Quasi-Sturmian Functions in Continuum Spectrum Problems

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Abstract

Quasi-Sturmian (QS) functions are proposed as an expansion basis to describe continuum states of a quantum system. A closed analytic representation of QS functions is derived. A two-body scattering example is given to demonstrate advantages of the method.

Keywords: *Inhomogeneous Schrödinger equation, Sturmian basis, Coulomb Green's function*

1 Introduction

The three-body Coulomb scattering is one of the fundamental unresolved problem. In atomic physics two-electrons systems are of great interest. In the one-electron continuum problem (e. g., when the electron is scattered by a bound pair) an expansion on the bispherical basis is applicable. In this case an expansion of the partial wave function on the basis of square integrable functions (of the electron coordinates r_1 and r_2) is recognized to be suitable. In the J-matrix method [1] as well as in the converge-close coupling (CCC) approach [2] the Laguerre basis functions are used for this purpose. Recently a new version of the Sturmian approach [3] has been developed, based upon an expansion on the so called generalized Sturmian functions (see, e. g., the papers [4, 5] and references therein) which are eigensolutions for integral or differential Sturm–Liouville equations with the outgoing- and incoming-wave boundary conditions. The Coulomb interaction within all these approaches is involved in the construction of the basis functions into the unperturbed part of the two-body Hamiltonian. In the framework of the J-matrix, the Coulomb Green's function have been obtained in a suitable analytic form [6, 7] in terms of hyper-geometric functions. In turn, the short-ranged operator of the potential energy is represented here in a finite subspace of L^2 basis functions. As a result, e. g., the phase shift corresponding to this truncated model potential, oscillates as the number of used basis functions increases [8]. Thus an application of the J-matrix method to the two-body scattering problem yet requires additional efforts in order to improve the convergence. The Sturmian function approach is free from such flaws. However these basis functions are calculated numerically, so the generation of the basis poses a problem as difficult as the original scattering problem.

In this paper, basis functions are proposed which we call Quasi Sturmians (QS). The QS functions formally are the solutions of the inhomogeneous Schrödinger equation

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whose right-hand-side contains the Laguerre L^2 functions. Hence, unlike the Sturmian functions, the QS functions with an appropriate asymptotic behavior can be obtained in a closed analytic form.

The atomic units are assumed throughout.

2 Quasi Sturmians

Let us consider the motion of a particle of mass μ in a potential $V(r) = V_C(r) + U(r)$ which is represented by the sum of the Coulomb potential $V_C(r) = \frac{Z_1 Z_2}{r}$ and a short-range one U. The scattering wave function $\Psi_\ell^{(+)}$ (we consider the outgoing-wave boundary condition) satisfies the Schrödinger equation

$$\left[-\frac{1}{2\mu}\left(\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2}\right) + V(r) - E\right]\Psi_\ell^{(+)}(r) = 0. \tag{1}$$

To solve the scattering problem, we express the wave function as a sum of the Coulomb wave and of the so-called scattering wave $\Psi_{sc}^{(+)}$:

$$\Psi(k,r) = \Psi_\ell^C(k,r) + \Psi_{sc}^{(+)}(k,r), \tag{2}$$

where Ψ_ℓ^C is the regular Coulomb solution [9]:

$$\Psi_\ell^C(k,r) = \frac{1}{2}(2kr)^{\ell+1}\, e^{-\pi\alpha/2}\, e^{ikr}\, \frac{|\Gamma(\ell+1+i\alpha)|}{(2\ell+1)!}\, {}_1F_1(\ell+1+i\alpha; 2\ell+2; -2ikr). \tag{3}$$

Here $\alpha = \frac{\mu Z_1 Z_2}{k}$ is the Sommerfeld parameter, the energy is defined as $E = \frac{k^2}{2\mu}$.

Inserting (2) into (1) yields the following inhomogeneous equation for $\Psi_{sc}^{(+)}$:

$$\left[-\frac{1}{2\mu}\left(\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2}\right) + \frac{Z_1 Z_2}{r} + U(r) - E\right]\Psi_{sc}^{(+)}(k,r) = -U(r)\Psi_\ell^C(k,r). \tag{4}$$

We suggest to find the solution $\Psi_{sc}^{(+)}$ of the Driven Equation (4) in form of the expansion

$$\Psi_{sc}^{(+)}(r) = \sum_{n=0}^{N-1} c_{n,\ell}\, Q_{n,\ell}^{(+)}(r). \tag{5}$$

The functions $Q_{n,\ell}^{(+)}$ satisfy the inhomogeneous equation

$$\left[-\frac{1}{2\mu}\left(\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2}\right) + \frac{Z_1 Z_2}{r} - E\right] Q_{n,\ell}^{(+)}(r) = \frac{1}{r}\phi_{n,\ell}(r), \tag{6}$$

where the Laguerre basis functions

$$\phi_{n,\ell}(\lambda, r) = \sqrt{\frac{n!}{(n+2\ell+1)!}}\, e^{-\lambda r}\, (2\lambda r)^{\ell+1} L_n^{2\ell+1}(2\lambda r) \tag{7}$$

are used; λ is the scale parameter of the basis.

We call the functions $Q_{n,\ell}^{(+)}$ Quasi Sturmians due to their analogy with (using as a basis) Sturmian functions. QS with appropriate asymptotic properties can be obtained (unlike the Sturmian functions) in a closed form.

QS functions can be presented as an integral:

$$Q_{n,\ell}^{(+)}(r) = \int_0^\infty dr'\, G^{\ell(\pm)}(k; r, r')\, \frac{1}{r'}\, \phi_{n,\ell}(\lambda, r'). \tag{8}$$

The Green function operator $\hat{G}^{\ell(+)}$ kernel is expressed in terms of the Whittaker functions [10]:

$$G^{\ell(\pm)}(k;r,r') = \mp\frac{\mu}{ik}\frac{\Gamma(\ell+1\pm i\alpha)}{(2\ell+1)!}\,\mathcal{M}_{\mp i\alpha;\ell+1/2}(\mp ikr_<)\,\mathcal{W}_{\mp i\alpha;\ell+1/2}(\mp ikr_>). \tag{9}$$

Explicit expressions for the matrix elements

$$G^{\ell(\pm)}_{m,n}(k;\lambda) = \int\limits_0^\infty\int\limits_0^\infty drdr'\,\frac{1}{r}\,\phi_{m,\ell}(\lambda,r)\,G^{\ell(\pm)}(k;r,r')\,\frac{1}{r'}\,\phi_{n,\ell}(\lambda,r') \tag{10}$$

have been obtained in Ref. [6] (see also Ref. [7]) using two linear independent J-matrix solutions [11]:

$$G^{\ell(\pm)}_{m,n}(k;\lambda) = \frac{2\mu}{k}\,\mathcal{S}_{n_<,\ell}(k)\,\mathcal{C}^{(\pm)}_{n_>,\ell}(k). \tag{11}$$

The coefficients of the QS function expansion in terms of the Laguerre basis functions (7) are calculated by multiplying Eq. (8) by $\frac{1}{r}\phi_{n,\ell}(\lambda,r)$ and integrating over r. As a result, in view of Eq. (10), we obtain

$$Q^{(\pm)}_{n,\ell}(r) = \sum_{m=0}^{\infty}\phi_{m,\ell}(\lambda,r)\,G^{\ell(\pm)}_{m,\,n}(k;\lambda). \tag{12}$$

3 Example

Let us consider an s-wave scattering of a particle of mass $\mu = 1$ and momentum $k = 1$ by the combination of the Coulomb potential with $Z_1Z_2 = 1$ and Yukawa potential

$$U(r) = b\,\frac{e^{-ar}}{r}, \quad a = 1.3, \;\; b = 1. \tag{13}$$

We study the expansion (5) convergence with increasing N. The functions $Q^{(+)}_{n,0}$ oscillate with different frequencies within the range of the potential U (see Fig. 1) while the Sturmians possess the same behavior up to the amplitude factor outside the range.

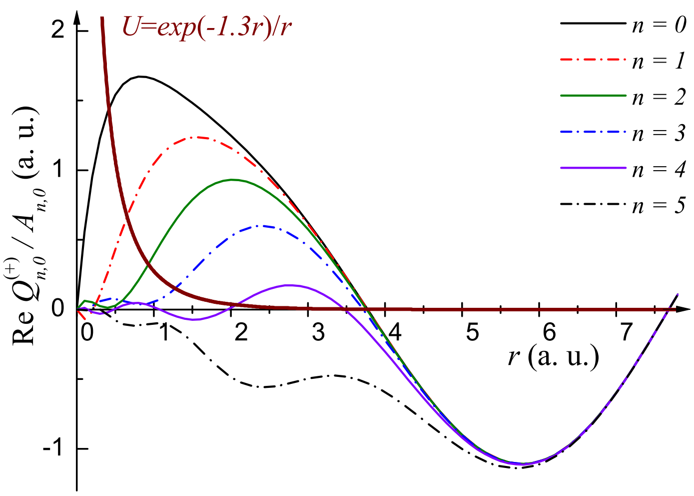

Figure 1: Real parts of the first six QS functions for a particle of mass $\mu = 1$ and momentum $k = 1$ in the Coulomb potential $V_C = \frac{1}{r}$. The scale parameter of the basis $\lambda = 2.6$.

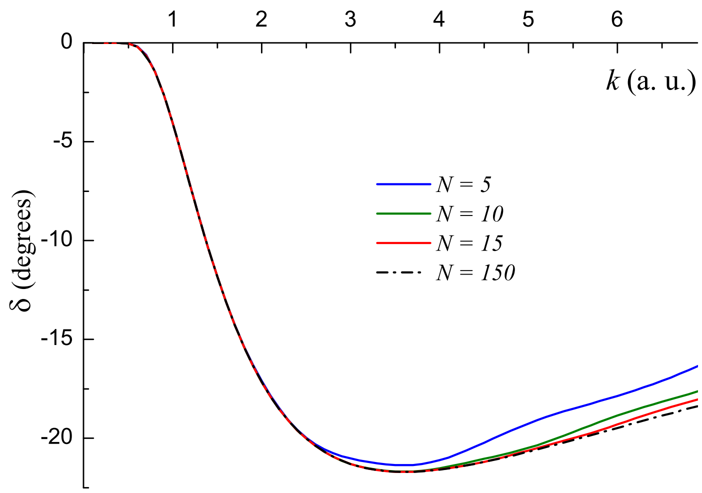

Figure 2: Convergence of the phase shift with N.

We insert the expansion (5) into Eq. (4), multiply the resulting expression by $\phi_{n,\ell}(\lambda, r)$ and integrate over r to obtain a discrete equation for the coefficients $c_{n,\ell}$:

$$[\mathbf{I} + \mathcal{U}]\,\mathbf{c} = \mathbf{d}. \tag{14}$$

The components d_m, $m = 0, \ldots, N-1$ of the vector $\mathbf{d}$ in the right-hand-side of Eq. (14) are defined as

$$d_m = -\int_0^\infty dr\,\phi_{m,0}(\lambda, r)\,U(r)\,\Psi_0^C(r), \tag{15}$$

the elements $\mathcal{U}_{m,n}$ of the $N \times N$ matrix $\mathcal{U}$ are defined as

$$\mathcal{U}_{m,n} = \int_0^\infty dr\,\phi_{m,0}(\lambda, r)\,U(r)\,Q_{n,0}^{(+)}(r) \tag{16}$$

The unit matrix I present in the left-hand-side of Eq. (14) appears due to the orthogonality relation for the Laguerre basis.

Convergence of the s-wave phase shift $\delta_0(k)$ with N is shown in Fig. 3.

4 Conclusion

A comparison of the phase shift obtained by our method with the phase shift from the J-matrix calculations shows advantages of the proposed approach over the J-matrix method.

In this work we suggested the Quasi-Sturmian functions and showed that their application to the two-body scattering problem is quite efficient. The convergence rate appeared to be comparable or even higher than that achieved in the J-matrix method and generalized Sturmian approach. Moreover, the QS functions have an obvious advantage that they can be expressed in a closed analytic form. An explicit representation of the basis QS function in terms of known special functions may be useful in applications to the Coulomb three-body problem.

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