Representing continuum wave functions with complex Gaussian functions

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The advantage of Gaussian functions in simplifying multi-center integrals is known since the work of Boys [1]. Their use has become pivotal in molecular calculations of bound states functions (see for example ref. [2]). The representation of continuum wave functions with Gaussians, on the other hand, has been much less studied. In 1990 Nestmann and Peyerimhoff [3] applied a nonlinear least square approach in an attempt to fit Bessel functions with Gaussians. While this approach is robust for low energy functions, the accuracy is poor when the functions are oscillating fast, especially at large distances. This drawback is related to the nodeless nature of real Gaussians. On the contrary complex Gaussians, *i.e.* Gaussians with complex exponents, have an intrinsic oscillating behavior which renders them more appropriate to represent oscillating functions.

In this work we generalized the approach of Nestmann and Peyerimhoff to complex Gaussians using a quadratic approximation method [4] to perform the optimization. An illustration of the representation, with both real and complex Gaussians, is shown in the figure for the case of a pure Coulomb continuum function. As a physical application we have considered the ionization of Hydrogen by a photon or an electron, and performed cross section calculations comparing to benchmark values.

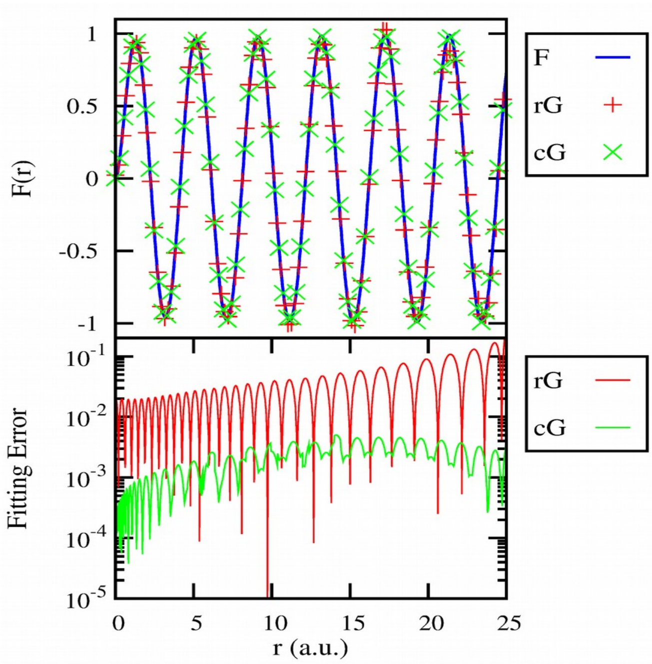

Figure : Upper panel : Curve of a simple Coulomb function (in blue) for wave number k = 1.5 a.u. with its fitting by either 30 real Gaussians (rG) or 30 complex Gaussians (cG) up to a distance of 25 a.u. . In the bottom panel we show the corresponding absolute errors.

[1] S. F. Boys *Proc. R. Soc.* A **200** 542 (1950).
[2] J. G. Hill *J. Quantum Chem.* **113** 21 (2013).
[3] B. M. Nestmann and S. D. Peyerimhoff *J. Phys. B: At. Mol. Opt. Phys.* **23** 773 (1990).
[4] M. G. D. Powell *Univ. Cambridge* **DAMTP NA06** (2009).