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Numerical transforms from position to momentum space via Gaussian quadrature in the complex plane

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ABSTRACT

A method for the numerical evaluation of integrals involving Bessel functions of the first kind, via non-standard Gaussian quadrature, is appraised. This method uses specialized Gaussian quadratures based on weight functions which are modified Bessel functions of the third kind. We apply the method to calculate momentum space radial wave functions of the two-dimensional hydrogen atom and harmonic oscillator, via two-dimensional Fourier or Hankel transforms of the position space functions. Results show that the method performs best for the asymptotic or large p regions of the hydrogen atom. We also illustrate that accurate results can be obtained for the smaller argument regions with the use of higher-order quadratures. On the other hand, the method fails in its application to the harmonic oscillator. A discussion of the strengths and weaknesses of the method is presented.

1. Introduction

The task of numerically computing Bessel function integrals of the form,

$$I(\eta, \nu, p) = \int_0^\infty x^\eta h(x) J_\nu(px)\mathrm{d}x, \tag{1}$$

is of great interest in science and engineering, especially in fields where wave phenomena are common. The problem lies in the evaluation of Eq. (1) for slowly decaying functions at large values of the argument p, where the integrand oscillates rapidly [1–14]. These integrals are particular examples of the more general problem of the appropriate methodology for the numerical calculation of integrals involving integrands with highly oscillatory behavior [15–18].

Of particular interest among these applications is the two-dimensional Fourier transform of a function, $f(\mathbf{r}) = f(r,\phi)$, in polar coordinates, which can be written as a product of radial and angular parts $f(r,\phi) = f(r)e^{\imath m\phi}$. Its Fourier transform is given as [19–21]

$$\begin{aligned}\tilde{f}(\mathbf{p}) &= \frac{1}{2\pi}\int f(\mathbf{r})e^{\imath\mathbf{p}\cdot\mathbf{r}}d\mathbf{r}\\ &= \frac{1}{2\pi}\int_0^\infty\int_0^{2\pi} f(r)e^{\imath m\phi}e^{-\imath pr\cos(\phi-\phi_p)}rdrd\phi\end{aligned} \tag{2}$$

where ϕ_p is the angle between the resulting vector and the $\phi = 0$ axis. Substituting $\theta = \phi - \phi_p$, and using the periodicity of the integrand over the angular variable yields

$$\begin{aligned}\tilde{f}(\mathbf{p}) &= \imath^m e^{\imath m\phi_p}\int_0^\infty f(r)rdr\left[\int_0^{2\pi} e^{\imath m\theta}e^{\imath pr\cos\theta}d\theta\right]\\ &= \imath^m e^{\imath m\phi_p}\int_0^\infty f(r)J_m(pr)rdr.\end{aligned} \tag{3}$$

The parenthesis is the integral representation of the m-th order Bessel function with argument pr, multiplied by $2\pi\imath^m$. The last integral above is known as the m-th order Hankel transform of the radial function $f(r)$. Thus the two dimensional Fourier transform is related to the Hankel transform of the radial function.

Two dimensional Fourier transforms are necessary to transform two-dimensional wave functions from position space to momentum space. Momentum space perspectives offer a complementary avenue in the analysis of electronic systems [22].

The solutions to the two-dimensional Schrödinger equation in position space for the hydrogen atom [23–25] are

$$\Psi_{n,m}(r,\phi) = \frac{N_{n,m}}{\sqrt{2\pi}}(2p_0 r)^{|m|}e^{-p_0 r}L^{2|m|}_{n-|m|-1}(2p_0 r)e^{\imath m\phi}, \tag{4}$$

where $p_0 = \frac{2Z}{2n-1}$, $L^{2|m|}_{n-|m|-1}$ are the associated Laguerre polynomials, and the normalization constant is $N_{n,m} = 2p_0\left[\frac{(n-|m|-1)!}{2\pi(2n-1)[(n+|m|-1)!]^3}\right]^{1/2}$. Note that the m quantum number is not the same as that found

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in three dimensional systems. One can also find it referred to as l in the literature [23].

The momentum space representations are [25]

$$\widetilde{\Psi}_{n,m}(p,\phi_p) = \imath^m(-1)^{n-1}\frac{\sqrt{8}p_0^2}{(p_0^2+p^2)^{3/2}}Y_{n-1,m}(\theta,\phi_p). \tag{5}$$

The dependence on the θ variable in the spherical harmonics is given in terms of sines and cosines as [26]

$$\sin\theta = \frac{2p_0p}{(p_0^2+p^2)}, \quad \cos\theta = \frac{(p_0^2-p^2)}{(p_0^2+p^2)}. \tag{6}$$

Position space solutions of the harmonic oscillator are [27]

$$\Psi_{n,m}(r,\phi) = \frac{N_{n,m}}{\sqrt{2\pi}}r^m e^{-\frac{\lambda r^2}{2}}L_n^m(\lambda r^2)e^{\imath m\phi}, \tag{7}$$

with radial normalization constant $N_{n,m} = \left[\frac{2n!\lambda^{m+1}}{\Gamma(n+m+1)}\right]^{1/2}$. The wave function in the momentum space representation is [27]

$$\widetilde{\Psi}_{n,m}(p,\phi_p) = \frac{\widetilde{N}_{n,m}}{\sqrt{2\pi}}p^m e^{-\frac{p^2}{2\lambda}}L_n^m\left(\frac{p^2}{\lambda}\right)e^{\imath m\phi_p}, \tag{8}$$

where the normalization constant is $\widetilde{N}_{n,m} = \left[\frac{2n!\lambda^{-m-1}}{\Gamma(n+m+1)}\right]^{1/2}$.

Radial position and momentum space wave functions of the hydrogen atom and harmonic oscillator are tabulated in Tables 1 and 2. The radial functions in momentum space are related to the position space ones by

$$\widetilde{R}_{n,m}(p) = \imath^m\int_0^\infty R_{n,m}(r)J_\nu(pr)rdr. \tag{9}$$

Closed form solutions to these integrals are available [9]. The analytical representations of the momentum space functions can be used to test numerical procedures for obtaining the transforms of the position space functions.

2. Quadratures with Bessel weight functions

In the numerical evaluation of the integral in Eq. (1), one could think of using a composite Gauss-Legendre quadrature, transformed to consider the intervals between the nodes of the integrand. However, the convergence would be slow depending on the value of p. Another option is developing and applying a specialized Gaussian quadrature with weight function $J_\nu(t)$ $(t = px)$ over the interval $[0,\infty]$. The problem with this is that the usual route to Gaussian quadrature, via the associated orthogonal polynomials and their three-term recurrence relationship [28], is not obvious since the weight function of the orthogonal polynomial system normally obeys $w(t) \geqslant 0$ in the defined interval. $J_\nu(t)$ does not obey this requirement. Moreover, the higher-order moments of the weight function do not exist.

Another route lies in the formulation of the problem of obtaining abscissae and weights of the Gaussian quadrature as the solution to a system of non-linear equations. The moments of the auxiliary distribution, $\int_0^\infty t^{\beta+\eta}J_\nu(t)e^{-t}dt$, where the exponential factor has been added to force the convergence of the integrals, do exist. This problem is difficult since it implies finding the solution of a system of n non-linear equations in two variables. Furthermore, the vector containing the weights and abscissas can be complex-valued [29].

Another alternative into the complex plane lies in the use of integral representations of the Bessel function to formulate the problem as a double integral. Gauss-Laguerre and Gauss-Chebyshev quadratures can then be used, with the Gauss-Laguerre quadratures transformed into the complex plane [30]. Complex plane methods for the evaluation of integrals have been proposed and are of current interest in the literature [31–34].

The principal issue in developing Gaussian quadrature based on weight functions, $J_\nu(t)$, is that the Bessel functions can be negative-valued in the $[0,\infty]$ interval. Wong [35] was able to circumvent this problem by using a known expression of the Bessel functions of the first kind, $J_\nu(t)$, in terms of the Hankel functions

$$J_\nu(t) = \frac{1}{2}\left\{H_\nu^{(1)}(t) + H_\nu^{(2)}(t)\right\}. \tag{10}$$

In turn, the Hankel functions are defined in terms of $K_\nu(t)$, the modified Bessel functions of the third kind,

$$H_\nu^{(1)}(t) = \frac{2}{\pi\imath}e^{-\imath\pi\nu/2}K_\nu(-\imath t) \tag{11}$$

$$H_\nu^{(2)}(t) = -\frac{2}{\pi\imath}e^{\imath\pi\nu/2}K_\nu(\imath t). \tag{12}$$

The benefit is that the modified Bessel function of the third kind is non-negative in the $[0,\infty]$ interval, hence orthogonal polynomials and Gaussian quadrature can be constructed with $K_\nu(x)$ $[x = \pm\imath t]$ as the weight function. This leads to quadrature rules which are real-valued. $K_\nu(x)$ is also known as the modified Bessel function of the second kind.

Table 1
Radial wave functions for the hydrogen atom in two dimensions $R_{n,m}(r)$ with $Z = 1$ [25]. Radial momentum space wave functions are $\widetilde{R}_{n,m}(p)$.

n	m	$R_{n,m}(r)$	$\widetilde{R}_{n,m}(p)$
1	0	$2e^{-p_0r}p_0$	$\frac{4\sqrt{\frac{2}{\pi}}}{(4+p^2)^{3/2}}$
2	0	$\left[\frac{2}{\sqrt{3}}\right]e^{-p_0r}p_0(1-2p_0r)$	$\frac{12\sqrt{\frac{6}{\pi}}(9p^2-4)}{(4+9p^2)^{5/2}}$
2	±1	$\left[\frac{4}{\sqrt{6}}\right]e^{-p_0r}p_0^2r$	$-\frac{144\imath\sqrt{\frac{3}{\pi}}p}{(4+9p^2)^{5/2}}$
3	0	$\left[\frac{1}{\sqrt{5}}\right]e^{-p_0r}p_0(2-8p_0r+4p_0^2r^2)$	$\frac{20\sqrt{\frac{10}{\pi}}(16-400p^2+625p^4)}{(4+25p^2)^{7/2}}$
3	±1	$\left[\frac{4}{\sqrt{30}}\right]e^{-p_0r}p_0^2r(3-2p_0r)$	$-\frac{400\imath\sqrt{\frac{15}{\pi}}p(25p^2-4)}{(4+25p^2)^{7/2}}$
3	±2	$\left[\frac{8}{\sqrt{120}}\right]e^{-p_0r}p_0^3r^2$	$-\frac{4000\sqrt{\frac{15}{\pi}}}{(4+25p^2)^{7/2}}$
4	0	$\left[\frac{1}{3\sqrt{7}}\right]e^{-p_0r}p_0(6-36p_0r+36p_0^2r^2-8p_0^3r^3)$	$\frac{28\sqrt{\frac{14}{\pi}}(117649p^6-86436p^4+7056p^2-64)}{(4+49p^2)^{9/2}}$
4	±1	$\left[\frac{1}{\sqrt{21}}\right]e^{-p_0r}p_0^2r(12-16p_0r+4p_0^2r^2)$	$-\frac{748\imath\sqrt{\frac{42}{\pi}}p(16-588p^2+2401p^4)}{(4+49p^2)^{9/2}}$
4	±2	$\left[\frac{4}{\sqrt{210}}\right]e^{-p_0r}p_0^3r^2(5-2p_0r)$	$-\frac{10976\sqrt{\frac{105}{\pi}}p^2(49p^2-4)}{(4+49p^2)^{9/2}}$
4	±3	$\left[\frac{4}{3\sqrt{35}}\right]e^{-p_0r}p_0^4r^3$	$\frac{153664\imath\sqrt{\frac{70}{\pi}}p^3}{(4+49p^2)^{9/2}}$