Non homogeneous solution to a Coulomb Schrödinger equation as a basis set for scattering problems

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Synopsis Quasi-Sturmians, a mainly analytical tool for solving scattering problems, are introduced and their performance is compared with the Generalized Sturmian Function method.

Very recently Quasi-Sturmian (QS) functions in parabolic coordinates were introduced and used to solve a three-body model problem [1]. Spherical Quasi-Sturmian basis functions are presented in this work. Although ultimately intended for usage in three body problems, we present first here their definitions and applications on two-body scattering problems described by a driven equation as the following

$$[T_l + V_L(r) - E]\,\psi_{sc}(r) = -V_R(r)\,\phi(r)\,. \quad (1)$$

Radial QS functions are the solution of equation

$$[T_l + \bar{V}(r) - E]\,\psi^{+}_{n,l}(r) = \mathcal{U}_g(r)\varphi_{n,l}(\lambda, r). \quad (2)$$

The QS functions $\psi^{+}_{n,l}(r)$ can be understood as a generalization of the Green's function where instead of Dirac delta functions, the elements of a complete basis set $\{\varphi_{n,l}(\lambda, r)\}$ are considered on the on the right-hand-side (RHS). Different type of asymptotic behaviors can be imposed to $\psi^{+}_{n,l}(r)$: incoming, outgoing and standing-wave. It can be shown that the QS functions form a complete basis set on the configuration space.

We study here the solutions of Eq. (2) for the case where $\bar{V}(r)$ is a Coulomb potential. We consider on the RHS Laguerre and Slater-type basis functions. For these cases, closed form analytical solutions can be derived. We present various analytical representations and for various asymptotic behaviors. We also present a high order finite difference method that allows us to derive solutions of (2) for any arbitrary $\bar{V}(r)$, basis set $\varphi_{n,l}(\lambda, r)$ and $\mathcal{U}_g(r)$. The method employs a matricial finite difference scheme. It is a higher order analogous to the startup procedure implemented in the Sturmian obtention technique presented in [2].

The main advantage of these functions over the Sturmian ones is that, for Coulombic $\bar{V}(r)$ potential, analytical solutions are available almost for any RHS. This allow us to go an step ahead on the understanding of the analytical properties of three-body wave functions.

To prove that the efficiency of the QS functions is at least equivalent to that of the Generalized Sturmian functions, we solve the driven equation (1). We consider for that the scattering of a particle in a combined Coulomb potential of charge $z_1 z_2 = -2$ plus a Yukawa potential. In this case the solution of (1) is expanded as $\sum a_n \psi^{+}_{n,l}(r)$ where outgoing behavior is considered. The convergence rate found was even better than that of the Sturmian Functions. With 10 Quasi-Sturmian functions the scattering solution was already converged, while it took 30 Sturmian Functions to achieve the same accuracy. The RHS expansions obtained with both, Sturmians and Quasi-Sturmian methodologies were indistinguishable from the original RHS. Results were checked with an independent finite difference code.

In addition, we will outline the use of the QS for constructing three-body scattering wave functions.

References

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