B-splines in atomic physics

the reason of their success and some applications to He photoionization

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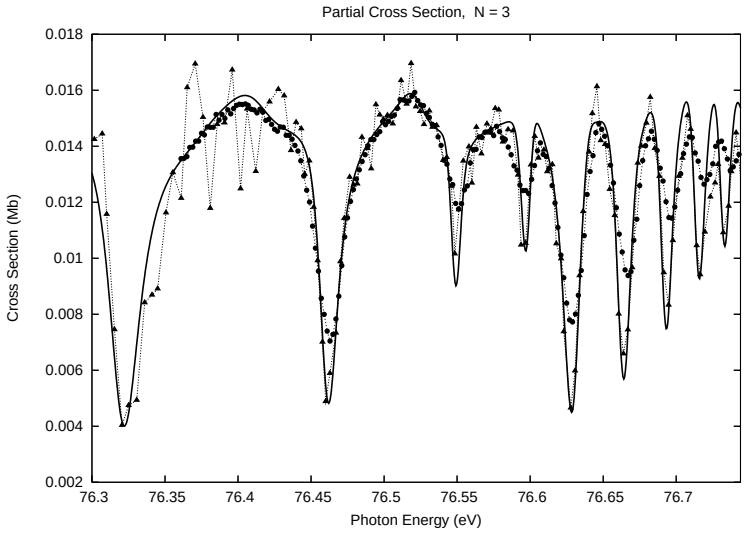
When an atom is struck by an X-ray photon, it often breaks up, emitting one or more electrons. In the process, the system may pass through metastable states where many electrons are temporarily captured in collective excitations. The interference between direct and resonant fragmentation paths gives rise to complicated spiky profiles in the photoionization spectrum. An example is given in the figure.



Cross section for the $\mathrm{He}+\gamma \rightarrow \mathrm{He}^+(3\ell) + e^-$ photoionization below N=5 He^+ threshold. $\bullet\cdots\bullet$: experimental results by Mentzel *et al* [1]; $\blacktriangle\cdots\blacktriangle$: experimental results by Jiang *et al* [2]; continuous line: B-spline K-matrix calculation by Argenti *et al* [3].

The interpretation of such spectra requires sophisticated computational schemes and versatile basis functions, in order to reproduce simultaneously quantum dynamics as diverse as tightly bound states, diffuse metastable states, scattering waves and short range correlated electron motions.

Thanks to their capability of approaching completeness without spoiling numerical accuracy (effective completeness), and to their flexibility, B-splines, basis for $\mathcal{C}^k$ piecewise polynomials, are recognized today as one of the most powerful tools to simulate the ionization of atoms [4].

The K-matrix method, a configuration interaction in the continuum, takes advantage of B-splines flexibility to the full: Rydberg satellites expanding well beyond the quantization box realize autoionizing multiplets of unprecedented excitation. The continuous line shown in the figure gives an example of the close agreement between B-spline K-matrix predictions and experimental data.

In this seminar I will survey the main properties of B-splines from the perspective of atomic physics, with particular reference to effective completeness [5]. As an application to a practical problem, I will outline the contruction of a B-spline basis suitable to reproduce a specific photofragmentation process.

References

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[2] Y. H. Jiang *et al*, Phys. Rev. A **69**, 042706 (2004)
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[5] L. Argenti and R. Colle, *in preparation*