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The Green's Function for the Tridimensional Harmonic Oscillator

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A closed representations for the Green's function of the Schrödinger equation with a tridimensional isotropic harmonic oscillator potential is obtained by means of the Sturm-Liouville expansion method.

Calcula-se uma representação fechada da função de Green para a equação de Schrödinger com um potencial tipo oscilador harmônico isotrópico tridimensional usando-se o método de expansão de Sturm-Liouville.

1. INTRODUCTION

The present paper contains a derivation of the Green's function for the Schrödinger equation for tridimensional harmonic oscillator. Titchmarsh[1] calculated the Green's function for the one -dimensional harmonic oscillator by means of the Sturm-Liouville expansion. An integral representation for N-dimensional isotropic harmonic oscillator was calculated by Bellandi-Caetano Neto[2] using a spectral decomposition of the Green's functions in terms of the harmonic oscillator wave functions.

We calculate the tridimensional harmonic oscillator Green's function by means of the Sturm-Liouville expansion[3] in section 2,

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where we present a closed integral representation and in section 3 is showed how to obtain a closed representation in terms of the product of two Whittaker functions.

2. INTEGRAL REPRESENTATION

The Sturm-Liouville method[3] consists in writing the Green's function in terms of two linearly independent solutions of the corresponding homogeneous equation. Consider the Schrödinger equation

$$(H - E)\ \Psi(x) = 0$$

where

$$H = -\frac{\hbar^2}{2m}\ \frac{1}{f}\ \frac{d}{dx}\ (f\ \frac{d}{dx}) + V(x)\ .$$

where f=1 in the one-dimensional case and $f = x^2$ for the radial equation. We shall assume that the boundary conditions are defined at the singular points of the potential $V(x)$ and we denote by $\Psi^a(x)$ a solution that is regular as $x \to a$ and by $\Psi^b(x)$ the solution that is regular as $x \to b$ $(a \lesssim x \lesssim b)$.

The Green's function that satisfies

$$(H - E)G(x,x';E) = -\frac{1}{\sqrt{f(x)f(x')}}\ \delta(x-x')$$

is given by

$$G(x,x'E) = -\frac{2m}{\hbar^2}\frac{1}{\Delta}\ \ \Psi^a(x_<)\Psi^b(x_>)\ \ ,$$

where $x_<$ and $x_>$ are the min (x,x') and max (x,x') respectively. The constant $\Delta = f(x)W[\Psi^a(x),\ \Psi^b(x)]$, where W is the Wronskian of the two solutions.

The Green's function of the Schrödinger equation for the tridimensional isotropic harmonic oscillator satisfies the following inhomogeneous differential equation

$$(-\frac{\hbar^2}{2m}\nabla^2 + \frac{kr^2}{2} - E)\ \ G(\vec{r},\vec{r}\,';E) = -\ \delta(\vec{r}-\vec{r}\,')\ . \tag{1}$$

To apply the Sturm-Liouville method, we shall firstly make a partial wave expansion for the Green's function

$$G(r,r'E) = \sum_{\ell=0}^{\infty} \frac{2\ell + 1}{4\pi} P_\ell(\cos\gamma)\, G_\ell(r,r';E) \qquad (2)$$

where $P_\ell(\cos\gamma)$ are the Legendre Polynomial, $\cos\gamma = (\vec{r}.\vec{r}')/rr'$ and $G_\ell(r,r';E)$ is the radial Green's function, that satisfies the following differential Equation.

$$\left[-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right) + \frac{kr^2}{2} - E + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}\right] G_\ell(r,r';E) = -\frac{1}{rr'}\,\delta(r-r')$$

(3)

Changing the variables to $z = (\frac{m\omega}{\hbar})^{1/2} r$, $\omega^2 = k/m$, $\lambda = E/\hbar\omega$ and defining

$$G_\ell(r,r';E) = \left(\frac{4\omega m^3}{\hbar^5}\right)^{1/2} g_\ell(z,z';\lambda)$$

in Eq.3 we get

$$\left[\frac{d^2}{dz^2} + \frac{2}{z}\frac{d}{dz} - z^2 + 2\lambda - \frac{\ell(\ell+1)}{z^2}\right] g_\ell(z,z';\lambda) = \frac{1}{zz'}\,\delta(z-z') .$$

(4)

The solution of this equation calculated by means of the Sturm-Liouville expansion is

$$G_\ell(r,r';E) = \frac{(rr')^{-3/2}}{\hbar\omega}\,\Gamma\left(\frac{2\ell+3-2\lambda}{4}\right) M_{\lambda/2;\frac{2\ell+1}{4}}\left(\frac{m\omega}{\hbar} r_<^2\right) W_{\lambda/2;\frac{2\ell+1}{4}}\left(\frac{m\omega}{\hbar} r_>^2\right)$$

(5)

where M and W are the Whittaker functions, M is regular as $r \to 0$ and W is regular as $r \to \infty$; $r_<(r_>)$ is min (r,r') (max (r,r')).

The sum in Eq. 2 can be performed if we use an integral representation for the product of the Whittaker functions[4]

$$M_{\lambda/2;\frac{2\ell+1}{4}}(\frac{m\omega}{\hbar}r^2)\ W_{\lambda/2;\frac{2\ell+1}{4}}(\frac{m\omega}{\hbar}r'^2) =$$

$$= \frac{m\omega}{\hbar}(rr')\ \frac{1}{\Gamma(\frac{2\ell+3-2\lambda}{4})}\int_0^\infty e^{-\frac{m\omega}{\hbar}\frac{r^2+r'^2}{2}\cosh v}\ I_{\ell+1/2}(\frac{m\omega}{\hbar}rr'\,\mathrm{sh}v)\coth^{\lambda}v/2dv \tag{6}$$

which $r' > r$ and Re $(\frac{2\ell+3-2\lambda}{4}) > 0$.

Where $I_{\ell+1/2}$ is the modified Bessel function, and the following Newman expansion for the Bessel function[5]

$$z^{\nu}e^{\alpha z} = 2^{\nu}\Gamma(\nu)\sum_{n=0}^{\infty}(\nu+n)\ C_n^{\nu}(\cos\alpha)I_{\nu+n}(z). \tag{7}$$

We obtain for the total Green's function

$$G(r,r;E) = (\frac{m\omega}{\pi\hbar})^{3/2}\frac{1}{\hbar\omega}\int_0^1 d\xi\ \xi^{-\lambda+1/2}(1-\xi^2)^{-3/2}\exp\left[-\frac{r^2+r'^2}{2}+\right.$$

$$\left.+\frac{2r.r'\xi-(r^2+r'^2)\ \xi^2}{1-\xi^2}\right] \tag{8}$$

where Re$(3/2-\lambda) \gtrsim 0$. In this equation we use the variables defined by $\cosh v = \frac{1+\xi^2}{1-\xi^2}$. This is exactly the expression obtained by Bellandi--Caetano Neto[2] using the generalized Mehler formula.

In order to compare the two methods we can use in Eq.5 the following addition theorem for the product of the Whittaker functions[5]

$$\Gamma(-\nu+\mu+\tfrac{1}{2})\ M_{\nu,\mu}(x)\ W_{\nu,\mu}(y) =$$

$$= -\sum_{n=0}^{\infty}\frac{1}{\nu-n-\mu-\frac{1}{2}}\ \frac{\Gamma(2\mu+n+1)}{n!}\ M_{n+\mu+1/2;\mu}(x)M_{n+\mu+1/2;\mu}(y) \tag{9}$$

and remember that the M Whittaker function is related to the Laguerre polynomials by the expression[4]

$$M(n + \frac{1+\mu}{2})_{\mu/2}(z) = \frac{n!}{\Gamma(1+n+\mu)} z^{\frac{1+\mu}{2}} e^{-z/2} L_n^{\mu}(z) \tag{10}$$

and then compare with the radial wave function of the tridimensional harmonic oscillator . We see that we can transform Eq.2 into

$$G(\vec{r},\vec{r}\,';E) = \sum_{n=0}^{\infty} \frac{1}{E_n - E} \Psi_n(\vec{r}) \Psi_n^*(\vec{r}\,') \tag{11}$$

which is the spectral decomposition used by Bellandi-Caetano Neto[2].

3. A CLOSED REPRESENTATION IN TERMS OF WHITTAKER'S FUNCTIONS

The total Green's function $G(\vec{r},\vec{r}\,';E)$ can be written in the following way

$$G(\vec{r},\vec{r}\,';E) = -\frac{m(rr')^{-1/2}}{\pi\hbar^2} \frac{1}{2\pi i} \int_{\infty}^{1^+} dy (y+1)^{\frac{\lambda}{2}-\frac{1}{2}} (y-1)^{-\frac{\lambda}{2}-\frac{1}{2}}$$

$$\exp(\frac{m\omega}{\hbar} \frac{r^2 + r'^2}{2} y) \, . \sum_{\ell=0}^{\infty} \frac{2\ell+1}{4} P_\ell(\cos\gamma) \Gamma(\frac{2\ell+3-2\lambda}{4})$$

$$\exp\left[i\pi (\frac{\lambda}{2} - \frac{\ell}{2} + \frac{1}{4})\right] \Gamma(\frac{\lambda}{2} - \frac{\ell}{2} + \frac{1}{4}) I_{\ell+1/2} (\frac{m\omega}{\hbar} rr' \sqrt{y^2-1}) \tag{12}$$

where the integration contour begins at $y = +\infty$, runs down the positive real axis to a point on the right at $y = +1$ circles the point $y = +1$ in the positive (counter clock-wise) sense, and returns along the positive real axis to $y = +\infty$. The angle of $(y \pm 1)$ are determined along the contour by continuity, their initial values at $y = +\infty$ being arc $(y \pm 1) = 0$.

We can perform the sum in Eq.12 using another Newman expansion[7] for the modified Bessel function

$$\left(\frac{1}{2}\,kz\right)^{\mu-\nu}\; I_\nu(kz)\Gamma(\nu+1) =$$

$$= k^\mu \sum_{n=0}^{\infty} (-1)^n\;(2n+\mu)\,\frac{\Gamma(\mu+n)}{\Gamma(n+1)}\;{}_2F_1\;(-n,n+\mu,\nu+1;k^2)\,I_{2n+\mu}(z) \tag{13}$$

and

$$P_{2n}(z) = \frac{\pi^{1/2}}{n!\,\Gamma(\frac{1}{2}-n)}\;{}_2F_1(-n,n+\frac{1}{2},\,\frac{1}{2}\,,z^2) \tag{14}$$

$$P_{2n+1}(z) = -\,\frac{2z\pi^{1/2}}{n!\,\Gamma(-\frac{1}{2}-n)}\;{}_2F_1\;(-n,n+\frac{3}{2},\frac{3}{2};z^2) \tag{15}$$

we get

$$G(\vec{r},\vec{r}\,';E) = -\,\frac{m(rr')^{-1/2}}{\pi\hbar^2}\,\frac{1}{2\pi i}\int_{\infty}^{1^+} dy\,(y+1)^{\frac{\lambda}{2}-\frac{1}{2}}\,(y-1)^{-\frac{\lambda}{2}-\frac{1}{2}}$$

$$\exp\left(-\,\frac{m\omega}{\hbar}\,\frac{r^2+r'^2}{2}\;y\right).S \tag{16}$$

where

$$S = \frac{\pi}{4}\exp\left(\frac{i\pi\lambda}{2}\right)\,x^{1/2}\;\beta\Big[\sin^{-1}\frac{\pi}{4}\,(2\lambda+1)\exp(i\pi/4)\;I_{-1/2}(x\beta)\;+$$

$$+\,\sin^{-1}\frac{\pi}{4}\,(2\lambda-1)\exp(-i\pi/4)\,I_{1/2}(x\beta)\Big]$$

with

$$x = \cos\gamma \quad\text{and}\quad \beta = \frac{m\omega}{\hbar}\,rr'\,\sqrt{y^2-1}\;\;.$$

Using for the modified Bessel function the relation[7]

$$\sqrt{x}\,\beta I_{\mp}(x\beta) = \frac{d}{dx}\left[\sqrt{x}\;I_{\pm 1/2}\;(x\beta)\right] \tag{17}$$

we can writte

$$G(\vec{r},\vec{r}\,',E) = \frac{1}{4\pi\hbar\omega}\frac{d}{d(\xi\xi')}\left[\frac{1}{\sqrt{\xi\xi'}}\Gamma(\tfrac{3}{4}-\tfrac{\lambda}{2})\, M_{\frac{\lambda}{2},\frac{1}{4}}(\tfrac{m\omega}{\hbar}\xi^2)\, W_{\frac{\lambda}{2},\frac{1}{4}}(\tfrac{m\omega}{\hbar}\xi'^2) + \right.$$

$$\left. + \frac{1}{\sqrt{\xi\xi'}}\Gamma(\tfrac{1}{4}-\tfrac{\lambda}{2})\, M_{\frac{\lambda}{2}-\frac{1}{4}}(\tfrac{m\omega}{\hbar}\xi^2)\, W_{\frac{\lambda}{2}-\frac{1}{4}}(\tfrac{m\omega}{\hbar}\xi'^2)\right] \qquad (18)$$

where

$$2\xi = \sqrt{|\vec{r}+\vec{r}\,'|^2} - \sqrt{|\vec{r}\,'-\vec{r}|^2} \quad \text{and} \quad 2\xi' = \sqrt{|\vec{r}\,'+\vec{r}|^2} + \sqrt{|\vec{r}\,'-\vec{r}|^2} .$$

This expresses the total Green's function for the tridimensional isotropic harmonic oscillator in terms of the Whittaker functions.

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