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Computation of resonant states using explicitly correlated coordinates in Be-like atomic systems

Juan Carlos Cardona[*, 1] **and José Luis Sanz-Vicario**[*, 2]

[*]Grupo de Física Atómica y Molecular, Instituto de Física, Universidad de Antioquia, Medellín, Colombia

Synopsis We present an efficient computational method to obtain accurate values for energy positions and widths of autoionizing states in Be-like atomic systems. The two-active (outer) electron wavefunction is expanded in terms of Hylleraas-type correlated configurations. The interaction with the $1s^2$ frozen core is represented through a model potential and the unphysical $1sn\ell$ series of virtual core states are removed by using a Phillips-Kleinman pseudopotential projector. A novel feature is that all matrix elements can be written in closed form. We illustrate the performance of our approach in computing doubly-excited states in Be and Ne^{6+} by using the stabilization method.

The accurate computation of the electronic structure in atoms and molecules remains to be a major aim of quantum theory since its early days. In spite of today's computational resources, the precise calculation of quantum states and of their related physical processes in many-electron atoms are still far from completeness, in particular when the electronic continuum is involved. The configuration interaction (CI) method provides a rigorous way to compute approximate, but accurate, variational energies and wavefunctions, as proved by the Hylleraas-Undheim-McDonald theorem. Nevertheless, the convergence of classical (central-symmetry) CI methods depends upon the size of both radial and angular expansions and it shows to be slow rated. Consequently, very large expansions (radial and angular) are usually required when one is interested in computing super-excited states. The acceleration of the convergence may be achieved by moving to expansions in terms of explicitly correlated coordinates.

In this communication we present details of our implementation for a Hylleraas configuration interaction method (HyCI), specifically applied to obtain resonance parameters for autoionizing states in Be-like systems [1]. The Hamiltonian for the four-electron atomic system (two electrons outside a frozen $1s^2$ core) reads

$$H_m = \sum_i h_m(i) + \frac{1}{r_{12}} + V_{PS}$$

where

$$h_m = -\frac{1}{2}\nabla^2 - \frac{Z}{r} + V_m(r)$$

represents the one-electron Hamiltonian that includes a model potential V_m which accounts for the electrostatic interaction produced by the core

$1s^2$. We use the simple form

$$V_m(r) = \frac{2}{r} - \frac{2}{r}(1 + \gamma r)e^{-2\gamma r}$$

where γ is the effective charge felt by the valence electrons due to the core which and it is the only adjusted parameter. The term V_{PS} corresponds to a Phillips-Kleinman pseudo-potential, i.e., $V_{PS} = M\mathcal{P}$, where $\mathcal{P}$ is a two-electron projection operator whose effect is to shift upwards in energy by a quantity M the non physical $1sn\ell$ series of virtual core states. The total HyCI wavefunction is constructed as a linear combination of antisymmetrized correlated configurations which have the form $\Psi_i(1,2) = \mathcal{A}\{\phi_i(\mathbf{r}_1, \mathbf{r}_2)\chi(1,2)\}$ where the spatial wavefunctions is built by using correlated STOs basis and usual vector coupled spherical harmonics, $\phi_i(\mathbf{r}_1, \mathbf{r}_2) = r_1^n r_2^m r_{12}^j e^{-\alpha r_1 - \beta r_2}\mathcal{Y}_{LM}(\mathbf{r}_1, \mathbf{r}_2)$. All the radial and angular integrals involved in our approach are solved in closed form, at variance with other prescriptions [2] where radial integrals must be computed with recursion relations (sometimes numerically unstable). For the sake of illustrating the effectiveness of our method we choose to use the stabilization method [3] to uncover the lowest resonances in Be and Ne^{6+} for $^{1,3}S^e$ symmetries for which we give accurate positions and widths.

References

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[1]E-mail: jcardona@fisica.udea.edu.co
[2]E-mail: sanjose@fisica.udea.edu.co