

High-precision methods for Coulomb, linear confinement and Cornell potentials in momentum space

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In Memory of Professor Nikolai Shumeiko

We use special quadrature formulas for singular and hypersingular integrals to numerically solve the Schrödinger equation in momentum space with the linear confinement potential, Coulomb and Cornell potentials. It is shown that the eigenvalues of the equation can be calculated with high accuracy, far exceeding other calculation methods.

In Memory of Professor Nikolai Shumeiko



**Professor Nikolai Maksimovich Shumeiko
(02.09.1942–15.06.2016).**

A numerical study of some relativistic QCD-motivated models is reduced to solving the problems in momentum space (for instance, Bethe–Salpeter equation [Bete:1951], spinless Salpeter equation [Salpeter:1952], CST model [Savkli:1999me], Poincaré-invariant quantum mechanics (or relativistic Hamiltonian dynamics) approach for description of bound states [Keister:1991] and others. Typically these equations are an integral equations and reduced to the Schrödinger equation in the nonrelativistic limit.

Advantages of using momentum representation for solving physics problems have long attracted the attention of researchers for a long time [Salpeter:1957, Eyre:1986]. In momentum space, in contrast to coordinate space, relativistic effects are much simpler. For example there is no need for additional constructions related to the definition of the relativistic kinetic energy operator $T(k)$.

The momentum space code has an additional advantage of being easily adaptable to relativistic equations. It is also relatively easy to obtain a relativistic interaction potential with the use of appropriate elastic scattering amplitudes [Lucha:1991], since the calculation is carried out initially in momentum space, which here arises naturally. In momentum space formulation is also flexible means of incorporating such dynamical effects as finite size of particles, vacuum polarization and so on.

However, the problem of using momentum space is aggravated by the fact that even the simplest interaction potentials in the momentum representation lead to integrals with singularities.

At present, there are many papers devoted to the solution of integral equations for bound states with singular kernels. So in the Refs. [Gammel:1973, Kwon:1978, Mainland:2001, Norbury:1994, Norbury:1994a, Maung:1993, J.Chen:2013] various methods of numerical solution of equations with a logarithmic singularity are developed.

Equations with linear confinement potentials containing a double-pole singularity are considered in Refs. [Eyre:1986, Spence:1993, Hersbach:1993, Norbury:1992, Tang:2001, Deloff:2006, J.Chen:2013-14, J.Chen:2012, Leitao:2014]. The subtraction technique (Landé-subtracted approach) that isolates the singularity in an integral that can be evaluated analytically is most often used.

Therefore, the accuracy of solutions for a number of problems with Coulomb and linear confining potentials was relatively low ($10^{-4} \div 10^{-6}$) [Norbury:1992, Norbury:1994, Tang:2001, Deloff:2006], though it is possible to reach a higher accuracy in coordinate space $\sim 10^{-11} \div 10^{-13}$ [Kang:2006].

The problem of accuracy in calculating characteristics of the bound quantum systems has more than just an academic nature. A high precise calculation of various energy corrections of the hydrogen-like systems is an relevant problem since the experimental measurements of such values are performed with high accuracy $\sim 10^{-13}$ [Udem:1997, Liu:1999].

Thus, when calculating characteristics of the bound quantum systems, one should allocate the problem of developing computational methods and the development of mathematical methods, which would allow one to simplify the calculation schemes and obtain results with a high degree of accuracy required for the experiment.

The most promising method to increase the accuracy of solution of integral equations of bound systems with singular kernels, is the method of quadratures, where the weight factors depend upon the location of the singularity.

The idea of inclusion of singularities into the weight factors is not new and it is actively used in the numerical calculations of singular integrals [Chan:2003, Bichi:2014, Z.Chen:2011, Sheshko:1976, et al.]. In [Deloff:2007], such an approach was used in solving Schrödinger equation with the Coulomb potential (logarithmic singularity), which allowed one to increase an accuracy of solution up to $\sim 10^{-13} \div 10^{-14}$.

The aim of this work is to develop methods for the precision calculation of energy spectra of the bound state equations in the momentum representation with Coulomb, linear confining, and Cornell potentials.

The Schrödinger equation for centrally symmetric potentials $\tilde{V}(|\mathbf{r}|) = \tilde{V}(r)$ after partial expansion can be written as follows:

$$\frac{k^2}{2\mu} \phi_{n\ell}(k) + \int_0^{\infty} V_{\ell}(k, k') \phi_{n\ell}(k') k'^2 dk' = E_{n\ell} \phi_{n\ell}(k), \quad k = |\mathbf{k}|, \quad (2.1)$$

where wave function $\phi_{n\ell}(k)$ is the radial part of $\phi(\mathbf{k})$ and $V_{\ell}(k, k')$ denotes the ℓ -th partial wave projection of the centrally symmetric potential

$$V_{\ell}(k, k') = \frac{2}{\pi} \int_0^{\infty} j_{\ell}(k' r) j_{\ell}(k r) \tilde{V}(r) r^2 dr, \quad (2.2)$$

where $j_{\ell}(x)$ is the spherical Bessel function.

The numerical solution of integral equation (2.1) will be turned into a finite matrix equation with help of the quadrature formulas for the integrals in this equation. At the first stage we make the transition from the semi-infinite interval of integration $(0, \infty[$ to the “standard” interval $[-1, 1]$ by means of the change of variables

$$\int_0^{\infty} f(k) dk = \int_{-1}^1 f(k(t)) \frac{dk}{dt} dt. \quad (2.3)$$

The function $k(t)$ satisfies the boundary conditions

$$k(t = -1) = 0, \quad k(t = 1) = \infty. \quad (2.4)$$

Among various possibilities, the following mappings of the domain $(0, \infty)$ onto $(-1, 1)$ are used more frequently [Bielefeld:1999, Savkli:1999me, Tang:2001, van Iersel:2000, Deloff:2006]:

$$k(t) = \beta_0 \frac{1+t}{1-t}, \quad (2.5)$$

$$k(t) = \beta_0 \sqrt{\frac{1+t}{1-t}}, \quad (2.6)$$

where β_0 is a numeric parameter. It can be used for the additional control of the convergence rate of numerical process.

The standard approach is based on the approximation of integral (2.3) by means of the quadrature formula

$$\int_0^{\infty} f(k) dk \approx \sum_{j=1}^N \tilde{\omega}_j f(k_j) , \quad (2.7)$$

where N is the number of abscissas and the $\tilde{\omega}_j$ are related to the tabulated ω_j weight factors for the interval $(-1, 1)$ by the relationship: $\tilde{\omega}_j = (dk/dt)_j \omega_j$.

As a result, the numerical solution of integral equation (2.1) can be reduced to the eigenvalue problem for the matrix H which arises when using the quadrature formulas of type (2.7) for the integrals:

$$\sum_{j=1}^N H(k_i, k_j) \phi(k_j) = \sum_{j=1}^N H_{ij} \phi_j = E^{(N)} \phi_i , \quad (2.8)$$

where $E^{(N)} \approx E_{nl}$ and the matrix-elements H_{ij} are given by:

$$H_{ij} = \frac{k_j^2}{2\mu} \delta_{i,j} + \tilde{\omega}_j k_j^2 V_l(k_i, k_j) . \quad (2.9)$$

However, the description of bound states in momentum space has a singular kernel for both the Coulomb and linear confinement potentials. Let us illustrate this statement.

The Coulomb potential $\tilde{V}(r) = -\frac{\alpha}{r}$ in momentum space has the form

$$V_{\ell}(k, k') = -\frac{\alpha Q_{\ell}(y)}{\pi(kk')}, \quad (2.10)$$

where the coupling parameter α is dimensionless.

Parameter y in (2.10) is the combination of momenta

$$y = \frac{k^2 + k'^2}{2kk'}, \quad (2.11)$$

and the $Q_\ell(y)$ is Legendre polynomial of the second kind:

$$Q_\ell(y) = P_\ell(y)Q_0(y) - w_{l-1}(y), \quad (2.12)$$

$$Q_0(y) = \frac{1}{2} \log \left| \frac{1+y}{1-y} \right|, \quad w_{l-1}(y) = \sum_{n=1}^l \frac{1}{n} P_{n-1}(y) P_{l-n}(y). \quad (2.13)$$

In Eq. (2.12) $P_\ell(y)$ is the Legendre polynomial of the first kind.

From (2.12) and (2.13) it follows that potential (2.10) has a logarithmic singularity in the case where $k = k' (y = 1)$.

The linear confinement potential $V(r) = \sigma r$ with parameter σ in momentum space is written in the form

$$V_\ell(k, k') = \frac{\sigma Q'_\ell(y)}{\pi(k k')^2}. \quad (2.14)$$

With the help of (2.12) and (2.13) we find that the derivative $Q'_\ell(y)$ in Eq. (2.14) is given by the relation

$$Q'_\ell(y) = P'_\ell(y)Q_0(y) + P_\ell(y)Q'_0(y) - w'_{l-1}(y), \quad (2.15)$$

$$Q'_0(y) = \frac{1}{1-y^2} = - \left(\frac{2kk'}{k'+k} \right)^2 \frac{1}{(k'-k)^2}. \quad (2.16)$$

As follows from (2.16), the function $Q'_\ell(y)$ is hypersingular in the case $k = k'$, and $V_\ell(k, k')$ consequently the potential itself is also hypersingular.

As follows from the above, the problem of calculating the elements (2.9) for the Coulomb and linear confinement potentials is not complex if $i \neq j$. However, for $i = j$ ($k = k'$) it is not possible to directly compute H_{ij} due to the presence of singularities.

To obtain the solution, the most frequently used method assumes the “reduction” of the singularity with the help of a counter term (the Landé subtraction method) [Kahana:1993, Norbury:1992, Hersbach:1993, Tang:2001, J.Chen:2012, Leitao:2014].

The maximum possible accuracy in solving the Schrödinger equation in momentum space reaches $\sim 10^{-6}$ for both Coulomb and linear potential, though in coordinate space one may reach a considerably higher accuracy $\sim 10^{-11} \div 10^{-13}$ [Kang:2006]. It is therefore necessary to find such methods of finding the eigenvalues that are comparable with the accuracy of solutions obtained in coordinate space.

In contrast to the Landé-subtracted approaches used in solving the Schrödinger equation, the main feature of the developed approach, which should increase the accuracy of solving Eq. with singular potentials, is the inclusion of singularities into the weight factors ω_i of the quadrature formula of type (2.7).

Furthermore, we consider the general calculation method of such weight factors using the interpolation polynomial

$$G_i(t) = \frac{P_N^{(\alpha,\beta)}(t)}{(t - \xi_{i,N}) P_N'^{(\alpha,\beta)}(\xi_{i,N})}, \quad (3.1)$$

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

$$P_N^{(\alpha,\beta)}(\xi_{i,N}) = 0 \quad (i = 1, 2, \dots, N). \quad (3.2)$$

Of all Jacobi polynomials $P_N^{(\alpha,\beta)}(z)$, it is better to take polynomials with $\alpha, \beta = \pm 1/2$. These polynomials $P_N^{(\pm 1/2, \pm 1/2)}(z)$ associated with Chebyshev polynomials. There are several kinds of Chebyshev polynomials. These include the Chebyshev polynomials of the first $T_n(x)$, second $U_n(x)$, third $V_n(x)$ and fourth $W_n(x)$ kinds [Mason:2002].

Let's introduce a function $K_n^{(\alpha,\beta)}(z)$ that generalizes the Chebyshev polynomials by defining

$$K_n^{(\alpha,\beta)}(z) = \begin{cases} T_n(z), & \alpha = \beta = -1/2, \\ U_n(z), & \alpha = \beta = 1/2, \\ V_n(z), & \alpha = -\beta = -1/2, \\ W_n(z), & \alpha = -\beta = 1/2. \end{cases} \quad (3.3)$$

For these polynomials, the convergence of quadratures is maximal relative to other Jacobi polynomials. Moreover, the zeroes of polynomials can be easily calculated (there are analytical expressions) and many integrals for the weight factors with singularities are given by relatively simple formulas [Kaya:1987, Golberg:1990, Mason:1999, Sheshko:1976].

Quadrature scheme

Let us find the quadrature formula for the integral

$$I(z) = \int_{-1}^1 F(t)w(t)g(t,z) dt \quad (4.1)$$

where $g(t,z)$ is the singular function at $t = z$ and $F(t), w(t)$ are the part of the kernel without singularities for all $-1 < t, z < 1$.

For this purpose, the function $F(t)$ in (4.1) is replaced by the following expression with the help of interpolation polynomial (3.1)

$$F(t) \approx \sum_{i=1}^N G_i(t) F(\xi_{i,N}), \quad (4.2)$$

where $\xi_{i,N}$ are the zeroes of Jacobi polynomial (see (3.2)).

Substituting expansion (4.2) into $I(z)$, the quadrature formula for the integral takes the form

$$I(z) \approx \sum_{i=1}^N \omega_i(z) F(\xi_{i,N}) \quad (4.3)$$

with

$$\omega_i(z) = \frac{\tilde{\omega}_N(z, \xi_{i,N})}{P_N^{(\alpha, \beta)}(\xi_{i,N})}, \quad (4.4)$$

where additional function are introduced to simplify the notation

$$\tilde{\omega}_j(z, \xi) = \int_{-1}^1 g(t, z) w(t) \frac{P_j^{(\alpha, \beta)}(t)}{t - \xi} dt. \quad (4.5)$$

The use of the Christoffel-Darboux formula for the Jacobi polynomials

$$\begin{aligned} & \sum_{m=0}^n \frac{1}{h_m} P_m^{(\alpha, \beta)}(x) P_m^{(\alpha, \beta)}(y) \\ &= \frac{k_n}{k_{n+1} h_n} \frac{P_{n+1}^{(\alpha, \beta)}(x) P_n^{(\alpha, \beta)}(y) - P_n^{(\alpha, \beta)}(x) P_{n+1}^{(\alpha, \beta)}(y)}{x - y}, \end{aligned} \quad (4.6)$$

where

$$\begin{aligned} k_m &= \frac{\Gamma(2m + \alpha + \beta + 1)}{2^m \Gamma(m + \alpha + \beta + 1) \Gamma(m + 1)}, \\ h_m &= \frac{2^{\alpha + \beta + 1} \Gamma(m + \alpha + 1) \Gamma(m + \beta + 1)}{(2m + \alpha + \beta + 1) \Gamma(m + 1) \Gamma(m + \alpha + \beta + 1)}. \end{aligned} \quad (4.7)$$

gives the result for the weight factor in the form

$$\omega_i(z) = \lambda_{i,N}^{(\alpha, \beta)} \sum_{m=0}^{N-1} \frac{1}{h_m} P_m^{(\alpha, \beta)}(\xi_{i,N}) J_m^{(\alpha, \beta)}(z). \quad (4.8)$$

The Christoffel symbols $\lambda_{m,N}^{(\alpha,\beta)}$ in (4.8) for the Jacobi polynomials are defined by the relation [G. Szegő:1993]

$$\begin{aligned} \lambda_{m,N}^{(\alpha,\beta)} &= \int_{-1}^1 \frac{w^{(\alpha,\beta)}(t) P_m^{(\alpha,\beta)}(t)}{P_N^{(\alpha,\beta)}(\xi_{i,N})(x - \xi_{i,N})} dt \\ &= \frac{2^{\alpha+\beta+1} \Gamma(N + \alpha + 1) \Gamma(N + \beta + 1)}{\Gamma(N + 1) \Gamma(N + \alpha + \beta + 1)} \\ &\quad \times \frac{1}{(1 - \xi_{i,N}^2) [P_N^{(\alpha,\beta)}(\xi_{i,N})]^2}, \end{aligned} \quad (4.9)$$

then the integral $J_m^{(\alpha,\beta)}(z)$ takes up the form

$$J_m^{(\alpha,\beta)}(z) = \int_{-1}^1 g(t, z) w(t) P_m^{(\alpha,\beta)}(t) dt. \quad (4.10)$$

The coefficient $\lambda_{i,N}^{(\alpha,\beta)}$ is the weight factor for the integral $I(z)$ without the singular function $g(t, z)$, i.e.

$$\int_{-1}^1 F(t) w^{(\alpha,\beta)}(t) dt \approx \sum_{i=1}^N \lambda_{i,N}^{(\alpha,\beta)} F(\xi_{i,N}), \quad (4.11)$$

where the function $w^{(\alpha,\beta)}(t)$ is a weight function of the Jacobi polynomial $P_N^{(\alpha,\beta)}(x)$

$$w^{(\alpha,\beta)}(t) = (1-t)^\alpha (1+t)^\beta, \quad \alpha, \beta > -1. \quad (4.12)$$

The important case of practical interest is that in which $w(t) = 1$ and we have

$$\int_{-1}^1 F(t) dt \approx \sum_{i=1}^N \omega_i^{\text{st}} F(\xi_{i,N}) \quad (4.13)$$

with the weights

$$\omega_i^{\text{st}} = \frac{1}{P_N^{(\alpha,\beta)}(\xi_{i,N})} \int_{-1}^1 \frac{P_i^{(\alpha,\beta)}(t)}{t - \xi_{i,N}} dt . \quad (4.14)$$

Using Eqs. (4.8) and (4.10) with $g(t, z) = w(t) = 1$ the weights in (4.14) read

$$\omega_i^{\text{st}} = \lambda_{i,N}^{(\alpha,\beta)} \sum_{m=0}^{N-1} \frac{1}{h_m} P_m^{(\alpha,\beta)}(\xi_{i,N}) J_m^{(\alpha,\beta)} , \quad (4.15)$$

where

$$J_m^{(\alpha,\beta)} = \frac{2}{m + \alpha + \beta} \left[\binom{m + \alpha}{m + 1} + (-1)^m \binom{m + \beta}{m + 1} \right] . \quad (4.16)$$

For example, when $\alpha = \beta = -1/2$ the relation (4.15) is transformed to the form [Deloff:2007]

$$\omega_i^{\text{st}} = -\frac{4}{N} \sum_{k=0}^{[(N-1)/2]} / \frac{T_{2k}(\xi_{i,N})}{4k^2 - 1}, \quad (4.17)$$

where the sign / indicate that the first term in the sum is divided by two. The $[n]$ symbol means that the integer part of the number n is taken.

Therefore, the calculation of (4.4) or (4.10) makes it possible to find the weight factors for quadrature formula (4.3) with singularities. One important fact is the calculation of the analytical expressions, since only in this case it is possible to increase the accuracy of calculations.

Analytical expressions of weights with a singularity

Consider the possibility of analytical calculation of the weights for various forms of singularities, i.e., depending on the form of the function $g(t, z)$.

Cauchy integral

The most known variant of (4.1) in the literature is the Cauchy integral (sign f)

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

There are many works for this case (see, for example [Golberg:1990, Sheshko:1976]), in which the different variants of quadrature formulas are proposed. Therefore, it is possible to obtain formulas for weight factors (4.4) by the direct calculation of the integral

$$\omega_N(z, \xi_{i,N}) = \frac{1}{P_N^{(\alpha,\beta)}(\xi_{i,N})} \int_{-1}^1 \frac{w(t) P_N^{(\alpha,\beta)}(t)}{(t - \xi_{i,N})(t - z)} dt. \quad (5.1)$$

The coefficients (5.1) reduce to the form

$$\omega_N(z, \xi_{i,N}) = \frac{1}{P_N'^{(\alpha,\beta)}(\xi_{i,N})} \begin{cases} \frac{\Pi_N^{(\alpha,\beta)}(z) - \Pi_N^{(\alpha,\beta)}(\xi_{i,N})}{(z - \xi_{i,N})} & , z \neq \xi_{i,N} , \\ \Pi_N'^{(\alpha,\beta)}(\xi_{i,N}) & , z = \xi_{i,N} , \end{cases} \quad (5.2)$$

where

$$\Pi_n^{(\alpha,\beta)}(z) = \int_{-1}^1 w(t) \frac{P_n^{(\alpha,\beta)}(t)}{(t-z)} dt . \quad (5.3)$$

For calculating coefficients

$$\omega_i(z) = \frac{\omega_N(z, \xi_{i,N})}{P_N'^{(\alpha,\beta)}(\xi_{i,N})} \quad (5.4)$$

with high degree of accuracy, it is necessary to evaluate integral (5.3) analytically for various forms of the function $w(t)$.

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

The most known representation of $w(t)$ is the form with the Jacobi polynomial weight function $P_n^{(\alpha,\beta)}(t)$; that is,

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

Then for integral (5.3) one obtains

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

where

$$\bar{Q}_n^{(\alpha,\beta)}(z) = \int_{-1}^1 (1-t)^\alpha (1+t)^\beta \frac{P_n^{(\alpha,\beta)}(t)}{(t-z)} dt . \quad (5.5)$$

In the most general case at arbitrary α and β , the function $\bar{Q}_n^{(\alpha,\beta)}(z)$ is related to the second order Jacobi polynomials $Q_n^{(\alpha,\beta)}(z)$ by the relationship

$$\bar{Q}_n^{(\alpha,\beta)}(z) = (-2)(z-1)^\alpha (z+1)^\beta Q_n^{(\alpha,\beta)}(z) , \quad (5.6)$$

where [Bateman:1953]

$$Q_n^{(\alpha, \beta)}(z) = 2^{\alpha + \beta + n} \frac{\Gamma(n + \alpha + 1)\Gamma(n + \beta + 1)}{\Gamma(2n + \alpha + \beta + 2)} (z + 1)^{-\beta} \\ \times (z - 1)^{-\alpha - n - 1} {}_2F_1\left(n + 1, n + \alpha + 1; 2n + \alpha + \beta + 2; \frac{2}{1 - z}\right). \quad (5.7)$$

$$w(t) = 1$$

Consider the integral (5.3), when $w(t) = 1$. This is the most economical and natural choice for practical calculations.

The subtraction procedure leads us to the relation

$$\begin{aligned} \Pi_n^{(\alpha,\beta)}(z) &= \mathcal{P}_N^{(\alpha,\beta)}(z) = \int_{-1}^1 \frac{P_N^{(\alpha,\beta)}(t)}{(t-z)} dt \\ &= \int_{-1}^1 \frac{P_N^{(\alpha,\beta)}(t) - P_N^{(\alpha,\beta)}(z)}{(t-z)} dt + P_N^{(\alpha,\beta)}(z) \log\left(\frac{1-z}{1+z}\right) \end{aligned} \quad (5.8)$$

Consider equation (5.8) when $\alpha = \beta = \pm 1/2$. We can received that

$$\begin{aligned} \mathcal{P}_N^{(\alpha,\beta)}(z) &= K_N^{(\alpha,\beta)}(z) \log\left(\frac{1-z}{1+z}\right) \\ &+ 4 \sum_{i=0}^{\lfloor \frac{N-1}{2} \rfloor} \frac{K_{N-2i-1}^{(\alpha,\beta)}(z)}{2i+1}, \quad (\alpha, \beta = \pm 1/2) \end{aligned} \quad (5.9)$$

to the form for all cases, except in the case $\alpha = \beta = -1/2$.

Hypersingular variant

Consider a hypersingular variant of integral (4.4), where $g(t, z) = 1/(t - z)^2$.

The concept of calculation of the finite part of hypersingular integral was first put forward by Hadamard (J. Hadamard, Lectures on Cauchy's Problem in Linear Partial Differential Equations, 1923) and developed in [Shia:1999, Kaya:1987, Kutt:1975, et al.]. The finite part of hypersingular integral marked by the sign \oint is related to the Cauchy integral by the equation [Kaya:1987]

$$\oint_{-1}^1 \frac{w(t)F(t)}{(t-z)^2} dt = \frac{d}{dz} \left[\int_{-1}^1 \frac{w(t)F(t)}{t-z} dt \right], \quad -1 < z < 1. \quad (5.10)$$

Useful in applications can be a subtraction, in which the hypersingular version of the equation (4.1) is expressed as

$$\oint_{-1}^1 \frac{F(t)w(t)}{(t-z)^2} dt = \int_{-1}^1 (F(t) - F(z)) \frac{w(t)}{(t-z)^2} dt + F(z) \oint_{-1}^1 \frac{w(t)}{(t-z)^2} dt. \quad (5.11)$$

Correspondingly, the weight factors of the quadrature formula

$$\oint_{-1}^1 \frac{w(t)F(t)}{(t-z)^2} dt = \sum_{i=1}^N \omega_i^H(z) F(\xi_{i,N}) \quad (5.12)$$

are related to coefficients (5.2) by the relation

$$\omega_i^H(z) = \frac{d}{dz} [\omega_i^C(z)] = \frac{1}{P_N^{(\alpha,\beta)}(\xi_{i,N})} \frac{d}{dz} [\tilde{\omega}_N^C(z, \xi_{i,N})] . \quad (5.13)$$

Then the weight factors of integral (5.12) can be calculated by the formulas [Andreev:2017]

$$\omega_i^H(z) = \frac{1}{P_N^{(\alpha,\beta)}(\xi_{i,N})} \begin{cases} \frac{\Pi_N^{(\alpha,\beta)}(z)}{(z-\xi_{i,N})} - \frac{\Pi_N^{(\alpha,\beta)}(z) - \Pi_N^{(\alpha,\beta)}(\xi_{i,N})}{(z-\xi_{i,N})^2} & , z \neq \xi_{i,N} \\ \frac{1}{2} \Pi_N^{\prime\prime(\alpha,\beta)}(\xi_{i,N}) & , z = \xi_{i,N} \end{cases} \quad (5.14)$$

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

For the Cauchy integral at $\alpha = -\beta = -1/2$, the quadrature formula for hypersingular integral has the form [Andreev:2017]

$$\oint_{-1}^1 \sqrt{\frac{1+t}{1-t}} \frac{F(t)}{(t-z)^2} dt \approx \sum_{i=1}^N \omega_i^{HV}(z) F(\xi_{i,N}), \quad (5.15)$$

where

$$\omega_i^{HV}(z) = \frac{\pi}{V_N'(\xi_{i,N})} \times \begin{cases} \frac{W_N'(z)}{(z - \xi_{i,N})} - \frac{W_N(z) - W_N(\xi_{i,N})}{(z - \xi_{i,N})^2} & , z \neq \xi_{i,N} , \\ \frac{1}{2} W_N''(\xi_{i,N}) & , z = \xi_{i,N} . \end{cases} \quad (5.16)$$

and function $V_n(z)$ and $W_n(z)$ are the Chebyshev polynomials of the third and fourth order, correspondingly [Mason:2002].

$$w(t) = \sqrt{1-t^2}$$

The quadrature formula for a hypersingular integral with weight function $w(t) = \sqrt{1-t^2}$ are readily determined in a similar way from the Eq. (5.15).

The appropriate quadrature, takes the form

$$\oint_{-1}^1 \frac{F(t)}{(t-z)^2 \sqrt{1-t^2}} dt \approx \sum_{i=1}^N \omega_i^{HT}(z) F(\xi_{i,N}), \quad (5.17)$$

where

$$\omega_i^{HT}(z) = \frac{\pi}{NU_{N-1}(\xi_{i,N})} \times \begin{cases} \frac{2C_{N-2}^{(2)}(z)}{(z-\xi_{i,N})} - \frac{U_{N-1}(z) - U_{N-1}(\xi_{i,N})}{(z-\xi_{i,N})^2} & , z \neq \xi_{i,N} , \\ 4C_{N-3}^{(3)}(\xi_{i,N}) & , z = \xi_{i,N} . \end{cases} \quad (5.18)$$

or

$$\omega_i^{HT}(z) = \frac{4\pi}{N} \sum_{k=2}^{N-1} \cos[(k-1/2)\pi/N] C_{k-2}^{(2)}(z), \quad (5.19)$$

where $C_n^{(\alpha)}(z)$ are Gegenbauer polynomials.

Special case

In practice, a quadrature formula with subtraction can be useful

$$\int_{-1}^1 \frac{F(t) - F(z)}{(t-z)^2} dt \approx \sum_{i=1}^N \omega_i^{HS}(z) F(\xi_{i,N}). \quad (5.20)$$

Using (4.8), we find a formula for calculating weight factor with the singularity $\omega_i^{HS}(z)$ in the form

$$\omega_i^{HS}(z) = \lambda_{i,N}^{(\alpha,\beta)} \sum_{m=0}^{N-1} \frac{1}{h_m} P_m^{(\alpha,\beta)}(\xi_{i,N}) J_m^H(z), \quad (5.21)$$

where

$$J_m^H(z) = \int_{-1}^1 \frac{P_m^{(\alpha,\beta)}(t) - P_m^{(\alpha,\beta)}(z)}{t-z} dt + P_m'^{(\alpha,\beta)}(z) \log\left(\frac{1-z}{1+z}\right). \quad (5.22)$$

This integral can be calculated in principle for arbitrary values of α and β . When solving physical problems, we can restrict ourselves to $\alpha, \beta = \pm 1/2$. Here we give the formula for the case $\alpha = \beta = -1/2$

$$\omega_i^{HS}(z) = \frac{2}{N} \sum_{m=1}^N {}' T_{m-1}(\xi_{i,N}) J_{m-1}^H(z), \quad (5.23)$$

where

$$J_m^H(z) = mU_{m-1}(z) \log\left(\frac{1-z}{1+z}\right) + 4 \sum_{j=0}^{b_m} \left(\frac{m}{2j+1} - 1\right) U_{m-2j-2}(z) c_j^m(b_m), \quad b_m = \left[\frac{m-1}{2}\right]. \quad (5.24)$$

the presence of a function $c_j^m(n)$ indicate that the last term in the sum is divided by two, if m is an odd number.

Eqs.(5.15), (5.16), (5.18) and (5.23) for the weight factors makes it possible to calculate them with high accuracy and, correspondingly, it can be used for solving the Schrödinger equation with linear potential in momentum space.

Logarithmic singularity

Let us consider weight coefficient (4.4) for polynomials $K_n^{(\alpha,\beta)}(z)$ (3.3), when $g(t, z) \sim \log |t - z|$ and $w(t) = 1, \sqrt{(1+t)/(1-t)}$.

Variant $w(t) = 1$

Let us consider the singular function of the form

$$g(t, z) = \log |t - z| . \quad (5.25)$$

Using (4.4), (4.5), we find a formula for calculating weight factor with the logarithmic singularity $\omega_i^{\log}(z)$.

As a result, for the integral with a logarithmic singularity (5.25), we obtain the quadrature formula

$$\int_{-1}^1 \log |t - z| F(t) dt \approx \sum_{i=1}^N \omega_i^{\log}(z) F(\xi_{i,N}) , \quad (5.26)$$

where

$$\omega_i^{\log}(z) = \frac{2}{K_N^{(\alpha,\beta)}(\xi_{i,N})} \sum_{m=0}^{N-1} \frac{K_{N-1-m}^{(\alpha,\beta)}(\xi_{i,N})}{m+1} \times \left\{ (-1)^m \log(z+1) + \log(1-z) - T_{m+1}(z) \log\left(\frac{1-z}{1+z}\right) - 4 \sum_{k=0}^{\lfloor \frac{m}{2} \rfloor} \frac{T_{m-2k}(z)}{2k+1} c_k^m(\lfloor m/2 \rfloor) \right\}, \quad (5.27)$$

$$c_k^m(n) = \begin{cases} 1/2, & k = n \text{ and } m \text{ is odd number,} \\ 1, & k = n \text{ and } m \text{ is even number,} \\ 1, & k \neq n \end{cases}. \quad (5.28)$$

If $\alpha = \beta = -1/2$, then the summation in (5.27) (index m) the last term is divided by two.

Structure-analogous coefficients were obtained for $T_N(t)$ polynomials in [Deloff:2007] and used to solve the Schrödinger equation with the Coulomb potential in momentum space [Deloff:2006].

Variante $w(t) = w^{(\alpha, \beta)}(t) = \sqrt{(1+t)/(1-t)}$

The Chebyshev polynomial $V_n(t)$ of the third kind is defined by [Mason:2002]

$$V_n(t) = \frac{\cos[(n + 1/2) \arccos(t)]}{\cos[\arccos(t)/2]} . \quad (5.29)$$

Hence, the zeros of $V_n(t)$ occur at

$$\xi_{i,N} = \cos \theta_{i,N} = \cos \left(\frac{2i - 1}{2N + 1} \right) , \quad (i = 1, \dots, N) . \quad (5.30)$$

Then for integrals with a logarithmic singularity (5.25) we obtain the following quadrature formula

$$\int_{-1}^1 \log |t - z| \sqrt{\frac{1+t}{1-t}} F(t) dt \approx \sum_{i=1}^N \omega_i^V(z) F(\xi_{i,N}) , \quad (5.31)$$

where

$$\begin{aligned} \omega_i^V(z) = & -\frac{4\pi}{2N+1} \cos\left(\frac{\theta_{i,N}}{2}\right) \left[(\log 2 + z) \cos\left(\frac{\theta_{i,N}}{2}\right) \right. \\ & \left. + \sum_{m=1}^{N-1} \cos\left[\left(m + \frac{1}{2}\right) \theta_{i,N}\right] \left(\frac{T_k(z)}{k} + \frac{T_{k+1}(z)}{k+1}\right) \right]. \end{aligned} \quad (5.32)$$

Variant $w(t) = \sqrt{1-t^2}$

For convenience, we consider not only the case $\alpha = -\beta = 1/2$ but also the case when $\alpha = \beta = -1/2$. In this case the weight factors of the quadrature formula for integrals with a logarithmic singularity of the form

$$\int_{-1}^1 \log|t-z| \frac{F(t)}{\sqrt{1-t^2}} dt \approx \sum_{i=1}^N \omega_i^T(z) F(\xi_{i,N}), \quad (5.33)$$

are obtained from the Eq.(4.8) and can be written in the form

$$\omega_i^T(z) = -\frac{\pi}{N} \left[\ln 2 + 2 \sum_{k=1}^{N-1} \frac{1}{k} T_k(\xi_{i,N}) T_k(z) \right]. \quad (5.34)$$

Special case

Let us consider weight coefficient (4.4) when

$$g(t, z) = Q_0(t, z) = \log \left| \frac{1 - tz + \sqrt{(1-t^2)(1-z^2)}}{t-z} \right| \quad (5.35)$$

and $\alpha, \beta = \pm 1/2$, $w(t) = 1$.

Quadrature formula for the integral with logarithmic singularity of type (5.35)

$$\int_{-1}^1 F(t) \log \left| \frac{1 - tz + \sqrt{(1-t^2)(1-z^2)}}{t-z} \right| dt \approx \sum_{i=1}^N \omega_i^{Q_0}(z) F(\xi_{i,N}) \quad (5.36)$$

contains the weight factors

$$\omega_i^{Q_0}(z) = \frac{2\pi \sqrt{1-z^2}}{K_N^{(\alpha,\beta)}(\xi_{i,N})} \sum_{k=0}^{N-1} K_{N-1-k}^{(\alpha,\beta)}(\xi_{i,N}) \frac{U_k(z)}{k+1}. \quad (5.37)$$

The weight coefficients (5.27), (5.32), (5.34) and (5.37) despite the cumbersome form, can be calculated with a sufficient degree of accuracy and used to solve the equations.

Energy spectrum for Coulomb potential

The equation with Coulomb potential we transform to the form

$$\tilde{k}^2 \phi_{nl}(\tilde{k}) - \frac{2}{\pi \tilde{k}} \int_0^{\infty} Q_l(y) \tilde{k}' \phi_{nl}(\tilde{k}') d\tilde{k}' = \varepsilon_{nl} \phi_{nl}(\tilde{k}), \quad (6.1)$$

where

$$k = \beta \tilde{k}, \quad \phi_{nl}(\tilde{k}) = \beta^{3/2} \phi_{nl}(k), \quad \beta = \mu \alpha, \quad E_{nl} = \frac{\beta^2}{2\mu} \varepsilon_{nl}. \quad (6.2)$$

In the case of Coulomb potential, the exact values of energies are known, namely,

$$\varepsilon_{nl}^C = -1/n^2. \quad (6.3)$$

The accuracy of solving the equation will be determined using the relative error

$$\delta_{nl} = \left| \frac{\varepsilon_{nl} - \varepsilon_{nl}^{(N)}}{\varepsilon_{nl}} \right|, \quad (6.4)$$

where ε_{nl} are exact eigenvalues and $\varepsilon_{nl}^{(N)}$ is the energy spectrum obtained by the numerical solution of the eigenvalues problem for matrix H at the given number of N

$$\sum_{j=1}^N H_{ij} \phi_{nl}(\xi_{j,N}) = \varepsilon_{nl}^{(N)} \phi_{nl}(\xi_{i,N}). \quad (6.5)$$

The calculations were carried out in the Wolfram Mathematica system [S.Wolfram:2003], and the chosen accuracy of the weight factors and zeros was equal to 90. For all calculations, we assume that numeric parameter $\beta_0 = 0.999992$.

Quadrature rules for $\ell \geq 0$

For the numerical solution of the Schrödinger equation with the logarithmic singularity, we use three realizations of the eigenvalue problem with the help of quadrature rules.

In the first method (Method I) we use the Chebyshev polynomials of the third kind $V_n(t)$ with the function $w(t) = \sqrt{(1+t)/(1-t)}$ and, respectively, the weight factors (5.32) to eliminate the logarithmic singularity. The second method (Method II) includes using Chebyshev polynomials of the first kind $T_n(t)$ with the function $w(t) = 1$ and weight factors (5.27) for integrals with a logarithmic singularity. In Method III, we apply the quadrature rule with weights factors (4.17) to all integrals in the subtracted integral equation (Landé subtraction method). Some characteristics of the methods are presented in the Table 1.

Table 1: Characteristics of methods.

Method	$P_n^{(\alpha, \beta)}(t)$	$\xi_{i,n}$	ω_i
I	$V_n(t)$	$\cos\left(\frac{2i-1}{2n+1}\pi\right)$	$\omega_i^V(z), \quad (5.32)$
II	$T_n(t)$	$\cos\left(\frac{i-1/2}{n}\pi\right)$	$\omega_i^{\log}(z), \quad (5.27)$
III	$T_n(t)$	$\cos\left(\frac{i-1/2}{n}\pi\right)$	$\omega_i^{\text{st}}, \quad (4.17)$

By making use of mapping (2.5)

$$\tilde{k} = \beta_0 \frac{1+z}{1-z}, \quad \tilde{k}' = \beta_0 \frac{1+t}{1-t}, \quad (6.6)$$

we transform Eq. (6.1) to

$$\begin{aligned} & \frac{4\beta_0}{\pi} \frac{1-z}{1+z} \int_{-1}^1 Q_\ell(y(z,t)) \left(\frac{1+t}{1-t} \right) \phi_{n\ell}(t) \frac{dt}{(1-t)^2} \\ &= \left(\beta_0^2 \left(\frac{1+z}{1-z} \right)^2 - \varepsilon_{n\ell} \right) \phi_{n\ell}(z), \end{aligned} \quad (6.7)$$

where

$$Q_\ell(y(z,t)) = P_\ell(y(z,t)) \log \left| \frac{1-tz}{t-z} \right| - w_{\ell-1}(y(z,t)), \quad (6.8)$$

and

$$y(z,t) = \frac{2(t-z)^2}{(1-t^2)(1-z^2)} + 1. \quad (6.9)$$

To shorten the notation in this section, we introduce functions

$$\bar{k}_i = \left(\frac{1 + \xi_{i,N}}{1 - \xi_{i,N}} \right), \quad d\bar{k}_i = \frac{1}{(1 - \xi_{i,N})^2}. \quad (6.10)$$

Consider the numerical solution to Eq. (6.7) by means of the quadrature formulas. Employing the Method I and putting that $z = \xi_{i,N}$ and $t = \xi_{j,N}$, the integral Eq. (6.7) can be approximated by the matrix equation (6.5) with

$$H_{ij} = \beta_0 \left[\beta_0 \delta_{i,j} \bar{k}_j^2 - \frac{4}{\pi} (1/\bar{k}_i) \sqrt{\bar{k}_j} Q_\ell^V(y_{ij}) d\bar{k}_j \right], \quad (6.11)$$

where

$$Q_\ell^V(y_{ij}) = \lambda_{j,N}^{(-1/2, 1/2)} \left[P_\ell(y_{ij}) \log |1 - \xi_{i,N} \xi_{j,N}| - w_{\ell-1}(y_{ij}) \right] \\ - \omega_j^{\log}(\xi_{i,N}) P_\ell(y_{ij}), \quad y_{ij} = y(\xi_{i,N}, \xi_{j,N}). \quad (6.12)$$

The weight factors $\lambda_{j,N}^{(-1/2,1/2)}$ and $\omega_j^V(\xi_{i,N})$ are determined by the Eqs. (??) and (5.32), respectively, and the values of $\xi_{i,N}$ by the formula (see Table 1)

$$\xi_{i,N} = \cos \left(\frac{2i-1}{2N+1} \pi \right). \quad (6.13)$$

Calculations using the Method II adduce to a matrix of the form

$$H_{ij} = \beta_0 \left[\beta_0 \delta_{i,j} \bar{k}_j^2 - \frac{4}{\pi} (\bar{k}_j / \bar{k}_i) Q_\ell^T(y_{ij}) \bar{d}k_j \right], \quad (6.14)$$

where

$$\begin{aligned} Q_\ell^T(y_{ij}) &= \omega_j^{\text{st}} \left[P_\ell(y_{ij}) \log |1 - \xi_{i,N} \xi_{j,N}| - w_{\ell-1}(y_{ij}) \right] \\ &- \omega_j^{\log}(\xi_{i,N}) P_\ell(y_{ij}). \end{aligned} \quad (6.15)$$

The weight factor ω_j^{st} and $\omega_j^{\text{log}}(\xi_{i,N})$ are determined by the Eqs.(4.17) and (5.27), respectively, and the values of $\xi_{i,N}$ by the relationship

$$\xi_{i,N} = \cos\left(\frac{i-1/2}{N}\pi\right). \quad (6.16)$$

The matrix elements H_{ij} of Landé-subtracted integral equation with a Coulomb potential are

$$\begin{aligned} H_{ii} &= \beta_0 \left[\beta_0 \bar{k}_i^2 - \frac{2}{\pi} C_\ell \bar{k}_i + \frac{4}{\pi} \sum_{r=1}^N \omega_r^{\text{st}} Q_\ell(y_{ri} \neq 1) \left(\frac{\bar{k}_i}{\bar{k}_r}\right) \overline{dk}_r \right], \\ H_{ij} &= -\frac{4\beta_0}{\pi} \omega_j^{\text{st}} \left(\frac{\bar{k}_j}{\bar{k}_i}\right) Q_\ell(y_{ij}) \overline{dk}_j, \quad (i \neq j). \end{aligned} \quad (6.17)$$

The diagonal matrix elements H_{ii} of Eqs.(6.11), (6.14) are finite and all singularities are under control.

Numerical results calculated by three methods are compared with each other (see Table 2).

Table 2: Relative errors $\delta_{n\ell}$ (6.4) on the computed Coulomb binding energies. Index I, II, III denotes that Methods I, II, III are used for calculation of $\varepsilon_{n\ell}^N$ respectively and $7.1(-16) \equiv 7.1 \times 10^{-16}$.

$\ell = 0$					
N	$n = 1$	$n = 2$	$n = 3$	$n = 4$	$n = 5$
50^{I}	2.3(-12)	2.3(-9)	1.8(-8)	7.5(-8)	2.3(-7)
100^{I}	3.7(-14)	3.7(-11)	2.9(-10)	1.2(-9)	3.7(-9)
150^{I}	3.3(-15)	3.3(-12)	2.5(-11)	1.1(-10)	3.3(-10)
150^{II}	1.1(-16)	6.7(-15)	1.1(-13)	8.6(-13)	4.1(-12)
150^{III}	7.1(-7)	1.4(-5)	1.2(-4)	5.3(-4)	1.8(-3)
$\ell = 1$					
N	$n = 1$	$n = 2$	$n = 3$	$n = 4$	$n = 5$
50^{I}	2.2(-14)	1.0(-12)	1.4(-11)	1.1(-10)	4.4(-10)
100^{I}	2.3(-17)	1.0(-15)	1.5(-14)	1.1(-13)	5.8(-13)
150^{I}	4.0(-19)	1.8(-17)	2.6(-16)	2.0(-15)	1.0(-14)
150^{II}	4.7(-16)	9.2(-15)	8.7(-14)	4.5(-13)	1.8(-12)
150^{III}	4.2(-5)	1.7(-4)	3.6(-4)	4.3(-4)	1.2(-4)

Table 3: Continuation of the table

$\ell = 2$					
N	$n = 1$	$n = 2$	$n = 3$	$n = 4$	$n = 5$
50^{I}	2.2(-14)	1.0(-12)	1.4(-11)	1.1(-10)	4.4(-10)
100^{I}	2.3(-17)	1.0(-15)	1.5(-14)	1.1(-13)	5.8(-13)
150^{I}	4.0(-19)	1.8(-17)	2.6(-16)	2.0(-15)	1.0(-14)
150^{II}	1.7(-19)	4.7(-18)	6.1(-17)	4.7(-16)	2.6(-15)
150^{III}	1.4(-5)	1.1(-4)	4.8(-4)	1.6(-3)	4.3(-3)

As follows from the results of the calculation, Methods I and II have excellent convergence with increasing N and significantly exceed the accuracy of Method III. In addition, the accuracy of Methods I and II increases with the increase of orbital number ℓ , unlike Method III.

Therefore, quadrature formulas (5.32) and (5.27), in which the logarithmic singularities of integrals are included into the weight factors, make it possible to solve the Schrödinger equation with Coulomb potential in momentum space with high accuracy.

Special case for $\ell = 0$

Using mapping (2.6)

$$\tilde{k} = \beta_0 \sqrt{\frac{1+z}{1-z}}, \quad \tilde{k}' = \beta_0 \sqrt{\frac{1+t}{1-t}}, \quad (6.18)$$

Eq.(6.1) for $\ell = 0$ is given by

$$\begin{aligned} & \frac{2\beta_0}{\pi} \sqrt{\frac{1-z}{1+z}} \int_{-1}^1 \phi_{n0}(t) \log \left| \frac{1-tz + \sqrt{(1-t^2)(1-z^2)}}{t-z} \right| \frac{dt}{(1-t)^2} \\ &= \left(\beta_0^2 \left(\frac{1+z}{1-z} \right) - \varepsilon_{n0} \right) \phi_{n0}(z) . \end{aligned} \quad (6.19)$$

Consider the numerical solution to Eq.(6.19) by means of the quadrature formula (5.36) with the weights (5.37) (see, [Andreev:2017]). Using (5.36), integral equation (6.7) reduces to the eigenvalues problem

$$\sum_{j=1}^N H_{ij} \phi_{n0}(\xi_{j,N}) = \varepsilon_{n0}^{(N)} \phi_{n0}(\xi_{i,N}) , \quad (6.20)$$

where the matrix elements of H are given by the formula

$$H_{ij} = \beta_0 \left[\beta_0 \delta_{i,j} \bar{k}_j - \frac{2}{\pi} \frac{d\bar{k}_j}{\bar{k}_i^{1/2}} \omega_j^{Q_0}(\xi_{i,N}) \right]. \quad (6.21)$$

The matrix $\omega_j^{Q_0}(\xi_{i,N})$ is calculated by means of (5.37) and the functions \bar{k}_i , $d\bar{k}_i$ are determined by the Eq. (6.10).

We carry out the calculations for two sets of polynomials: the first-order Chebyshev polynomials $T_n(t)$ ($\alpha = \beta = -1/2$) and the third-order Chebyshev polynomials $V_n(t)$ ($\alpha = -1/2$, $\beta = 1/2$). The values of relative error (6.4), obtained as a result of numerical solution, are given in Table 4, depending on the number of nodes N .

Table 4: The five relative errors δ_{n0} with $\ell = 0$ for polynomials $V_n(t)$, obtained by solving Eq. (6.19).

N	$n = 1$	$n = 2$	$n = 3$	$n = 4$	$n = 5$
50	0.0(-90)	9.5(-41)	3.0(-21)	4.6(-12)	8.8(-7)
100	0.0(-90)	3.0(-87)	1.7(-49)	1.1(-31)	4.7(-21)
150	0.0(-90)	0.0(-90)	1.6(-78)	2.0(-52)	8.4(-37)

The solution of Eq. (6.19) for the first-order Chebyshev polynomials $T_n(t)$ leads to analogous results (see Table 5).

Table 5: Relative error δ_{n0} for polynomials $T_n(t)$.

N	$n = 1$	$n = 2$	$n = 3$	$n = 4$	$n = 5$
50	0.0(-90)	8.0(-40)	1.1(-20)	1.1(-11)	1.6(-6)
100	0.0(-90)	2.7(-86)	6.5(-49)	2.8(-31)	9.6(-21)
150	0.0(-90)	0.0(-90)	6.3(-78)	5.3(-52)	1.8(-36)

As follows from the results, “nearly exact” quadrature formula for the integral in the Schrödinger equation allows one to reproduce the energy spectrum ε_{n0} with a high degree of accuracy, greatly surpassing the analogous calculations [Deloff:2006, Tang:2001, J.Chen:2013].

Results for the linear potential

We write the Schrödinger equation with linear confinement potential in the form

$$\tilde{k}^2 \phi_{nl}(\tilde{k}) + \frac{1}{\pi \tilde{k}^2} \int_0^{\infty} Q'_l(y) \phi_{nl}(\tilde{k}') d\tilde{k}' = \varepsilon_{nl} \phi_{nl}(\tilde{k}) \quad (7.1)$$

using the replacements

$$k = \beta \tilde{k}, \quad E = \frac{\beta^2}{2\mu} \varepsilon, \quad \beta = (2\mu\sigma)^{1/3}, \quad \phi_{nl}(\tilde{k}) = \beta^{3/2} \phi_{nl}(k). \quad (7.2)$$

We may deduce from Eq.(2.15) and Landé subtraction term

$$\int_0^{\infty} dk Q'_0(y) = 0, \quad (7.3)$$

that the Schrödinger equation (7.1) is

$$\begin{aligned} & (\varepsilon_{n\ell} - \tilde{k}^2) \phi_{n\ell}(\tilde{k}) \\ &= \frac{1}{\pi \tilde{k}^2} \int_0^{\infty} \left[Q'_0(y) \left\{ P_\ell(y) \phi_{n\ell}(\tilde{k}') - \phi_{n\ell}(\tilde{k}) \right\} - w'_{\ell-1}(y) \phi_{n\ell}(\tilde{k}') \right] d\tilde{k}' \\ &+ \frac{1}{\pi \tilde{k}^2} \int_0^{\infty} Q_0(y) P'_\ell(y) \phi_{n\ell}(\tilde{k}') d\tilde{k}'. \end{aligned} \quad (7.4)$$

To test the accuracy of calculations of the energy spectrum, we use the equation (6.4). In the particular case $\ell = 0$ the exact result is known and the binding energy is

$$\varepsilon_{n0}^L = -z_n, \quad n = 1, 2, 3 \dots, \quad (7.5)$$

where z_n are zeroes of the Airy functions $\text{Ai}(z)$.

In contrast to Coulomb potential, there are no exact analytical solutions with linear potential for $\ell \geq 1$. For $\ell \geq 1$ the values marked as exact have been computed by solving the Schrödinger equation in configuration space. For this purpose we used the variational method of solving with trial pseudo-Coulomb wave functions [Fulcher:1993]

$$\psi_{n\ell}^C(\mathbf{r}, \beta) = \sqrt{\frac{n!}{(n + 2\ell + 2)!}} (2\beta)^{3/2} (2\beta r)^\ell e^{-\beta r} L_n^{2\ell+2}(2\beta r), \quad (7.6)$$

where $L_n^\ell(z)$ are the Laguerre polynomials with $n, \ell \geq 0$. In [Fulcher:1993], the analytical expressions for the integrals with functions (7.6) arising in coordinate space were obtained. This makes it possible to carry out calculations with a high degree of accuracy.

Therefore, the numerical solution in momentum space for $\ell \geq 1$ will be compared to the solution of this equation in coordinate space.

Quadrature rules $\ell \geq 0$

To solve the Schrödinger equation in a momentum space with a linear potential, we use quadrature formulas (5.17) and (5.20). The methods of solving the equation with the help of formulas (5.20) and (5.17) will be called as Method A and B, respectively.

Let us now explain a method of solution (Method A) of the integral equation (7.4). Employing the variable transformation (2.5)

$$\tilde{k} = \beta_0 \left(\frac{1+z}{1-z} \right), \quad \tilde{k}' = \beta_0 \left(\frac{1+t}{1-t} \right) \quad (7.7)$$

and then using quadrature relationships (5.17) and (5.20) with the weight factors (5.26) and (5.23), respectively, the subtracted integral equation (7.4) is approximated by the matrix equation (6.5), where the matrix elements are

$$H_{ij} = \beta_0^2 T_{ij} + \frac{1}{\beta_0 \pi} (1/\bar{k}_i^2) \left(V_{ij}^H + V_{ij}^{\text{Log}} \right). \quad (7.8)$$

In Eq (7.8)

$$\begin{aligned}
 T_{ij} &= \delta_{i,j} \bar{k}_j^2, \\
 V_{ij}^H &= 2 \left[\omega_j^{HS}(\xi_{i,N}) P_\ell(y_{ij}) Z_{ij} - \delta_{i,j} \sum_{k=1}^N \omega_k^{HS}(\xi_{j,N}) Z_{kj} \right. \\
 &\quad \left. - \omega_j^{\text{st}} w'_{\ell-1}(y_{ij}) \right] \bar{d}k_j, \\
 V_{ij}^{\text{Log}} &= 2 P'_\ell(y_{ij}) \left[\omega_j^{\text{st}} \log |1 - \xi_{i,N} \xi_{j,N}| - \omega_j^{\text{log}}(\xi_{i,N}) \right] \bar{d}k_j, \quad (7.9)
 \end{aligned}$$

where

$$Z_{ij} = -\frac{1}{4} \left[\frac{(1 - \xi_{i,N}^2)(1 - \xi_{j,N}^2)}{(1 - \xi_{i,N} \xi_{j,N})} \right]^2, \quad (7.10)$$

$$y_{ij} = \frac{2(\xi_{i,N} - \xi_{j,N})^2}{(1 - \xi_{i,N}^2)(1 - \xi_{j,N}^2)} + \delta_{i,j}. \quad (7.11)$$

Weight factors ω_j^{st} , $\omega_j^{\text{HS}}(\xi_{i,N})$ and $\omega_j^{\text{log}}(\xi_{i,N})$ are determined by the Eqs. (4.17), (5.23) and (5.26), respectively. The numbers $\xi_{i,N}$ are the zeros of the Chebyshev polynomial of the first kind $T_n(t)$ (see the Eq.(6.16)).

Next we describe a quick method of solution (Method B) of the hypersingular integral equation (7.1). The characteristic (specific) features of Method B consist in using the change of variables (6.18) and quadrature formulas (5.17) and (5.33) with the weight function $w(t) = \sqrt{1-t^2}$ of the Chebyshev polynomial $T_n(t)$.

As a result, the matrix \tilde{H} for calculating the energy spectrum using the Method B is determined by the following relation

$$\tilde{H}_{ij} = \beta_0^2 \tilde{T}_{ij} + \frac{1}{\beta_0 \pi} (1/\bar{k}_i) \left(\tilde{V}_{ij}^{\text{H}} + \tilde{V}_{ij}^{\text{Log}} \right). \quad (7.12)$$

In Eq. (7.12)

$$\begin{aligned}\tilde{T}_{ij} &= \delta_{i,j} \bar{k}_j, \\ \tilde{V}_{ij}^{\text{H}} &= \omega_j^{\text{HT}}(\xi_{i,N}) P_\ell(y_{ij}^T) (\xi_{i,N}^2 - 1) (1 + \xi_{j,N}) - \frac{\pi}{N} w'_{\ell-1}(y_{ij}^T),\end{aligned}\quad (7.13)$$

$$\begin{aligned}\tilde{V}_{ij}^{\text{Log}} &= \frac{P'_\ell(y_{ij}^T)}{(1 - \xi_{j,N})} \\ &\times \left[\frac{\pi}{N} \log \left| 1 - \xi_{i,N} \xi_{j,N} + \sqrt{1 - \xi_{i,N}^2} \sqrt{1 - \xi_{j,N}^2} \right| - \omega_j^T(\xi_{i,N}) \right]\end{aligned}\quad (7.14)$$

where

$$y_{ij}^T = \frac{1 - \xi_{i,N} \xi_{j,N}}{\sqrt{1 - \xi_{i,N}^2} \sqrt{1 - \xi_{j,N}^2}}. \quad (7.15)$$

Weight factors $\omega_j^{\text{HT}}(\xi_{i,N})$ and $\omega_j^T(\xi_{i,N})$ are determined by the Eqs. (5.19) and (5.34), respectively.

The numerical results calculated by the Methods A and B are compared with each other (see Table 6).

Table 6: Relative errors $\delta_{n\ell}$ (6.4) on the computed linear binding energies. Index A, B denotes that Methods A, B are used for calculation of $\varepsilon_{n\ell}^N$ respectively and $7.6(-13) \equiv 7.6 \times 10^{-13}$.

$\ell = 0$					
N	$n = 1$	$n = 2$	$n = 3$	$n = 4$	$n = 5$
100 ^A	2.9(-15)	1.1(-14)	2.2(-14)	3.7(-14)	5.4(-14)
150 ^A	1.1(-16)	4.1(-16)	8.6(-16)	1.4(-15)	2.1(-15)
150 ^B	2.6(-27)	6.2(-26)	5.5(-24)	8.8(-23)	6.2(-22)
$\ell = 1$					
N	$n = 1$	$n = 2$	$n = 3$	$n = 4$	$n = 5$
100 ^A	8.0(-14)	8.3(-14)	1.6(-13)	1.7(-13)	2.4(-13)
150 ^A	7.0(-15)	7.1(-15)	1.4(-14)	1.4(-14)	2.1(-14)
150 ^B	2.6(-10)	7.4(-10)	1.4(-9)	2.2(-9)	3.1(-9)
$\ell = 2$					
N	$n = 1$	$n = 2$	$n = 3$	$n = 4$	$n = 5$
100 ^A	6.5(-13)	2.3(-13)	5.6(-13)	1.5(-12)	8.0(-12)
150 ^A	5.5(-14)	1.8(-14)	9.9(-14)	3.3(-14)	1.4(-13)
150 ^B	1.5(-14)	6.5(-14)	1.7(-13)	3.5(-13)	6.2(-13)

As follows from the results of calculations, Method A gives a more accurate result than method B for $\ell \geq 1$.

Thus, a special quadrature formula (5.20) based on the use of a counter term and an analytical calculation of weight factors involving a singularity gives a highly accurate solution of the Schrödinger equation in momentum space for a linear potential. It should be noted that the accuracy of calculating the spectrum of the Schrödinger equation with a linear potential in the momentum space of both methods far exceeds the accuracy of the solution in the approaches proposed in the papers [J.Chen:2013-14, Deloff:2006, Hersbach:1993, Leitao:2014, Tang:2001, J.Chen:2013].

Special case for $\ell = 0$

By making use of mapping

$$\tilde{k} = \beta_0 \sqrt{\frac{1+z}{1-z}}, \quad \tilde{k}' = \beta_0 \sqrt{\frac{1+t}{1-t}}, \quad (7.16)$$

we transform Eq. (7.1) to

$$\begin{aligned} & \frac{1}{\pi \beta_0} \left(\frac{1-z}{1+z} \right) \int_{-1}^1 Q'_\ell(y(t, z)) \frac{\phi_{n\ell}(t) dt}{(1-t)\sqrt{1-t^2}} \\ & = \left(\varepsilon_{n\ell} - \beta_0^2 \left(\frac{1+z}{1-z} \right) \right) \phi_{n\ell}(z). \end{aligned} \quad (7.17)$$

In the case $\ell = 0$, equation (7.17) after simplifications is written in the form

$$\begin{aligned}
 & -\frac{1}{\pi\beta_0} (1-z)^2 \int_{-1}^1 \phi_{n0}(t) \sqrt{\frac{1+t}{1-t}} \frac{dt}{(t-z)^2} \\
 & = \left(\varepsilon_{n0} - \beta_0^2 \frac{1+z}{1-z} \right) \phi_{n0}(z) .
 \end{aligned} \tag{7.18}$$

Starting from the structure of the integral equation, the most suitable interpolation polynomial for the quadrature formula is the polynomial $V_n(t)$, and the weight function can be chosen in the form

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

As a result, the matrix of the eigenvalues problem takes the form [Andreev:2017]:

$$H_{ij} = \left[\beta_0^2 \delta_{i,j} \bar{k}_j - \frac{\omega_j^H(\xi_{i,N})}{\pi \beta_0 \bar{d}k_i} \right], \quad (7.19)$$

where $\xi_{i,N}$ are the zeros of the polynomial $V_N(t)$ (see, Eq. (6.13)) and the matrix elements $\omega_j^H(\xi_{i,N})$ are calculated with the help of Eq.(5.16).

Therefore, it is possible to compare the results of numerical calculations with matrix (7.19) and exact values $-z_n$ (7.5). Table 7 lists the values of the relative error (6.4)

$$\delta = \left| \frac{\varepsilon_{n0}^L - \varepsilon_n^{(N)}}{\varepsilon_{n0}^L} \right|, \quad (7.20)$$

where $\varepsilon_n^{(N)}$ is the energy spectrum obtained by the numerical solution of the eigenvalues problem for matrix (7.19) at the given number of N .

Table 7: Relative error δ_{n0} of solving Eq.(7.18).

N	$n = 1$	$n = 2$	$n = 3$	$n = 4$	$n = 5$
50	3.4(-22)	3.6(-20)	3.2(-17)	2.9(-15)	8.0(-14)
100	1.7(-39)	1.1(-35)	1.5(-32)	4.3(-31)	5.2(-28)
150	4.5(-54)	8.2(-50)	4.8(-47)	1.3(-43)	5.9(-42)

Note, however, that the special method presented here gives high-precision results only in the case $\ell = 0$. If $\ell \geq 1$, the kernel of Eq. (7.18) changes, which leads to a sharp decrease of accuracy [Andreev:2017].

Energy spectrum for Cornell potential

We are going to consider the case where both the Coulomb and the linear confinement potential are present. For the Cornell potential $V(r) = -\alpha/r + \sigma r$, there are no analytical solutions. Therefore, the numerical solution in momentum space will be compared to the solution of this equation in coordinate space.

The method for estimating the accuracy of the solution will be the same as for the case of a linear confinement potential.

Quadrature scheme for $\ell \geq 0$

From an analysis of the methods for solving the Schrödinger equation in momentum space for the Coulomb and linear potentials, the most optimal is the use of quadrature formulas (5.20) and (5.26) in which the weight factors $\omega_i^{HS}(z)$ (5.23) and $\omega_i^{\log}(z)$ (5.27) depend on double-pole and logarithmic singularities.

Using (7.2) and subtraction term (7.3), the Schrödinger equation with Cornell potential $V(r) = -\alpha/r + \sigma r$ in momentum space is written in the form

$$\begin{aligned}
 (\varepsilon_{nl} - \tilde{k}^2) \phi_{nl}(\tilde{k}) &= \frac{1}{\pi \tilde{k}^2} \int_0^\infty \left\{ Q'_\ell(y) \phi_{nl}(\tilde{k}') - Q'_0(y) \phi_{nl}(\tilde{k}) \right\} d\tilde{k}' \\
 - \frac{\lambda}{\pi \tilde{k}} \int_0^\infty Q_\ell(y) \phi_{nl}(\tilde{k}') \tilde{k}' d\tilde{k}' , & \quad (8.1)
 \end{aligned}$$

where

$$\lambda = \frac{\alpha (2\mu)^{2/3}}{\sigma^{1/3}} . \quad (8.2)$$

The results of calculation are presented in Table 8. To determine the energy spectrum the appropriate Schrödinger equation was solved in both the momentum and the coordinate space. As seen from Table 8 there is excellent agreement between these two methods of calculation.

Table 8: Relative errors $\delta_{n\ell}$ (6.4) on the computed Cornell binding energies with $\lambda = 1$.

$\ell = 0$					
N	$n = 1$	$n = 2$	$n = 3$	$n = 4$	$n = 5$
50	6.7(-13)	2.4(-12)	4.9(-12)	1.9(-10)	4.7(-9)
100	2.7(-15)	9.6(-15)	2.0(-14)	3.5(-14)	5.2(-14)
150	1.1(-16)	3.7(-16)	7.9(-16)	1.4(-15)	2.0(-15)
$\ell = 1$					
N	$n = 1$	$n = 2$	$n = 3$	$n = 4$	$n = 5$
50	3.0(-12)	1.4(-11)	1.4(-10)	4.7(-10)	3.2(-8)
100	3.2(-14)	7.4(-14)	1.1(-14)	1.5(-13)	3.1(-14)
150	3.2(-15)	6.0(-15)	1.8(-15)	1.2(-14)	1.4(-15)
$\ell = 2$					
N	$n = 1$	$n = 2$	$n = 3$	$n = 4$	$n = 5$
50	1.7(-10)	1.8(-9)	2.7(-9)	1.3(-7)	9.3(-7)
100	4.1(-16)	1.1(-15)	1.6(-15)	3.2(-15)	1.0(-13)
150	3.2(-17)	7.2(-17)	1.4(-16)	2.2(-16)	3.3(-16)

Thus, the use of the quadrature rules on the base of Eqs.(5.20) and (5.26) will allow us to find the spectrum of the system with the Cornell potential with a relative error of 10^{-15} for $\ell = 0$ and 10^{-22} for $\ell > 1$.

Special quadrature scheme for $\ell = 0$

Using (6.21) and (7.19) , matrix H_{ij} for the equation with Cornell potential at $\ell = 0$ is written in the form (see, [Andreev:2017])

$$H_{ij} = \beta_0^2 \delta_{i,j} \bar{k}_j - \frac{\omega_j^H(\xi_{i,N})}{\pi \beta_0 \bar{d}k_i} - \frac{\lambda \beta_0}{\pi} \frac{\bar{d}k_j}{\bar{k}_i^{1/2}} \omega_j^{Q_0}(\xi_{i,N}) , \quad (8.3)$$

Table 9 represents the values

$$\delta_{n0} = \left| \frac{\tilde{\varepsilon}_{n0} - \varepsilon_n^{(N)}}{\tilde{\varepsilon}_{n0}} \right| , \quad (8.4)$$

where $\tilde{\varepsilon}_{n0}$ are the eigenvalues obtained in coordinate space.

Table 9: Value of δ_{n0} for polynomials $V_N(t)$ with $\lambda = 1$.

N	$n = 1$	$n = 2$	$n = 3$	$n = 4$	$n = 5$
50	4.9(-23)	5.6(-20)	1.7(-17)	1.5(-15)	9.7(-14)
100	8.5(-40)	2.7(-36)	9.6(-34)	1.9(-30)	3.9(-28)
150	5.0(-55)	8.7(-51)	2.8(-47)	1.5(-44)	1.4(-41)

This method, as in the case of a special quadrature rules for a linear potential (7.19), is highly accurate only for $\ell = 0$ [Andreev:2017]. It is to be noted that numerical calculations with the help of (8.3) completely agree with results [Kang:2006].

Conclusions

In this paper, we solve numerically the Schrödinger equation in momentum space with the Coulomb, linear confinement and Cornell potentials by using new quadrature rules.

The numerical results demonstrate the efficiency of the created method. The new quadrature formulas, in which the singularities of integrals are included into the weight functions, make it possible to solve the Schrödinger equation for the momentum space with high accuracy.

The achieved accuracy of calculations is many orders of magnitude higher than in similar calculations in momentum space conducted in the papers [J.Chen:2013-14, Deloff:2006, Hersbach:1993, Leitao:2014, Tang:2001, J.Chen:2013]. Special high-precision methods of solution for states with zero orbital angular momentum are considered.

These methods are easily generalized to the relativistic equations, where the potentials are generally derived in momentum space. Consequently, the developed procedure to obtain the energy spectra can be used to study and calculate various effects in the two-body quantum systems, such as hydrogen-like atoms, hadronic atoms and bound quark systems.

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Thanks for your time !!!

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