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High Intensity 800nm Laser Simulations

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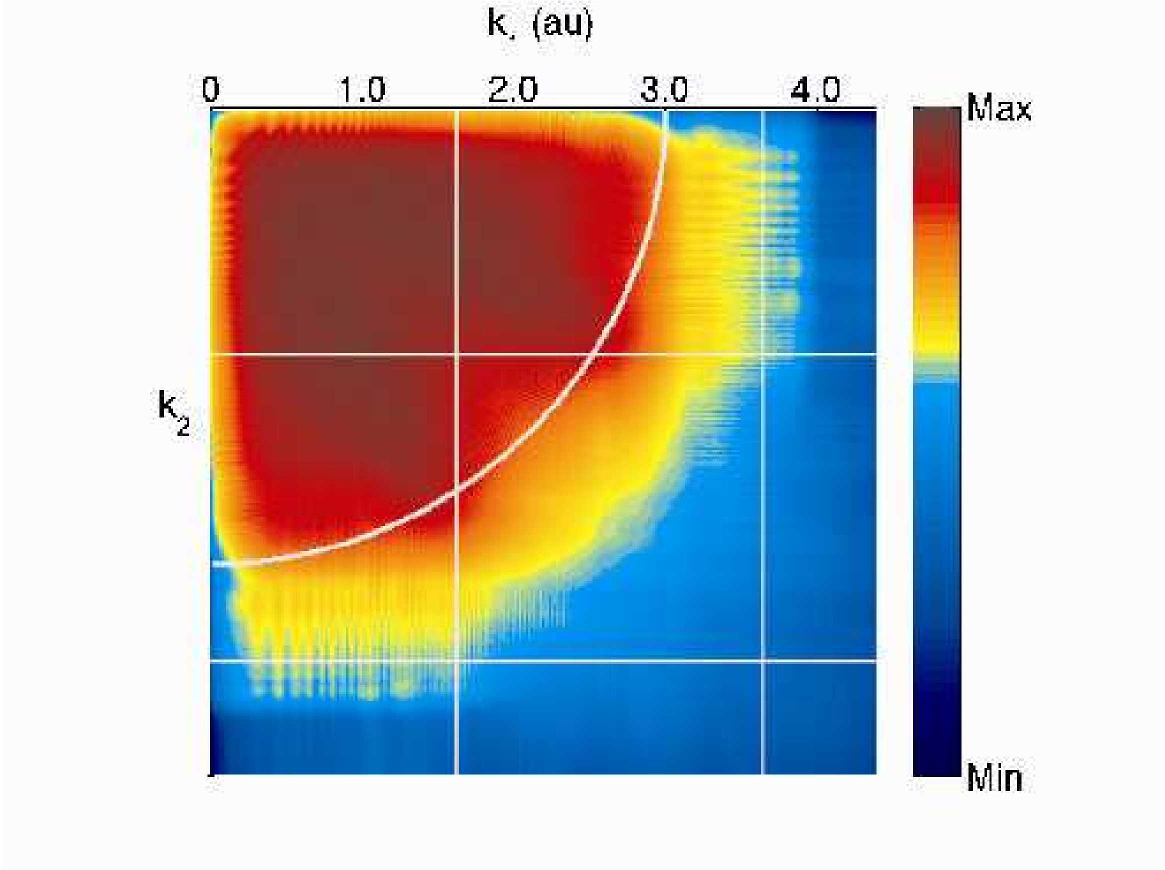

Figure 1

Abstract. The full-dimensional time-dependent Schrödinger equation for laser-driven helium is integrated to high numerical accuracy in order to obtain quantitatively correct data on double-electron ionization in the high intensity limit. Double-electron ionization is a subtle effect, deeply buried within the integrated wavefunction, but it reveals in detail important features of the ionization dynamics of correlated quantum mechanical systems. In order to discriminate double- from the dominant single-ionization it was necessary to limit integration truncation errors to less than 1 part in a billion. We report two successful integrations on 16110 cores.

Introduction

The laser-driven helium atom is a nearly ideal system for both experimental and theoretical exploration of quantum mechanical correlation and quantum mechanical energy exchange between matter and light. Non-classical correlation (also called entanglement) is one of the most mysterious and anti-intuitive features of the quantum mechanical universe. For example correlation, in the form of entangled qubits, is at the heart of most formulations of quantum computing, and correlated photons are what makes quantum cryptography feasible. Correlation is something shared between particles. In the case of laser-driven helium we are concerned with correlation between pairs of electrons ejected from the atom by the strong laser fields. In the present research the analysis has been directed toward understanding the exchange of energy between the laser and atom during the production of these correlated pairs.

Helium - the simplest of all multi-electron atoms - is the only multi-electron atom for which rigorous (quantitatively correct) numerical solutions of the full-dimensional equations of motion (Schrödinger's equation) can be obtained. Laser-driven hydrogen is similarly susceptible to rigorous study numerically, but hydrogen's single electron cannot exhibit the correlation effects that make multi-electrons of such interest. The physics of single electron atoms driven by high intensity laser radiation has been well understood for many decades. Helium turned out to be very different in this respect - every high integrity solution of the Schrödinger's equation we obtained revealed effects that were unpredicted, surprising and unexplained.

HELIUM is a code that calculates solutions to the Schrödinger equation for a two-electron atom or ion exposed to an intense linearly-polarized laser field – a time-dependent 5-dimensional partial differential equation. It began development on the Cray T3D in 1994. In this time-propagation, the accuracy of the solution must be maintained to 9-12 decimal places at all time-steps and at each point in space. This is in order that very small components of the wavefunction, contributing especially to double ionization processes, can be discriminated against single ionization components that are typically 4 to 8 orders of magnitude larger. To this end we have pioneered the use of high-order Arnoldi propagator methods in HELIUM.

From the very beginning of experimental studies on laser-driven helium in the early 90s, the phenomenon of double ionization of the atom has yielded many surprises. Except for a few notable exceptions, most experimental work has used the Ti:sapphire fundamental wavelength of 800 nm, one of the most commonly used lasers in atomic physics, industry and medicine. The numerical integrations we perform scale as the cube of the wavelength in running time and in memory requirements. Integrations performed on early parallel machines were limited to UV frequencies, something of the order 200 nm. Compared to the 200 nm runs, the 800 nm runs we report here are at the very minimum a factor of 64 more laborious in most measures of computational overhead.

The integrations discussed here could not have been performed without both the memory and the computational capacity of HECToR – both of the 800 nanometer runs required 16,110 cores of the Phase IIa service- near the maximum available on HECToR.

The Scientific Achievements

Figure 1 shows the momentum-space probability distribution of the two ejected electrons at the end of a 7 field period 800 nm laser pulse. The log of the joint-probability density is plotted. The two vertical lines are lines of constant momentum k_1 for the first electron. The kinetic energy $K = (k_1^2 / 2)$ associated with these two lines is 2 U_p and 10 U_p. The ponderomotive energy U_p is $E^2 / (4 w^2)$, where E is the peak electric field. Along the circular arc total kinetic energy K is constrained to $K = 6.8\ U_p = k_1^2/2 + k_2^2/2$.

These results are consistent with the ~$7U_p$ law in the intense field limit at 800 nm. The results are significant because 800 nm is (near) infra-red, a limit in which physics of atom-laser interactions is often very different from that observed at optical and UV wavelengths. Our previous results at 800 nm were preliminary in the sense that we were unable to test the convergence properties of the grid and basis used in the numerical integration. The present results, carried out as part of this project, were the first high-integrity integrations in this difficult limit, and provided some confirmation that previous results were integrated using numerically converged basis sets. The results were of additional significance to us because they helped extend the range of data into a limit that is of some importance in the physics of atom-laser interactions. The high-intensity limit that this project explores is the limit in which the rescattering electron returns to the parent ion with sufficient energy to free the tightest bound electron of the parent ion. One of the interesting features of the cut-off energies that concern us here is their sensitivity to the energy of the rescattering electron. The present data is consistent with our initial theoretical explanation for the cut-off law. A full theory of the cut-off law remains elusive, despite much interest world-wide. At present there is no reliable way of predicting what the cut-off will be at higher intensities and lower frequencies. The joint probability distribution provides us with a graphical representation of the various ways in which momentum is shared between the two electrons after they have been ejected from the helium atom by the laser fields. Straight vertical or horizontal linear features are the result of ionization processes in which one electron acquires momentum from the laser entirely independently of the absorption of momentum by the other electron. Processes that exhibit this kind of independence are by definition uncorrelated. The circular white arc marks the high-energy extent of the dominant 2-electron ionization process, which appears as black (highest probability) in the figure. The maximum kinetic energy K absorbed by these electron pairs is the radius of the white circular arc, as explained in the figure caption. This we call the high-energy cut-off. In the figure it is clear that this high energy feature is associated with two jets emanating from the (black) high-probability region. The maximum extent of these jets is weakly intensity dependent, but appears to follow a similar law in all of the cases we have explored, from 800 nm to 195 nm. The existence of this feature was discovered by our group using HELIUM on massively parallel processors. It was subsequently confirmed experimentally. Simplified models of atom-laser interaction failed to predict this process. Progress in understanding the physics of atom-laser interaction has been largely a result of full-dimensional integrations of the exact Schroedinger equation, which has become possible in recent years only as a result of the introduction of massively parallel computers and their provision to the scientific community. The helium-laser interactions we have focussed on here are presently under intensive experimental study world-wide.

Both of the 800 nanometer runs (at intensities 3.8 x 10^{14} W/cm^2 and 4.8 x 10^{14} W/cm^2) were successful. The results confirmed our present understanding of the high-energy cutoff law (~7 U_p in the intense field limit). The results were consistent with results at 390 nm, 248 nm, and 195 nm.

The Technical Achievements

Producing checkpoint data is important to not only this but many other codes. It is important to allow long runs to be restarted but also to provide information on the evolution of the problem. The Cray Centre of Excellence for HECToR worked on improving the performance of this phase. An I/O server approach was taken where the responsibility for performing the checkpoints was the responsibility of dedicated processes.

This approach effectively reduced the time to complete the checkpoint to zero and allow the rest of the computation to continue. Figure 2 shows this improvement and shows the increasing return that is observed with the very large core counts.

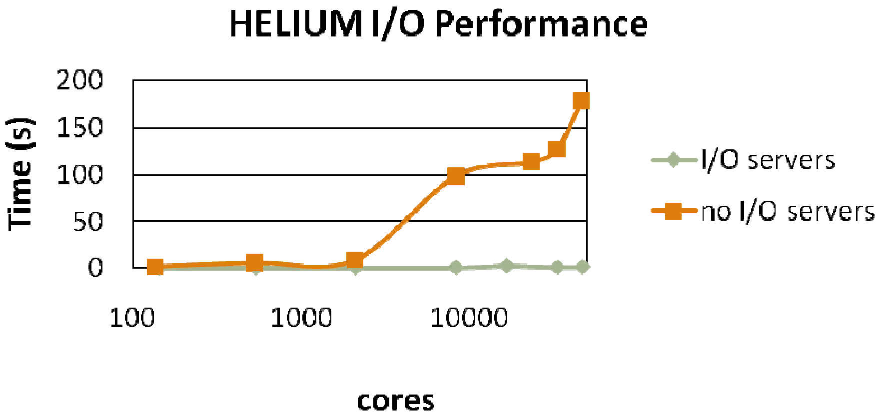

Figure 2. Shows the amount of time saved using I/O servers. The checkpoints are implemented efficiently in both cases but become noticeable on over 2000 cores, at this point the I/O server approach provides significant improvements.

Conclusions

In summary we completed two successful integrations of the time-dependent helium Schrödinger equation in an extreme limit, each requiring over 130 wall-clock hours on 16,110 cores of hector. Over 32 million AUs were used. The results confirm the existence of a previously unknown energy exchange process in atom-laser interactions, whose most prominent characteristic is a ~7 U_p energy cutoff, and which appears as a pair of jets in the momentum-space joint-probability distribution of the two correlated electrons ejected in the intense laser radiation. Results are being prepared for publication in Physical Review Letters.

During the course of this work we developed a collaboration with Dr Agapi Emmanouilidou, an EPSRC Career-acceleration Fellow newly appointed at University College London in October 2009. We successfully prevailed on Dr Emmanouilidou to carry out calculations for laser-driven helium using her full-dimensionality classical mechanics formulation. This was done initially to see how results from a full-dimensionality classical treatment would simply compare with our benchmark quantum ones for double ionization. We motivated Dr Emmanouilidou with quantum *results at 400 nm we already had in hand. The agreement between classical and quantum results turned out to be quantitative rather than (as we actually expected) merely qualitative. This gave us a very considerable further motivation to try and link energy cutoff behaviour in double ionization (common to both quantum and classical results) to underlying classical electron dynamics. This has been accomplished successfully. The findings of this collaborative work mark a major advance in our understanding of the double ionization process and will be shortly submitted for publication in Physical Review Letters. It is a priority with us now to inspire Dr Emmanouilidou to perform classical calculations complementary to the quantum ones this project has made possible for 800 nm.*

HELIUM was the essential application software (unrivalled world-wide) to the accomplishment of the Science in this CoE project, but the granted HECToR resource was equally essential. The project has enabled the UK to maintain a commanding lead in this area of Science. It is also particularly pleasing that the new collaboration with Dr Emmanouilidou has linked our work with the world-leading classical approach (also from the UK) with a consequence major advance in understanding of the double ionization process.

We would like to thank and acknowledge the support of the University of Edinburgh and EPSRC for the resources required to complete this project. Some results and resources were used during this project on JaguarPF, the fastest computer in the world, with the approval of the Oak Ridge National Laboratory Leadership Computing Division.