Introducing a phase factor for the two-electron continuum representation

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Synopsis We propose an approach to describe three-body Coulomb continuum wave functions in the entire space. It makes use of expansions on Convoluted Quasi Sturmian (CQS) basis, modified by an adequate phase factor as to possess an asymptotic form very close to the formal one. To show numerically that they constitute a suitable set of basis functions we consider the two-electron continuum case (e.g., electron impact double ionization of helium): a considerable improvement of the partial transition amplitudes' convergence rate is indeed observed.

The continuum spectrum of three charged particles in Coulomb interaction is notoriously difficult to describe. When solving atomic or molecular ionization problems, imposing the cumbersome boundary conditions to the wave function constitutes one of the primary mathematical and numerical difficulty. Besides, the long range nature of the Coulomb interaction implies solving Schrödinger's equation on relatively large spatial domains, which eventually translates into using large basis sets and a high computational cost. Ideally, such a domain should be extended up to the boundary of the asymptotic region (Ω_0) where all interparticle distances are large.

Only few *ab initio* methods (see, e.g., the review [2] and Introduction of [3]) have been and are being developed for constructing three-body continuum wave functions. In this contribution, we would like put forward a numerical approach in which the solution is obtained in the entire space so that the ionization amplitude is extracted from the expansion coefficients. The key idea is to use an expansion on a basis set of functions whose asymptotic behavior is as close as possible to the formal one in the Ω_0 region [1].

The proposed basis set contains two ingredients. First, it uses two-particle functions, named Convoluted Quasi Sturmian (CQS) in Ref. [3]; these behave asymptotically as a six-dimensional outgoing (incoming) spherical wave, meaning that they already possess intrinsically some three-body features. While promising, truncated expansions on CQS functions failed to converge satisfactorily with increasing basis size. The reason behind it is that they miss out an important term in the large hyperradius ($\rho = \sqrt{r_1^2 + r_2^2}$) domain: a Coulomb logarithmic phase which corresponds to the interelectronic potential. This brings us to the second ingredient, which consists in introducing – from the outset – an appropriate phase factor into the basis set. The modified CQS functions possess then an asymptotic behavior closer to the formal one, and lead to a considerable convergence improvement in numerical results.

For the sake of simplicity, we consider the two-electron continuum that occurs, for example, in the electron-impact double ionization of helium. To first order, the process can be described by a three-body Schrödinger driven equation. We seek a solution in the form of a truncated partial wave expansion on modified CQS. The desired phase is obtained as to cancel out at best the Coulomb potential $1/r_{12}$.

As we focus on the region Ω_0 we consider, as a numerical test case, typical experimental kinematical conditions with two electrons escaping with 10 eV each. We first investigate the compatibility of introducing a phase factor when using truncated expansions with a two-channel case with total angular momentum $L = 0$. We construct a suitable formula for the phase, and show that it indeed accelerates significantly the convergence of the calculated amplitudes as the number of basis functions is increased. We then consider total angular momentum $L = 1$, which provides the dominant contribution to the cross sections [4]. It is found that the introduction of the phase factor (with just two parameters) is again effective in obtaining satisfactory convergence of the partial transition amplitudes on a basis set of reasonable size. Thus, we expect the CQS basis combined with the proposed phase method to provide an effective tool for the study of full $(e,3e)$ processes as well.

References

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