Photoelectron Spectra Calculated from Absorption with Applications

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In this talk I will present the photoelectron spectra calculated from absorption via the density operator (PESCADO) method with applications.

Here we augment the time-dependent Schrödinger equation with a complex absorbing potential, which will remove any part of the wavefunction with a spatial overlap with the absorber. Then we aggregate the outgoing waves by rewriting the state in terms of a density operator, and coherently accumulate its diagonal elements of interest. Within such a formulation, any global phase factor becomes superfluous. This allows us to study photoelectrons using much smaller numerical domains.

Applications involve modelling photoionisation of a hydrogen atom exposed to a laser pulse in the moderately ultraviolet region. Here PESCADO performed favourably compared to similar methods, which can be seen in Fig. 1.

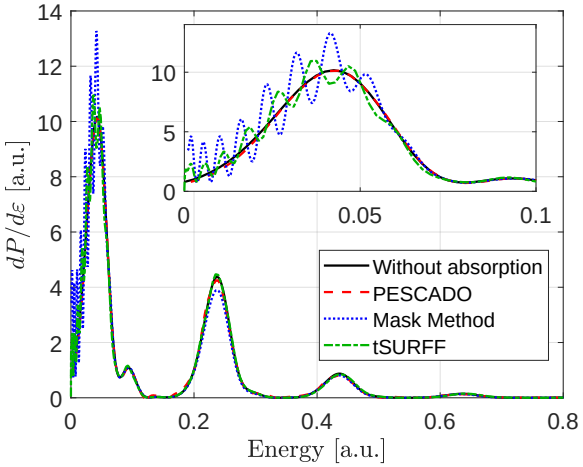

Figure 1: Energy probability distributions for photoionisation of a hydrogen atom exposed to a laser pulse in the moderately ultraviolet region. We compare the PESCADO method with the Mask and tSURFF methods, as well as results with an untruncated numerical domain

We have also used PESCADO to model Autler–Townes splitting during photoionisation. We then used machine learning to optimise the asymmetry between resulting energy peaks, by chaining the parameters of a shaped laser pulse.

In a recent paper we formulated PESCADO in a semianalytical manner, which allows us to extrapolate to infinite times after the interaction with the external field. In addition we also demonstrated how—and when—the absorber may be seen as a detector, distorting the angular distributions when the detector is placed in the extreme vicinity of the atom.