

## tSURFF — *ab initio* solutions to the time-dependent non-perturbative half-scattering problem

A. Zielinski, V. P. Majety, and A. Scrinzi,<sup>† 1</sup>

Department of Physics, Ludwig Maximilians University, Munich, Germany

**Synopsis** A new approach to the half-scattering problem is introduced and demonstrated on several of the challenging applications in laser-matter interaction: precision single photo-electron spectra, fully differential double-emission spectra at near IR wave-length, and emission from multi-electron systems. A long-standing discrepancy between theory and measurement in the orientation dependence of  $CO_2$  ionization is resolved. Application to many-body systems will be demonstrated and extension to the full scattering problem will be discussed.

The *ab initio* computation of particle emission spectra from systems that undergo strong, time-dependent perturbations require that the solutions are followed until the perturbation ceases and final energies and emission channels can be established. For determining spectra, the asymptotics of the solution must be computed and analyzed. Only in the case of potential scattering, spectral decomposition suffices.

In a series of papers we have introduced a new approach to this problem. It combines mathematically and computationally perfect absorption [1] with the time-dependent analysis of outgoing flux [2] and the time-evolution of the emission channels including double continuum channels [3]. The power of this “time-dependent surface flux” (tSURFF) approach has allowed us to solve key problems in strong laser-matter interaction: (1) the computation of precision photo-electron spectra at elliptic polarization (attoclock, [4]) and at wave-length up to  $2\mu m$ , (2) accurate fully differential (angle-resolved) double emission spectra from the He atom and from  $H_2$  with polarization parallel to the molecular axis, (3) single photo-emission from the  $CO_2$  molecule in dependence of molecular orientation. In all cases we can provide dependable accuracy estimates.

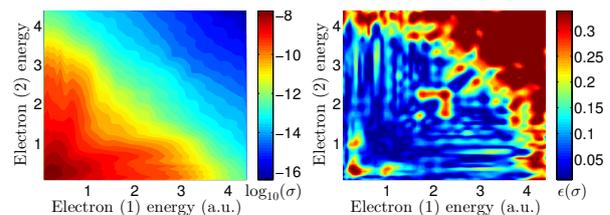
The attoclock results strictly show that the measured deflection angles in elliptically polarized near-infrared pulses are not compatible with solutions of the single-electron Schrödinger equation, implying that an effect of either exchange or multi-electron dynamics is observed.

An example of precision near-IR double emission calculations is shown in Fig. 1.

For computing emission from molecules, strong field dynamics is combined with quantum chemical structure (COLUMBUS, [5]) including full interchannel coupling and exchange

[6]. We find that including exchange is crucial: it explains the observed orientation dependence of ionization of  $CO_2$ . Multi-electron effects can clearly be detected, but have no influence on the peak emission angle at  $45^\circ$ .

In addition to these examples, we will present extensions of the method to many-body physics and discuss its potential for applications in standard scattering problems.



**Figure 1.** Double emission spectra of He by a 3 cycle 730nm pulse at intensity  $3 \times 10^{14} W/cm^2$  (left) and estimate of the relative error (right). Sequential and non-sequential emission is clearly distinguishable. The fully 6-dimensional calculation was performed during two days on 96 CPUs. The error is  $\leq 10\%$  in large part of the spectrum.

### References

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<sup>†</sup>E-mail: [armin.scrinzi@lmu.de](mailto:armin.scrinzi@lmu.de)

