Journal of Physics: Conference Series **635** (2015) 082005 doi:10.1088/1742-6596/635/8/082005

Quasi Sturmian basis functions in hyperspherical coordinates

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Synopsis Quasi-Sturmian functions are an alternative set of basis functions useful to describe time-independent three body scattering problems. Their analytical closed form, for the Coulomb case, and some of their properties are presented here in hyperspherical coordinates.

An important theoretical issue when dealing with time-independent three-body scattering processes is how to impose the correct asymptotic behavior to the wave function. Many spectral methods use two-body basis functions that generally do not possess the correct behavior at large distances. One exception are the Generalized Sturmian Functions (GSF) [1], defined as to take into account the interactions of the problem, thus making them an efficient basis set.

In this work we propose a different set of functions, named Quasi Sturmian Functions (QSF). Like GSF, they posses the correct asymptotic behavior and, as an advantage, it is possible to express them with analytical representations. The definition, the properties and the efficiency of this alternative basis set (compared to GSF) have been presented for the two-body case [2].

For the three-body case, QSF in parabolic coordinates have been introduced [3]. We are interested here in using hyperspherical coordinates, consisting in one hyperradial (ρ) and five angular variables. Considering the latter as parameters, the hyperradial part of QSF is obtained by a generalization of the method presented in [2]. For a Temkin-Poet model, only the hyperangle $\alpha = \tan^{-1}(r_2/r_1)$ is retained, and we define the QSF to be the solutions of the non-homogeneous differential equation

$$\left[-\frac{1}{2\mu}\frac{d^2}{d\rho^2} + \frac{\lambda(\lambda+1)}{2\mu\rho^2} + \frac{C(\alpha)}{\rho} - E\right] Q_n^{(\pm)}(\alpha,\nu;\rho) = \frac{1}{\rho}\,\phi_{n,\lambda}(\nu;\rho)$$

where E is the total energy of the problem, λ and ν are fixed parameters and $C(\alpha)/\rho$ is the interaction potential. If $\phi_{n,\lambda}(\nu;\rho)$ is a Laguerre-type function, the QSF, and consequently its asymptotic behavior, have an analytical expression. For $\rho \to \infty$ we have:

$$\frac{Q_n^{(\pm)}(\nu,\alpha;\rho)}{\mathcal{Q}_n^{as}(\nu,\alpha)} \sim e^{\pm i\left(k\rho - \frac{\mu C(\alpha)}{k}\ln(2k\rho) + \sigma_\lambda - \frac{\lambda\pi}{2}\right)} \qquad (1)$$

where σ_λ is the Coulomb phase shift and $\mathcal{Q}_n^{as}(\nu,\alpha)$ can be expressed in terms of a Gauss hypergeometric function. This is the expected Coulomb behavior for a α-dependent charge $C(\alpha)$, and it is illustrated in the figure.

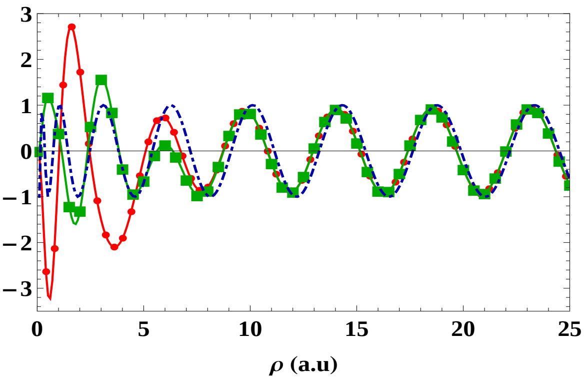

Figure 1. Real part of QSF (actually the ratio (1)), for $n = 4$ (line with solid dots) and $n = 7$ (line with solid squares), as function of ρ and for fixed $\alpha = \pi/4$. The dot-dashed line represents the real part of the asymptotic exponential function (1).

Taking advantage of their adequate asymptotic behavior, we plan to apply QSF basis sets to solve three-body scattering problems, such as double ionization processes, starting with a Temkin-Poet model. In particular, we will analyze the differences between standard extrapolation techniques and through QSF to extract the transition amplitude at infinite hyperradii.

References

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