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Harmonic oscillator Green functions

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Abstract. The Green function for the Schrödinger equation with an isotropic, three-dimensional harmonic-oscillator potential is given in closed form. A similar closed form is obtained when the Schrödinger equation also contains a magnetic interaction and the magnetic field is such that the precession and oscillation frequencies are equal. The latter Green function is used to obtain energy and Sturmian eigenvalues that occur in the theory of atom–atom collisions.

1. Introduction

The harmonic oscillator is one of the most widely used model interactions in physics and is fundamental to many quantum systems. Much is known about the wavefunctions, eigenvalues and time-dependent propagator for the Schrödinger equation with harmonic-oscillator potentials. The mathematical apparatus for this model seems complete [1], yet there is one function that is conspicuously absent, namely, the time-independent, hereafter called the stationary, Green function $G(\mathbf{r}, \mathbf{r}', E)$. The Green function is known in closed form only for one dimension. Expressions for the stationary Green function in three dimensions have only appeared in the literature as sums over partial waves [2]. To the best of our knowledge, the sums themselves have not yet been evaluated in closed form. The purpose of this manuscript is to derive closed-form expressions for the Green functions for the Schrödinger equation with an isotropic harmonic-oscillator potential. Atomic units with $e = m = \hbar = 1$ are used throughout.

Our interest in the harmonic-oscillator potential derives from its appearance in the mapping of the time-dependent free-particle Schrödinger equation via a scaling transformation. In this transformation, the Schrödinger equation is written in a coordinate system where the lengthscale varies with time [3]. Coordinates \mathbf{r} of particles scale according to $\mathbf{r} = \mathbf{q}R(t)$, where $R(t)$ is a function chosen for its relevance to specific physical situations. In the situation of interest for our work, this coordinate is the distance between two positively charged ions following a classical trajectory $R(t)$ and \mathbf{r} is the coordinate of a negative electron. The scaling transformation has also been applied to a particle in a box where the walls of the box move with time [5], and to the models where atomic potentials are replaced by zero-range potentials [6].

In three dimensions the length $R(t)$ varies with time and the internuclear axis rotates. Transformations to rotating frames are standard and are represented by the rotation operator

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$\exp[i\Theta(t)\mathbf{n}\cdot\mathbf{L}]$. Such transformations introduce a factor $i\Theta\mathbf{n}\cdot\mathbf{L}$ in the Schrödinger equation, while the scale transformation introduces an oscillator potential. Thus the Green function for the oscillator together with the rotation term is pertinent to physical applications. For that reason, we consider the Green function for a three-dimensional (3D) oscillator without and with rotation. In the latter case the spring constant of the oscillator Ω^2 is the square of the angular frequency Ω of rotation. For $R(t) = \sqrt{b^2 + v^2 t^2}$, where b and v are constants the transformed Schrödinger equation is stationary, i.e. H is time independent. This transformation of the Schrödinger equation is reviewed in section 3.1.

The Green function is the Laplace transform of the well known propagator $K(\mathbf{r}, T; \mathbf{r}', 0)$, thus computing the Green function is accomplished by evaluating a Laplace integral. The propagator and its relation to the Green function is reviewed in section 2. Computation of a Laplace integral is the main task and is reported in section 2.2. The Laplace integral is then used to compute the Green function without rotation in section 2.3 and with rotation in section 2.4. A particular case of this latter function, of importance for zero-range potentials, has the coordinate y' equal to zero, and is therefore referred to as the in-plane Green function. The in-plane Green function is derived in section 2.5 and employed in section 3 to compute energy and Sturmian eigenvalues for the harmonic oscillator with two zero-range potentials.

2. Oscillator Green functions in 3D

2.1. General

We begin with the propagator [1] for a 3D oscillator with the frequency Ω

$$K(\mathbf{r}, T, \mathbf{r}', 0) = \left(\frac{\Omega}{2\pi i \sin \Omega T}\right)^{3/2} \exp\left(\frac{i\Omega}{2 \sin \Omega T}[(r^2 + r'^2) \cos \Omega T - 2\mathbf{r} \cdot \mathbf{r}']\right). \quad (1)$$

The propagator equation (1) satisfies the Schrödinger equation

$$\left[-\frac{1}{2}\nabla_r^2 + \frac{1}{2}\Omega^2 r^2\right]K(\mathbf{r}, T, \mathbf{r}', 0) = i\frac{\partial}{\partial T}K(\mathbf{r}, T, \mathbf{r}', 0) \quad (2)$$

with the initial condition

$$K(\mathbf{r}, T, \mathbf{r}', 0)|_{T=0} = \delta(\mathbf{r} - \mathbf{r}'). \quad (3)$$

The Green function is

$$G(\mathbf{r}, \mathbf{r}', E) = \lim_{\eta \rightarrow +0} i \int_0^\infty \exp[i(E + i\eta)T]K(\mathbf{r}, T, \mathbf{r}', 0) dT \quad (4)$$

it satisfies the stationary inhomogeneous equation

$$\left[-\frac{1}{2}\nabla_r^2 + \frac{1}{2}\Omega^2 r^2 - E\right]G(\mathbf{r}, \mathbf{r}', E) = \delta(\mathbf{r} - \mathbf{r}'). \quad (5)$$

The Green function is not completely specified by the Schrödinger equation, since appropriate boundary conditions must be imposed. One such boundary condition is that $G(\mathbf{r}, \mathbf{r}')$ is regular everywhere except at the singular point $\mathbf{r} = \mathbf{r}'$, in particular $G(\mathbf{r}, \mathbf{r}')$ is regular at the origin. The function also satisfies boundary conditions at infinite distance. In the absence of the harmonic-oscillator potential $G(\mathbf{r}, \mathbf{r}')$ satisfies outgoing wave boundary conditions, but because of the attractive harmonic-oscillator potential $G(\mathbf{r}, \mathbf{r}')$ of equation (5) it is exponentially damped. With the definition (4) the boundary conditions at infinity are

$$\lim_{r \rightarrow \infty} \frac{1}{rG} \frac{\partial(rG)}{\partial r} = -\sqrt{\Omega^2 r^2 - 2(E + i\eta)}. \quad (6)$$

The small imaginary part $i\eta$ is retained in the equation (6) in order to assure that the Green function is uniquely specified for $\Omega = 0$. The uniqueness of solutions of the Schrödinger equation is needed in order to assure that the expression we obtain by solving equation (5) is identical to the expression needed to evaluate the Laplace transform in equation (4).

2.2. Evaluation of an integral

From equation (4) it follows that the Green functions are proportional to the integral, which cannot be found in standard tables such as [7],

$$F_E(\alpha, \beta) = i \int_0^\infty \exp(iET) \left(\frac{\Omega}{2\pi i \sin \Omega T} \right)^{3/2} \exp\left(\frac{i\Omega}{2 \sin \Omega T} (\alpha \cos \Omega T + \beta) \right) dT. \quad (7)$$

We present a method to calculate such integrals in this manuscript. Our method employs the well known expression for the s-wave component of the Green function.

Expanding the Green function over spherical harmonics and projecting onto the s-wave component gives

$$\int G(\mathbf{r}, \mathbf{r}', E) Y_{00}(\hat{\mathbf{r}}') d\hat{\mathbf{r}}' = \frac{1}{\sqrt{4\pi}} \frac{g_E(r_>) f_E(r_<)}{r'^2 W(g_E(r'), f_E(r'))} \quad (8)$$

where $W(g_E(r'), f_E(r'))$ is the Wronskian of the functions g_E and f_E . The function on the right-hand side of equation (8) is a solution of the equation

$$\left[-\frac{1}{2} \left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} - \Omega^2 r^2 \right) - E \right] \frac{g_E(r_>) f_E(r_<)}{r'^2 W(g_E(r'), f_E(r'))} = \frac{1}{r^2} \delta(r - r') \quad (9)$$

with appropriate boundary conditions.

The functions f and g are given explicitly by

$$g_E(r) = \exp(-\Omega r^2/2) U\left(\frac{3}{4} - \frac{E}{2\Omega}, \frac{3}{2}, \Omega r^2 \right) \quad (10)$$

$$f_E(r) = \exp(-\Omega r^2/2) M\left(\frac{3}{4} - \frac{E}{2\Omega}, \frac{3}{2}, \Omega r^2 \right) \quad (11)$$

where M and U are confluent hypergeometric functions [8]. The Wronskian is calculated directly, and we find

$$\frac{1}{r'^2 W(g_E(r'), f_E(r'))} = 2\sqrt{\frac{\Omega}{\pi}} \Gamma\left(\frac{3}{4} - \frac{E}{2\Omega} \right). \quad (12)$$

Equation (8) together with equation (12) is a closed-form expression for the s-wave Green function. It is also a closed-form expression for the Laplace transform of the spherical average of the propagator. Because the mathematical expression for the spherical average of the propagator is similar to that for the propagator itself, the s-wave Green function, with appropriate variables, can be used to write a closed-form expression for the 3D Green function $G(\mathbf{r}, \mathbf{r}')$. We first compute the s-wave Green function directly from the definition equation (4) to obtain equation (16) below. This result is then used to calculate the general integral $F_E(\alpha, \beta)$ of equation (7) and the various 3D Green functions of sections 2.3–2.5.

The propagator equation (1) has the following form

$$K(\mathbf{r}, T, \mathbf{r}', 0) = \left(\frac{\Omega}{2\pi i \sin \Omega T} \right)^{3/2} \exp\left(\frac{i\Omega}{2 \sin \Omega T} [A \cos \Omega T - B\mu] \right) \quad (13)$$

where $A = r^2 + r'^2$, $B = 2rr'$, and $\mu = \hat{r} \cdot \hat{r}'$. In addition we need the inverse relations

$$2r_{>}^2 = A + \sqrt{A^2 - B^2} \tag{14}$$

$$2r_{<}^2 = A - \sqrt{A^2 - B^2}. \tag{15}$$

Substituting equations (4) and (13) into equation (8), and performing the integration over μ one obtains

$$\begin{aligned} & i \int_0^\infty \exp(iET) \left(\frac{\Omega}{2\pi i \sin \Omega T} \right)^{3/2} \frac{2 \sin \Omega T}{i\Omega} \\ & \times \left[\exp \left(\frac{i\Omega}{2 \sin \Omega T} [A \cos \Omega T + B] \right) - \exp \left(\frac{i\Omega}{2 \sin \Omega T} [A \cos \Omega T - B] \right) \right] dT \\ & = 2B\Lambda(\Omega, E)g_E(r_{>})f_E(r_{<}) \end{aligned} \tag{16}$$

where

$$\Lambda(\Omega, E) = \frac{1}{2\pi r'^2 W(g_E(r'), f_E(r'))} \equiv \frac{1}{2\Omega} \left(\frac{\Omega}{\pi} \right)^{3/2} \Gamma \left(\frac{3}{4} - \frac{E}{2\Omega} \right). \tag{17}$$

Forming the partial derivative of equation (16) with respect to B and taking into account definition of $F_E(\alpha, \beta)$ equation (7) gives our first relation

$$F_E(A, B) + F_E(A, -B) = 2\Lambda(\Omega, E) \frac{\partial}{\partial B} [Bg_E(r_{>})f_E(r_{<})]. \tag{18}$$

Alternatively we can use

$$\exp(iEt) \sin \Omega t = \frac{1}{2i} \{ \exp[i(E + \Omega)t] - \exp[-i(E - \Omega)t] \} \tag{19}$$

in equation (16) to write a second equation

$$\begin{aligned} & F_{E+\Omega}(A, B) - F_{E-\Omega}(A, B) - [F_{E+\Omega}(A, -B) - F_{E-\Omega}(A, -B)] \\ & = -2\Omega\Lambda(\Omega, E)Bg_E(r_{>})f_E(r_{<}). \end{aligned} \tag{20}$$

In a similar fashion we can take the derivative of equation (16) with respect to A and use

$$\exp(iEt) \cos \Omega t = \frac{1}{2} \{ \exp[i(E + \Omega)t] + \exp[-i(E - \Omega)t] \} \tag{21}$$

to obtain a third independent equation

$$\begin{aligned} & F_{E+\Omega}(A, B) + F_{E-\Omega}(A, B) - [F_{E+\Omega}(A, -B) + F_{E-\Omega}(A, -B)] \\ & = 4\Lambda(\Omega, E)B \frac{\partial}{\partial A} [g_E(r_{>})f_E(r_{<})]. \end{aligned} \tag{22}$$

Adding equations (20) and (22), and changing $E \rightarrow E - \Omega$ gives

$$\begin{aligned} & F_E(A, B) - F_E(A, -B) = 2\Lambda(\Omega, E - \Omega) \\ & \times B \left(\frac{\partial}{\partial A} [g_{E-\Omega}(r_{>})f_{E-\Omega}(r_{<})] - \frac{\Omega}{2} g_{E-\Omega}(r_{>})f_{E-\Omega}(r_{<}) \right) \end{aligned} \tag{23}$$

and the desired result is obtained by adding equations (18) and (23)

$$\begin{aligned} & F_E(A, B) = \Lambda(\Omega, E) \left(\frac{\partial}{\partial B} [Bg_E(r_{>})f_E(r_{<})] \right) \\ & + \Lambda(\Omega, E - \Omega) B \left(\frac{\partial}{\partial A} [g_{E-\Omega}(r_{>})f_{E-\Omega}(r_{<})] - \frac{\Omega}{2} g_{E-\Omega}(r_{>})f_{E-\Omega}(r_{<}) \right). \end{aligned} \tag{24}$$

Instead of summing equations (20) and (22), we can subtract them and change $E \rightarrow E + \Omega$, to obtain the alternative form

$$F_E(A, B) = \Lambda(\Omega, E) \left(\frac{\partial}{\partial B} [B g_E(r_{>}) f_E(r_{<})] \right) + \Lambda(\Omega, E + \Omega) B \left(\frac{\partial}{\partial A} [g_{E+\Omega}(r_{>}) f_{E+\Omega}(r_{<})] + \frac{\Omega}{2} g_{E+\Omega}(r_{>}) f_{E+\Omega}(r_{<}) \right). \tag{25}$$

Equations (24) and (25) are the main results of this section. They provide closed form expressions for the Laplace integral of equation (7) with arbitrary values of the parameters α and β .

2.3. 3D Green functions without rotation

By inspection of the propagator equation (1) it is easy to see that the Green function is obtained from equation (25) when the parameters α and β are chosen according to

$$\alpha = r^2 + r'^2 \tag{26}$$

$$\beta = -2\mathbf{r} \cdot \mathbf{r}'. \tag{27}$$

It is convenient to introduce a new pair of variables†

$$\xi = \frac{\Omega}{2} (r^2 + r'^2 + |\mathbf{r} - \mathbf{r}'| |\mathbf{r} + \mathbf{r}'|), \tag{28}$$

$$\eta = \frac{\Omega}{2} (r^2 + r'^2 - |\mathbf{r} - \mathbf{r}'| |\mathbf{r} + \mathbf{r}'|) \tag{29}$$

which are connected with α and β as follows

$$\alpha = \frac{1}{\Omega} (\xi + \eta) \tag{30}$$

$$\beta = -\text{sign}(\mathbf{r} \cdot \mathbf{r}') \frac{2}{\Omega} \sqrt{\xi \eta}. \tag{31}$$

Transforming equation (25) to new variables (ξ, η) , gives the Green function

$$G(\mathbf{r}, \mathbf{r}', E) = \exp\left(-\frac{\xi + \eta}{2}\right) \left\{ \Lambda(\Omega, E) \left(1 + \frac{2\xi\eta}{\xi - \eta} \left[\frac{\partial}{\partial \eta} - \frac{\partial}{\partial \xi} \right] \right) U_E(\xi) M_E(\eta) + \text{sign}(\mathbf{r} \cdot \mathbf{r}') \Lambda(\Omega, E + \Omega) \frac{2\sqrt{\xi\eta}}{\xi - \eta} \left[\eta \frac{\partial}{\partial \eta} - \xi \frac{\partial}{\partial \xi} \right] U_{E+\Omega}(\xi) M_{E+\Omega}(\eta) \right\} \tag{32}$$

where $\Lambda(\Omega, E)$ is given by equation (17), and

$$U_E(\xi) = U\left(\frac{3}{4} - \frac{E}{2\Omega}, \frac{3}{2}, \xi\right) \tag{33}$$

$$M_E(\eta) = M\left(\frac{3}{4} - \frac{E}{2\Omega}, \frac{3}{2}, \eta\right). \tag{34}$$

Equation (32) is the desired closed-form expression for the 3D Green function. Using equations (28) and (29) it is straightforward to show that the Green function equation (32) has the required singularity when $\mathbf{r} \rightarrow \mathbf{r}'$, i.e.

$$G(\mathbf{r}, \mathbf{r}', E) \sim \frac{1}{2\pi |\mathbf{r} - \mathbf{r}'|} \quad \text{when } \mathbf{r} \rightarrow \mathbf{r}'. \tag{35}$$

† Variables ξ and η correspond to $r_{>}^2$ and $r_{<}^2$ given by equations (14) and (15).

Using the N -dimensional propagator for harmonic oscillator

$$K(\mathbf{r}, T, \mathbf{r}', 0) = \left(\frac{\Omega}{2\pi i \sin \Omega T} \right)^{N/2} \exp \left(\frac{i\Omega}{2 \sin \Omega T} [(r^2 + r'^2) \cos \Omega T - 2\mathbf{r} \cdot \mathbf{r}'] \right) \quad (36)$$

equation (4) for the Green function, and closed form in 3D equation (32) it is possible to obtain closed forms for harmonic oscillator Green functions with arbitrary *odd* number of dimensions. Introducing $\mu = \hat{\mathbf{r}} \cdot \hat{\mathbf{r}}'$, and denoting the dimensionality by a superscript, we obtain

$$G^{(2N+3)}(\mathbf{r}, \mathbf{r}', \mu) = \frac{1}{(2\pi r r')^N} \frac{\partial^N}{\partial \mu^N} G^{(3)}(\mathbf{r}, \mathbf{r}', \mu) \quad (37)$$

where $G^{(3)}(\mathbf{r}, \mathbf{r}', \mu)$ is given by equation (32) with $(2N + 3)$ -dimensional vectors \mathbf{r} and \mathbf{r}' .

The importance of the closed forms for Green functions in atomic physics stems from the possibility to take into account exactly all partial waves in the problem. It is relatively easy to write partial-wave expansions for Green functions, but their usefulness is limited to the cases where only several partial waves are important. There are very few nontrivial examples of 3D Green functions known in closed forms. One of them is the Coulomb Green function derived in closed form by Hostler and Pratt [9]. The Coulomb Green function found many applications in atomic physics; to mention a few: in calculating dynamic polarizabilities of alkali-metal atoms [10], or in the theory of ion-pair formation in Rydberg atom collisions [11].

We believe that the harmonic-oscillator Green function given by equation (32) will prove to be equally useful, since the harmonic oscillator is one of the most wide-spread model potentials in modern physics. In section 3 we give an application of the harmonic-oscillator Green function in ion-atom collisions. An additional oscillator potential appears in the Schrödinger equation when one constructs explicitly Galilean-invariant theory according to Solov'ev [3]. However, the Solov'ev's Galilean-invariant theory requires taking account of the internuclear axis rotation. In the next two sections we derive closed forms for the oscillator Green functions in the coordinate systems rotating with the frequency of the oscillator.

The final remark is in order here to avoid possible confusion. Even though we use the well known s-wave component of the oscillator Green function to evaluate the integral in equation (7), it does not mean that our final result equation (32) is limited to the s-wave. In fact equation (32) is exact and contains all partial waves, as can be seen from the limiting case equation (35), for example. This remark pertains to all Green functions derived in this paper.

2.4. 3D Green functions with rotation

In the theory of atom-atom collisions (see section 3 below) one deals with the oscillator in a reference frame rotating with the fundamental frequency of the oscillator. In this section we derive a Green function for this case.

The propagator with rotation is simply

$$K_{\text{rot}}(\mathbf{r}, T, \mathbf{r}', 0) = \exp(i\Omega T \hat{L}_y) K(\mathbf{r}, T, \mathbf{r}', 0) \quad (38)$$

where \hat{L}_y is the projection of the angular momentum operator on the axis of rotation (chosen to be the y -axis here). Using the explicit form equation (1) and performing the indicated transformation to the rotating frame gives

$$K_{\text{rot}}(\mathbf{r}, T, \mathbf{r}', 0) = \left(\frac{\Omega}{2\pi i \sin \Omega T} \right)^{3/2} \exp[-i\Omega(z'x - x'z)]$$

$$\times \exp\left(\frac{i\Omega}{2\sin\Omega T}[(r^2 + r'^2 - 2(xx' + zz'))\cos\Omega T - 2yy']\right). \quad (39)$$

The propagator with rotation satisfies the differential equation

$$[-\frac{1}{2}\nabla_r^2 + \frac{1}{2}\Omega^2 r^2 + \Omega\hat{L}_y]K_{\text{rot}}(\mathbf{r}, T, \mathbf{r}', 0) = i\frac{\partial}{\partial T}K_{\text{rot}}(\mathbf{r}, T, \mathbf{r}', 0) \quad (40)$$

with the same initial condition as the propagator without rotation (see equation (3)). The Green function is given by equation (4) and satisfies the equation

$$[-\frac{1}{2}\nabla_r^2 + \frac{1}{2}\Omega^2 r^2 + \Omega\hat{L}_y - E]G_{\text{rot}}(\mathbf{r}, \mathbf{r}', E) = \delta(\mathbf{r} - \mathbf{r}'). \quad (41)$$

The Green function is proportional to the integral in equation (7), but with different parameters α and β . Introducing new variables

$$\xi_r = \frac{\Omega}{2}(|\mathbf{r} - \mathbf{r}'|^2 + 2yy' + |\mathbf{r} - \mathbf{r}'||\mathbf{r} - \mathbf{r}'_{xz}|) \quad (42)$$

$$\eta_r = \frac{\Omega}{2}(|\mathbf{r} - \mathbf{r}'|^2 + 2yy' - |\mathbf{r} - \mathbf{r}'||\mathbf{r} - \mathbf{r}'_{xz}|) \quad (43)$$

where $\mathbf{r}'_{xz} = (x', -y', z')$ (the reflection of \mathbf{r}' in the xz -plane), we can write the Green function with rotation in the form similar to equation (32)

$$G_{\text{rot}}(\mathbf{r}, \mathbf{r}', E) = \exp[-i\Omega(z'x - x'z)] \exp\left(-\frac{\xi_r + \eta_r}{2}\right) \quad (44)$$

$$\times \left\{ \Lambda(\Omega, E) \left(1 + \frac{2\xi_r\eta_r}{\xi_r - \eta_r} \left[\frac{\partial}{\partial\eta_r} - \frac{\partial}{\partial\xi_r}\right]\right) U_E(\xi_r)M_E(\eta_r) \right. \\ \left. + \text{sign}(yy')\Lambda(\Omega, E + \Omega) \frac{2\sqrt{\xi_r\eta_r}}{\xi_r - \eta_r} \left[\eta_r \frac{\partial}{\partial\eta_r} - \xi_r \frac{\partial}{\partial\xi_r}\right] U_{E+\Omega}(\xi_r)M_{E+\Omega}(\eta_r) \right\} \quad (45)$$

where functions U_E and M_E are defined above by equations (33) and (34).

2.5. In-plane 3D Green functions with rotation

In atom-atom collisions to a very good approximation the nuclei move in the plane perpendicular to the total angular momentum. Therefore, the in-plane Green function is important for applications. It is obtained from the general formula equation (45) by taking the limit $y' \rightarrow 0$, which in terms of ξ_r and η_r corresponds to

$$\xi_r \rightarrow \Omega|\mathbf{r} - \mathbf{r}'|^2 \quad \text{and} \quad \eta_r \rightarrow 0. \quad (46)$$

The in-plane Green function then takes a very concise form

$$G_{\text{rot}}^{y'=0}(\mathbf{r}, \mathbf{r}', E) = \frac{\exp(i[\mathbf{r}' \times \boldsymbol{\Omega}] \cdot \mathbf{r})}{2\pi|\mathbf{r} - \mathbf{r}'|} \frac{U\left(-\frac{E}{\Omega}, \sqrt{2\Omega}|\mathbf{r} - \mathbf{r}'|\right)}{U\left(-\frac{E}{\Omega}, 0\right)} \quad (47)$$

where $U(a, x)$ is a parabolic cylinder function defined in [8].

This simple result can also be obtained by other means. First of all, when $y' = 0$, one can perform the integration directly [7] in equation (4) without using equation (25). Second, the equation for the Green function equation (41) can be solved by introducing two new variables

$$\rho = |\mathbf{r} - \mathbf{r}'| \quad (48)$$

$$\sigma = \frac{\Omega}{|\mathbf{r} - \mathbf{r}'|}(x'z - z'x) \quad (49)$$

and separating them in a way similar to one employed by Hostler and Pratt [9] to find the Coulomb Green function. It is reassuring that three different methods give the same result equation (47) for the in-plane Green function with rotation.

In atomic collision applications (section 3) we will need the regularized Green function defined by

$$G_r(\mathbf{r}, \mathbf{r}, E) = G_{\text{rot}}^{y'=0}(\mathbf{r}, \mathbf{r}', E) - \frac{1}{2\pi|\mathbf{r} - \mathbf{r}'|}. \quad (50)$$

It is easy to find the explicit expression for the limit of the regularized in-plane Green function as $\mathbf{r}' \rightarrow \mathbf{r}$:

$$G_r(E) = \lim_{\mathbf{r}' \rightarrow \mathbf{r}} G_r(\mathbf{r}, \mathbf{r}, E) = \frac{\sqrt{2\Omega} U'(-\frac{E}{\Omega}, 0)}{2\pi U(-\frac{E}{\Omega}, 0)}. \quad (51)$$

In this case $G_r(E)$ does not depend on coordinates, therefore we omit reference to \mathbf{r} in equation (51).

Finally, it should be noted that Green functions with rotation have slightly different symmetry with respect to permutation of \mathbf{r} and \mathbf{r}' :

$$G_{\text{rot}}(\mathbf{r}, \mathbf{r}') = G_{\text{rot}}^*(\mathbf{r}', \mathbf{r}). \quad (52)$$

Green functions with rotation are complex conjugated under permutations of \mathbf{r} and \mathbf{r}' , whereas ordinary Green functions do not change at all.

3. Oscillator Green functions in atomic collision theory

3.1. Solov'ev-Vinitsky transformation

Consider an atomic collision with two nuclei moving along a classical trajectory $\mathbf{R}(t)$ with the initial velocity v and impact parameter b (figure 1), and one electron described by a time-dependent Schrödinger equation

$$\left[-\frac{1}{2}\nabla_r^2 + V(\mathbf{r}, \mathbf{R}(t)) \right] \psi(\mathbf{r}, t) = i \frac{\partial \psi(\mathbf{r}, t)}{\partial t}. \quad (53)$$

The Solov'ev-Vinitsky transformation [3] of the above equation involves the change of variables

$$\mathbf{q} = \frac{\mathbf{r}}{R(t)} \quad (54)$$

$$\tau = \int_{-\infty}^t \frac{dt'}{R^2(t')} \quad (55)$$

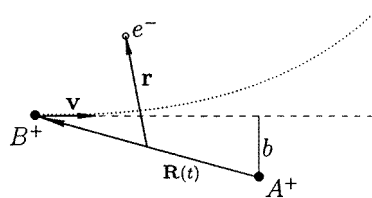


Figure 1. Collision scheme.

and the transformation of the wavefunction

$$\psi(\mathbf{r}, t) = \frac{1}{R^{\frac{3}{2}}(\tau)} \exp\left(\frac{i\dot{R}(\tau)}{2R(\tau)}q^2\right) \varphi(\mathbf{q}, \tau) \quad \text{where } R^2(\tau) = \frac{dt}{d\tau}. \quad (56)$$

In a reference frame that rotates with frequency Ω we obtain a new Schrödinger equation

$$\left[-\frac{1}{2}\nabla_{\mathbf{q}}^2 + \frac{1}{2}\Omega^2q^2 + \Omega\hat{L}_y + R^2(\tau)V(\mathbf{q}, R(\tau))\right]\varphi(\mathbf{q}, \tau) = i\frac{\partial\varphi(\mathbf{q}, \tau)}{\partial\tau}. \quad (57)$$

A thorough introduction to the Solov'ev-Vinitsky transformation in ion-atom collisions can be found elsewhere [4]. Such an introduction is rather beyond the scope of this paper, but several remarkable features of the Solov'ev-Vinitsky transformation should be mentioned here.

(1) In the original physical coordinates $\{\mathbf{r}, t\}$ the nuclei move along a trajectory $\mathbf{R}(t)$, therefore the interaction between the electron and the nuclei depends on the direction of the vector $\mathbf{R}(t)$. In the Solov'ev-Vinitsky space $\{\mathbf{q}, \tau\}$, the nuclei no longer move either in a radial or in an angular sense; they are fixed at the distance of 1 au from each other on the q_z -axis. Consequently, the potential in the transformed coordinates no longer depends on the direction of $\mathbf{R}(t)$. The dynamical effects are described by the scalar function $R(\tau)$ and two additional terms in the new Hamiltonian: a simple harmonic-oscillator term and an angular-momentum operator. The fact that nuclei do not move in the new representation leads to the following very important property.

(2) If v is the relative velocity of the collision, b , impact parameter, and $vt \gg b$, then functions $\varphi(\mathbf{q}, \tau)$ are Galilean invariant under translations in the plane of v and \mathbf{R} , therefore *there is no need for translation factors*, i.e. phase factors that are required to write $\psi(\mathbf{r}, t)$ in frames moving relative to a particular reference frame.

(3) For straight-line trajectories the frequency Ω does not depend on τ , and

(4) for Coulomb potentials one has effectively $R^2(\tau)V(\mathbf{q}, R(\tau)) = R(\tau)V(\mathbf{q})$ so that, in some cases, all dependence on τ in equation (57) comes from the factor $R(\tau)$ multiplying the potential. A similar statement can be made for zero-range potentials (ZRP): the parameter of a ZRP is changed according to $\alpha \rightarrow \alpha R(\tau)$ in scaled coordinates $\mathbf{q} = \mathbf{r}/R(t)$ (equations (58) and (59) below) and, in some cases, all dependence on τ comes from the multiplicative factor $R(\tau)$ in the boundary conditions.

The last property simplifies the Schrödinger equation and suggests the use of Sturmian eigenfunctions where the coefficient of $V(\mathbf{q})$ is an eigenvalue. The Galilean invariance of $\varphi(\mathbf{q}, \tau)$ means that basis functions do not have to be modified in an *ad hoc* way by attaching the translation factors, and that they are therefore orthogonal.

3.2. Adiabatic and Sturmian solutions for zero-range potentials

A ZRP with an eigenenergy $\varepsilon_\alpha = -\alpha^2/2$ is equivalent to $V = 0$ in equation (53) and the following boundary condition [6]

$$\psi(\mathbf{r}, t)|_{r_j \rightarrow 0} = N_\psi(t) \left(\frac{1}{r_j} - \alpha\right) \quad (58)$$

where $r_j = |\mathbf{r} - \mathbf{r}_{j0}|$, and \mathbf{r}_{j0} is the ZRP's position. Systems of several ZRPs can be considered, and we attach an additional index j to distinguish between positions of different ZRPs. A coefficient $N_\psi(t)$ in (58) might depend on t , but not on \mathbf{r} .

In scaled coordinates $\mathbf{q} = \mathbf{r}/R(t)$, boundary conditions equation (58) become

$$\varphi(\mathbf{q}, \tau)|_{q_j \rightarrow 0} = N_\varphi(\tau) \left(\frac{1}{q_j} - \alpha R(\tau)\right) \quad (59)$$

where $N_\varphi(\tau)$ does not depend on \mathbf{q} .

To solve the time-dependent problem equation (57) one can expand the solution over adiabatic or Sturmian functions. In the next section, both basis sets for ZRPs are found in closed form in terms of the oscillator Green functions with rotation. For simplicity we consider two identical ZRPs.

3.2.1. Adiabatic basis for two ZRPs. The adiabatic functions $\Phi_n(\mathbf{q}; R)$ (R is a parameter) satisfy the equation

$$[-\frac{1}{2}\nabla_{\mathbf{q}}^2 + \frac{1}{2}\Omega^2 q^2 + \Omega\hat{L}_y]\Phi_n(\mathbf{q}; R) = E_n(R)\Phi_n(\mathbf{q}; R) \quad (60)$$

with the boundary conditions

$$\Phi_n(\mathbf{q}; R)|_{q_{\pm} \rightarrow 0} = \text{constant} \times \left(\frac{1}{q_{\pm}} - \alpha R \right) \quad q_{\pm} = |\mathbf{q} \mp \hat{\mathbf{R}}/2| \quad (61)$$

and

$$\lim_{q \rightarrow \infty} \frac{1}{q\Phi_n(\mathbf{q}; R)} \frac{\partial(q\Phi_n(\mathbf{q}; R))}{\partial q} = -\sqrt{\Omega^2 q^2 - 2(E_n(R) + i\eta)}. \quad (62)$$

Since we work in scaled coordinates, the two ZRPs are located at $\pm\hat{\mathbf{R}}/2$ and the distance between them is unity. For simplicity of notation, we have introduced the eigenvalue $E_n(R)$ of the scaled equation which relates to the usual adiabatic eigenvalue $\varepsilon_n(R)$ according to $E_n(R) = \varepsilon_n(R)R^2$.

To find closed forms for the adiabatic states, we write the wave functions Φ_n in the form

$$\Phi_n(\mathbf{q}; R) = aG_{\text{rot}}^{y'=0}(\mathbf{q}, \hat{\mathbf{R}}/2, E_n^{\pm}(R)) + bG_{\text{rot}}^{y'=0}(\mathbf{q}, -\hat{\mathbf{R}}/2, E_n^{\pm}(R)). \quad (63)$$

The functions (63) satisfy equation (60), and have correct singularities at ZRP positions $\mathbf{q} = \pm\hat{\mathbf{R}}/2$. The boundary condition equation (62) is satisfied by virtue of the boundary condition equation (6) on the Green function. The coefficients a and b in equation (63) should be chosen so that the boundary conditions equation (61) are satisfied. Substituting equation (63) into equation (61) one obtains homogeneous algebraic equations with respect to a and b . Adiabatic energy values are defined by the requirement that these equations are self-consistent. The equation for the adiabatic energies $E_n(R)$ is then

$$G_r(E) \pm \sqrt{G_{\text{rot}}^{y'=0}(\hat{\mathbf{R}}/2, -\mathbf{R}/2, E)G_{\text{rot}}^{y'=0}(-\hat{\mathbf{R}}/2, \mathbf{R}/2, E)} = -\frac{\alpha R}{2\pi} \quad (64)$$

where $G_r(E)$ is the regularized Green function defined by equation (50).

Assuming that self-consistency condition equation (64) is satisfied, we find explicit expressions for adiabatic wavefunctions:

$$\Phi_n^{\pm}(\mathbf{q}; R) = N_a^{\pm}(G_{\text{rot}}^{y'=0}(\mathbf{q}, \hat{\mathbf{R}}/2, E_n^{\pm}(R)) \pm G_{\text{rot}}^{y'=0}(\mathbf{q}, -\hat{\mathbf{R}}/2, E_n^{\pm}(R))) \quad (65)$$

where N_a^{\pm} is a constant, and $G_{\text{rot}}^{y'=0}$ is given by equation (47).

The eigenvalue equation generally has an infinite number of solutions, giving an infinite set of adiabatic eigenfunctions. Using equations (47), (51) and (64) one easily finds that these functions have the proper behaviour near the ZRPs;

$$\Phi_n^{\pm}(\mathbf{q}; R)|_{q \rightarrow \pm\hat{\mathbf{R}}/2} = \frac{N_a^{\pm}}{2\pi} \left[\frac{1}{|\mathbf{q} \mp \hat{\mathbf{R}}/2|} - \alpha R \right] \quad (66)$$

which is equivalent to equation (61). The constants N_a^{\pm} for the adiabatic functions are defined by the usual normalization condition

$$\langle \Phi_n^{\pm}(R) | \Phi_n^{\pm}(R) \rangle = 1. \quad (67)$$

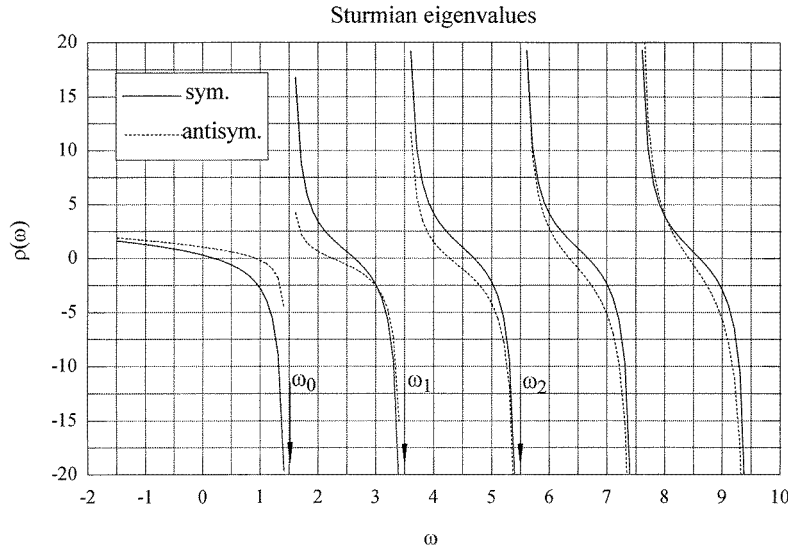


Figure 2. Sturmiian eigenvalues for two ZRPs plus oscillator in a rotating reference frame calculated by equation (71). The frequency of the oscillator and of the rotation is $\Omega = 1$. The ZRP parameters are $\alpha = 1$, $E_{ZRP} = -\alpha^2/2$. Poles of the eigenvalues $\omega_0, \omega_1, \omega_2 \dots$, are discussed in the text. Full curves, symmetric Sturmiian eigenvalues; broken curves, antisymmetric ones.

3.2.2. *Sturmiian basis for two ZRPs.* The Sturmiian functions $S(\mathbf{q}; \omega)$, where ω is a parameter, satisfy the equation

$$\left[-\frac{1}{2}\nabla_{\mathbf{q}}^2 + \frac{1}{2}\Omega^2 q^2 + \Omega \hat{L}_y\right]S(\mathbf{q}; \omega) = \omega S(\mathbf{q}; \omega) \tag{68}$$

with the boundary conditions

$$S(\mathbf{q}; \omega)|_{q_{\pm} \rightarrow 0} = \text{constant} \times \left(\frac{1}{q_{\pm}} - \alpha\rho(\omega)\right) \tag{69}$$

and

$$\lim_{q \rightarrow \infty} \frac{1}{qS(\mathbf{q}; \omega)} \frac{\partial(qS(\mathbf{q}; \omega))}{\partial q} = -\sqrt{\Omega^2 q^2 - 2(\omega + i\eta)} \tag{70}$$

where $\rho(\omega)$ is the Sturmiian eigenvalue. The eigenvalues can be readily found from equation (64) by making substitutions $R \rightarrow \rho(\omega)$ and $E_n(R) \rightarrow \omega$:

$$\rho^{\pm}(\omega) = -\frac{1 \pm U(-\omega/\Omega, \sqrt{2\Omega}) + \sqrt{2\Omega}U'(-\omega/\Omega, 0)}{\alpha U(-\omega/\Omega, 0)}. \tag{71}$$

In contrast to the adiabatic case, there is only one Sturmiian eigenvalue $\rho^{\pm}(\omega)$ for each symmetry. It follows that the Sturmiian set for ZRPs is not complete, yet it is possible to write the exact solution of the time-dependent equation in terms of the two Sturmiian functions. The solution of the time-dependent equation is beyond the scope of this report, thus we will not demonstrate how exact solutions are written in terms of the Sturmiian functions.

The Sturmiian functions are written in closed form, similar to the adiabatic case

$$S^{\pm}(\mathbf{q}; \omega) = N_s^{\pm}(G_{\text{rot}}^{y'=0}(\mathbf{q}, \hat{\mathbf{R}}/2, \omega) \pm G_{\text{rot}}^{y'=0}(\mathbf{q}, -\hat{\mathbf{R}}/2, \omega)) \tag{72}$$

where N_s^{\pm} are some constants, and $G_{\text{rot}}^{y'=0}$ is given by equation (47).

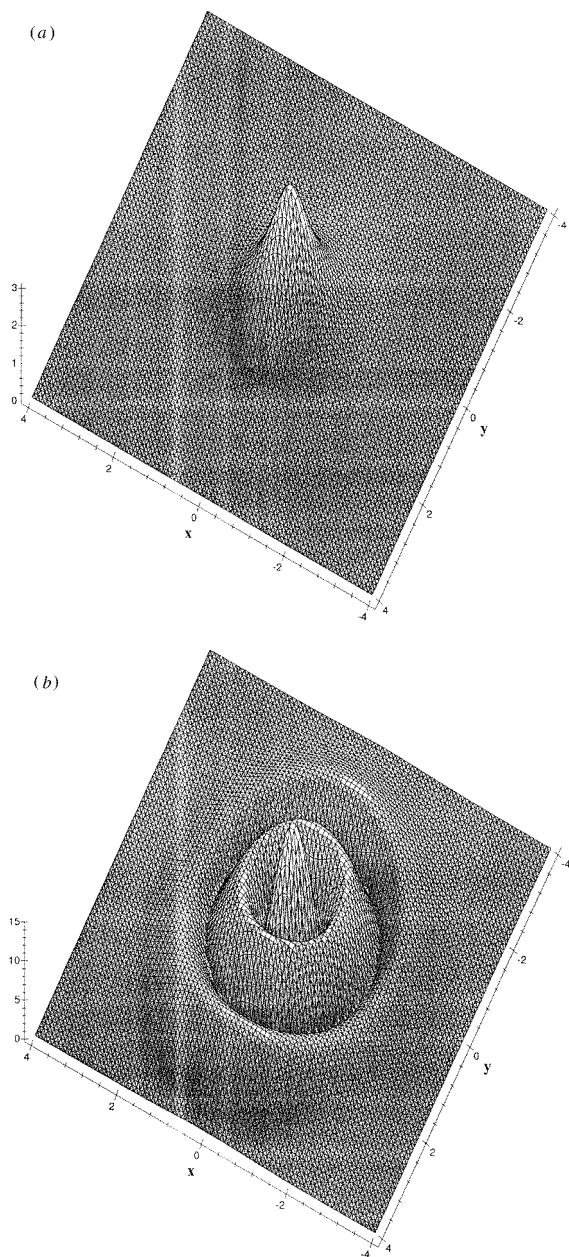


Figure 3. Moduli of the Sturmian functions given by equation (72) in the equatorial plane ($z = 0$) as functions of x and y . (a)–(c) show symmetric Sturmians for $\omega = -0.11, 5.11, 11.11$ respectively. (d)–(f) show antisymmetric Sturmians for the same values of ω .

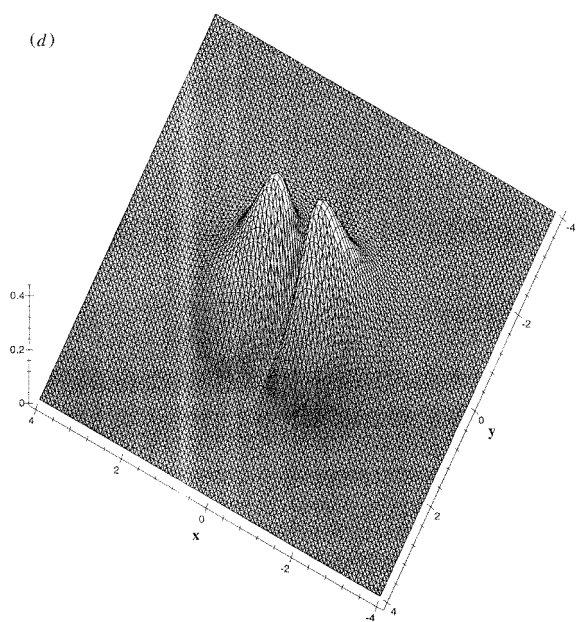
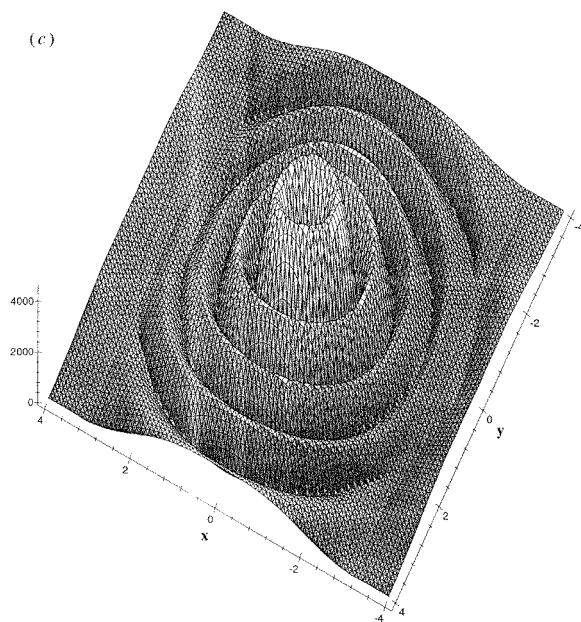
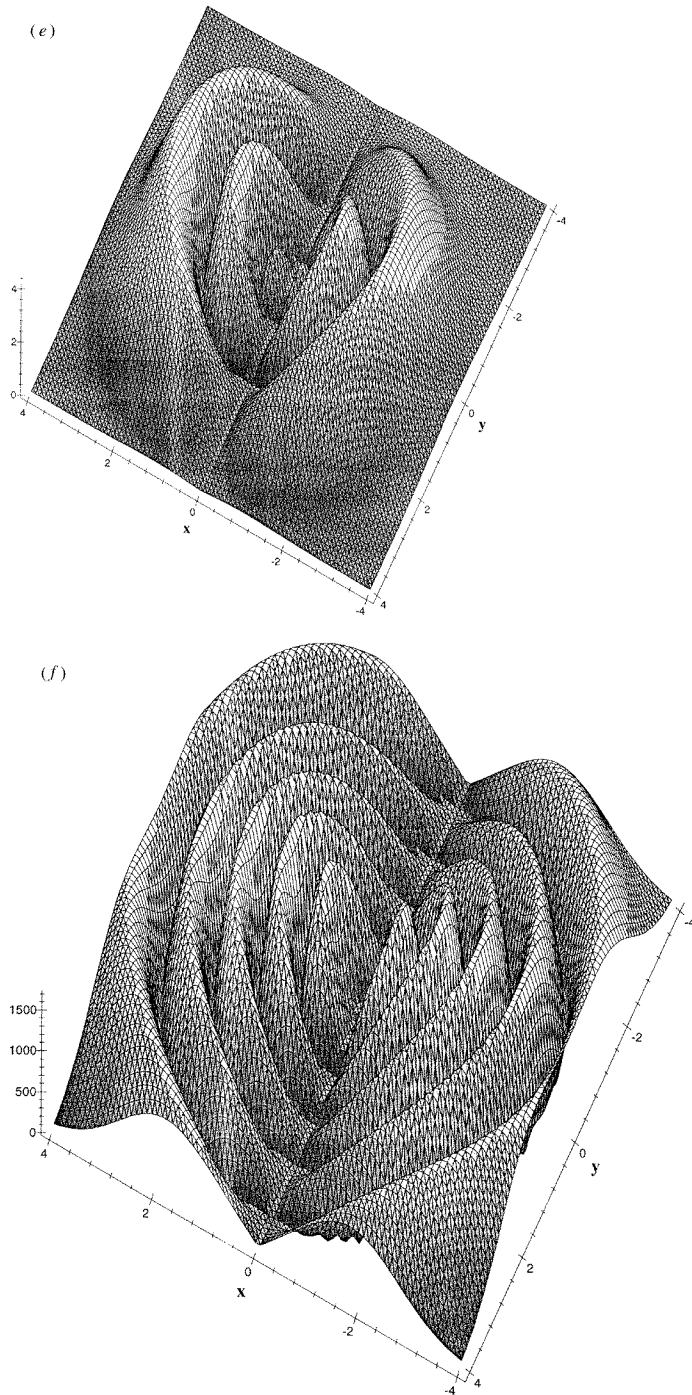


Figure 3. (Continued)

**Figure 3.** (Continued)

The Sturmians are better suited for solving the time-dependent problem equation (57) than the adiabatic functions, but, again, such solutions are beyond the scope of this manuscript. However, it is appropriate to consider properties of the Sturmians themselves (equation (72)), since they are not so commonly used in atomic physics as adiabatic functions equation (65).

First of all, it should be noted that there are only two Sturmian functions for this physical system: symmetric and antisymmetric. This should be compared with the adiabatic case where equation (64) has infinitely many solutions, thus generating infinitely many adiabatic functions. The symmetric and antisymmetric Sturmian eigenvalues equation (71) are plotted in figure 2 as functions of ω . One can see immediately that these eigenvalues have infinitely many poles. To understand the physical meaning of these poles, let us turn to figure 3, where moduli of the Sturmians equation (72) are plotted in the equatorial plane ($z = 0$) as functions of x and y for different values of ω . Note that for $\omega < \omega_0$, where ω_0 is the first pole of $\rho^\pm(\omega)$ equation (71), the symmetric Sturmian has no nodes, and the antisymmetric one has only one node (figures 3(a) and (d)). This topology of the Sturmian functions remains the same for all $\omega < \omega_0$. The topology changes, namely, another node is added, when $\omega_0 < \omega < \omega_1$, where ω_1 is the next pole of $\rho^\pm(\omega)$. Again, this new topology does not change until ω becomes greater than ω_1 . In general, every time ω increases and crosses a pole of $\rho^\pm(\omega)$ another node appears in the Sturmian functions. This situation is illustrated in figures 3(b) and (e), where the symmetric Sturmian exhibits two nodes, and the antisymmetric one has three nodes at $\omega = 5.11$.

The spatial extent of the Sturmian functions increases as ω becomes large and positive. Compare figures 3(a) and (d) at $\omega = -0.11$ with figures 3(c) and (f) at $\omega = 11.11$. It can be seen that at $\omega = -0.11$ the distribution is contained completely within a 2×2 square in the xy -plane, while at $\omega = 11.11$ it does not quite fit into a 4×4 square in the same coordinates. The spatial extent of the Sturmian functions becomes infinite as $\omega \rightarrow +\infty$. Thus, a single Sturmian function describes well both bound states and the continuum of the system. This property makes Sturmians especially useful for description of various ionization processes.

4. Conclusions

In this work we have derived analytic formulae for mathematical objects that are widely applicable in modern physics, namely nonrelativistic Green function for isotropic harmonic oscillators. Green functions in closed form often allow us to find exact analytical solutions to many nontrivial 3D problems of quantum mechanics. When exact solutions are not possible, closed forms for Green functions can be employed to build effective approximations with all partial waves taken into account explicitly. These properties make closed forms for Green functions very valuable in quantum physics. Unfortunately, very few 3D Green functions are known in closed forms: free particle, Coulomb field and electric field. We believe that our derivation of the harmonic-oscillator Green functions makes an important addition to that short list.

Our particular motivation was to find a suitable basis to solve time-dependent collisional problems. The requirement of Galilean invariance of the basis, insured in the Solov'ev-Vinitsky representation, leads to harmonic-oscillator potentials in the Schrödinger equation. Closed-form expressions for the adiabatic and Sturmian functions in 3D greatly simplifies the analysis of this equation. Such closed-form expressions have been obtained here using our expressions for the harmonic-oscillator Green function.

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