On solving the Schrodinger equation with hypersingular kernel in momentum space

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Abstract

This paper shows that the Schrödinger equation in the momentum representation for a linear confining potential for states with zero orbital angular momentum can be solved with high accuracy (far superior to other methods) using the special quadrature formulas for hypersingular integral.

1 Methods of solution of integral equations

After partial decomposition Schrödinger equation in the momentum space for centrally symmetric potentials, takes the form:

$$\frac{k^2}{2\mu}\phi_\ell(k) + \int\limits_0^\infty V_\ell(k,k')\phi_\ell(k')k'^2\mathrm{d}k' = E\phi_\ell(k)\ , \tag{1}$$

where $\mu = m_1 m_2/(m_1+m_2)$ is the reduced mass; m_1, m_2 are mass of the constituents of a bound system; $\mathbf{k}$ is the momentum of the relative motion ($|\mathbf{k}| = k$); $\phi_\ell(k)$ is the radial part of the Fourier transform of the wave function in the coordinate representation; $V_\ell(k,k')$ is the operator ℓ -th component of the partial decomposition of the interaction potential; E is binding energy.

However, the description of bound states in the momentum representation is complicated by necessity of solving the integral equation (1), containing singular terms. So for a linear confining potential $V(r) = \sigma r$ we have that

$$V_\ell(k,k') = \frac{\sigma}{\pi(kk')^2}Q'_\ell\left(\frac{k^2+k'^2}{2kk'}\right)\ . \tag{2}$$

where function $Q_\ell(y)$ is Legendre polynomial of 2nd kind. Since the function Q'_ℓ hypersingular if $k = k'$, then the potential $V_\ell(k,k')$ is also hypersingular. Standard methods of numerical solution of the equation (1) with the potential (2) gives relatively low accuracy of [1, 2]. The numerical solution of the integral equation (1) can be reduced to a problem on the eigenvalues, which arises when using quadrature formulas for the integrals in the equation.

As a result, the integral equation of the form (1) can be reduced to the problem

$$\sum_{j=1}^{N} H\left(k_i,k_j\right)\phi(k_j) = \sum_{j=1}^{N} H_{ij}\phi(k_j) = E\phi(k_i)\ , \tag{3}$$

where to obtain the eigenvalues and vectors need to know the elements of H_{ij}. And if $i \neq j$, the problem of calculating the elements H_{ij} for a linear confining potential is not complex, then the $i = j$ $(k = k')$ directly to do this is not possible, due to the presence of singularities.

2 Quadrature formulas for singular integrals

Receive quadrature formula for the integral

$$I(z) = \int_{-1}^{1} F(t) w(t) g(t, z)\, \mathrm{d}t \tag{4}$$

where $g(t, z)$ is function is singular at $t = z$. The functions $F(t)$ and $w(t)$ is part of the kernel that does not contain the singularities for all $-1 < t, z < 1$.

For this the function $F(t)$ in (4) with the help of interpolation polynomial

$$G_i(t) = \frac{P_N^{(\alpha,\beta)}(t)}{(t - \xi_{i,N})\, P_N'^{(\alpha,\beta)}(\xi_{i,N})} \tag{5}$$

replaced the expansion

$$F(t) \approx \sum_{i,=1}^{N} G_i(t)\, F(\xi_{i,N}) \ , \tag{6}$$

where $\xi_{i,N}$ are the roots of the Jacobi polynomial

$$P_N^{(\alpha,\beta)}(\xi_{i,N}) = 0 \quad (i = 1, 2, \ldots, N) \ . \tag{7}$$

Substituting the expansion (6) in a ratio of $I(z)$ we find that the quadrature formula for the integral takes the form

$$I(z) \approx \sum_{i=1}^{N} \omega_i(z)\, F(\xi_{i,N}) \ , \tag{8}$$

where

$$\omega_i(z) = \frac{1}{P_N'^{(\alpha,\beta)}(\xi_{i,N})} \int_{-1}^{1} g(t, z)\, w(t)\, \frac{P_N^{(\alpha,\beta)}(t)}{t - \xi_{i,N}} \mathrm{d}t \ . \tag{9}$$

Thus the calculation of (9) will help you find the weight coefficients for the quadrature formula (4), the singular values.

3 The analytical form of weighting factors

Consider the possibility of analytical calculation of the weighting factors for different types of singularities that is, depending on the function $g(t, z)$.

3.1 The singular Cauchy integral

The most famous option (4) in the literature is the Cauchy integral

$$g(t, z) = \frac{1}{t - z} \ , \quad -1 < z < 1 \ .$$

For this case, there are a large number of works (see for examples [3, 4, 5]), which offered various options for quadrature formulas. In this case, you can get a formula for the weighting factors (9) direct calculation of the integral

$$\omega_i^C(z) = \int_{-1}^{1} \frac{w(t)}{P_N'^{(\alpha,\beta)}(\xi_{i,N})} \frac{P_N^{(\alpha,\beta)}(t)}{(t - \xi_{i,N})(t - z)} \mathrm{d}t \ . \tag{10}$$

With the help of identity

$$\frac{1}{(t-\xi_{i,N})\,(t-z)}=\frac{1}{z-\xi_{i,N}}\left[\frac{1}{t-z}-\frac{1}{t-\xi_{i,N}}\right] \tag{11}$$

coefficients (10)reducible to the form

$$\omega_i^C\,(z)=\begin{cases}\dfrac{1}{P_N'^{(\alpha,\beta)}\,(\xi_{i,N})}\dfrac{\Pi_N^{(\alpha,\beta)}\,(z)-\Pi_N^{(\alpha,\beta)}\,(\xi_{i,N})}{(z-\xi_{i,N})}\ , & \text{if } z\neq\xi_{i,N}\ ,\\ \dfrac{\Pi_N'^{(\alpha,\beta)}\,(\xi_{i,N})}{P_N'^{(\alpha,\beta)}\,(\xi_{i,N})}\ , & \text{if } z=\xi_{i,N}\end{cases}\ , \tag{12}$$

where

$$\Pi_n^{(\alpha,\beta)}\,(z)=\int\limits_{-1}^{1}w(t)\frac{P_n^{(\alpha,\beta)}\,(t)}{(t-z)}\mathrm{d}t\ . \tag{13}$$

To calculate the coefficients of $\omega_i^C\,(z)$ with a high degree of accuracy to be calculated analytically integral (13) for a variety of functions $w(t)$.

The most famous variant is the version of the function $w(t)$ is weight function of the Jacobi polynomial $P_n^{(\alpha,\beta)}\,(t)$ that is

$$w(t)=w^{(\alpha,\beta)}\,(t)\equiv(1-t)^{\alpha}\,(1+t)^{\beta}\ .$$

Then the integral (13) have the form

$$\Pi_n^{(\alpha,\beta)}\,(z)=\mathcal{Q}_n^{(\alpha,\beta)}\,(z)\ ,$$

where

$$\mathcal{Q}_n^{(\alpha,\beta)}\,(z)=\int\limits_{-1}^{1}(1-t)^{\alpha}\,(1+t)^{\beta}\,\frac{P_n^{(\alpha,\beta)}\,(t)}{(t-z)}\,\mathrm{d}t\ . \tag{14}$$

In the most general case for arbitrary α and β, the function $\mathcal{Q}_n^{(\alpha,\beta)}\,(z)$ connected with the Jacobi polynomials of the second kind $Q_n^{(\alpha,\beta)}\,(z)$ ratio

$$\mathcal{Q}_n^{(\alpha,\beta)}\,(z)=(-2)\,(z-1)^{\alpha}\,(z+1)^{\beta}\,Q_n^{(\alpha,\beta)}\,(z)\ , \tag{15}$$

where

$$Q_n^{(\alpha,\beta)}\,(z)=2^{\alpha+\beta+n}\,\frac{\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{\Gamma(2n+\alpha+\beta+2)}\times$$
$$\times(z+1)^{-\beta}(z-1)^{-\alpha-n-1}\,{}_2F_1\left(n+1,n+\alpha+1;2n+\alpha+\beta+2;\frac{2}{1-z}\right)\ .$$

3.2 Hypersingular variant

Consider hypersingular variant the integral (9), when the function is $g(t,z)=1/(t-z)^2$. The concept of the final calculation of the integrals of this type was first introduced by Hadamard (J. Hadamard, Lectures he Cauchy's Problem in Linear Partial Differential Equations, Yale University Press (1923).) and developed in the papers [6, 7, 8].

The final part hypersingular integral can be written as

$$\oint_{-1}^{1} \frac{f(t)}{(t-z)^2}\,\mathrm{d}t = \frac{\mathrm{d}}{\mathrm{d}z}\left[\int_{-1}^{1} \frac{f(t)}{t-z}\,\mathrm{d}t\right] \;,\quad -1 < z < 1\,. \tag{16}$$

Therefore, the weighting coefficients of the quadrature formula

$$\int_{-1}^{1} \frac{f(t)}{(t-z)^2}\,\mathrm{d}t = \sum_{i=1}^{N} \omega_i^H(z)\, f(\xi_{i,N}) \tag{17}$$

are related with coefficients (ref fz3) ratio

$$\omega_i^H(z) = \frac{\mathrm{d}}{\mathrm{d}z}\left[\omega_i^C(z)\right]\;. \tag{18}$$

Then the weights for the integral (4) function $g(t,z) = 1/(t-z)^2$ can be calculated by formulas

$$\omega_i^H(z) = \begin{cases} \dfrac{1}{P_N'^{(\alpha,\beta)}(\xi_{i,N})}\left\{\dfrac{\Pi_N'^{(\alpha,\beta)}(z)}{(z-\xi_{i,N})} - \dfrac{\Pi_N^{(\alpha,\beta)}(z) - \Pi_N^{(\alpha,\beta)}(\xi_{i,N})}{(z-\xi_{i,N})^2}\right\}\;, & \text{if } z \neq \xi_{i,N}\;, \\ \dfrac{\Pi_N''^{(\alpha,\beta)}(\xi_{i,N})}{2P_N'^{(\alpha,\beta)}(\xi_{i,N})}\;, & \text{if } z = \xi_{i,N}\;. \end{cases} \tag{19}$$

For the Cauchy integral ($g(t,z) = 1/(t-z)$) with $\alpha = -\beta = -1/2$, we have

$$\Pi_n^{(-1/2,1/2)}(z) = \int_{-1}^{1} \sqrt{\frac{1+t}{1-t}}\,\frac{V_n(t)}{(t-z)}\mathrm{d}t = \pi W_n(z)\;, \tag{20}$$

where $V_n(z)$ and $W_n(z)$ are Chebyshev polynomials 3 and 4 of kind, respectively (see [9]).

Then the quadrature formula for the Cauchy integral is of the form:

$$\int_{-1}^{1} \sqrt{\frac{1+t}{1-t}}\,\frac{f(t)}{(t-z)}\mathrm{d}t \approx \sum_{i=1}^{N} \omega_i^C(z)\, f(\xi_{i,N})\;, \tag{21}$$

where

$$\omega_i^C(z) = \begin{cases} \dfrac{\pi}{V_N'(\xi_{i,N})}\,\dfrac{W_N(z) - W_N(\xi_{i,N})}{(z-\xi_{i,N})}\;, & \text{if } z \neq \xi_{i,N}\;, \\ \pi\,\dfrac{W_N'(\xi_{i,N})}{V_N'(\xi_{i,N})}\;, & \text{if } z = \xi_{i,N} \end{cases}\;. \tag{22}$$

Quadrature formula for hypersingular integral has the form:

$$\int_{-1}^{1} \sqrt{\frac{1+t}{1-t}}\,\frac{f(t)}{(t-z)^2}\mathrm{d}t \approx \sum_{i=1}^{N} \omega_i^H(z)\, f(\xi_{i,N})\;, \tag{23}$$

where

$$\omega_i^H(z) = \begin{cases} \dfrac{\pi}{V_N'(\xi_{i,N})}\left\{\dfrac{W_N'(z)}{(z-\xi_{i,N})} - \dfrac{W_N(z) - W_N(\xi_{i,N})}{(z-\xi_{i,N})^2}\right\}\;, & \text{if } z \neq \xi_{i,N}\;, \\ \dfrac{\pi}{2}\,\dfrac{W_N''(\xi_{i,N})}{V_N'(\xi_{i,N})}\;, & \text{if } z = \xi_{i,N}\;. \end{cases} \tag{24}$$

Formula (24) to calculate weight coefficients allows to them with high accuracy and hence can be used to solve the Schrödinger equation with a linear confining potential in momentum space.

4 The calculation of the energy spectrum for a linear confining potential with $\ell = 0$

The Schrödinger equation with a linear confining potential

$$\frac{k^2}{2\mu}\phi_\ell(k) + \frac{\sigma}{\pi k^2}\int\limits_0^\infty Q'_\ell(y)\,\phi_\ell(k')\mathrm{d}k' = E\phi_\ell(k)\ ,\ \ y = \frac{k^2 + {k'}^2}{2kk'}\ , \tag{25}$$

reducible to the form

$$\tilde{k}^2\,\phi_\ell(\tilde{k}) + \frac{1}{\pi\,\tilde{k}^2}\int\limits_0^\infty Q'_\ell(y)\,\tilde{k}'\phi_\ell(\tilde{k}')\mathrm{d}\tilde{k}' = \varepsilon\,\phi_\ell(\tilde{k}) \tag{26}$$

with the help of replacements

$$k = \beta\tilde{k}\ ,\ \ E = \frac{\beta^2}{2\mu}\varepsilon\ ,\ \ \beta = (2\mu\sigma)^{1/3}\ . \tag{27}$$

Using the mapping

$$\tilde{k} = \beta_0\sqrt{\frac{1+z}{1-z}}\ ,\tilde{k}' = \beta_0\sqrt{\frac{1+t}{1-t}}\ , \tag{28}$$

we find that the equation (26) is transformed into

$$\frac{1}{\pi\beta_0}\left(\frac{1-z}{1+z}\right)\int\limits_{-1}^{1} Q'_\ell(y(t,z))\,\frac{\phi_\ell(t)\mathrm{d}t}{(1-t)\sqrt{1-t^2}} = \left(\varepsilon - \beta_0^2\frac{1+z}{1-z}\right)\phi_\ell(z)\ . \tag{29}$$

For the case of $\ell = 0$ the equation (29) after simplifications can be written as follows:

$$-\frac{1}{\pi\beta_0}\,(1-z)^2\int\limits_{-1}^{1}\phi_{\ell=0}(t)\sqrt{\frac{1+t}{1-t}}\,\frac{\mathrm{d}t}{(t-z)^2} = \left(\varepsilon - \beta_0^2\frac{1+z}{1-z}\right)\phi_{\ell=0}(z)\ . \tag{30}$$

Thus, for a linear confining potential we have hypersingular kernel $\sim 1/(t-z)^2$ and therefore for the numerical solution is necessary to use weighting factors(24).

Function $w(t)$ naturally chosen in the form

$$w(t) = \sqrt{\frac{1+t}{1-t}}\ .$$

As a result, the matrix for eigenvalue problems It takes the form:

$$H_{ij} = \left[\beta_0^2\,\delta_{ij}\,\left(\frac{1+\xi_{j,N}}{1-\xi_{j,N}}\right) - \frac{\omega_j^H\,(\xi_{i,N})}{\pi\,\beta_0}\,(1-\xi_{i,N})^2\right]\ , \tag{31}$$

where $z \to \xi_{i,N}$ and $t \to \xi_{j,N}$, $\xi_{i,N}$ are zeros of the polynomial $V_N(t)$ and matrix $\omega_j^H\,(\xi_{i,N})$ is calculated using the (24).

For a linear confining potential in the $\ell = 0$ is known that

$$\varepsilon = -z_n\ ,\ \ n = 1, 2, 3\ldots \tag{32}$$

where z_n are the zeros of the Airy function $Ai(z)$. Therefore, it is possible to compare the results of numerical calculations of the matrix (31) and accurate values (see, table 1)

Thus, the choice of weighting coefficients in which the singularity treated analytically and functions $w(t)$ associated with interpolating polynomials $P_N^{(\alpha,\beta)}(t)$ allows us to solve the equation (25) for $\ell = 0$ in momentum space with high accuracy.

The accuracy of calculations many orders of magnitude higher than similar calculations in momentum space [10, 11, 12, 13, 1]

Table 1: Relative error of δ of the solution of equation (31) ($\beta_0 = 0{,}9999$)

N	$n = 1$	$= 2$	$n = 3$	$n = 4$	$n = 5$
50	3×10^{-22}	4×10^{-20}	3×10^{-17}	3×10^{-15}	8×10^{-14}
80	5×10^{-33}	2×10^{-29}	1×10^{-26}	3×10^{-24}	4×10^{-22}
100	2×10^{-39}	1×10^{-35}	1×10^{-32}	4×10^{-31}	5×10^{-28}
150	4×10^{-54}	8×10^{-50}	5×10^{-47}	1×10^{-43}	6×10^{-42}

5 Conclusion

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