but the simplist problems in atomic physics. The large number of independent variables in a complex atom requires the use of an approximation. The challenge is to maximize the return on a computational investment given the technology available.

Increases in computer speed have been matched by similar improvements in memory. Indeed, the "core" or direct access memory which can be rapidly accessed by programs is expanding seemingly without limit. Even smaller machines often have huge "virtual" memories made available by clever programming and special machine instructions. Problems that just a few years ago required a large mainframe computer can now be comfortably handled by an advanced desktop machine. Moreover, problems that exceeded the theorists' most diligent economies can now fit on the newest generation of supercomputers, opening new avenues of research.

The range of topics which fall under the heading "atomic scattering physics" is very broad. High energy heavy ion accelerators can produce close collisions between high-Z nuclei in which super-critical fields are reached. At the opposite extreme, slow collisions with surfaces are of interest both as probes of the complex surface layer and as practical means of "atomic engineering" in microelectronic fabrication. The talks which comprise this symposium look at a variety of topics in scattering physics, each of which exploits supercomputer technology for the solutions of hitherto unapproachable problems.

Electron-atom collisions are among the more simple collision processes to describe theoretically, in that the atomic nucleus provides a center of symmetry. Nevertheless, the complexity of atomic structure can make an accurate calculation very difficult. In the relatively straightforward distorted wave approximation the target wavefunction is frozen and the continuum wave is computed in an approximate scattering potential. The

approximate scattering potential. The interaction between the scattering electron and the target can then be computed via perturbation theory to yield a cross section. The distorted wave approximation breaks down when there is significant interaction between the continuum electron and the target.

In more sophisticated approximations, the interaction of the scattering electron and the target atom is described by a compound state represented in terms of an expansion over single atom states plus some type of distorted continuum wave. Two major computational methods have been developed to treat electron scattering from complex atoms: the close coupling approximation and the R-matrix method. In the close coupling approximation a set of coupled equations for low lying states of the atom + continuum complex are solved to model the total wavefunction. Because the computational labor increases rapidly with the number of states, considerable care is used in defining the basis states so as to reproduce accurate optical oscillator strengths, energies, etc. In expansion methods problems in convergence can occur which effectively limit the number of basis states, making the final answer somewhat dependent on the cleverness with which the basis is chosen. Calculations with 9-15 states are now commonplace, although rigorous proof of the convergence of the expansion remains an open question. In particular, the difficulty of treating continuum components continues to be a problem.

The R-matrix method is based on a diagonalization of the target+scattering electron Hamiltonian in a basis set defined within some finite volume surrounding the atom. The boundary of this volume is chosen such that the electron-atom interaction has reached its asymptotic form, so that the solution in the exterior region is known analytically. The diagonalization process produces a coupled wavefunction which can then be used in scattering cross section calculations. As with any finite basis expansion, the accuracy of the R-matrix method depends on the completeness of the basis set.

Both the close coupling approximation and the R-matrix approximation have been applied to problems in electron excitation and photoionization, but run into difficulties when applied to electron ionization or other processes containing two or more continuum electrons in the final state. The interaction of multiple continuum electrons represents higher order terms in a Born-type expansion. Here the problem is more than obtaining computational resources sufficient to handle the complexity of interacting long range orbitals. Rather there is the lack of a fundamental theory to guide the calculations. More information on the close coupling and R-matrix methods can be found in invited lectures included in this volume.

The collision of two atoms or ions introduces an additional level of complexity owing to the loss of a single center of symmetry. At low scattering energies the trajectories of the atoms can be significantly perturbed by electronic interactions, requiring a self-consistent treatment of ion and electronic motion. At higher energies one may employ an approximate form of the interatomic interaction to determine the trajectories and concentrate on electronic transitions such as excitation, ionization, or charge transfer. To describe such processes one can employ much of the language and methodology of quantum chemistry to describe level crossings and other resonant phenomena important for the determination of cross sections. A finite basis expansion of the total wavefunction based on nucleus-centered states is usually performed, sometimes with the addition of auxiliary functions located between the nuclei or at other strategic locations. As with any basis expansion method, the two-electron Coulomb operator with its four orbital components causes the size of the

basis set size. For any but the simplest atoms one can rapidly fill a supercomputer memory. Kulander et al.[2] among others has developed a time dependent Hartree-Fock approximation for the description of atomic and molecular scattering.

With the completion of the heavy ion accelerator at GSI Darmstat atomic physicists have the opportunity to observe very close collisions of heavy nuclei containing no or only a few electrons. Clearly any "atomic" states which might exist during such collisions will be strongly influenced by the changing nuclear configuration as well as by large relativistic and QED effects. During close collisions "quasi-molecular" states can occur in which bound electrons are shared among the nearby nuclei. During the collision of two heavy nuclei it is possible for the local electrostatic field to exceed the critical value, i.e., that which would correspond to a nucleus with Z=137. In the supercritical field regime, pair production is possible, and has been observed. At the present time there is still debate concerning the physical mechanism for this pair production, since it is sometimes observed to occur after the nuclei have moved sufficiently apart to drop the local electrostatic field below the critical level. Modeling such phenomena requires a robust methodology which is capable of describing the three dimensional motion of the nuclear configurations as a function of time. Bottcher et al.[3] have applied basis spline techniques to such problems with exciting results. In these calculations space is divided into a large number of discrete volume elements, the physics in which is determined by the usual equations of QED. A variety of methods can be used to propagate solutions in time so that overall rate coefficients can be determined.

Atomic collisions with surfaces is a subject of considerable practical importance for the semiconductor industry. In the drive for ever more sophisticated microelectronics "atomic engineering" is being performed wherein monoatomic layers are deposited on surfaces to perform special functions. With the advent of advanced electron microscopes, we can map the surfaces of materials down to the level of individual atoms, providing fascinating images of the subject under study. As one might expect, the theoretical treatment of atom-surface interactions is exceptionally complex, owing both to the discontinuous nature of the surface itself and the complex interactions possible between the surface and a scattering atom. Garcia et al.[4] have developed a method which they have applied to atomic scattering from hard surfaces and from "jellium." They are able to describe the time-dependent distortion of the atomic wavefunction as it interacts with the surface and is repelled. Figure 2 shows the result of one of their calculations of a hydrogen atom being reflected from a hard barrier.

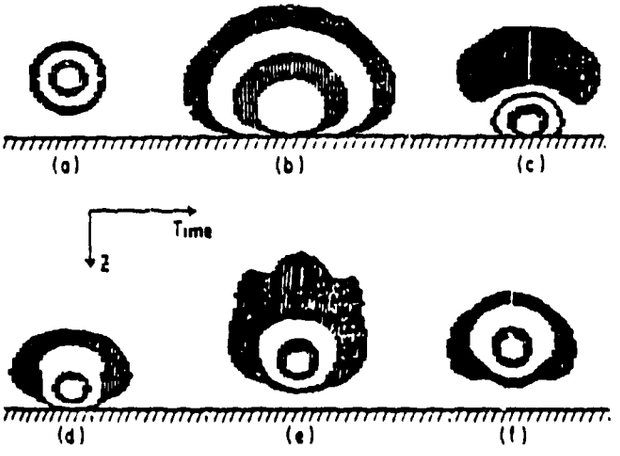

Figure 2. Density contours of the electronic wavefunction of a hydrogen atom scattering off of a hard barrier. The initial energy of the atom was 25 eV.(Ref. 4.)

With more computer power it is possible to construct a computational model consisting of several atomic layers with some type of realistic boundary condition to model the deeper material. The incident atom can then be projected against the surface at different angles and impact parameters to generate probabilities for sticking, reflection, and transmission into the solid.

A fascinating practical problem which borrows heavily from quantum chemistry is that of scattering in a dense liquid or solid. Here the complication of many simultaneous interactions is present. In a liquid, there is the additional complexity of a disordered asymptotic boundary. Recent calculations performed with an approximate time-dependent Hartree-Fock code have demonstrated that many-atom interactions in liquids soften the interatomic interaction compared to what one would observe in binary collisions. The origin of this softening is the self-consistent redistribution of the electronic charge density during close collisions. Although such calculations which treat 30 or more atoms can take many thousands of minutes even on a supercomputer, they demonstrate that new phenomena await the computational theorist, and that with advances in computer hardware, problems of great complexity can be handled in a more less direct fashion.[5]

Midway between few-atom collisions and liquids lies the domain of clusters. Cluster physics has undergone a tremendous boom in recent years as new experimental techniques have been developed both to produce and examine the properties of clusters with well characterized numbers of atoms. On the theoretical side, Car and Parrinello[6] have developed an efficient computational theory for clusters based on the local density approximation. The electronic wavefunction is expanded over a plane wave basis set and the time dependent Schrodinger equation is solved for the motion of the nuclei. By imparting a velocity distribution to the nuclei they were able to study structural transitions in small clusters as a function of temperature. A particularly interesting finding was that at high temperatures the density of states increases dramatically, i.e. there are a very large number of nearly degenerate bound configurations. Hence rather than "melting" of the sample into a true disordered liquid state, they identified transitions into a large but countable number of discrete bound configurations.

Increasing the temperature to where a plasma forms brings another class of problems. In contrast to the low temperature case, where only the ground state or some set of low lying states is populated, in a plasma the electronic population may be spread over many hundreds or thousands of energy levels. The level populations are controlled by a complex series of excitation, ionization, and recombination processes which involve ions, electrons, and photons. To model an atom embedded in a plasma it is necessary to have detailed rate coefficients for all of these processes for all of the ionization stages expected to be important for the kinetics. This information is fed into a rate equation solver which yields the populations of individual levels. Such a procedure is challenging even for simple atoms. For complex atoms, such as rare earths, it becomes impractical owing to the many thousands of levels involved. Here one may employ a statistical approximation which deals with entire arrays of transitions rather than the individual lines themselves. Klapisch et al[7] have developed such an unresolved transition array (UTA) approximation which has been successfully applied to a wide class of problems in laser interactions and plasma physics.

The immense complexity of rare earth and other heavy element spectra and the need to develop useful approximations is one indicator that increased computational power alone is

increased computational power alone is not the answer to every atomic physics problem. Equally important is the development of realistic theoretical structures which efficiently treat the dominant interactions in a way that will allow solutions to be obtained in a reasonable amount of time. As we approach even more complicated problems, such as the simulation of macromolecular interactions, we will be forced either to break the calculation into manageable parts or to use one or more simplifying assumptions in the calculation. Thus, far from reducing physics to mere computation, the development of computational atomic physics will require a new level of creativity to model a wide range of phenomena in pure and applied research. Theoretical approximations and numerical algorithms developed for past generations of single processor computers may not be the most suitable ones for the next generations of multi-processor machines. For example, rather than fretting over the completeness of highly optimized basis sets used in expansion methods, it may be easier to use a many-body perturbation theory approach which computes a very large number of correlation diagrams automatically given a reasonably realistic starting Hamiltonian.

As atomic physicists begin to harness the power of supercomputers for their own interests, they are also noting the similarities between their problems and those from a wide variety of other scientific disciplines. The connection between atomic and molecular scattering and quantum chemistry is an old example. More recently, however, recognition has been increasing that the methods developed for dense plasma interactions also have application to the quark gluon plasma expected to be formed in ultrarelativistic nuclear collisions. Similarly, workers who are approaching the liquid state from a traditional atomic-molecular level are deriving guidance from the statistical mechanics community. In the study of electronic phenomena occurring during the collision of heavy nuclei one must explicitly consider the time dependent development of nuclear shapes during the collision.

The recognition that numerical recipes and algorithms can be applied to a wide variety of problems in seemingly disparate fields of physics, chemistry, and material science is opening new vistas to the computational physicist. In effect, the computer is becoming a theoretical laboratory where numerical experiments can be conducted over a wide range of physical parameters. Exciting similarities between phenomena at the eV and GeV range are being uncovered, revealing common mechanisms operating over unprecedented ranges of time, space, and energy.

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