A first meeting-ground with laboratory experiment enabled by turing

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Turing has now made possible the first comparison between results from a full-dimensional numerical model of multiphoton-double-ionization of helium and those from laboratory experiment.

The comparison is displayed in Figure 1 which plots the ratio of He^{++} yield to He^{+} yield as a function of laser intensity at a wavelength of 390 nm. The experimental results were obtained by Dr DiMauro and his group at the Brookhaven National Laboratory in the USA.

After discussions with Dr DiMauro at the 8th International Laser Physics Workshop in Budapest in early July 1999, the Queen's University Belfast group got their complementary calculations pushed through turing by the end of September in time to be presented in an Invited Talk by Professor Taylor at the 8th International Conference on Multiphoton Processses held in Monterey, California in early October 1999.

The importance of the theoretical and complementary laboratory work is that reliable quantitative knowledge can thus be gained on the dynamics of a fundamental three-body charged particle quantum mechanical system (i.e. two electrons and a bare nucleus) as it is driven far from equilibrium by a strongly time-dependent force. The light electrons of the system respond dramatically to this force -supplied by the very high-intensity femto-second laser pulse- whereas the much heavier nucleus makes oscillations of negligible amplitude. A full-dimensionality treatment of the electronic motion is essential to properly account for both the angular momentum absorbed from the laser pulse and the repulsive interaction between the two electrons.

The Time-dependent Schrodinger Equation (TDSE) governs the dynamics of the system. This is a partial differential equation (PDE), first order in the time and, when written in full-dimensionality for laser-driven helium, involves dependence on no less than 5 spatial variables. The Belfast group has over the past six years been developing, and exploiting, state-of-the-art algorithms to solve such a multi-dimensionality PDE on massively parallel supercomputers.

Each of the 5 calculated points on Figure 1 is obtained by solving the TDSE at the given laser intensity and frequency. The general rule is as follows: the longer the laser wavelength and/or the higher the laser intensity, the more computationally demanding are the calculations. A wavelength of 390 nm proves an excellent meeting-ground between laboratory experiment and calculation now possible with turing. Most experiments on helium are carried out at the Ti-Sapphire fundamental wavelength of 780 nm which unfortunately is still completely inaccessible for full-dimensionality calculations - even with the power of turing!- at sufficiently high intensities for double ionization to be possible. The work at 390 nm brought almost the entire power of turing into play especially for the two highest intensity points plotted in Figure 1. Thus the highest intensity point required runs accumululating to 48 wall-clock hours using simultaneously 455 of the 576 processors.

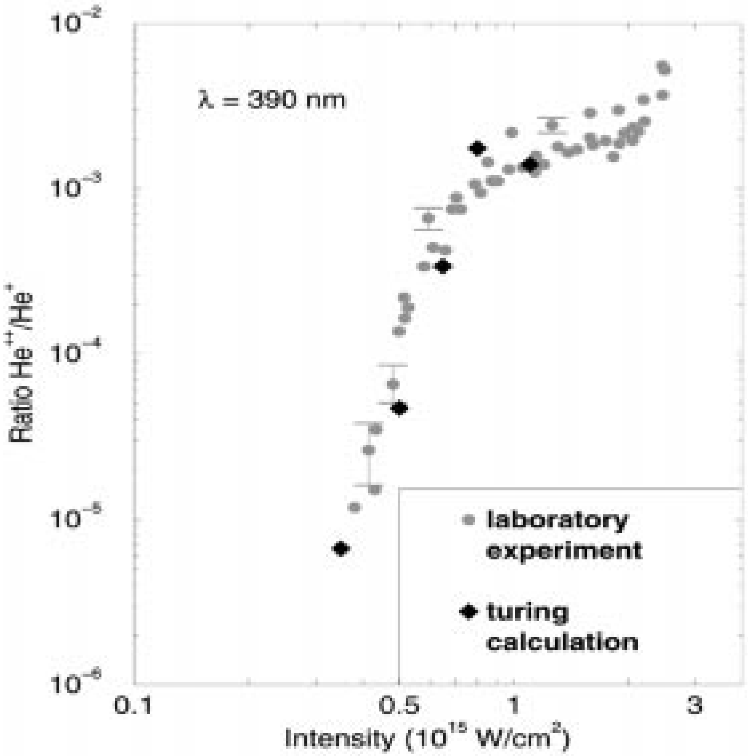

Figure 1. The ratio of the probability for doubly ionizing the helium atom to that for singly ionizing it plotted against laser intensity. The laboratory experiment is that reported by B Sheehy, R Lafon, M Widmer, B Walker and L F DiMauro Phys Rev A58, 3942 (1998) and the turing calculation is by Jonathan Parker, Laura Moore and Ken Taylor of Queen's University Belfast. All experimental points have been moved up in intensity by a global 23% which is within the stated uncertainty in the laboratory determination of laser intensity.

The laser pulse after an initial ramp-on over 4 cycles is allowed to oscillate at a constant amplitude of electric field for at least a further 20 cycles to ensure no transient character in the electronic response remains.

The electrons of helium start out in their ground state but, controlled by the TDSE, evolve rapidly into one- and two-electron ionizing wavepackets leaving the atom. For the middle point plotted on Figure 1 (at intensity 6.5 X 10^{14} W/cm^2 Figures 2(a) and (b) display respectively the time-dependence of the single and double ionization yield these wavepacket motions give rise to. Note that on each half-cycle of the laser pulse there is an additional step-wise contribution to each yield corresponding to the liberation of wavepackets. What is plotted in Figure 1 is the essentially constant value of the ratio between these yield rates once the initial laser ramp-on is over.

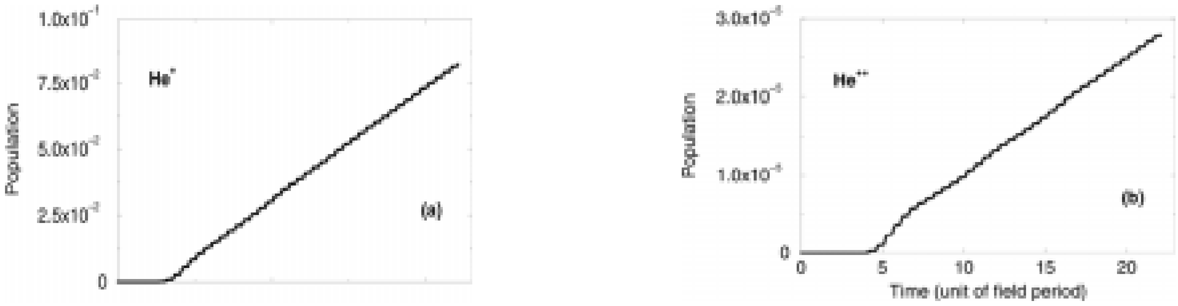

Figure 2. The cumulative ionization yields as a function of time for single ionization (a) and for double ionization(b) of helium for the turing calculation in Figure 1 at a laser intensity of 6.5 X 10^{14} W/cm^2.

The analysis of the data produced in the turing calculations brings out much richer information on the dynamicsof this three-body system than emerges from the Stoneybrook experiment. In this analysis, scientific visualisation methods have played a crucial role and these have also been developed for this problem in recent years by the Belfast group, most notably by Dr Daniel Dundas. For laser pulses of wavelength between 248 and 390 nm it has been possible from this scientific visualisation analysis to determine, for example, that in the two-electron ionizing wavepackets both electrons emerge on the *same* side of the nucleus and with near zero angle initially between their directions of motion. This result is *contrary* to that predicted by many other,less complete,theoretical approaches.

However new results from two German experiments reported at the Monterey meeting have provided the first experimental confirmation of the two-electron wavepacket dynamics found in the turing calculations.

Although these German experiments operated at 780 nm, there is no physical reason for the electronic dynamics to be qualitatively different from those explored in the turing calculations at 390 nm.

The electronic response of helium can however be expected to be very different for substantially shorter laser wavelengths e.g. in the vicinity of 20 nm. Free-electron laser sources in Germany and elsewhere are now making this new shorter wavelength range available to experimentalists. At traditionally used wavelengths (e.g. 390 nm) at intensities around 1.0 X 10^{15} W/cm^2 the atom ionizes overwhelmingly in a sequential manner. At the much shorter wavelength of 20 nm, physical considerations borne out by exploratory calculations on turing indicate the contrary. Indeed the response of the less-tightly-bound outer two electrons of alkaline earth atoms can be expected to be much less sequential when exposed to laser pulses at standard wavelengths operating at lower intensities around 1.0 X 10^{15} W/cm^2

The Belfast group, through the full-dimensionality approach developed on massively parallel machines, is now uniquely well-placed to investigate the qualitatively new physics arising in these cases.

The work at Belfast described above forms part of the activity of the Multiphoton and Electron Collision Processes HPC Consortium operating at CSAR.