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ON POTENTIALS INTEGRATED BY NIKIFOROV–UVAROV METHOD

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Abstract. We discuss basic potentials of the nonrelativistic and relativistic quantum mechanics that can be integrated in the Nikiforov and Uvarov paradigm with the aid of a computer algebra system. This consideration may help the readers to study analytical methods of quantum physics.

Building on ideas of de Broglie and Einstein, I tried to show that the ordinary differential equations of mechanics, which attempt to define the co-ordinates of a mechanical system as functions of the time, are no longer applicable for "small" systems; instead there must be introduced a certain *partial* differential equation, which defines a variable ψ ("wave function") as a function of the co-ordinates and the time.

Erwin Schrödinger [31]

1. Introduction

Discovery of the relativistic and nonrelativistic Schrödinger equations [28], [29], [30], [31] is discussed in [2] (see also the references therein). Finding of the energy levels and the corresponding normalized wave functions of various systems is one of the basic problems of quantum physics. Only in a few elementary cases the exact solutions are known. They are usually investigated by different techniques. Nonetheless, those completely integrable problems are important in creation of mathematical models for complex quantum systems. Moreover, they may provide a useful testing ground for verification of numerical methods.

We assemble analytical solutions for a range of potentials in the nonrelativistic and relativistic quantum mechanics that are available in the literature. Data for most of the potentials that can be studied, in a unified way, by the so-called Nikiforov–Uvarov method [24] are collected, independently verified, and completed with the help of the Mathematica computer algebra system. Only bound states are discussed. On the contrary, in a traditional approach, for each of those problems one has to identify and factor out the singularities of the corresponding square integrable wave functions and find the remaining terminating power series expansions or use algebraic methods (see, for example, [3], [5], [6], [8], [10], [15], [16], [20], [32], [33]). As a result, each of such problems has to be treated separately, which is not suitable for a unified computer algebra approach.

The article is organized as follows. In the next section, we introduce the basics of the Nikiforov–Uvarov approach and then, successively, apply it to the main problems of introductory quantum mechanics, such as harmonic oscillators, Bessel functions, Coulomb problems, Pöschl–Teller potential holes, Kratzer's molecular potential, Hulthén potential, and Morse potentials, in the forthcoming sections. All calculations are verified in a complementary Mathematica notebook that can serve both educational and research purposes. Appendices A and B contain, for the reader's convenience,

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the data for classical orthogonal polynomials and a useful integral evaluation, respectively, in order to make our presentation as self-contained as possible.

This article is written for those who study quantum mechanics and would like to see more details than in the classical textbooks. It is motivated by an introductory course in mathematics of quantum mechanics which one of the authors (SKS) has been teaching at Arizona State University for more than two decades.

2. Summary of the Nikiforov–Uvarov approach

The generalized equation of the hypergeometric type

$$u'' + \frac{\widetilde{\tau}(x)}{\sigma(x)}u' + \frac{\widetilde{\sigma}(x)}{\sigma^2(x)}u = 0 \tag{2.1}$$

($\sigma(x)$, $\widetilde{\sigma}(x)$ are polynomials of degrees at most 2 and $\widetilde{\tau}(x)$ is a polynomial degree at most one) by the substitution

$$u = \varphi(x)y(x) \tag{2.2}$$

can be reduced to the form

$$\sigma(x)y'' + \tau(x)y' + \lambda y = 0 \tag{2.3}$$

if:

$$\frac{\varphi'}{\varphi} = \frac{\pi(x)}{\sigma(x)}, \qquad \pi(x) = \frac{1}{2}\left(\tau(x) - \widetilde{\tau}(x)\right) \tag{2.4}$$

(or, $\tau(x) = \widetilde{\tau} + 2\pi$, for later),

$$k = \lambda - \pi'(x) \qquad (\text{or, } \lambda = k + \pi'), \tag{2.5}$$

and

$$\pi(x) = \frac{\sigma' - \widetilde{\tau}}{2} \pm \sqrt{\left(\frac{\sigma' - \widetilde{\tau}}{2}\right)^2 - \widetilde{\sigma} + k\sigma} \tag{2.6}$$

is a linear function. (Use the choice of the constant k to complete the square under the radical sign; see [24] and our argument below for more details.)

In Nikiforov–Uvarov's method, the energy levels can be obtained from the quantization rule:

$$\lambda + n\tau' + \frac{1}{2}n(n-1)\sigma'' = 0 \qquad (n = 0, 1, 2, \dots) \tag{2.7}$$

and the corresponding square-integrable solutions are classical orthogonal polynomials, up to a factor. They can be found by the *Rodrigues-type formula* [24]:

$$y_n(x) = \frac{B_n}{\rho(x)}\left(\sigma^n(x)\rho(x)\right)^{(n)}, \qquad (\sigma\rho)' = \tau\rho, \tag{2.8}$$

where B_n is a constant (see also [35] and Table 15).

(The corresponding data for basic nonrelativistic and relativistic problems are presented in the Tables 1–14 below.)

Let us try to transform the differential equation (2.1) to the simplest form by the change of unknown function $u = \varphi(x)\, y$ with the help of some special choice of function $\varphi(x)$.

Substituting $u = \varphi(x)\, y$ in (2.1) one gets

$$y'' + \left(\frac{\widetilde{\tau}}{\sigma} + 2\frac{\varphi'}{\varphi}\right) y' + \left(\frac{\widetilde{\sigma}}{\sigma^2} + \frac{\widetilde{\tau}}{\sigma}\frac{\varphi'}{\varphi} + \frac{\varphi''}{\varphi}\right) y = 0. \tag{2.9}$$

Equation (2.9) should not be more complicated than our original equation (2.1). Thus, it is natural to assume that the coefficient in front of y' has the form $\tau(x)/\sigma(x)$, where $\tau(x)$ is a polynomial of degree at most one. This implies the following first-order differential equation

$$\frac{\varphi'}{\varphi} = \frac{\pi(x)}{\sigma(x)} \tag{2.10}$$

for the function $\varphi(x)$, where

$$\pi(x) = \frac{1}{2}\left(\tau(x) - \widetilde{\tau}(x)\right) \tag{2.11}$$

is a polynomial of degree at most one. As a result, equation (2.9) takes the form

$$y'' + \frac{\tau(x)}{\sigma(x)}\, u' + \frac{\overline{\sigma}(x)}{\sigma^2(x)}\, u = 0, \tag{2.12}$$

where

$$\overline{\sigma}(x) = \widetilde{\sigma}(x) + \pi^2(x) + \pi(x)\left[\widetilde{\tau}(x) - \sigma'(x)\right] + \pi'(x)\sigma(x). \tag{2.13}$$

The functions $\tau(x)$ and $\overline{\sigma}(x)$ are polynomials of degrees at most one and two in x, respectively. Therefore, equation (2.12) is an equation of the same type as our original equation (2.1).

By using a special choice of the polynomial $\pi(x)$ we can reduce (2.12) to the simplest form assuming that

$$\overline{\sigma}(x) = \lambda\, \sigma(x), \tag{2.14}$$

where λ is some constant. Then equation (2.12) takes the form (2.3). We call equation (2.3) a *differential equation of hypergeometric type* and its solutions *functions of hypergeometric type.* In this context, it is natural to call equation (2.1) a *generalized differential equation of hypergeometric type.*

The condition (2.14) can be rewritten as

$$\pi^2 + \left(\widetilde{\tau} - \sigma'\right)\, \pi + \widetilde{\sigma} - k\sigma = 0, \tag{2.15}$$

where

$$k = \lambda - \pi'(z) \tag{2.16}$$

is a constant. Assuming that this constant is known, we can find $\pi(x)$ as a solution (2.6) of the quadratic equation (2.15). But $\pi(x)$ is a polynomial, therefore the second degree polynomial

$$p(x) = \left(\frac{\sigma'(x) - \widetilde{\tau}(x)}{2}\right)^2 - \widetilde{\sigma}(x) + k\sigma(x) \tag{2.17}$$

under the radical should be a square of a linear function and the discriminant of $p(x)$ should be zero. This condition gives an equation for the constant k, which is, generally, a quadratic equation. Given k as a solution of this equation, we find $\pi(x)$ by the quadratic formula (2.6), then $\tau(x)$ and λ by (2.11) and (2.16). Finally, we find the function $\varphi(x)$ as a solution of (2.10). It is clear that the reduction of equation (2.1) to the simplest form (2.3) can be accomplished by a few different ways in accordance with different choices of the constant k and different signs in (2.6) for $\pi(x)$.

A closed form for the constant k can be obtained as follows [2]. Let

$$p(x) = \left(\frac{\sigma' - \widetilde{\tau}}{2}\right)^2 - \widetilde{\sigma} + k\sigma = q(x) + k\sigma(x), \tag{2.18}$$

where

$$q(x) = \left(\frac{\sigma' - \widetilde{\tau}}{2}\right)^2 - \widetilde{\sigma}. \tag{2.19}$$

Completing the square, one gets

$$p(x) = \frac{p''}{2}\left(x + \frac{p'(0)}{p''}\right)^2 - \frac{\left(p'(0)\right)^2 - 2p''p(0)}{2p''}, \tag{2.20}$$

where the last term must be eliminated:

$$\left(p'(0)\right)^2 - 2p''p(0) = 0. \tag{2.21}$$

Therefore,

$$\left(q'(0) + k\sigma'(0)\right)^2 - 2\left(q'' + k\sigma''\right)\left(q(0) + k\sigma(0)\right) = 0, \tag{2.22}$$

which results in the following quadratic equation:

$$ak^2 + 2bk + c = 0. \tag{2.23}$$

Here,

$$a = \left(\sigma'(0)\right)^2 - 2\sigma''\sigma(0), \tag{2.24}$$

$$b = q'(0)\sigma'(0) - \sigma''q(0) - \sigma(0)q'', \tag{2.25}$$

$$c = \left(q'(0)\right)^2 - 2q''q(0). \tag{2.26}$$

Solutions are

$$k_0 = -\frac{c}{2b}, \qquad \text{if} \quad a = 0 \tag{2.27}$$

and

$$k_{1,2} = \frac{-b \pm \sqrt{d}}{a}, \qquad \text{if} \quad a \neq 0. \tag{2.28}$$

Here,

$$d = b^2 - ac = \left(\sigma(0)q'' - \sigma''q(0)\right)^2 - 2\left(\sigma'(0)q'' - \sigma''q'(0)\right)\left(\sigma(0)q'(0) - \sigma'(0)q(0)\right). \tag{2.29}$$

As a result,

$$p(x) = \left[\frac{p''}{2}\left(x + \frac{p'(0)}{p''}\right)^2\right]_{k=k_{0,1,2}}, \tag{2.30}$$

which allows evaluating the linear function $\pi(x)$ in the Nikiforov–Uvarov technique.

Examples, for the most integrable cases that are available in the literature, are presented in the Tables 1–14 below, where all these analytical arguments are implemented in a supplementary Mathematica notebook.

3. Harmonic Oscillator

Let us consider the one-dimensional stationary Schrödinger equation for the harmonic oscillator:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+\frac{1}{2}m\omega^2x^2\psi=E\psi \tag{3.1}$$

with the orthonormal real-valued wave function

$$\int_{-\infty}^{\infty}\psi^2(x)\ dx=1. \tag{3.2}$$

Introducing dimensionless variables

$$\psi(x)=u(\xi), \qquad x=\xi\sqrt{\frac{\hbar}{m\omega}}, \quad E=\hbar\omega\varepsilon \tag{3.3}$$

one gets

$$u''+\left(2\varepsilon-\xi^2\right)u=0. \tag{3.4}$$

Here, $\sigma(\xi)=1$, $\widetilde{\tau}(\xi)=0$, and $\widetilde{\sigma}(\xi)=2\varepsilon-\xi^2$. Therefore,

$$\pi(\xi)=\pm\sqrt{k-2\varepsilon+\xi^2}=\pm\xi, \qquad k=2\varepsilon. \tag{3.5}$$

We pick $\pi=-\xi$, which gives a negative derivative for

$$\tau(\xi)=\widetilde{\tau}(\xi)+2\pi(\xi)=-2\xi. \tag{3.6}$$

Then

$$\frac{\varphi'}{\varphi}=\frac{\pi(\xi)}{\sigma(\xi)}=-\xi, \qquad \varphi(\xi)=e^{-\xi^2/2} \tag{3.7}$$

and $\lambda=2\varepsilon-1$, $\rho(\xi)=e^{-\xi^2}$. The energy levels are $\varepsilon=\varepsilon_n=n+1/2$, $(n=0,1,2,\dots)$ from (2.7). The eigenfunctions,

$$y_n(\xi)=B_ne^{\xi^2}\frac{d^n}{d\xi^n}\left(e^{-\xi^2}\right), \tag{3.8}$$

are, up to a normalization, the Hermite polynomials (Table 15).

As a result, the orthonormal wave functions are given by [29], [31], [20]

$$\psi(x)=\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{2^nn!}}\exp\left(-\frac{m\omega}{2\hbar}x^2\right)H_n\left(x\sqrt{\frac{m\omega}{\hbar}}\right), \tag{3.9}$$

corresponding to the discrete energy levels

$$E_n=\hbar\omega\left(n+\frac{1}{2}\right) \qquad (n=0,1,2,\dots), \tag{3.10}$$

in Gaussian units. (More general, “missing”, solutions of the time-dependent Schrödinger equation are discussed in [17], [18], and [21].)

$\sigma(\xi)$	1
$\widetilde{\sigma}(\xi)$	$2\varepsilon-\xi^2$
$\widetilde{\tau}(\xi)$	0
k	2ε
$\pi(\xi)$	$\pm\xi$
$\tau(\xi)=\widetilde{\tau}+2\pi$	-2ξ
$\lambda=k+\pi'$	$2\varepsilon-1$
$\varphi(\xi)$	$e^{-\xi^2/2}$
$\rho(\xi)$	$e^{-\xi^2}$
$y_n(\xi)$	$C_nH_n(\xi)$
C_n^2	$\dfrac{1}{\sqrt{\pi}\,2^n n!}$

TABLE 1. Stationary Schrödinger equation for the harmonic potential $U(x)=\frac{1}{2}m\omega^2x^2$.

4. Bessel Functions

Let us also mention some solutions of the *Bessel equation*:

$$z^2u''+zu'+\left(z^2-\nu^2\right)u=0. \tag{4.1}$$

With the aid of the change of the function $u=\varphi(z)y$ when $\varphi(z)=z^\nu e^{iz}$ this equation can be reduced to the hypergeometric form

$$zy''+(2iz+2\nu+1)y'+i(2\nu+1)y=0 \tag{4.2}$$

(Table 2) and one can obtain the *Poisson integral representations* for the Bessel functions of the first kind, $J_\nu(z)$, and the Hankel functions of the first and second kind, $H_\nu^{(1)}(z)$ and $H_\nu^{(2)}(z)$:

$$J_\nu(z)=\frac{(z/2)^\nu}{\sqrt{\pi}\,\Gamma(\nu+1/2)}\int_{-1}^{1}\left(1-t^2\right)^{\nu-1/2}\cos(zt)\,dt, \tag{4.3}$$

$$H_\nu^{(1,2)}(z)=\sqrt{\frac{2}{\pi z}}\,\frac{e^{\pm i\left(z-\frac{\pi}{2}\nu-\frac{\pi}{4}\right)}}{\Gamma(\nu+1/2)}\int_0^\infty e^{-t}t^{\nu-1/2}\left(1\pm\frac{it}{2z}\right)^{\nu-1/2}dt, \tag{4.4}$$

where $\operatorname{Re}\nu>-1/2$. It is then possible to deduce from these integral representations all the remaining properties of these functions. (For details, see [24] and [35] or [37] and [38]).

5. Central Field: Spherical Harmonics

The stationary Schrödinger equation in the central field with the potential energy $U(r)$ is given by

$$\Delta\psi+\frac{2m}{\hbar^2}\left(E-U(r)\right)\psi=0. \tag{5.1}$$

$\sigma(z)$	z
$\widetilde{\sigma}(z)$	$z^2 - \nu^2$
$\widetilde{\tau}(z)$	1
k	$\pm 2i\nu$
$\pi(z)$	$\pm\nu \pm iz$
$\tau(z) = \widetilde{\tau} + 2\pi$	$1 + 2\nu + 2iz$
$\lambda = k + \pi'$	$i(2\nu + 1)$
$\varphi(z)$	$z^{\pm\nu} e^{\pm iz}$
$\rho(z)$	$z^{2\nu} e^{2iz}$

TABLE 2. Bessel's equation.

The Laplace operator in the spherical coordinates r, θ, φ has the form [23], [24]:

$$\Delta = \Delta_r + \frac{1}{r^2}\Delta_\omega \tag{5.2}$$

with

$$\Delta_r = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right), \qquad \Delta_\omega = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}. \tag{5.3}$$

and separation of the variables $\psi = R(r)Y(\theta,\varphi)$ gives

$$\Delta_\omega Y(\theta,\varphi) + \mu Y(\theta,\varphi) = 0, \tag{5.4}$$

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR(r)}{dr}\right) + \left(\frac{2m}{\hbar^2}\left(E - U(r)\right) - \frac{\mu}{r^2}\right)R(r) = 0. \tag{5.5}$$

Bounded single-valued solutions of equation (5.4) on the sphere S^2 exist only when $\mu = l(l+1)$ with $l = 0, 1, 2, \dots$. They are the spherical harmonics $Y = Y_{lm}(\theta,\varphi)$.

Looking for solutions in the form $Y = e^{im\varphi}f(\theta)$ with $m = 0, \pm1, \pm2, \dots$ one gets

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{dg}{d\theta}\right) - \frac{m^2}{\sin^2\theta}\,g + \mu g = 0. \tag{5.6}$$

The following change of variables $\xi = \cos\theta$ and $F(\xi) = f(\theta)$ results in the generalized equation of hypergeometric type:

$$\left(1-\xi^2\right)F'' - 2\xi F' + \left(\mu - \frac{m^2}{1-\xi^2}\right)F = 0, \tag{5.7}$$

with $\sigma(\xi) = 1 - \xi^2$, $\widetilde{\tau}(\xi) = -2\xi$ and $\widetilde{\sigma}(\xi) = \mu\left(1-\xi^2\right) - m^2$, which can be reduced to the simpler form by the standard substitution $F = \varphi\, y$:

$$\left(1-\xi^2\right)y'' - 2\left(|m|+1\right)\xi\, y' + \left(\mu - |m|\left(|m|+1\right)\right)y = 0 \tag{5.8}$$

Indeed, by (2.6)

$$\pi(\xi) = \pm\sqrt{(\mu-k)\xi^2 + k + m^2 - \mu}, \tag{5.9}$$

or

$$\pi(\xi)=\begin{cases}\pm|m|, & k=\mu\\ \pm|m|\,\xi, & k=\mu-m^2\end{cases} \tag{5.10}$$

where we should choose the case when the linear function $\tau=\widetilde{\tau}+2\pi$ will have a negative derivative and a zero on the interval $(-1,1)$.

Then

$$\frac{\varphi'}{\varphi}=\frac{-|m|\xi}{1-\xi^2},\qquad \ln\varphi=-|m|\int\frac{\xi\,d\xi}{1-\xi^2}=\frac{1}{2}\ln\left(1-\xi^2\right) \tag{5.11}$$

and

$$\varphi(\xi)=\left(1-\xi^2\right)^{|m|/2}=(\sin\theta)^{|m|}. \tag{5.12}$$

(see our complementary Mathematica notebook and Table 3 for further details of calculations).

The final result is given by

$$Y_{l\,m}(\theta,\varphi)=A_m\,\frac{e^{im\varphi}}{2^{|m|}\,l!}\sqrt{\frac{2l+1}{4\pi}\,(l-m)!(l+m)!}\;(\sin\theta)^{|m|}\;P_{l-|m|}^{(|m|,|m|)}(\cos\theta). \tag{5.13}$$

Here, $P_n^{(\alpha,\,\alpha)}(\xi)$ are the Jacobi polynomials (Table 15); $A_m=(-1)^m$, $m\geq 0$ and $A_m=1$, $m<0$. (See [23], [24], [36] for more details.)

$\sigma(\xi)$	$1-\xi^2,\qquad \xi=\cos\theta,\quad 0\leq\theta\leq\pi$
$\widetilde{\sigma}(\xi)$	$\mu(1-\xi^2)-m^2$
$\widetilde{\tau}(\xi)$	-2ξ
k	$\mu-m^2$
$\pi(\xi)$	$-\|m\|\xi$
$\tau(\xi)=\widetilde{\tau}+2\pi$	$-2\,(\|m\|+1)\,\xi$
$\lambda=k+\pi'$	$\mu-\|m\|\,(\|m\|+1)$
$\varphi(\xi)$	$(1-\xi^2)^{\|m\|/2}=(\sin\theta)^{\|m\|}$
$\rho(\xi)$	$(1-\xi^2)^{\|m\|}$
$y_n(\xi)$	$N_{l\,m}\,P_{l-\|m\|}^{(\|m\|,\,\|m\|)}\,(\cos\theta)\,,\quad n=l-\|m\|$
$N_{l\,m}$	$\dfrac{1}{2^{\|m\|}\,l!}\sqrt{\dfrac{2l+1}{2}\,(l-m)!(l+m)!}$

TABLE 3. Equation for spherical harmonics.

6. Nonrelativistic Coulomb Problem

In view of identity

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)=\frac{1}{r}\frac{d^2}{dr^2}\,(rR)\,, \tag{6.1}$$

the substitution $F(r) = rR(r)$ into (5.5) results in the standard radial equation

$$F'' + \left[\frac{2m_e}{\hbar^2}\left(E - U(r)\right) - \frac{l(l+1)}{r^2}\right] F = 0, \quad U(r) = -\frac{Ze^2}{r} \tag{6.2}$$

for the nonrelativistic Coulomb problem in spherical coordinates. In dimensional units,

$$F(r) = u(x), \quad x = \frac{r}{a_0}, \quad \varepsilon_0 = \frac{E}{E_0} \quad \left(a_0 = \frac{\hbar^2}{m_e e^2}, \quad E_0 = \frac{e^2}{a_0}\right) \tag{6.3}$$

the radial equation is a generalized equation of hypergeometric type,

$$u'' + \left[2\left(\varepsilon_0 + \frac{Z}{x}\right) - \frac{l(l+1)}{x^2}\right] u = 0, \tag{6.4}$$

where

$$\sigma(x) = x, \qquad \widetilde{\tau}(x) = 0, \qquad \widetilde{\sigma}(x) = 2\varepsilon_0 x^2 + 2Zx - l(l+1). \tag{6.5}$$

Therefore, one can utilize Nikiforov and Uvarov's approach in order to determine the corresponding wave functions and discrete energy levels.

We transform (6.4) to the equation of hypergeometric type (2.3). The linear function $\pi(x)$ takes the form

$$\pi(x) = \frac{1}{2} \pm \sqrt{\frac{1}{4} - 2\varepsilon_0 x^2 - 2x + l(l+1) + kx}, \tag{6.6}$$

or

$$\pi(x) = \frac{1}{2} \pm \left\{ \begin{array}{ll} \sqrt{-2\varepsilon_0}\ x + l + 1/2, & k = 2Z + (2l+1)\sqrt{-2\varepsilon_0} \\ \sqrt{-2\varepsilon_0}\ x - l - 1/2, & k = 2Z - (2l+1)\sqrt{-2\varepsilon_0} \end{array} \right. \tag{6.7}$$

where we should choose the case when the linear function $\tau = \widetilde{\tau} + 2\pi$ will have a negative derivative and a zero on $(0, +\infty)$:

$$\tau(x) = 2\left(l + 1 - x\sqrt{-2\varepsilon_0}\right).$$

This choice corresponds to

$$\pi(x) = l + 1 - x\sqrt{-2\varepsilon_0}, \quad \varphi(x) = x^{l+1} \exp\left(-x\sqrt{-2\varepsilon_0}\right)$$

and

$$\lambda = k + \pi' = 2\left[Z - (l+1)\sqrt{-2\varepsilon_0}\ \right].$$

The energy values are given by (2.7):

$$\varepsilon_0 = \frac{E}{E_0} = -\frac{Z^2}{2\left(n_r + l + 1\right)^2}, \qquad E_0 = \frac{e^2}{a_0}. \tag{6.8}$$

Here, $n = n_r + l + 1$ is known as the principal quantum number.

In order to use the Rodrigues formula, one finds

$$\frac{\rho'}{\rho} = \frac{\tau - \sigma'}{\sigma} = \frac{2l+1}{x} - \frac{2Z}{n},$$

or

$$\rho(x) = x^{2l+1} \exp\left(-\frac{2Z}{n} x\right), \qquad x = \frac{r}{a_0}.$$

Therefore,

$$y_{n_r}(x) = \frac{B_{n_r}}{x^{2l+1} e^{-\eta}} \frac{d^{n_r}}{dx^{n_r}} \left(x^{n_r + 2l + 1} e^{-\eta}\right) = L_{n_r}^{2l+1}(\eta), \tag{6.9}$$

where

$$\eta = \frac{2Z}{n} x = \frac{2Z}{n} \left(\frac{r}{a_0} \right) = 2x\sqrt{-2\varepsilon_0},$$

and, up to a constant,

$$F(r) = rR(r) = C_{nl}\ \eta^{l+1} e^{-\eta/2} L_{n_r}^{2l+1}(\eta). \tag{6.10}$$

In view of the normalization condition

$$1 = \int_0^\infty F^2\ dr = C_{nl}^2 \left(\frac{na_0}{2Z} \right) \int_0^\infty \eta^{2l+2} e^{-\eta} \left[L_{n_r}^{2l+1}(\eta) \right]^2\ d\eta,$$

the three-term recurrence relation

$$\eta L_n^\alpha = -(n+1) L_{n+1}^\alpha + (\alpha + 2n + 1) L_n^\alpha - (\alpha + n) L_{n-1}^\alpha,$$

and the orthogonality property of the Laguerre polynomials (Table 15), one gets

$$C_{nl}^2 = \frac{Z}{a_0 n^2} \frac{(n-l-1)!}{(n+l)!}. \tag{6.11}$$

More details can be found in [24] and [35]. (See also Appendices A and B.)

As a result, the nonrelativistic Coulomb wave functions obtained by the method of separation of the variables in spherical coordinates, see above, are

$$\psi = \psi_{nlm}(\mathbf{r}) = R_{nl}(r)\ Y_{lm}(\theta, \varphi), \tag{6.12}$$

where $Y_{lm}(\theta, \varphi)$ are the spherical harmonics, the radial functions $R_{nl}(r)$ are given in terms of the Laguerre polynomials [3], [8], [20], [24], [32]

$$R(r) = R_{nl}(r) = \frac{2}{n^2} \left(\frac{Z}{a_0} \right)^{3/2} \sqrt{\frac{(n-l-1)!}{(n+l)!}}\ e^{-\eta/2} \eta^l\ L_{n-l-1}^{2l+1}(\eta) \tag{6.13}$$

with

$$\eta = \frac{2Z}{n} \left(\frac{r}{a_0} \right), \qquad a_0 = \frac{\hbar^2}{m_e e^2} \tag{6.14}$$

and the normalization is

$$\int_0^\infty R_{nl}^2(r) r^2\ dr = 1. \tag{6.15}$$

Here $n = 1, 2, 3, \dots$ is the principal quantum number of the hydrogen-like atom in the nonrelativistic Schrödinger theory; $l = 0, 1, \dots, n-1$ and $m = -l, -l+1, \dots, l-1, l$ are the quantum numbers of the angular momentum and its projection on the z-axis, respectively. The corresponding discrete energy levels in the cgs units are given by Bohr's formula [28]:

$$E = E_n = -\frac{m_e Z^2 e^4}{2\hbar^2 n^2}, \tag{6.16}$$

where $n = 1, 2, 3, \dots$ is the principal quantum number; they do not depend on the quantum number of the orbital angular momenta l.

Remark. In the original Nikiforov–Uvarov approach, the variable coefficients $\sigma(x)$ and $\tau(x)$ in (2.3) should not depend on the eigenvalue λ. Here, we obtain

$$xy'' + 2\left(l + 1 - x\sqrt{-2\varepsilon_0} \right) y' + 2\left(Z - (l+1)\sqrt{-2\varepsilon_0} \right) y = 0. \tag{6.17}$$

$\sigma(x)$	x
$\widetilde{\sigma}(x)$	$2\varepsilon_0\, x^2 + 2Z\, x - l(l+1), \quad \varepsilon_0 = E/E_0$
$\widetilde{\tau}(x)$	0
k	$2Z - (2l+1)\sqrt{-2\varepsilon_0}$
$\pi(x)$	$l + 1 - \sqrt{-2\varepsilon_0}\, x$
$\tau(x) = \widetilde{\tau} + 2\pi$	$2\left(l + 1 - \sqrt{-2\varepsilon_0}\, x\right)$
$\lambda = k + \pi'$	$2\left(Z - (l+1)\sqrt{-2\varepsilon_0}\right)$
$\varphi(x)$	$x^{l+1} e^{-x\sqrt{-2\varepsilon_0}}$
$\rho(x)$	$x^{2l+1} e^{-(2Z\ x)/n}, \quad x = r/a_0$
$y_{n_r}(x)$	$C_{n_r} L_{n_r}^{2l+1}(\eta), \quad \eta = \dfrac{2Z}{n} x = \dfrac{2Z}{n}\left(\dfrac{r}{a_0}\right)$
$C_{n_r}^2$	$\dfrac{Z}{a_0 n^2} \dfrac{(n-l-1)!}{(n+l)!}, \quad n_r = n - l - 1$

TABLE 4. Schrödinger equation for the Coulomb potential $U(r) = -\dfrac{Ze^2}{r}$. Dimensionless quantities:

$$r = a_0 x, \quad a_0 = \frac{\hbar^2}{m_e e^2} \simeq 0.5 \cdot 10^{-8} \text{ cm}, \quad E_0 = \frac{e^2}{a_0}; \quad R(r) = F(x) = \frac{u(x)}{x}.$$

Nonetheless, the change of variables $y(x) = Y(\eta)$ with $\eta = 2x\sqrt{-2\varepsilon_0}$ results in

$$\eta Y'' + (2l + 2 - \eta)\, Y' + \left(\frac{Z}{\sqrt{-2\varepsilon_0}} - l - 1\right) Y = 0. \tag{6.18}$$

Thus the Nikiforov–Uvarov method can be applied and the uniqueness of square integrable solutions holds.

In a similar fashion, one can consider solution of the Kepler problem in the so-called parabolic coordinates, which is important in the theory of Stark effect [30], [20].

7. Relativistic Schrödinger Equation

The stationary relativistic Schrödinger equation has the form [2], [6], [15], [32]:

$$\left(E + \frac{Ze^2}{r}\right)^2 \chi = \left(-\hbar^2 c^2 \Delta + m^2 c^4\right) \chi. \tag{7.1}$$

We separate the variables in spherical coordinates, $\chi(r, \theta, \varphi) = R(r) Y_{lm}(\theta, \varphi)$, where $Y_{lm}(\theta, \varphi)$ are the spherical harmonics with familiar properties [36]. As a result,

$$\frac{1}{r^2} \frac{d}{dr}\left(r^2 \frac{dR}{dr}\right) + \left[\frac{\left(E + Ze^2/r\right)^2 - m^2 c^4}{\hbar^2 c^2} - \frac{l(l+1)}{r^2}\right] R = 0 \qquad (l = 0, 1, 2, \dots). \tag{7.2}$$

In the dimensionless quantities,

$$\varepsilon = \frac{E}{mc^2}, \qquad x = \beta r = \frac{mc}{\hbar} r, \qquad \mu = \frac{Ze^2}{\hbar c}, \tag{7.3}$$

for the new radial function,

$$R(r) = F(x) = \frac{u(x)}{x}, \tag{7.4}$$

one gets

$$\frac{1}{x^2}\frac{d}{dx}\left(x^2 \frac{dF}{dx}\right) + \left[\left(\varepsilon + \frac{\mu}{x}\right)^2 - 1 - \frac{l(l+1)}{x^2}\right] F = 0. \tag{7.5}$$

Given the identity $(x^2F')' = x(xF)''$, we obtain

$$u'' + \left[\left(\varepsilon + \frac{\mu}{x}\right)^2 - 1 - \frac{l(l+1)}{x^2}\right] u = 0. \tag{7.6}$$

This is the generalized equation of hypergeometric form (2.1), when

$$\sigma(x) = x, \qquad \widetilde{\tau}(x) \equiv 0, \qquad \widetilde{\sigma}(x) = \left(\varepsilon^2 - 1\right) x^2 + 2\mu\varepsilon x + \mu^2 - l(l+1) \tag{7.7}$$

The normalization condition takes the form:

$$\int_0^\infty R^2(r) r^2 \, dr = 1, \qquad \text{or} \qquad \int_0^\infty u^2(x)\, dx = \beta^3, \quad \beta = \frac{mc}{\hbar}. \tag{7.8}$$

Here, $u = \varphi\, y$. For further computational details, see our supplementary Mathematica notebook, as well as Refs. [2] and [24]. Final results are presented in Table 5.

In particular, one gets Schrödinger's fine structure formula (for a charged spin-zero particle in the Coulomb field):

$$E = E_{n_r} = \frac{mc^2}{\sqrt{1 + \left(\dfrac{\mu}{n_r + \nu + 1}\right)^2}} \qquad (n = n_r = 0, 1, 2, \dots). \tag{7.9}$$

Here,

$$\mu = \frac{Ze^2}{\hbar c}, \qquad \nu = -\frac{1}{2} + \sqrt{\left(l + \frac{1}{2}\right)^2 - \mu^2}. \tag{7.10}$$

The corresponding eigenfunctions are given by the Rodrigues-type formula

$$y_n(x) = \frac{B_n}{x^{2\nu+1} e^{-2ax}} \frac{d^n}{dx^n}\left(x^{n+2\nu+1} e^{-2ax}\right) = C_n L_n^{2\nu+1}(2ax). \tag{7.11}$$

Up to a constant, they are Laguerre polynomials (Table 15). In view of the normalization condition (7.8):

$$\begin{aligned} \beta^3 &= \int_0^\infty u^2(x)\, dx = C_n^2 \int_0^\infty \left[\varphi(x) L_n^{2\nu+1}(2ax)\right]^2 \, dx \\ &= \frac{C_n^2}{(2a)^{2\nu+3}} \int_0^\infty e^{-\xi}\, \xi^{2\nu+2} \left(L_n^{2\nu+1}(\xi)\right)^2 \, d\xi, \quad \xi = 2ax. \end{aligned} \tag{7.12}$$

The corresponding integral is given by (see [34], [35], and Appendix B):

$$I_1 = J_{nn1}^{\alpha\alpha} = \int_0^\infty e^{-x} x^{\alpha+1} \left(L_n^\alpha(x)\right)^2 \, dx = (\alpha + 2n + 1)\frac{\Gamma(\alpha + n + 1)}{n!}. \tag{7.13}$$

As a result,

$$C_n = 2(a\beta)^{3/2}(2a)^{\nu}\sqrt{\frac{n!}{\Gamma(2\nu+n+2)}}. \tag{7.14}$$

The normalized radial eigenfunctions, corresponding to the relativistic energy levels (7.9), are explicitly given by

$$R(r) = R_{n_r}(r) = 2(a\beta)^{3/2}\sqrt{\frac{n_r!}{\Gamma(2\nu+n_r+2)}}\, \xi^{\nu} e^{-\xi/2}\, L_{n_r}^{2\nu+1}(\xi), \tag{7.15}$$

where

$$\xi = 2ax = 2a\beta r = 2\sqrt{1-\varepsilon^2}\,\frac{mc}{\hbar}\, r. \tag{7.16}$$

(More details can be found in [2], [6], [32].)

Let us analyze a nonrelativistic limit of Schrödinger's fine structure formula (7.9)–(7.10):

$$\begin{aligned}\varepsilon_{\text{Schrödinger}} = \frac{E_{n_r,l}}{mc^2} &= \frac{1}{\sqrt{1+\dfrac{\mu^2}{\left(n_r+\frac{1}{2}+\sqrt{\left(l+\frac{1}{2}\right)^2-\mu^2}\right)^2}}} \\ &= 1-\frac{\mu^2}{2n^2}-\frac{\mu^4}{2n^4}\left(\frac{n}{l+1/2}-\frac{3}{4}\right)+\mathrm{O}(\mu^6), \quad \mu\to 0, \end{aligned} \tag{7.17}$$

which can be derived by a direct Taylor expansion and/or verified by a computer algebra system (see our supplementary Mathematica notebook). Here, $n = n_r+l+1$ is the corresponding nonrelativistic principal quantum number. The first term in this expansion is simply the rest mass energy $E_0 = mc^2$ of the charged spin-zero particle, the second term coincides with the energy eigenvalue in the nonrelativistic Schrödinger theory and the third term gives the so-called fine structure of the energy levels, which removes the degeneracy between states of the same n and different l.

Once again, our equation,

$$xy'' + 2(\nu+1-ax)y' + 2\left(\mu\varepsilon-(\nu+1)a\right)y = 0, \tag{7.18}$$

by the change of variables $y(x) = Y(\xi)$ with $\xi = 2ax$ can be transformed into the required form:

$$\xi Y'' + (2\nu+2-\xi)Y'\left(\frac{\mu\varepsilon}{\sqrt{1-\varepsilon^2}}-\nu-1\right)Y = 0. \tag{7.19}$$

Therefore, the set of the square integrable solutions above is unique.

8. Relativistic Coulomb Problem: Dirac Equation

8.1. **System of radial equations.** The radial Dirac equations are derived in Refs. [24], [34], and [35] by separation of variables in spherical coordinates (see also [3], [6], [8], [10], and [15]). Then the radial functions $F(r)$ and $G(r)$ satisfy the system of two first-order ordinary differential equations

$$\frac{dF}{dr} + \frac{1+\kappa}{r}\, F = \frac{mc^2+E-U(r)}{\hbar c}\, G, \tag{8.1}$$

$$\frac{dG}{dr} + \frac{1-\kappa}{r}\, G = \frac{mc^2-E+U(r)}{\hbar c}\, F, \tag{8.2}$$

$\sigma(x)$	x
$\widetilde{\sigma}(x)$	$(\varepsilon^2-1)\ x^2+2\mu\varepsilon\ x+\mu^2-l(l+1)$
$\widetilde{\tau}(x)$	0
k	$2\mu\varepsilon-(2\nu+1)\sqrt{1-\varepsilon^2}, \quad \nu=-\dfrac{1}{2}+\sqrt{\left(l+\dfrac{1}{2}\right)^2-\mu^2}$
$\pi(x)$	$\nu+1-a\ x, \qquad a=\sqrt{1-\varepsilon^2}$
$\tau(x)=\widetilde{\tau}+2\pi$	$2\left(\nu+1-a\ x\right), \quad \tau'<0$
$\lambda=k+\pi'$	$2\left(\mu\varepsilon-(\nu+1)a\right)$
$\varphi(x)$	$x^{\nu+1}e^{-a\ x}$
$\rho(x)$	$x^{2\nu+1}e^{-2a\ x}$
$y_{n_r}(x)$	$C_{n_r}L_{n_r}^{2\nu+1}(\xi), \quad \xi=2ax=2a\beta r=2\sqrt{1-\varepsilon^2}\dfrac{mc}{\hbar}r$
C_{n_r}	$2(a\beta)^{3/2}(2a)^{\nu}\sqrt{\dfrac{n_r!}{(\nu+n_r+1)\Gamma(2\nu+n_r+2)}}$

TABLE 5. Relativistic Schrödinger equation for the Coulomb potential $U(r)=-\dfrac{Ze^2}{r}$. Dimensionless quantities:

$$\varepsilon=\frac{E}{mc^2}, \quad x=\beta r=\frac{mc}{\hbar}r, \quad \mu=\frac{Ze^2}{\hbar c}; \qquad R(r)=F(x)=\frac{u(x)}{x}.$$

where $\kappa=\kappa_\pm=\pm(j+1/2)=\pm1,\pm2,\pm3,\ldots$ respectively. For the relativistic Coulomb problem, when $U=-Ze^2/r$, we introduce the dimensionless quantities

$$\varepsilon=\frac{E}{mc^2}, \qquad x=\beta r=\frac{mc}{\hbar}r, \qquad \mu=\frac{Ze^2}{\hbar c} \tag{8.3}$$

and change the variable in radial functions

$$f(x)=F(r), \qquad g(x)=G(r). \tag{8.4}$$

The Dirac radial system becomes

$$\frac{df}{dx}+\frac{1+\kappa}{x}\ f=\left(1+\varepsilon+\frac{\mu}{x}\right)g, \tag{8.5}$$

$$\frac{dg}{dx}+\frac{1-\kappa}{x}\ g=\left(1-\varepsilon-\frac{\mu}{x}\right)f. \tag{8.6}$$

(One can show later that in the nonrelativistic limit, $c\to\infty$, the following estimate holds: $|f(x)|\gg|g(x)|$; see, for example, Refs. [24], [34], and [35] for more details.)

8.2. **Decoupling of the radial system.** We follow [24] with somewhat different details. Let us rewrite the system (8.5)–(8.6) in a matrix form. If

$$u = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \begin{pmatrix} xf(x) \\ xg(x) \end{pmatrix}, \qquad u' = \begin{pmatrix} u_1' \\ u_2' \end{pmatrix}. \tag{8.7}$$

Then

$$u' = Au, \tag{8.8}$$

where

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} = \begin{pmatrix} -\dfrac{\kappa}{x} & 1+\varepsilon+\dfrac{\mu}{x} \\ 1-\varepsilon-\dfrac{\mu}{x} & \dfrac{\kappa}{x} \end{pmatrix}. \tag{8.9}$$

To find $u_1(x)$, we eliminate $u_2(x)$ from the system (8.8), obtaining a second-order differential equation

$$\begin{aligned} u_1'' - \left(a_{11} + a_{22} + \frac{a_{12}'}{a_{12}}\right) u_1' \\ + \left(a_{11}a_{22} - a_{12}a_{21} - a_{11}' + \frac{a_{12}'}{a_{12}}\, a_{11}\right) u_1 = 0. \end{aligned} \tag{8.10}$$

Similarly, eliminating $u_1(x)$, one gets an equation for $u_2(x)$:

$$\begin{aligned} u_2'' - \left(a_{11} + a_{22} + \frac{a_{21}'}{a_{21}}\right) u_2' \\ + \left(a_{11}a_{22} - a_{12}a_{21} - a_{22}' + \frac{a_{21}'}{a_{21}}\, a_{22}\right) u_2 = 0. \end{aligned} \tag{8.11}$$

The components of the matrix A have the following generic form

$$a_{ik} = b_{ik} + c_{ik}/x, \tag{8.12}$$

where b_{ik} and c_{ik} are constants. Equations (8.10) and (8.11) are not generalized equations of hypergeometric type (2.1). Indeed,

$$\frac{a_{12}'}{a_{12}} = -\frac{c_{12}}{c_{12}x + b_{12}x^2},$$

and the coefficients of $u_1'(x)$ and $u_1(x)$ in (8.10) are

$$\begin{aligned} a_{11} + a_{22} + \frac{a_{12}'}{a_{12}} &= \frac{p_1(x)}{x} - \frac{c_{12}}{c_{12}x + b_{12}x^2}, \\ a_{11}a_{22} - a_{12}a_{21} - a_{11}' + \frac{a_{12}'}{a_{12}}a_{11} &= \frac{p_2(x)}{x^2} - \frac{c_{12}(c_{11} + b_{11}x)}{(c_{12} + b_{12}x)x^2}, \end{aligned}$$

where $p_1(x)$ and $p_2(x)$ are polynomials of degrees at most one and two, respectively (see supplementary Mathematica notebook for their explicit forms). Equation (8.10) will become a generalized equation of hypergeometric type (2.1) with $\sigma(x) = x$ if either $b_{12} = 0$ or $c_{12} = 0$.

8.3. **Similarity transformation.** The following consideration helps. By a linear transformation

$$\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = C \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} \tag{8.13}$$

with a nonsingular matrix C that is independent of x, we transform the original system (8.8) to a similar one

$$v' = \widetilde{A} v, \tag{8.14}$$

where

$$v = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}, \qquad \widetilde{A} = CAC^{-1} = \begin{pmatrix} \widetilde{a}_{11} & \widetilde{a}_{12} \\ \widetilde{a}_{21} & \widetilde{a}_{22} \end{pmatrix}.$$

The new coefficients $\widetilde{a}_{ik}$ are linear combinations of the original ones a_{ik}. Hence they have a similar form

$$\widetilde{a}_{ik} = \widetilde{b}_{ik} + \widetilde{c}_{ik}/x, \tag{8.15}$$

where $\widetilde{b}_{ik}$ and $\widetilde{c}_{ik}$ are constants.

The equations for $v_1(x)$ and $v_2(x)$ are similar to (8.10) and (8.11):

$$\begin{aligned} v_1'' &- \left(\widetilde{a}_{11} + \widetilde{a}_{22} + \frac{\widetilde{a}_{12}'}{\widetilde{a}_{12}} \right) v_1' \\ &+ \left(\widetilde{a}_{11}\widetilde{a}_{22} - \widetilde{a}_{12}\widetilde{a}_{21} - \widetilde{a}_{11}' + \frac{\widetilde{a}_{12}'}{\widetilde{a}_{12}}\, \widetilde{a}_{11} \right) v_1 = 0, \end{aligned} \tag{8.16}$$

$$\begin{aligned} v_2'' &- \left(\widetilde{a}_{11} + \widetilde{a}_{22} + \frac{\widetilde{a}_{21}'}{\widetilde{a}_{21}} \right) v_2' \\ &+ \left(\widetilde{a}_{11}\widetilde{a}_{22} - \widetilde{a}_{12}\widetilde{a}_{21} - \widetilde{a}_{22}' + \frac{\widetilde{a}_{21}'}{\widetilde{a}_{21}}\, \widetilde{a}_{22} \right) v_2 = 0. \end{aligned} \tag{8.17}$$

The calculation of the coefficients in (8.16) and (8.17) is facilitated by a similarity of the matrices A and $\widetilde{A}$:

$$\widetilde{a}_{11} + \widetilde{a}_{22} = a_{11} + a_{22}, \qquad \widetilde{a}_{11}\widetilde{a}_{22} - \widetilde{a}_{12}\widetilde{a}_{21} = a_{11}a_{22} - a_{12}a_{21}.$$

By a previous consideration, in order for (8.16) to be an equation of hypergeometric type, it is sufficient to choose either $\widetilde{b}_{12} = 0$ or $\widetilde{c}_{12} = 0$. Similarly, for (8.17): either $\widetilde{b}_{21} = 0$ or $\widetilde{c}_{21} = 0$. These conditions impose certain restrictions on our choice of the transformation matrix C. Let

$$C = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}. \tag{8.18}$$

Then

$$C^{-1} = \frac{1}{\Delta} \begin{pmatrix} \delta & -\beta \\ -\gamma & \alpha \end{pmatrix}, \qquad \Delta = \det C = \alpha\delta - \beta\gamma,$$

and

$$\widetilde{A} = CAC^{-1} \tag{8.19}$$

$$= \frac{1}{\Delta}\begin{pmatrix} a_{11}\alpha\delta - a_{12}\alpha\gamma + a_{21}\beta\delta - a_{22}\beta\gamma & a_{12}\alpha^2 - a_{21}\beta^2 + (a_{22}-a_{11})\alpha\beta \\ a_{21}\delta^2 - a_{12}\gamma^2 + (a_{11}-a_{22})\gamma\delta & a_{12}\alpha\gamma - a_{11}\beta\gamma + a_{22}\alpha\delta - a_{21}\beta\delta \end{pmatrix}.$$

(Here, we have corrected typos in Eqs. (3.74) of [35]; see also [24] and the supplementary Mathematica notebook.) For the Dirac system (8.8)–(8.9):

$$a_{11} = -\frac{\kappa}{x}, \qquad a_{12} = 1 + \varepsilon + \frac{\mu}{x},$$
$$a_{21} = 1 - \varepsilon - \frac{\mu}{x}, \qquad a_{22} = \frac{\kappa}{x}$$

and

$$\Delta\, \widetilde{a}_{12} = \alpha^2 - \beta^2 + \left(\alpha^2+\beta^2\right)\varepsilon + \frac{\left(\alpha^2+\beta^2\right)\mu + 2\alpha\beta\kappa}{x}, \tag{8.20}$$

$$\Delta\, \widetilde{a}_{21} = \delta^2 - \gamma^2 - \left(\delta^2+\gamma^2\right)\varepsilon - \frac{\left(\delta^2+\gamma^2\right)\mu + 2\gamma\delta\kappa}{x}. \tag{8.21}$$

The	condition	$\widetilde{b}_{12} = 0$	yields	$(1+\varepsilon)\alpha^2 - (1-\varepsilon)\beta^2 = 0,$
”	”	$\widetilde{c}_{12} = 0$	”	$\left(\alpha^2+\beta^2\right)\mu + 2\alpha\beta\kappa = 0,$
”	”	$\widetilde{b}_{21} = 0$	”	$(1+\varepsilon)\gamma^2 - (1-\varepsilon)\delta^2 = 0,$
”	”	$\widetilde{c}_{21} = 0$	”	$\left(\delta^2+\gamma^2\right)\mu + 2\gamma\delta\kappa = 0.$

We see that there are several possibilities to choose the elements α, β, γ, δ of the transition matrix C. All quantum mechanics textbooks use the original one, namely, $\widetilde{b}_{12} = 0$ and $\widetilde{b}_{21} = 0$, due to Darwin [7] and Gordon [14]. Nikiforov and Uvarov [24] take another path, they choose $\widetilde{c}_{12} = 0$ and $\widetilde{c}_{21} = 0$ and show that it is more convenient for taking the nonrelativistic limit $c \to \infty$. These conditions are satisfied if

$$C = \begin{pmatrix} \mu & \nu - \kappa \\ \nu - \kappa & \mu \end{pmatrix}, \tag{8.22}$$

where $\nu = \sqrt{\kappa^2 - \mu^2}$, and we finally arrive at the following system of first-order equations for $v_1(x)$ and $v_2(x)$:

$$v_1' = \left(\frac{\varepsilon\mu}{\nu} - \frac{\nu}{x}\right) v_1 + \left(1 + \frac{\varepsilon\kappa}{\nu}\right) v_2, \tag{8.23}$$

$$v_2' = \left(1 - \frac{\varepsilon\kappa}{\nu}\right) v_1 + \left(\frac{\nu}{x} - \frac{\varepsilon\mu}{\nu}\right) v_2. \tag{8.24}$$

Here

$$\operatorname{Tr}\, \widetilde{A} = \widetilde{a}_{11} + \widetilde{a}_{22} = 0, \quad \det \widetilde{A} = \varepsilon^2 - 1 + \frac{2\varepsilon\mu}{x} - \frac{\nu^2}{x^2}, \quad \nu^2 = \kappa^2 - \mu^2, \tag{8.25}$$

which is simpler than the original choice in [24]. The corresponding second-order differential equations (8.16)–(8.17) become

$$v_1'' + \frac{\left(\varepsilon^2-1\right)x^2 + 2\varepsilon\mu x - \nu(\nu+1)}{x^2}\, v_1 = 0, \tag{8.26}$$

$$v_2'' + \frac{\left(\varepsilon^2-1\right)x^2 + 2\varepsilon\mu x - \nu(\nu-1)}{x^2}\, v_2 = 0. \tag{8.27}$$

They are generalized equations of hypergeometric type (2.1) of the simplest form $\widetilde{\tau} = 0$, thus resembling the one-dimensional Schrödinger equation; the second equation can be obtained from the first one by replacing $\nu \to -\nu$ (see also Eqs. (3.81)–(3.82) in Ref. [35]).

8.4. **Nikiforov–Uvarov paradigm.** All details of further calculations are presented in Table 6 (see also our supplementary Mathematica notebook and Refs. [24], [34], and [35] for more details). Then the corresponding energy levels $\varepsilon = \varepsilon_n$ are determined by

$$\varepsilon\mu = a(\nu + n + 1), \tag{8.28}$$

and the eigenfunctions are given by the Rodrigues–type formula

$$y_n(x) = \frac{C_n}{\rho(x)} \left(\sigma^n(x)\rho(x)\right)^{(n)} = C_n\, x^{-2\nu-1} e^{2ax} \frac{d^n}{dx^n} \left(x^{2\nu+n+1} e^{-2ax}\right). \tag{8.29}$$

These functions are, up to certain constants, Laguerre polynomials $L_n^{2\nu+1}(\xi)$ with $\xi = 2ax$. The corresponding eigenfunctions have the form

$$v_1(x) = \begin{cases} 0, \qquad n = 0, \\ A_n \xi^{\nu+1} e^{-\xi/2} L_{n-1}^{2\nu+1}(\xi), \qquad n = 1, 2, 3, \dots \, . \end{cases} \tag{8.30}$$

They are square integrable functions on $(0, \infty)$. The counterparts are

$$v_2(x) = B_n \xi^{\nu} e^{-\xi/2} L_n^{2\nu-1}(\xi), \qquad n = 0, 1, 2, \dots \, . \tag{8.31}$$

It is easily seen that the solution $\varepsilon = -\nu/\kappa$ is included in this formula when $n = 0$.

As a result,

$$xf(x) = \frac{B_n}{2\nu(\kappa - \nu)} \xi^{\nu} e^{-\xi/2} \left(f_1 \xi L_{n-1}^{2\nu+1}(\xi) + f_2 L_n^{2\nu-1}(\xi)\right), \tag{8.32}$$

$$xg(x) = \frac{B_n}{2\nu(\kappa - \nu)} \xi^{\nu} e^{-\xi/2} \left(g_1 \xi L_{n-1}^{2\nu+1}(\xi) + g_2 L_n^{2\nu-1}(\xi)\right), \tag{8.33}$$

where

$$f_1 = \frac{a\mu}{\varepsilon\kappa - \nu}, \quad f_2 = \kappa - \nu, \quad g_1 = \frac{a(\kappa - \nu)}{\varepsilon\kappa - \nu}, \quad g_2 = \mu. \tag{8.34}$$

(These formulas remain valid for $n = 0$; in this case the terms containing $L_{-1}^{2\nu+1}(\xi)$ have to be taken to be zero.) Thus we derive the representation for the radial functions up to the constant B_n in terms of Laguerre polynomials. The normalization condition

$$\int_{\mathbb{R}^3} \psi^\dagger\ \psi\ dv = \int_0^\infty r^2 \left(F^2(r) + G^2(r)\right)\, dr = 1 \tag{8.35}$$

gives the value of this constant as follows [24]:

$$B_n = a\beta^{3/2} \sqrt{\frac{(\kappa - \nu)(\varepsilon\kappa - \nu)n!}{\mu\Gamma(n + 2\nu)}}. \tag{8.36}$$

(This is verified in Section 5.4 of Ref. [35]. Observe that Eq. (8.36) applies when $n = 0$.)

8.5. **Summary: wave functions and energy levels.** The end results, namely, the complete wave functions and the corresponding discrete energy levels, are given by Eqs. (3.11)–(3.17) of Ref. [35]. The WKB, or semiclassical, approximation for the Dirac equation with Coulomb potential is discussed in [2].

The relativistic energy levels of an electron in the central Coulomb field are given by

$$E = E_{n_r,j} = \frac{mc^2}{\sqrt{1+\mu^2/(n_r+\nu)^2}}, \quad \mu = \frac{Ze^2}{\hbar c} \quad (n_r = 0, 1, 2, \dots). \tag{8.37}$$

In Dirac's theory,

$$\nu = \nu_{\text{Dirac}} = \sqrt{(j+1/2)^2 - \mu^2}, \tag{8.38}$$

where $j = 1/2, 3/2, 5/2, \dots$ is the total angular momentum including the spin of the relativistic electron. More details on the solution of this problem, including the nonrelativistic limit, can be found in [24], [34], [35] (following Nikiforov–Uvarov's paradigm), or in classical sources [3], [6], [7], [10], [14], [32].

In Dirac's theory of the relativistic electron, the corresponding limit has the form [3], [6], [32], [35]:

$$\varepsilon_{\text{Dirac}} = \frac{E_{n_r,j}}{mc^2} = 1 - \frac{\mu^2}{2n^2} - \frac{\mu^4}{2n^4}\left(\frac{n}{j+1/2} - \frac{3}{4}\right) + \mathrm{O}(\mu^6), \quad \mu \to 0, \tag{8.39}$$

where $n = n_r + j + 1/2$ is the principal quantum number of the nonrelativistic hydrogenlike atom. Once again, the first term in this expansion is the rest mass energy of the relativistic electron, the second term coincides with the energy eigenvalue in the nonrelativistic Schrödinger theory and the third term gives the so-called fine structure of the energy levels — the correction obtained for the energy in the Pauli approximation which includes the interaction of the spin of the electron with its orbital angular momentum. (See our supplementary Mathematica notebook for a computer algebra proof.)

9. A Model of the 3D-confinement Potential

Looking for solutions of the Schrödinger equation (5.1) in spherical coordinates,

$$\psi = \frac{1}{r} R(r) Y_{lm}(\theta, \varphi), \tag{9.1}$$

with the following model central field potential,

$$U(r) = V_0 \left(\frac{r}{a} - \frac{a}{r}\right)^2, \tag{9.2}$$

one gets the radial equation of the form

$$R'' + \frac{2m}{\hbar^2}\left[(E + 2V_0) - V_0\left(\frac{a^2}{r^2} + \frac{r^2}{a^2}\right) - \frac{\hbar^2 l(l+1)}{2mr^2}\right] R = 0 \quad (l = 0, 1, 2, \dots). \tag{9.3}$$

This is not a generalized equation of hypergeometric type and, therefore, cannot be treated right away by the Nikiforov–Uvarov method. By using the substitution

$$R(r) = u(\xi), \qquad \xi = \alpha r^2, \qquad \alpha^2 = \frac{2mV_0}{\hbar^2 a^2}, \tag{9.4}$$

$\sigma(x)$	x
$\widetilde{\sigma}(x)$	$(\varepsilon^2-1)\ x^2+2\mu\varepsilon\ x-\nu(\nu+1);\ \nu=\sqrt{\kappa^2-\mu^2},\ \kappa=\pm\left(j+\dfrac{1}{2}\right)$
$\widetilde{\tau}(x)$	0
k	$2\mu\varepsilon\pm\sqrt{1-\varepsilon^2}(2\nu+1)$
$\pi(x)$	$\dfrac{1}{2}\pm\left(\sqrt{1-\varepsilon^2}\,x\pm\left(\nu+\dfrac{1}{2}\right)\right)$
$\tau(x)=\widetilde{\tau}+2\pi$	$2(\nu+1-a\ x),\quad a=\sqrt{1-\varepsilon^2};\quad \tau'<0$
$\lambda=k+\pi'$	$2\left(\mu\varepsilon-(\nu+1)a\right)$
$\varphi(x)$	$x^{\nu+1}e^{-a\ x}$
$\rho(x)$	$x^{2\nu+1}e^{-2a\ x}$
$y_n(x)$	$A_nL_n^{2\nu+1}(\xi);\ \xi=2ax=2a\beta r=2\sqrt{1-\varepsilon^2}\dfrac{mc}{\hbar}r,\ n=n_r=0,1,\dots$
$A_n=\dfrac{a}{\kappa\varepsilon-\nu}\,B_n$	$B_n=a\beta^{3/2}\sqrt{\dfrac{(\kappa-\nu)(\kappa\varepsilon-\nu)\,n!}{\mu\Gamma(2\nu+n)}}$

Table 6. Dirac equation for the Coulomb potential $U(r)=-\dfrac{Ze^2}{r}$.
Dimensionless quantities:
$\varepsilon=\dfrac{E}{mc^2}$, $x=\beta r=\dfrac{mc}{\hbar}r$, $\mu=\dfrac{Ze^2}{\hbar c}$; $F(r)=f(x)=\dfrac{u_1(x)}{x}$, $G(r)=g(x)=\dfrac{u_2(x)}{x}$.

we finally obtain equation (2.1) with the following coefficients:

$$\sigma(\xi)=\xi,\quad \widetilde{\tau}=\frac{1}{2},\quad \widetilde{\sigma}(\xi)=\frac{1}{4}\left[\frac{2m}{\alpha\hbar^2}(E+2V_0)\xi-\alpha^2a^4-l(l+1)-\xi^2\right]. \tag{9.5}$$

In the Nikiforov–Uvarov method, the energy levels and the corresponding radial wave functions can be obtained by (2.7) and (2.8). As a result, they are given by

$$E_{n,l}=\hbar\sqrt{\frac{8V_0}{ma^2}}\left[n+\frac{1}{2}+\frac{1}{2}\left(\sqrt{\frac{2mV_0a^2}{\hbar^2}+\left(l+\frac{1}{2}\right)^2}-\sqrt{\frac{2mV_0a^2}{\hbar^2}}\right)\right] \tag{9.6}$$

and

$$R(r)=R_{n,l}(r)=C_n\xi^{(\beta-1/2)/2}\exp(-\xi/2)L_n^{\beta}(\xi), \tag{9.7}$$

provided

$$\int_0^\infty R^2(r)\,dr=1, \tag{9.8}$$

respectively. Here

$$C_n^2=\frac{2n!\sqrt{\alpha}}{\Gamma(\beta+n+1)},\qquad \alpha=\frac{\sqrt{2mV_0}}{\hbar a},\qquad \beta=\sqrt{\frac{2mV_0a^2}{\hbar^2}+\left(l+\frac{1}{2}\right)^2}. \tag{9.9}$$

Details of the calculations are presented in Table 7. (The case $l = 0$ corresponds to a one-dimensional problem from [12].)

In this case, the spectrum is linear, as for the harmonic oscillator. There is no continuous spectrum thus resembling the confinement property in quantum chromodynamics.

$\sigma(\xi)$	ξ
$\widetilde{\sigma}(\xi)$	$\frac{1}{4}\left[\frac{2m}{\alpha\hbar^2}(E+2V_0)\xi - \alpha^2a^4 - l(l+1) - \xi^2\right]$
$\widetilde{\tau}(\xi)$	$1/2$
k	$\frac{1}{2}\left[\frac{m}{\alpha\hbar^2}(E+2V_0) \pm \sqrt{\alpha^2a^4+(l+1/2)^2}\right]$
$\pi(\xi)$	$\frac{1}{4} \pm \frac{\xi \pm \sqrt{\alpha^2a^4+(l+1/2)^2}}{2}$
$\tau(\xi) = \widetilde{\tau} + 2\pi$	$1+\beta-\xi, \quad \beta = \sqrt{\frac{2mV_0a^2}{\hbar^2}+\left(l+\frac{1}{2}\right)^2}$
$\lambda = k + \pi'$	$\frac{1}{2}\left[\frac{m}{\alpha\hbar^2}(E+2V_0) - \sqrt{\alpha^2a^4+(l+1/2)^2}\right] - \frac{1}{2}$
$\varphi(\xi)$	$\xi^{\nu/2}\exp(-\xi/2),\ \nu = \beta + \frac{1}{2} = \frac{1}{2} + \sqrt{\alpha^2a^4+\left(l+\frac{1}{2}\right)^2}$
$\rho(\xi)$	$\xi^{\beta}\exp(-\xi)$
$y_n(\xi)$	$C_nL_n^{\beta}(\xi), \quad \xi = \alpha r^2, \quad n = 0, 1, \ldots$
C_n^2	$\frac{2n!\sqrt{\alpha}}{\Gamma(\beta+n+1)}, \quad \alpha = \frac{\sqrt{2mV_0}}{\hbar a}$

TABLE 7. A model of the $3D$-confinement potential $U(r) = V_0\left(\frac{r}{a}-\frac{a}{r}\right)^2$. Dimensionless quantities:

$$\xi = \alpha r^2, \quad \alpha = \frac{\sqrt{2mV_0}}{\hbar a}, \quad R(r) = u(\xi).$$

10. $3D$-Spherical Oscillator

Looking for solutions of the Schrödinger equation (5.1) with harmonic potential

$$U(r) = \frac{1}{2}m\omega^2r^2 \tag{10.1}$$

in spherical coordinates (9.1), one gets the following radial equation:

$$R'' + \left[\frac{2mE}{\hbar^2} - \frac{m^2\omega^2}{\hbar^2}r^2 - \frac{l(l+1)}{r^2}\right]R = 0 \qquad (l = 0, 1, 2, \ldots). \tag{10.2}$$

Using the abbreviations [8]

$$\frac{2mE}{\hbar^2} = \kappa^2, \quad \frac{m\omega}{\hbar} = \mu, \quad \frac{\kappa^2}{2\mu} = \frac{E}{\hbar\omega} = \varepsilon, \tag{10.3}$$

the radial equation can be rewritten in the standard form

$$\frac{d^2R}{dr^2} + \left[\kappa^2 - \mu^2 r^2 - \frac{l(l+1)}{r^2}\right] R = 0. \tag{10.4}$$

Finally, the substitution $R(r) = u(\xi)$ with $\xi = \mu r^2$ results in the generalized equation of hypergeometric type with

$$\sigma(\xi) = \xi, \quad \widetilde{\tau}(\xi) = \frac{1}{2}, \quad \widetilde{\sigma}(\xi) = \frac{1}{4}\left[\frac{\kappa^2}{\mu}\xi - \xi^2 - l(l+1)\right]. \tag{10.5}$$

Therefore,

$$2k - \varepsilon = \pm\left(l + \frac{1}{2}\right), \quad \pi(\xi) = \frac{1}{4} \pm \frac{1}{2}\left[\xi \pm \left(l + \frac{1}{2}\right)\right]. \tag{10.6}$$

Further details of calculation are presented in Table 8 and in the corresponding Mathematica file.

As a result, the energy levels are given by

$$E_0 = \hbar\omega\left(2n + l + \frac{3}{2}\right), \quad n = 0, 1, 2, \dots \tag{10.7}$$

and the corresponding radial wave functions are related to the Laguerre polynomials (Table 15):

$$R_n(r) = C_n \xi^{l+1} \exp\left(-\frac{\xi}{2}\right) L_n^{l+1/2}(\xi), \quad n = 0, 1, 2, \dots . \tag{10.8}$$

Here,

$$\int_0^\infty R_n^2(r)\, dr = 1. \tag{10.9}$$

Extension to the case of n-dimensions is discusses in [23].

11. Pöschl–Teller Potential Hole

Let us consider the one-dimensional stationary Schrödinger equation:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U(x)\psi = E\psi, \tag{11.1}$$

where

$$U(x) = \frac{1}{2}V_0\left[\frac{a(a-1)}{\sin^2(\alpha x)} + \frac{b(b-1)}{\cos^2(\alpha x)}\right], \quad V_0 = \frac{\hbar^2\alpha^2}{m} \tag{11.2}$$

with real-valued parameters $a > 1$, $b > 1$ in the finite region $0 < x < \pi/(2\alpha)$ bounded by the singularities of $U(x)$ (see [8], [26], [27] for original references and applications). Here, we are looking for orthonormal real-valued wave functions:

$$\int_0^{\pi/(2\alpha)} \psi^2(x)\, dx = 1. \tag{11.3}$$

Introducing new quantities

$$\psi(x) = u(\xi), \qquad \xi = \sin^2(\alpha x), \quad 1 - \xi = \cos^2(\alpha x), \tag{11.4}$$

$\sigma(\xi)$	ξ
$\widetilde{\sigma}(\xi)$	$\dfrac{1}{4}\left[2\varepsilon\,\xi-\xi^2-l(l+1)\right], \quad \varepsilon=\dfrac{E}{\hbar\omega}$
$\widetilde{\tau}(\xi)$	$\dfrac{1}{2}$
k	$-\dfrac{1}{2}\left(l+\dfrac{1}{2}-\varepsilon\right)$
$\pi(\xi)$	$\dfrac{1}{2}(l+1-\xi)$
$\tau(\xi)=\widetilde{\tau}+2\pi$	$l+\dfrac{3}{2}-\xi$
$\lambda=k+\pi'$	$-\dfrac{1}{2}\left(l+\dfrac{3}{2}-\varepsilon\right)$
$\varphi(\xi)$	$\xi^{(l+1)/2}\exp\left(-\xi/2\right)$
$\rho(\xi)$	$\xi^{l+1/2}\exp\left(-\xi\right)$
$y_n(\xi)$	$C_nL_n^{l+1/2}(\xi), \quad n=0,1,\ldots$
C_n^2	$\dfrac{2n!\sqrt{\mu}}{\Gamma(l+n+3/2)}, \quad \mu=\dfrac{m\omega}{\hbar}$

TABLE 8. The $3D$-spherical harmonic oscillator potential: $U(x)=\frac{1}{2}m\omega^2r^2$. Substitution: $\xi=\mu r^2$, $\mu=\frac{m\omega}{\hbar}$, and $R(r)=u(\xi)$.

one gets the following generalized equation of hypergeometric type:

$$\xi(1-\xi)u''+\left(\frac{1}{2}-\xi\right)u' + \frac{1}{4}\left[\frac{c^2}{\alpha^2}-\frac{a(a-1)}{\xi}-\frac{b(b-1)}{1-\xi}\right]u=0, \quad c^2=\frac{2mE}{\hbar^2}. \tag{11.5}$$

Here,

$$\sigma(\xi)=\xi(1-\xi), \qquad \widetilde{\tau}(\xi)=\left(\frac{1}{2}-\xi\right), \qquad \widetilde{\sigma}(\xi)=\frac{1}{4}\left[\frac{c^2}{\alpha^2}\xi(1-\xi)-a(a-1)(1-\xi)-b(b-1)\xi\right] \tag{11.6}$$

and the boundary conditions take the form $u(0)=u(1)=0$.

Therefore,

$$p(\xi)=\frac{1}{4}\left[(\kappa+1)\xi^2-(\kappa+1+(a-b)(a+b-1))\xi+a(a-1)+\frac{1}{4}\right], \tag{11.7}$$

$$\kappa = \frac{c^2}{\alpha^2} - 4k.$$

Equation (2.21) takes the form

$$\left[\kappa + 1 + (a-b)(a+b-1)\right]^2 = (\kappa+1)\left[4a(a-1)+1\right]. \tag{11.8}$$

There are two solutions

$$\kappa_1 = (a+b)(a+b-2), \quad \kappa_2 = -(b-a-1)(b-a+1) \tag{11.9}$$

If one chooses

$$\frac{c^2}{\alpha^2} - 4k = (a+b)(a+b-2), \tag{11.10}$$

then

$$\pi(\xi) = \frac{1}{2}\left(\frac{1}{2} - \xi\right) - \left(\frac{a+b-1}{2}\xi - \frac{(2a-1}{4}\right) = \frac{a}{2} - \frac{a+b}{2}\xi \tag{11.11}$$

and

$$\tau(\xi) = a + \frac{1}{2} - (a+b+1)\xi, \qquad \lambda = \frac{1}{4}\left[\frac{c^2}{\alpha^2} - (a+b)^2\right]. \tag{11.12}$$

Further details of calculation are presented in Table 9 (see also the corresponding Mathematica file).

As a result, the energy levels are given by (2.7):

$$E_0 = \frac{1}{2}V_0(a+b+2n)^2, \quad n = 0, 1, 2, \dots \tag{11.13}$$

and the corresponding wave functions are related to the Jacobi polynomials:

$$\psi_n(x) = C_n \sin^a(\alpha x)\cos^b(\alpha x)\; P_n^{(a-1/2,\, b-1/2)}\left(\cos(2\alpha x)\right), \tag{11.14}$$

where C_n is the normalization constant.

Indeed, by the Rodrigues-type formula (2.8):

$$y_n = \frac{B_n}{\xi^{a-1/2}(1-\xi)^{b-1/2}}\frac{d^n}{d\xi^n}\left[\xi^{n+a-1/2}(1-\xi)^{n+b-1/2}\right] \tag{11.15}$$

and with the aid of the substitution $\eta = 1 - 2\xi = \cos(2\alpha x)$ one gets

$$\begin{aligned} y_n(\eta) &= \frac{(-1)^n}{2^n}\frac{B_n}{(1-\eta)^{a-1/2}(1+\eta)^{b-1/2}}\frac{d^n}{d\eta^n}\left[(1-\eta)^{n+a-1/2}(1+\eta)^{n+b-1/2}\right] \\ &= C_n\, P_n^{(a-1/2,\, b-1/2)}(\eta). \end{aligned} \tag{11.16}$$

Moreover, by the normalization condition:

$$\begin{aligned} 1 &= \int_0^{\pi/(2\alpha)} \psi_n^2(x)\,dx = \frac{C_n^2}{2\alpha}\int_{-1}^1 \left[P_n^{(a-1/2,\, b-1/2)}(\eta)\right]^2 \frac{\varphi^2\; d\eta}{(1-\eta)^{1/2}(1+\eta)^{1/2}} \\ &= \frac{C_n^2}{(2\alpha)2^{a+b}}\int_{-1}^1 \left[P_n^{(a-1/2,\, b-1/2)}(\eta)\right]^2 (1-\eta)^{a-1/2}(1+\eta)^{b-1/2}\; d\eta \\ &= \frac{C_n^2}{2\alpha}\frac{\Gamma(a+n+1/2)\Gamma(b+n+1/2)}{n!(a+b+2n)\Gamma(a+b+n)}. \end{aligned} \tag{11.17}$$

(Here, the value of the squared norm d_n^2 for the Jacobi polynomials has been taken from Table 15.) As a result,

$$C_n^2 = \frac{2\alpha n!(a+b+2n)\Gamma(a+b+n)}{\Gamma(a+n+1/2)\Gamma(b+n+1/2)}. \tag{11.18}$$

$\sigma(\xi)$	$\xi(1-\xi) = \xi - \xi^2$
$\widetilde{\sigma}(\xi)$	$-\frac{1}{4}\left[\frac{c^2}{\alpha^2}\xi^2 - \left(\frac{c^2}{\alpha^2} + (a-b)(a+b-1)\right)\xi + a(a-1)\right],\ c^2 = \frac{2mE}{\hbar^2}$
$\widetilde{\tau}(\xi)$	$\frac{1}{2} - \xi$
k	$\frac{1}{4}\left[\frac{c^2}{\alpha^2} - (a+b)(a+b-2)\right]$
$\pi(\xi)$	$\frac{1}{2}\left[a - (a+b)\,\xi\right]$
$\tau(\xi) = \widetilde{\tau} + 2\pi$	$(a+1/2) - (a+b+1)\xi$
$\lambda = k + \pi'$	$\frac{1}{4}\left[\frac{c^2}{\alpha^2} - (a+b)^2\right]$
$\varphi(\xi)$	$\xi^{a/2}(1-\xi)^{b/2} = \sin^a(\alpha x)\cos^b(\alpha x)$
$\rho(\xi)$	$\xi^{a-1/2}(1-\xi)^{b-1/2}$
$y_n(\xi)$	$C_n P_n^{(a-1/2,\,b-1/2)}\left((1-\xi)/2)\right) = C_n P_n^{(a-1/2,\,b-1/2)}\left(\cos(2\alpha x)\right)$
C_n^2	$\frac{2\alpha n!(a+b+2n)\Gamma(a+b+n)}{\Gamma(a+n+1/2)\Gamma(b+n+1/2)} \qquad (n = 0, 1, 2, \dots)$

TABLE 9. The Pöschl–Teller potential hole:

$$U(x) = \frac{1}{2}V_0\left[\frac{a(a-1)}{\sin^2(\alpha x)} + \frac{b(b-1)}{\cos^2(\alpha x)}\right], \quad V_0 = \frac{\hbar^2\alpha^2}{m} \qquad (a > 1,\ b > 1).$$

Substitution: $\xi = \sin^2(\alpha x),\ \psi(x) = u(\xi),\ 0 < x < \pi/(2\alpha)$.

12. Modified Pöschl–Teller Potential Hole

In order to solve the one-dimensional stationary Schrödinger equation (11.1) for the potential:

$$U(x) = -\frac{\hbar^2\alpha^2}{2m}\frac{a(a-1)}{\cosh^2(\alpha x)} \qquad (-\infty < x < \infty) \tag{12.1}$$

with $a > 1$, one can use the following substitution $\psi(x) = u(\xi)$, where $\xi = \cosh^2(\alpha x)$ [8], [26]. As a result, we arrive at the generalized equation of hypergeometric type

$$\xi(1-\xi)u'' + \left(\frac{1}{2} - \xi\right)u' + \frac{1}{4}\left[\frac{c^2}{\alpha^2} - \frac{a(a-1)}{\xi}\right]u = 0, \quad c^2 = \frac{2m(-E)}{\hbar^2}, \tag{12.2}$$

where

$$\sigma(\xi) = \xi(1-\xi), \qquad \widetilde{\tau}(\xi) = \left(\frac{1}{2} - \xi\right), \tag{12.3}$$
$$\widetilde{\sigma}(\xi) = \frac{1}{4}\left[\frac{c^2}{\alpha^2}\xi - a(a-1)\right](1-\xi).$$

Using the standard substitution $u = \varphi(\xi)y$ with $\varphi(\xi) = \xi^{(1-a)/2}$, one gets the hypergeometric differential equation of the form:

$$\xi(1-\xi)y'' + \left[\frac{3}{2} - a + (a-2)\xi\right]y' + \frac{1}{4}\left[\frac{c^2}{\alpha^2} - (a-1)^2\right]y = 0. \tag{12.4}$$

Here, we concentrate only on the bounded states (continuous spectrum is discussed in [8]).

There is a finite number of negative discrete energy levels that are explicitly given by

$$E = E_n = -\frac{\hbar^2\alpha^2}{2m}(1-a+2n)^2, \quad n = 0, 1, \ldots < (a-1)/2. \tag{12.5}$$

The corresponding orthonormal wave functions are related to a set of Jacobi polynomials with a negative value of one parameter that are orthogonal on an infinite interval $(1, +\infty)$. They are given by the Rodrigues-type formula (2.8) or in terms of a terminating hypergeometric series:

$$y_n(\xi) = \frac{(1/2)_n}{n!}\ {}_2F_1\left(-n,\ 1-a+n;\ \frac{1}{2};\ 1-\xi\right) \tag{12.6}$$
$$= P_n^{(-1/2,\,1/2-a)}\left(\cosh(2\alpha x)\right),$$

where $(1/2)_n = \Gamma(n+1/2)/\Gamma(1/2)$. Cauchy's beta integral,

$$\int_0^\infty \frac{t^{A-1}}{(1+t)^{A+B}}\,dt = \frac{\Gamma(A)\,\Gamma(B)}{\Gamma(A+B)}, \qquad \Re(A) > 0,\ \Re(B) > 0, \tag{12.7}$$

should be used in order to find the value of the normalization constant (see [35], Exercise 1.15 and [25], (5.12.3)). Further details of calculation are presented in Table 10 (see also the corresponding Mathematica file). As a result, for the bound states (12.5), the normalized wave functions are given by

$$\psi_n(x) = \sqrt{\alpha}\left[\frac{n!(a-1-2n)\,\Gamma(a-n-1/2)}{\Gamma(n+1/2)\,\Gamma(a-n)}\right]^{1/2} \tag{12.8}$$
$$\times \cosh^{1-a}(\alpha x)\,P_n^{(-1/2,\,1/2-a)}\left(\cosh(2\alpha x)\right).$$

13. Kratzer's Molecular Potential

In order to investigate the rotation-vibration spectrum of a diatomic molecule, the potential

$$U(r) = -2D\left(\frac{a}{r} - \frac{1}{2}\frac{a^2}{r^2}\right) \qquad D > 0, \tag{13.1}$$

with a minimum $U(a) = -D$, has been used [8]. Once again we are looking for solutions of the Schrödinger equation (5.1) in spherical coordinates (9.1) and introduce the dimensionless quantities:

$$x = \frac{r}{a}, \qquad \beta^2 = -\frac{2ma^2}{\hbar^2}\,E, \qquad \gamma^2 = \frac{2ma^2}{\hbar^2}\,D \tag{13.2}$$

$\sigma(\xi)$	$\xi(1-\xi)$
$\widetilde{\sigma}(\xi)$	$\frac{1}{4}\left[\frac{c^2}{\alpha^2}\xi - a(a-1)\right](1-\xi), \quad c^2 = \frac{2m(-E)}{\hbar^2}$
$\widetilde{\tau}(\xi)$	$\frac{1}{2} - \xi$
k	$\frac{1}{4}\left(\frac{c^2}{\alpha^2} + 1 - a^2\right)$
$\pi(\xi)$	$\frac{1-a}{2}(1-\xi)$
$\tau(\xi) = \widetilde{\tau} + 2\pi$	$\frac{3}{2} - a + (a-2)\xi$
$\lambda = k + \pi'$	$\frac{1}{4}\left[\frac{c^2}{\alpha^2} - (a-1)^2\right]$
$\varphi(\xi)$	$\xi^{(1-a)/2}$
$\rho(\xi)$	$\xi^{(1/2)-a}(\xi-1)^{-(1/2)}$
$y_n(\xi)$	$C_n P_n^{(-1/2,\,1/2-a)}\left(\cosh(2\alpha x)\right),\ n < (a-1)/2$
C_n^2	$\alpha \frac{n!(a-1-2n)\Gamma(a-n-1/2)}{\Gamma(n+1/2)\Gamma(a-n)}$

Table 10. The modified Pöschl–Teller potential hole:

$$U(x) = -\frac{\hbar^2\alpha^2}{2m}\frac{a(a-1)}{\cosh^2(\alpha x)} \quad (a > 1).$$

Substitution: $\xi = \cosh^2(\alpha x),\ \psi(x) = u(\xi)$.

together with the standard substitution: $R(r) = u(x)$.

For bound states $E < 0, \beta > 0$ and the radial equation takes the form

$$u'' + \left[-\beta^2 + \frac{2\gamma^2}{x} - \frac{\gamma^2 + l(l+1)}{x^2}\right]u = 0. \tag{13.3}$$

Further computational details are presented in Table 11 (see also the corresponding Mathematica file). This case is somewhat similar to Coulomb and relativistic Coulomb problems.

As a result, the bound states are given by

$$E_n = -\frac{2ma^2D^2}{\hbar^2}\frac{1}{(\nu+n)^2}, \tag{13.4}$$

where

$$\nu = \frac{1}{2} + \sqrt{\gamma^2 + \left(l + \frac{1}{2}\right)^2}, \qquad \gamma^2 = \frac{2ma^2}{\hbar^2}\ D. \tag{13.5}$$

We can obtain the same exact result with the aid of the Bohr–Sommerfeld quantization rule in the semiclassical approximation (the WKB-method [2], [19], [24], [33]).

The normalized radial wave functions,

$$\int_0^\infty R^2(r)\,dr = 1, \tag{13.6}$$

are related to the Laguerre polynomials:

$$R_n(r) = C_n\,x^\nu \exp(-\beta x) L_n^{2\nu-1}(2\beta x) \qquad \left(x = \frac{r}{a}\right), \tag{13.7}$$

where

$$C_n^2 = \frac{(2\beta)^{2\nu+1} n!}{a(2\nu+2n)\Gamma(2\nu+n)}. \tag{13.8}$$

Once again, we have used the integral (7.13). (See also [4], [16] for some applications of Kratzer's molecular potential and further references.)

$\sigma(x)$	x
$\widetilde{\sigma}(x)$	$2\gamma^2 x - \beta^2 x^2 - \gamma^2 - l(l+1)$
$\widetilde{\tau}(x)$	0
k	$2\gamma^2 \pm \beta(2\nu-1), \quad \nu = \dfrac{1}{2} + \sqrt{\gamma^2 + \left(l+\dfrac{1}{2}\right)^2}$
$\pi(x)$	$\nu - \beta x$
$\tau(x) = \widetilde{\tau} + 2\pi$	$2(\nu - \beta x)$
$\lambda = k + \pi'$	$2(\gamma^2 - \nu\beta)$
$\varphi(x)$	$x^\nu \exp(-\beta x)$
$\rho(x)$	$x^{2\nu-1} \exp\left(-2\beta x\right)$
$y_n(x)$	$C_n\ L_n^{2\nu-1}(2\beta x)$
C_n^2	$\dfrac{(2\beta)^{2\nu+1} n!}{a(2\nu+2n)\Gamma(2\nu+n)}$

Table 11. The Kratzer's molecular potential:

$$U(x) = -2D\left(\frac{a}{r} - \frac{1}{2}\frac{a^2}{r^2}\right), \quad D > 0.$$

Substitution: $x = r/a,\ R(r) = u(x)$; see also (13.2).

14. Hulthén Potential

We are looking for solutions of the Schrödinger equation (5.1) in spherical coordinates (9.1) for the following central field potential,

$$U(r) = -V_0 \frac{e^{-r/a}}{1 - e^{-r/a}} \qquad (0 \le r < \infty), \tag{14.1}$$

when $l = 0$. (See, for example, (6.2) with $F = R$ and use these data for an explicit form of the corresponding radial equation.)

With the aid of the substitution

$$R(r) = u(\xi), \qquad \xi = e^{-r/a}, \tag{14.2}$$

when

$$\alpha^2 = -\frac{2mE}{\hbar^2}a^2 > 0, \qquad \beta^2 = \frac{2mV_0}{\hbar^2}a^2 > 0 \tag{14.3}$$

with $\alpha > 0$ and $\beta > 0$, one obtains the following generalized equation of hypergeometric type,

$$\xi^2\frac{d^2u}{d\xi^2} + \xi\frac{du}{d\xi} + \left(-\alpha^2 + \beta^2\frac{\xi}{1-\xi}\right)u = 0, \tag{14.4}$$

where

$$\sigma(\xi) = \xi(1-\xi), \qquad \widetilde{\tau}(\xi) = 1-\xi, \tag{14.5}$$

and

$$\widetilde{\sigma}(\xi) = (1-\xi)\left(\left(\alpha^2+\beta^2\right)\xi - \alpha^2\right). \tag{14.6}$$

The boundary conditions are

$$R(0) = \lim_{r\to 0^+} R(r) = 0, \qquad R(\infty) = \lim_{r\to\infty} R(r) = 0, \tag{14.7}$$

or

$$u(0) = u(1) = 0. \tag{14.8}$$

We have

$$k = \beta^2 \mp \alpha, \qquad \pi(\xi) = -\frac{\xi}{2} \pm \left(-\alpha \pm \frac{\xi}{2} + \alpha\xi\right) \tag{14.9}$$

for all four possible combinations. The solutions can be found by putting [8]

$$u = \varphi(\xi)y(\xi) = \xi^\alpha(1-\xi)y(\xi), \tag{14.10}$$

which results in

$$\xi(1-\xi)y'' + \left[2\alpha+1-(2\alpha+3)\xi\right]y' - \left(2\alpha+1-\beta^2\right)y = 0 \tag{14.11}$$

(details of calculations are presented in Table 12 and in a complementary Mathematica file).

As one can see, a direct quantization in terms of the classical orthogonal polynomials by Nikiforov and Uvarov's approach is not applicable here, right away, because the second coefficient,

$$\tau(\xi) = 2\alpha+1-(2\alpha+3)\xi, \tag{14.12}$$

does depend on α and therefore on the energy E. We have to utilize the boundary conditions (14.8) instead, in a somewhat similar way to the consideration of a familiar case of an infinite well.

Equation (14.11) is a special case of the hypergeometric equation [1], [25],

$$\xi(1-\xi)u'' + \left[C-(A+B+1)\xi\right]u' - ABu = 0, \tag{14.13}$$

with

$$A = 1+\alpha+\gamma, \qquad B = 1+\alpha-\gamma, \qquad C = 2\alpha+1; \qquad \gamma = \sqrt{\alpha^2+\beta^2}. \tag{14.14}$$

The required solution, that is bounded at $\xi = 0$, has the form

$$y = {}_2F_1\left(\begin{matrix}A,\ B\\ C\end{matrix};\xi\right) = {}_2F_1\left(\begin{matrix}1+\alpha+\gamma,\ 1+\alpha-\gamma\\ 2\alpha+1\end{matrix};\xi\right), \tag{14.15}$$

up to a constant, and the first boundary condition is satisfied $u(0) = 0$, when $\alpha > 0$.

As is known [25],

$$\lim_{\xi\to 1^-} (1-\xi)^{A+B-C} {}_2F_1\left(\begin{matrix} A,\ B \\ C \end{matrix};\ \xi\right) = \frac{\Gamma(C)\,\Gamma(A+B-C)}{\Gamma(A)\,\Gamma(B)}, \tag{14.16}$$

provided $\Re\,(C-A-B)<0$. Thus

$$\begin{aligned} u(1) &= \lim_{\xi\to 1^-} (1-\xi)\ {}_2F_1\left(\begin{matrix} 1+\alpha+\gamma,\ 1+\alpha-\gamma \\ 2\alpha+1 \end{matrix};\xi\right) \\ &= \frac{\Gamma(2\alpha+1)\,\Gamma(1)}{\Gamma(1+\alpha+\gamma)\,\Gamma(1+\alpha-\gamma)} = 0, \end{aligned} \tag{14.17}$$

provided that

$$\alpha-\gamma = -n = -1, -2, -3,\ \dots, \tag{14.18}$$

or

$$\alpha = \alpha_n = \frac{\beta^2-n^2}{2n} > 0. \tag{14.19}$$

As a result, the discrete energy levels are given by

$$E_n = -V_0 \left(\frac{\beta^2-n^2}{2\beta n}\right)^2, \qquad n=1,2,3,\ \dots \quad \left(n^2<\beta^2\right). \tag{14.20}$$

There exists a minimum size of potential hole before any energy eigenvalue at all can be obtained, viz. $\beta^2=1$. Equation $1\le n^2\le\beta^2$ determines the finite number of eigenvalues in a potential hole of a given size [8].

The radial wave functions take the form

$$R_n(r) = C_n\ \xi^\alpha (1-\xi)\ {}_2F_1\left(\begin{matrix} 1-n,\ 1+2\alpha+n \\ 2\alpha+1 \end{matrix};\xi\right), \qquad \xi = e^{-r/a}, \tag{14.21}$$

where the hypergeometric series terminates and C_n is a constant to be determined. Thus, the energy levels can be obtained by the condition (2.7) and the corresponding wave functions are derived with the help of the Rodrigues-type formula (2.8) as follows:

$$\left(\xi^{2\alpha+n-1}(1-\xi)^n\right)^{(n-1)} = \frac{\Gamma(2\alpha+n)}{\Gamma(2\alpha+1)}\xi^{2\alpha}(1-\xi)\ {}_2F_1\left(\begin{matrix} 1-n,\ 2\alpha+n+1 \\ 2\alpha+1 \end{matrix};\xi\right). \tag{14.22}$$

This result follows also, as a special case, from (15.5.9) of [25].

Once again, we can use (13.6) for normalization of the radial wave function. Then

$$aC_n^2 \int_0^1 \xi^{2\alpha-1}(1-\xi)^2 y_n^2(\xi)\,d\xi = 1, \tag{14.23}$$

where

$$\xi^{2\alpha}(1-\xi)y_n(\xi) = \frac{\Gamma(2\alpha+1)}{\Gamma(2\alpha+n)}\left[\xi^{2\alpha+n-1}(1-\xi)^n\right]^{(n-1)} \tag{14.24}$$

by (14.22). Moreover,

$$(1-\xi)y_n(\xi) = {}_2F_1\left(\begin{matrix} -n,\ 2\alpha+n \\ 2\alpha+1 \end{matrix};\xi\right), \tag{14.25}$$

by the familiar transformation [24]:

$$ {}_2F_1\left(\begin{matrix} A,\ B \\ C \end{matrix}; \xi\right) = (1-\xi)^{C-A-B}\ {}_2F_1\left(\begin{matrix} C-A,\ C-B \\ C \end{matrix}; \xi\right) \tag{14.26} $$

with $A=-n$, $B=2\alpha+n$, $C=2\alpha+1$. Therefore,

$$ \begin{aligned} \int_0^1 \xi^{2\alpha-1}(1-\xi)^2 y_n^2(\xi)\, d\xi &= \frac{\Gamma(2\alpha+1)}{\Gamma(2\alpha+n)} \\ &\times \int_0^1 \left[\xi^{-1}\ {}_2F_1\left(\begin{matrix} -n,\ 2\alpha+n \\ 2\alpha+1 \end{matrix}; \xi\right)\right] \left[\xi^{2\alpha+n-1}(1-\xi)^n\right]^{(n-1)}\ d\xi, \end{aligned} \tag{14.27} $$

and integrating by parts $n-1$ times, one gets

$$ \begin{aligned} &\int_0^1 \xi^{-1}\ {}_2F_1\left(\begin{matrix} -n,\ 2\alpha+n \\ 2\alpha+1 \end{matrix}; \xi\right) \left[\xi^{2\alpha+n-1}(1-\xi)^n\right]^{(n-1)}\ d\xi \\ &= \left(\xi^{-1}\ {}_2F_1\left(\begin{matrix} -n,\ 2\alpha+n \\ 2\alpha+1 \end{matrix}; \xi\right) \left[\xi^{2\alpha+n-1}(1-\xi)^n\right]^{(n-2)}\right)\Bigg|_{\xi=0}^{1} \\ &\quad - \int_0^1 \left[\xi^{-1}\ {}_2F_1\left(\begin{matrix} -n,\ 2\alpha+n \\ 2\alpha+1 \end{matrix}; \xi\right)\right]' \left[\xi^{2\alpha+n-1}(1-\xi)^n\right]^{(n-2)}\ d\xi \\ &= \cdots = (-1)^{k-1}\left(\left[\xi^{-1}\ {}_2F_1\left(\begin{matrix} -n,\ 2\alpha+n \\ 2\alpha+1 \end{matrix}; \xi\right)\right]^{(k-1)} \left[\xi^{2\alpha+n-1}(1-\xi)^n\right]^{(n-k-1)}\right)\Bigg|_{\xi=0}^{1} \\ &\quad +(-1)^k \int_0^1 \left[\xi^{-1}\ {}_2F_1\left(\begin{matrix} -n,\ 2\alpha+n \\ 2\alpha+1 \end{matrix}; \xi\right)\right]^{(k)} \left[\xi^{2\alpha+n-1}(1-\xi)^n\right]^{(n-k-1)}\ d\xi \\ &= \cdots = (-1)^{n-1}\int_0^1 \left[\xi^{-1}\ {}_2F_1\left(\begin{matrix} -n,\ 2\alpha+n \\ 2\alpha+1 \end{matrix}; \xi\right)\right]^{(n-1)} \xi^{2\alpha+n-1}(1-\xi)^n\ d\xi, \end{aligned} \tag{14.28} $$

in view of the boundary conditions (14.7)–(14.8). By the power series expansion,

$$ \begin{aligned} \left[\xi^{-1}\ {}_2F_1\left(\begin{matrix} -n,\ 2\alpha+n \\ 2\alpha+1 \end{matrix}; \xi\right)\right]^{(n-1)} &= \left(\frac{1}{\xi}\right)^{(n-1)} + \cdots + \frac{(-n)_n(2\alpha+n)_n}{(n!)(2\alpha+1)_n}(\xi^{n-1})^{(n-1)} \\ &= (-1)^{n-1}\frac{(n-1)!}{\xi^n} + \cdots + \frac{(-n)_n(2\alpha+n)_n}{(n!)(2\alpha+1)_n}(n-1)!, \end{aligned} \tag{14.29} $$

and our integral evaluation can be completed with the aid of the following Euler beta integrals:

$$ \begin{aligned} \int_0^1 \xi^{2\alpha-1}(1-\xi)^{(n+1)-1} d\xi &= \frac{\Gamma(2\alpha)(n!)}{\Gamma(2\alpha+n+1)}, \\ \int_0^1 \xi^{2\alpha+n-1}(1-\xi)^{(n+1)-1} d\xi &= \frac{\Gamma(2\alpha+n)(n!)}{\Gamma(2\alpha+2n+1)}. \end{aligned} $$

The final result is given by

$$C_n = \frac{(2\alpha)_n}{n!}\sqrt{\frac{(\alpha+n)(2\alpha+n)}{(2\alpha)a}}, \qquad \alpha = \frac{\beta^2-n^2}{2n} \quad (n=1,2,3,\ \dots) \tag{14.30}$$

as a complementary normalization in (14.21) (Table 12). We were not able to find the value of this constant in the available literature (see, for example, [8]).

The Hulthén potential at small values of r behaves like a Coulomb potential $U_C = -V_0 a/r$, whereas for large values of r it decreases exponentially. See [8] for more details and a numerical example.

$\sigma(\xi)$	$\xi(1-\xi)$
$\widetilde{\sigma}(\xi)$	$(1-\xi)\left[\left(\alpha^2+\beta^2\right)\xi-\alpha^2\right]$
$\widetilde{\tau}(\xi)$	$1-\xi$
k	$\beta^2-\alpha$
$\pi(\xi)$	$\alpha-(\alpha+1)\xi$
$\tau(\xi)=\widetilde{\tau}+2\pi$	$2\alpha+1-(2\alpha+3)\xi$
$\lambda=k+\pi'$	$\beta^2-2\alpha-1$
$\varphi(\xi)$	$\xi^{\alpha}(1-\xi)$
$\rho(\xi)$	$\xi^{2\alpha}(1-\xi)$
E_n	$-V_0\left(\dfrac{\beta^2-n^2}{2\beta n}\right)^2, \qquad n=1,2,3,\ \dots \quad \left(n^2<\beta^2\right)$
$y_n(\xi)$	${}_2F_1(1-n,\ 1+2\alpha+n;\ 2\alpha+1;\ \xi)$
C_n	$\dfrac{(2\alpha)_n}{n!}\sqrt{\dfrac{(\alpha+n)(2\alpha+n)}{(2\alpha)a}}, \quad \alpha=\alpha_n=\dfrac{\beta^2-n^2}{2n}$

Table 12. The Hulthén potential:

$$U(r) = -V_0\frac{e^{-r/a}}{1-e^{-r/a}} \qquad (0\le r<\infty)$$

in the spherically symmetric case $l=0$.
Substitution:

$$R(r)=u(\xi), \quad \xi=\exp(-r/a), \quad \alpha^2=-\frac{2mE}{\hbar^2}\ a^2>0, \quad \beta^2=\frac{2mV_0}{\hbar^2}\ a^2>0.$$

15. Morse Potential

The following central field potential:

$$U(r) = D\left(e^{-2\alpha x}-2e^{-\alpha x}\right), \quad x=\frac{r-r_0}{r_0} \quad (0\le r<\infty) \tag{15.1}$$

is used for the study of vibrations of two-atomic molecules [8], [22]. The corresponding Schrödinger equation (5.1) can be solved in spherical coordinates (9.1) when $l=0$. Introducing new parameters

$$\beta^2 = -\frac{2mEr_0^2}{\hbar^2} > 0, \qquad \gamma^2 = \frac{2mDr_0^2}{\hbar^2} \tag{15.2}$$

$(\beta, \gamma > 0)$, with the help of the following substitution

$$R(r) = u(\xi), \qquad \xi = \frac{2\gamma}{\alpha} e^{-\alpha x}, \quad x = \frac{r - r_0}{r_0} \tag{15.3}$$

one gets

$$\xi^2 \frac{d^2u}{d\xi^2} + \xi \frac{du}{d\xi} + \left(-\frac{\beta^2}{\alpha^2} + \frac{\gamma}{\alpha}\xi - \frac{1}{4}\xi^2 \right) u = 0. \tag{15.4}$$

This is the generalized equation of hypergeometric type with

$$\sigma(\xi) = \xi, \qquad \widetilde{\tau}(\xi) = 1, \tag{15.5}$$

and

$$\widetilde{\sigma}(\xi) = -\frac{\beta^2}{\alpha^2} + \frac{\gamma}{\alpha}\xi - \frac{1}{4}\xi^2. \tag{15.6}$$

The substitution

$$u = \varphi(\xi) y(\xi) = \xi^{\beta/\alpha} e^{-\xi/2} y(\xi) \tag{15.7}$$

results in the confluent hypergeometric equations:

$$y'' + \left(\frac{2\beta}{\alpha} + 1 - \xi \right) y' + \left(\frac{\gamma - \beta}{\alpha} - \frac{1}{2} \right) y = 0 \tag{15.8}$$

with the following values of parameters:

$$c = 2\frac{\beta}{\alpha} + 1, \quad a = \frac{1}{2}c - \frac{\gamma}{\alpha} = \frac{1}{2} + \frac{\beta - \gamma}{\alpha} \tag{15.9}$$

(see Table 13 and the corresponding Mathematica file for more details).

The general solution of (15.8) has the form [24], [25]:

$$y = A\ {}_1F_1\left(\begin{matrix} a \\ c \end{matrix} ; \xi \right) + B\ \xi^{1-c}\ {}_1F_1\left(\begin{matrix} 1 + a - c \\ 2 - c \end{matrix} ; \xi \right). \tag{15.10}$$

Here, the second constant must vanish, $B = 0$, due to the boundary condition $\lim_{r\to\infty} R(r) = u(0) = 0$, because

$$1 - c + \frac{\beta}{\alpha} = -\frac{\beta}{\alpha} < 0. \tag{15.11}$$

The first constant A has to be determined by the normalization.

The second boundary condition, namely, $\lim_{r\to 0} R(r) = u(\xi_0) = 0$ with $\xi_0 = (2\gamma/\alpha)e^{\alpha}$, states

$${}_1F_1\left(\begin{matrix} a \\ c \end{matrix} ; \xi_0 \right) = 0, \tag{15.12}$$

where both coefficients depend on energy in view of (15.2) and (15.9). This transcendent equation for the discrete energy levels cannot be solved explicitly but for all real diatomic molecules $\xi_0 \gg 1$ [8]. This is why one can use the familiar asymptotic:

$$\begin{aligned} {}_1F_1\left(\begin{matrix} a \\ c \end{matrix};\xi\right) &= \frac{\Gamma(c)}{\Gamma(c-a)}(-\xi)^{-a}\left[1+\mathrm{O}\left(\frac{1}{\xi}\right)\right] \\ &+ \frac{\Gamma(c)}{\Gamma(a)}e^{\xi}\ \xi^{a-c}\left[1+\mathrm{O}\left(\frac{1}{\xi}\right)\right], \quad \xi\to\infty \end{aligned} \tag{15.13}$$

for the confluent hypergeometric function [24], [25].

By eliminating the largest asymptotic term with $\Gamma(a)=\infty$, an approximate quantization rule states: [1]

$$a=-v; \quad v=0,1,2,\ \dots; \quad v<\frac{\gamma}{\alpha}-\frac{1}{2} \tag{15.14}$$

(more details can be found in [8]). The corresponding approxiation to the discrete energy levels is given by

$$-\beta^2 = -\gamma^2 + 2\gamma\alpha\left(v+\frac{1}{2}\right) - \alpha^2\left(v+\frac{1}{2}\right)^2. \tag{15.15}$$

This result can also be obtained in the Nikiforov-Uvarov approach by (2.7). Hence, the approximate energy levels in terms of the vibrational quantum number v are

$$E_v = -D + \frac{\hbar^2}{2mr_0^2}\left[2\gamma\alpha\left(v+\frac{1}{2}\right) - \alpha^2\left(v+\frac{1}{2}\right)^2\right], \tag{15.16}$$

where the last term reflects the anharmonicity correction. This formula can be rewritten as follows [8]:

$$E_v = -D + \hbar\omega\left[\left(v+\frac{1}{2}\right) - \frac{\alpha}{2\gamma}\left(v+\frac{1}{2}\right)^2\right], \qquad \hbar\omega = \hbar^2\frac{\alpha\gamma}{mr_0^2} = \hbar\frac{\alpha}{r_0}\sqrt{\frac{2D}{m}}. \tag{15.17}$$

The first two terms in this formula are in complete agreement with the harmonic oscillator energy levels. The last term reflects the anharmonicity correction, which shows that the anharmonic term never exceeds the harmonic one [8].

The corresponding radial wave functions are given in terms of the Laguerre polynomials:

$$R(r) = R_v(r) = \sqrt{\frac{(2\beta)\ v!}{r_0\Gamma\left(2\beta/\alpha+v+1\right)}}\,\xi^{\beta/\alpha}e^{-\xi/2}\ L_v^{2\beta/\alpha}(\xi). \tag{15.18}$$

Here, we have used the following normalization:

$$\begin{aligned} \int_{r=0}^{\infty} R^2(r)\ dr &= \frac{r_0}{\alpha}\int_{\xi=0}^{\xi_0} \xi^{2\beta/\alpha-1}e^{-\xi}y^2(\xi)\ d\xi \\ &\approx C_v^2\frac{r_0}{\alpha}\int_{\xi=0}^{\infty} \xi^{2\beta/\alpha-1}e^{-\xi}\left(L_v^{2\beta/\alpha}(\xi)\right)^2\ d\xi = 1 \end{aligned} \tag{15.19}$$

[1] The values $v=0$ can be added because $\exp(-\xi_0/2)\ll 1$ and the upper bound is due to convergence of the normalization integral (15.19).

and the following integral:

$$I_{-1} = J^{\delta\delta}_{mm,-1} = \int_0^\infty e^{-\xi}\xi^{\delta-1}\left(L^\delta_m(\xi)\right)^2\ d\xi = \frac{\Gamma(\delta+m+1)}{m!\delta}. \tag{15.20}$$

Here $\delta = 2\beta/\alpha > 0$ (see [34], [35] and Appendix B; further details are left to the reader).

$\sigma(\xi)$	ξ
$\widetilde{\sigma}(\xi)$	$-\dfrac{\beta^2}{\alpha^2} + \dfrac{\gamma}{\alpha}\xi - \dfrac{1}{4}\xi^2$
$\widetilde{\tau}(\xi)$	1
k	$\dfrac{\gamma-\beta}{\alpha}$
$\pi(\xi)$	$\dfrac{\beta}{\alpha} - \dfrac{\xi}{2}$
$\tau(\xi) = \widetilde{\tau} + 2\pi$	$1 + \dfrac{2\beta}{\alpha} - \xi$
$\lambda = k + \pi'$	$\dfrac{\gamma-\beta}{\alpha} - \dfrac{1}{2}$
$\varphi(\xi)$	$\xi^{\beta/\alpha}e^{-\xi/2}$
$\rho(\xi)$	$\xi^{2\beta/\alpha}e^{-\xi}$
E_v	$-D + \dfrac{\hbar^2}{2mr_0^2}\left[2\gamma\alpha\left(v+\dfrac{1}{2}\right) - \alpha^2\left(v+\dfrac{1}{2}\right)^2\right]$
$y_v(\xi)$	$C_v\ L^{2\beta/\alpha}_v(\xi) = C_v\dfrac{\Gamma(2\beta/\alpha+v+1)}{v!\,\Gamma(2\beta/\alpha+1)}\ {}_1F_1(-v; 2\beta/\alpha+1\ ;\xi)$
C_v^2	$\dfrac{(2\beta)v!}{r_0\Gamma(2\beta/\alpha+v+1)}$

Table 13. The Morse potential:

$$U(r) = D\Big(e^{-2\alpha x} - 2e^{-\alpha x}\Big), \quad x = \frac{r-r_0}{r_0} \quad (0 \le r < \infty)$$

in the spherically symmetric case $l = 0$.
Substitution:

$$R(r) = u(\xi), \quad \xi = \frac{2\gamma}{\alpha}\exp(-\alpha x), \quad \beta^2 = -\frac{2mEr_0^2}{\hbar^2} > 0, \quad \gamma^2 = \frac{2mDr_0^2}{\hbar^2}.$$

16. Rotation Correction of Morse Potential

The standard centrifugal term [29]:

$$\frac{l(l+1)}{r^2} = \frac{l(l+1)}{r_0^2}\frac{1}{(1+x)^2}, \quad x = \frac{r-r_0}{r_0} \tag{16.1}$$

can be approximated, in the neighborhood of the minimum of the Morse potential $r=r_0$ (or $x=0$), as follows [8]:

$$\frac{l(l+1)}{r^2}\approx\frac{l(l+1)}{r_0^2}\left(C_0+C_1e^{-\alpha x}+C_2e^{-2\alpha x}\right), \tag{16.2}$$

where

$$C_0=1-\frac{3}{\alpha}+\frac{3}{\alpha^2},\quad C_1=\frac{4}{\alpha}-\frac{6}{\alpha^2},\quad C_2=-\frac{1}{\alpha}+\frac{3}{\alpha^2}. \tag{16.3}$$

Indeed,

$$\frac{1}{(1+x)^2}-\left(C_0+C_1e^{-\alpha x}+C_2e^{-2\alpha x}\right)=x^3\left(-\frac{2}{3}\alpha^2+3\alpha-4\right)+\mathrm{O}(x^4),\qquad x\to 0. \tag{16.4}$$

This consideration allows one to introduce a rotation correction to the Morse potential without changing the mathematical model much [9].

In this approximation, the radial Schrödinger equation (5.1) in spherical coordinates (9.1)

$$R''(r)+\left[\frac{2m}{\hbar^2}\left(E-D\left(e^{-2\alpha x}-2e^{-\alpha x}\right)\right)-\frac{l(l+1)}{r^2}\right]R(r)=0, \tag{16.5}$$

with the new variables

$$R(r)=u(\xi),\qquad \xi=\frac{2\gamma_2}{\alpha}e^{-\alpha x},\quad x=\frac{r-r_0}{r_0} \tag{16.6}$$

and with the modified parameters

$$\beta_1^2 = \beta^2+l(l+1)C_0,\qquad \beta^2=-\frac{2mEr_0^2}{\hbar^2}>0, \tag{16.7}$$

$$\gamma_1^2 = \gamma^2-\frac{1}{2}l(l+1)C_1,\quad \gamma_2^2=\gamma^2+l(l+1)C_2,\quad \gamma^2=\frac{2mDr_0^2}{\hbar^2}, \tag{16.8}$$

becomes the following generalized equation of hypergeometric type:

$$\xi^2u''+\xi u'+\left(-\frac{\beta_1^2}{\alpha^2}+\frac{\gamma_1^2}{\alpha\gamma_2}\xi-\frac{1}{4}\xi^2\right)u=0. \tag{16.9}$$

Here

$$\sigma(\xi)=\xi,\qquad \widetilde{\tau}(\xi)=1, \tag{16.10}$$

and

$$\widetilde{\sigma}(\xi)=-\frac{\beta_1^2}{\alpha^2}+\frac{\gamma_1^2}{\alpha\gamma_2}\xi-\frac{1}{4}\xi^2. \tag{16.11}$$

The following substitution

$$u=\xi^{\beta_1/\alpha}e^{-\xi/2}y(\xi) \tag{16.12}$$

results, once again, in the confluent hypergeometric equation

$$y''+\left(\frac{2\beta_1}{\alpha}+1-\xi\right)y'+\left(\frac{\gamma_1^2}{\alpha\gamma_2}-\frac{\beta_1}{\alpha}-\frac{1}{2}\right)y=0 \tag{16.13}$$

with the new values of the parameters:

$$c_1=2\frac{\beta_1}{\alpha}+1,\quad a_1=\frac{1}{2}c_1-\frac{\gamma_1^2}{\alpha\gamma_2}=\frac{1}{2}+\frac{\beta_1}{\alpha}-\frac{\gamma_1^2}{\alpha\gamma_2} \tag{16.14}$$

(see Table 14 and the corresponding Mathematica file for more details).

An approximate quantization rule states:

$$a_1 = -v; \quad v = 0, 1, 2, \ \ldots \ . \tag{16.15}$$

Therefore,

$$-\beta_1^2 = -\left[\frac{\gamma_1^2}{\gamma_2} - \alpha\left(v + \frac{1}{2}\right)\right]^2, \tag{16.16}$$

and, in the energy formula, one has to replace γ by

$$\frac{\gamma_1^2}{\gamma_2} \approx \gamma\left[1 - l(l+1)\frac{C_1 + C_2}{2\gamma^2}\right], \quad \gamma \gg 1. \tag{16.17}$$

As a result, we arrive at the following vibration-rotation energy levels:

$$\begin{aligned} E \ = \ E_{vl} = \frac{\hbar^2}{2mr_0^2}\Bigg[&-\gamma^2 + 2\gamma\alpha\left(v + \frac{1}{2}\right) - \alpha^2\left(v + \frac{1}{2}\right)^2 + l(l+1) \\ &-\frac{3(\alpha-1)}{\alpha\gamma}\left(v + \frac{1}{2}\right)l(l+1) - \frac{9(\alpha-1)^2}{4\alpha^4\gamma^2}l^2(l+1)^2\Bigg]. \end{aligned} \tag{16.18}$$

This formula can be presented in the form

$$\begin{aligned} E_{vl} \ = \ &-D + \hbar\omega\left[\left(v + \frac{1}{2}\right) - \frac{\alpha}{2\gamma}\left(v + \frac{1}{2}\right)^2\right] + \frac{\hbar^2 l(l+1)}{2mr_0^2} \\ &-\frac{3(\alpha-1)}{2\alpha^2 D}\hbar\omega\left(v + \frac{1}{2}\right)\frac{\hbar^2 l(l+1)}{2mr_0^2} - \frac{9(\alpha-1)^2}{4\alpha^2 D}\left(\frac{\hbar^2 l(l+1)}{2mr_0^2}\right)^2, \end{aligned} \tag{16.19}$$

where

$$\hbar\omega = \frac{\hbar^2\alpha\gamma}{mr_0^2} = \hbar\left(\frac{\alpha}{r_0}\sqrt{\frac{2D}{m}}\right). \tag{16.20}$$

The first three terms of this formula are exactly the same as those derived in the previous case; see (15.17). The fourth term can be interpreted as the molecule rotational energy at fixed distance r_0. The next term represents a coupling of the vibrations and rotations, which is negative because at higher vibrational quantum numbers the average nuclear distance increases beyond r_0 in consequence of the anharmonicity [8]. The last term can be thought of as a negative second-order correction to the rotation energy.

The corresponding radial wave functions are given in terms of the Laguerre polynomials:

$$R(r) = R_{vl}(r) = \sqrt{\frac{(2\beta_1)\ v!}{r_0\Gamma(2\beta_1/\alpha + v + 1)}}\,\xi^{\beta_1/\alpha}e^{-\xi/2}\ L_v^{2\beta_1/\alpha}(\xi). \tag{16.21}$$

Once again, we have used the normalization similar to (15.19). Further details on the rotational corrections of Morse formulas are discussed in [8], [9].

In a similar fashion, one can consider the Wood–Saxon potential and motion of the electron in magnetic field [8], [13] [20], and [24].

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$\sigma(\xi)$	ξ
$\widetilde{\sigma}(\xi)$	$-\dfrac{\beta_1^2}{\alpha^2}+\dfrac{\gamma_1^2}{\alpha\gamma_2}\xi-\dfrac{1}{4}\xi^2$
$\widetilde{\tau}(\xi)$	1
k	$\dfrac{\gamma_1^2}{\alpha\gamma_2}-\dfrac{\beta_1}{\alpha}$
$\pi(\xi)$	$\dfrac{\beta_1}{\alpha}-\dfrac{\xi}{2}$
$\tau(\xi)=\widetilde{\tau}+2\pi$	$1+\dfrac{2\beta_1}{\alpha}-\xi$
$\lambda=k+\pi'$	$\dfrac{\gamma_1^2}{\alpha\gamma_2}-\dfrac{\beta_1}{\alpha}-\dfrac{1}{2}$
$\varphi(\xi)$	$\xi^{\beta_1/\alpha}e^{-\xi/2}$
$\rho(\xi)$	$\xi^{2\beta_1/\alpha}e^{-\xi}$

Table 14. The rotation correction of Morse potential:

$$\frac{l(l+1)}{r^2}\approx\frac{l(l+1)}{r_0^2}\left(C_0+C_1e^{-\alpha x}+C_2e^{-2\alpha x}\right),\quad x=\frac{r-r_0}{r_0},$$

where the coefficients C_0, C_1, and C_2 are given by (16.3).

A. Data for the Classical Orthogonal Polynomials

The basic information about classical orthogonal polynomials, namely, for the Jacobi $P_n^{(\alpha,\beta)}(x)$, Laguerre $L_n^\alpha(x)$, and Hermite $H_n(x)$ polynomials, is presented, for the reader's convenience, in Table 15. It contains the coefficients of the differential equation (2.3), the intervals of orthogonality (a,b), the weight functions $\rho(x)$ and constants B_n in the Rodrigues-type formula (2.8), the leading terms:

$$y_n(x)=a_nx^n+b_nx^{n-1}+\dots \tag{A.1}$$

for these polynomials, their squared norms:

$$d_n^2=\int_a^b y_n^2(x)\rho(x)\,dx, \tag{A.2}$$

and the coefficients of the three-term recurrence relation:

$$x\,y_n(x)=\alpha_n\,y_{n+1}(x)+\beta_n\,y_n(x)+\gamma_n\,y_{n-1}(x), \tag{A.3}$$

where

$$\alpha_n=\frac{a_n}{a_{n+1}},\quad \beta_n=\frac{b_n}{a_n}-\frac{b_{n+1}}{a_{n+1}},\quad \gamma_n=\alpha_{n-1}\,\frac{d_n^2}{d_{n-1}^2}. \tag{A.4}$$

(More details can be found in [1], [23], [24], [25], and [35].)

$y_n(x)$	$P_n^{(\alpha,\beta)}(x)\ (\alpha>-1,\beta>-1)$	$L_n^{\alpha}(x)\ (\alpha>-1)$	$H_n(x)$
(a,b)	$(-1,1)$	$(0,\infty)$	$(-\infty,\infty)$
$\rho(x)$	$(1-x)^{\alpha}(1+x)^{\beta}$	$x^{\alpha}\,e^{-x}$	e^{-x^2}
$\sigma(x)$	$1-x^2$	x	1
$\tau(x)$	$\beta-\alpha-(\alpha+\beta+2)\,x$	$1+\alpha-x$	$-2x$
λ_n	$n(\alpha+\beta+n+1)$	n	$2n$
B_n	$\dfrac{(-1)^n}{2^n n!}$	$\dfrac{1}{n!}$	$(-1)^n$
a_n	$\dfrac{\Gamma(\alpha+\beta+2n+1)}{2^n n!\Gamma(\alpha+\beta+n+1)}$	$\dfrac{(-1)^n}{n!}$	2^n
b_n	$\dfrac{(\alpha-\beta)\Gamma(\alpha+\beta+2n)}{2^n(n-1)!\Gamma(\alpha+\beta+n+1)}$	$(-1)^{n-1}\dfrac{\alpha+n}{(n-1)!}$	0
d^2	$\dfrac{2^{\alpha+\beta+1}\Gamma(\alpha+n+1)\Gamma(\beta+n+1)}{n!(\alpha+\beta+2n+1)\Gamma(\alpha+\beta+n+1)}$	$\dfrac{\Gamma(\alpha+n+1)}{n!}$	$2^n n!\sqrt{\pi}$
α_n	$\dfrac{2(n+1)(\alpha+\beta+n+1)}{(\alpha+\beta+2n+1)(\alpha+\beta+2n+2)}$	$-(n+1)$	$\dfrac{1}{2}$
β_n	$\dfrac{\beta^2-\alpha^2}{(\alpha+\beta+2n)(\alpha+\beta+2n+2)}$	$\alpha+2n+1$	0
γ_n	$\dfrac{2(\alpha+n)(\beta+n)}{(\alpha+\beta+2n)(\alpha+\beta+2n+1)}$	$-(\alpha+n)$	n

TABLE 15. Data for the Jacobi $P_n^{(\alpha,\beta)}(x)$, Laguerre $L_n^{\alpha}(x)$, and Hermite $H_n(x)$ polynomials.

B. An Integral Evaluation

The following useful integral:

$$\begin{aligned} J_{nms}^{\alpha\beta} &= \int_0^{\infty} e^{-x}x^{\alpha+s}\ L_n^{\alpha}(x)L_m^{\beta}(x)\ dx \\ &= (-1)^{n-m}\frac{\Gamma(\alpha+s+1)\,\Gamma(\beta+m+1)\,\Gamma(s+1)}{m!\,(n-m)!\,\Gamma(\beta+1)\,\Gamma(s-n+m+1)} \\ &\quad\times\ {}_3F_2\left(\begin{matrix}-m,\ s+1,\ \beta-\alpha-s\\ \beta+1,\quad n-m+1\end{matrix};1\right),\qquad n\geq m,\end{aligned} \tag{B.1}$$

where parameter s may take some integer values and ${}_3F_2(1)$ is the generalized hypergeometric series [1], [25], has been evaluated in [34] and [35] (see also [30]). Special cases have been used above for the normalization of the wave functions; see (7.13) and (15.20).

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