Newton’s Method and Energy Eigenvalue Problems for the Schrödinger Equation

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Abstract
For a pedagogical example, we take up Newton’s method and energy eigenvalue problems for the Schrödinger equation. Newton’s method is systematically used to obtain energy eigenvalues and energy eigenfunctions of the Schrödinger equation.

The Schrödinger equation with the Woods-Saxon potential is considered for an S-state. One solution is obtained analytically by means of the hypergeometric series. Another one is obtained numerically using the Runge-Kutta method.

Because our approach makes the most of Newton’s method in this paper, our calculations would have pedagogical benefits for those undergraduate students beginning to learn practical computations actively in physics.

1 Introduction
As is well known, Newton’s method is very celebrated in mathematical analysis. However, it is less well-known in practical learnings of physics and chemistry. Therefore attempts to apply it to some topics of them seem to be very interesting. In order to use Newton’s method for exercises of Quantum mechanics, we take up an eigenvalue problem for the Schrödinger equation with the Woods-Saxon potential, which is very popular in the textbooks of nuclear physics, as a pedagogical example. We use two distinct approaches to deal with this problem. One solution was obtained analytically with the help of the hypergeometric series by T. Ishidzu [5]. Another one is obtained numerically using the fourth-order Runge-Kutta method [1]. We would like to stress that in both approaches the Newton’s method plays key roles.

Motivations of this paper consist of four viewpoints: to show how to solve a transcendental equation using Newton’s method without recourse to the graphical method, to show that the solution to the transcendental equation is fully compatible with the numerical one obtained by the distinct method using the Runge-Kutta method, to explain explicitly that Newton’s method plays key roles in obtaining these two solutions, and to show clearly, thanks to the transcendental equation, that when the diffuseness parameter of the Woods-Saxon potential gets closer and closer to zero, energy eigenvalues, as expected, converge to those of the 3-dimensional square-well potential.

Tools for our approaches are explained briefly in the following four sections after the introduction and section 6 is devoted to numerical calculations and results.

Newton’s method explained in this paper has been applied to the complex energy eigenvalues problems of kaonic atoms for the first time in the work of M. Atarashi et al. [2] and the present paper originated from their work.
2 Startup

The radial Schrödinger equation \( u(r) \) of a neutron in a symmetrical Woods-Saxon potential \( V(r) \) is given by

\[
\frac{d^2u(E,r)}{dr^2} + \frac{2m}{\hbar^2}(E-V(r) - \frac{l(l+1)\hbar^2}{2mr^2})u(E,r) = 0, \tag{1}
\]

where the total wave function \( \psi(r) \) for the neutron is represented by \( \psi(r) = r^{-1}u(r)Y_{l,m}(\theta,\phi) \), and \( V(r) \) is given by

\[
V(r) = \frac{V_0}{1 + e^{r/R}}. \tag{2}
\]

In this paper we take the parameters in the Woods-Saxon potential for convenience as

\[
A = 208, \quad Z = 82, \quad d = 0.67 \text{ fm}, \quad V_0 = (-51 + 33\frac{(N-Z)}{A}) \text{ MeV}, \quad R = 7.5247400137547205 \text{ fm.}
\]

These parameters are adopted from Blomqvist and Wahlborn \[3\] and give us

\[
V_0 = -44.01923076923077 \text{ MeV}, \quad R = 7.5247400137547205 \text{ fm.}
\]

Besides, the mass of neutron \( mc^2 = 940 \text{ MeV} \) and \( \hbar c = 197.3 \text{ MeV} \cdot \text{fm} \) are taken.

We note that for \( l \neq 0 \), equation (1) is easy to solve numerically but impossible to solve analytically. However, as Ishidzu calculated, only for \( l = 0 \) can we solve the equation analytically. For this reason, in this paper, we restrict our considerations to an S-state \( (l = 0) \). When \( E < 0 \) we solve equation (1) numerically with condition that

\[
u(E,r) = 0 \text{ at } r = 0 \quad \text{and} \quad u(E,r) \to 0 \text{ for } r \to \infty. \tag{4}
\]

With these boundary conditions we can determine the energy eigenvalues numerically.

3 Runge-Kutta method

In order to solve equation (1) numerically in case \( l = 0 \) we rewrite it as

\[
\frac{d^2u(E,r)}{dr^2} = g(E,r)u(E,r), \tag{5}
\]

where

\[
g(E,r) = -\frac{2m}{\hbar^2}(E - \frac{V_0}{1 + e^{r/R}}). \tag{6}
\]

If we put \( v(E,r) = du(E,r)/dr \), equation (5) is changed to a couple of the first-order differential equations as follows:

\[
\begin{aligned}
\frac{du(E,r)}{dr} &= v(E,r), \\
\frac{dv(E,r)}{dr} &= g(E,r)u(E,r).
\end{aligned} \tag{7, 8}
\]

We apply the fourth-order Runge-Kutta method \[1\] for solving the differential equations (7) and (8) numerically. Let \([a,b]\) stand for the interval where the equations are solved and we divide it into \( N \) intervals of width \( h \) each such that \( h = (b-a)/N \). Then we put \( r_0 = a, r_1 = r_0 + h, \ldots, r_N = b \) and set \( u_i(E) = u(E,r_i) \) and \( v_i(E) = v(E,r_i) \).

If we solve the recurrence relations resulting from the Runge-Kutta method numerically with the initial values \( u_0(E) = u(E,r_0) \) and \( v_0(E) = v(E,r_0) \), we can obtain every \( u_i(E), v_i(E) \) \( (i = 0, 1, \ldots, N) \).

4 Newton’s method

We find a solution \( x \) of a differentiable function \( f(x) = 0 \) numerically. Suppose \( x_0 \) is an approximate solution to \( f(x) = 0 \) and let \( \delta x_0 \) be the correction to \( x_0 \) such that \( f(x_0 + \delta x_0) = 0 \). We expand \( f(x_0 + \delta x_0) \) in powers of \( \delta x_0 \) as

\[
f(x_0 + \delta x_0) = f(x_0) + \delta x_0 f'(x_0) + \cdots. \tag{9}
\]

Keeping terms up to the first order in \( \delta x_0 \),

\[
f(x_0 + \delta x_0) = f(x_0) + \delta x_0 f'(x_0) = 0. \tag{10}
\]

Then we obtain

\[
\delta x_0 = -\frac{f(x_0)}{f'(x_0)}. \tag{11}
\]

Accordingly we obtain, by letting \( x_1 = x_0 + \delta x_0 \),

\[
x_1 = x_0 - \frac{f(x_0)}{f'(x_0)} \tag{12}
\]
If we replace \( x_0 \) and \( x_1 \) with \( x_n \) and \( x_{n+1} \) respectively, we obtain the recurrence relations
\[
x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} \quad (n = 0, 1, \cdots).
\] (13)

By iterating these recurrence relations, the sequence \( \{x_n\} \) is expected to converge to an exact solution. When we use these relations, a choice of the starting value \( x_0 \) is important. If \( f(x) \) has an analytic expression, we can calculate the derivative \( f'(x) \) analytically. Usually, we can easily compute the derivatives numerically using the following relations:
\[
f'(x_n) = \frac{f(x_n + h_n) - f(x_n - h_n)}{2h_n} \quad (n = 0, 1, \cdots),
\] (14)

where \( h_n \) are taken sufficiently small, and \( f(x_n + h_n) \) and \( f(x_n - h_n) \) are numerically computed.

5 Ishidzu’s analytical solution for S-state with the Woods-Saxon potential

In this section we explain briefly Ishidzu’s theory along the lines of his paper [5]. Putting
\[
r = R\rho, \quad d = \alpha R, \quad V_0 = -\frac{\alpha^2 h^2}{2mR^2}, \quad E = -\frac{\alpha^2 h^2}{2mR^2},
\] (15)

where \( \alpha, V_0, \) and \( \kappa \) are constants and furthermore changing the variables by
\[
x = -\exp \left\{ \frac{(1 - \rho)}{\alpha} \right\} = -\exp \left\{ \frac{(R - r)}{d} \right\},
\] (16)

\[
u(E, r) = e^{-\nu x} \chi(E, x),
\]

equation (1) becomes in case of \( l = 0 \)
\[
\chi''(E, x) + \frac{1 + 2\kappa a}{x} \chi'(E, x) + \frac{\alpha^2 \nu_0^2}{x^2 - 1} \chi(E, x) = 0 \quad (-e^{1/\kappa} < x < 0),
\] (17)

which can be solved by means of the hypergeometric series \([1]\). For the solution \( \chi(E, x) \) to this equation to take a finite value at \( x = 0 \) \((r \to \infty)\), \( \chi(E, x) \) must be
\[
\chi(E, x) = F(\mu, \nu; 1 + 2\kappa a|x|),
\] (18)

where \( F \) is the hypergeometric series \([1]\), and we put
\[
\mu = \alpha(x + i\kappa'), \quad \nu = \alpha(x - i\kappa'), \quad \kappa' = \sqrt{\nu_0^2 - \kappa^2}. \] (19)

The other boundary condition \( u(E, r) = e^{-\nu x} \chi(E, x) = 0 \) at \( r = 0 \) \((x = -e^{1/\kappa}) \) yields
\[
F(\mu, \nu; 1 + 2\kappa a|x| - e^{1/\kappa}) = 0.
\] (20)

Since generally \(| - e^{1/\kappa} | \gg 1 \), the function \( F \) must be continued analytically. By use of the relation between the hypergeometric series \([1]\):
\[
F(a, b; c|z)
= \frac{\Gamma(c)\Gamma(b - a)}{\Gamma(b)\Gamma(c - a)} (-z)^{-a}F(a, a - c + 1; a - b + 1|1/z)
+ \frac{\Gamma(c)\Gamma(a - b)}{\Gamma(a)\Gamma(c - b)} (-z)^{-b}F(b, b - c + 1; b - a + 1|1/z),
\] (21)

where \( \Gamma \) is the Gamma function, equation (20) is reduced to
\[
F(\mu, \nu; 1 + 2\kappa a|x| - e^{1/\kappa})
= \frac{\Gamma(1 + 2\kappa a)\Gamma(\mu - \nu)}{\Gamma(\mu + 1)}
\times e^{-\mu x}F(\mu, \mu - 2\kappa a; \mu - \mu + 1 - e^{-1/\kappa})
+ \frac{\Gamma(1 + 2\kappa a)\Gamma(\mu + \nu)}{\Gamma(\mu + 1)}
\times e^{-\nu x}F(\mu, \mu - 2\kappa a; \mu - \mu + 1 - e^{-1/\kappa}) = 0.
\] (22)

Since \( d = 0.67 \text{fm}, R = 7.52 \text{fm}, \) and \(| - e^{-1/\kappa} | = 1.34e^{-5} \ll 1 \), we keep only the first term of the expansion in powers of \((-e^{-1/\kappa})\) of the hypergeometric series \( F \). Therefore, the function \( F \) on the right-side of equation (22) can be approximated as unity to fairly good approximation. Consequently equation (22) becomes
\[
e^{-\kappa x}F(1 + 2\kappa a)
\times \left\{ \frac{\Gamma(-2i\kappa')}{\Gamma(\mu + 1)} e^{-ix} + \frac{\Gamma(2i\kappa')}{\Gamma(\mu + 1)} e^{ix} \right\} = 0,
\] (23)

where we have used equation (19) and have replaced the function \( F \) on the right-side of equation (22) with unity.

If we set
\[
\theta = \arg \frac{\Gamma(-2i\kappa')}{\Gamma(\mu + 1)}
\] (24)
where the notation $arg$ represents the argument of a complex number, equation (23) gives us significant relations

$$\begin{align*}
\cos(\theta - \kappa) &= 0, \\
\kappa' - \theta &= (n - \frac{1}{2})\pi \quad (n = 0, \pm 1, \pm 2, \cdots). \tag{25}
\end{align*}$$

With the help of equation (24), equations (25) become

$$\begin{align*}
\kappa' + arg\Gamma(2i\kappa') + arg\Gamma(\mu') + arg\Gamma(\bar{\mu} + 1) \\
= (n - \frac{1}{2})\pi \quad (n = 0, \pm 1, \pm 2, \cdots). \tag{26}
\end{align*}$$

As $\kappa, \kappa', \mu$ depend on $E$ through equations (15) and (19), the solutions $E_n$ to these transcendental equations (26) are energy eigenvalues.

### 6 Numerical calculations and the results

We consider Ishidzu’s approximate analytical expressions (26) and rewrite them, thanks to the mathematical properties of the Gamma function [1], as

$$\begin{align*}
\kappa' + arg\Gamma(1 + 2i\kappa') - 2arg\Gamma(\mu) - arg(\mu) \\
= n\pi \quad (n = 0, \pm 1, \pm 2, \cdots). \tag{27}
\end{align*}$$

we decompose equations (27) into two functions $arg(E)$ and $h(n) (n = 0, \pm 1, \pm 2, \cdots)$ such that

$$\begin{align*}
arg(E) &= \kappa' + arg\Gamma(1 + 2i\kappa') \\
- 2arg\Gamma(\mu) - arg(\mu), \tag{28}
h(n) &= n\pi \quad (n = 0, \pm 1, \pm 2, \cdots). \tag{29}
\end{align*}$$

We recognize that expression (28) is not yet well suited for our straightforward calculations. For that we deform it to a different form that is easy to calculate. By use of the following equation [4]:

$$\begin{align*}
\frac{\Gamma(x + iy)}{\Gamma(x)} &= e^{-i\gamma x} x(x + iy)^{-1} \prod_{m=1}^{\infty} \left[1 + iy/(x + m)\right] e^{iy/m}, \tag{30}
\end{align*}$$

where $\gamma$ is the Euler’s constant, the argument of $\Gamma(x + iy)$ is easily given by

$$\begin{align*}
arg(\Gamma(x + iy)) &= -\gamma y - \tan^{-1}\left(\frac{y}{x}\right) + \sum_{m=1}^{\infty} \left[\tan^{-1}\left(\frac{2\kappa'}{m}\right) - 2\tan^{-1}\left(\frac{\alpha\kappa'}{\alpha\kappa + m}\right)\right]. \tag{31}
\end{align*}$$

Thanks to this equation, equation (28) can be deformed to a tractable form

$$\begin{align*}
arg(E) &= \kappa' + \tan^{-1}\left(\frac{\kappa'}{\kappa}\right) \\
- \sum_{m=1}^{\infty} \left[\tan^{-1}\left(\frac{2\kappa'}{m}\right) - 2\tan^{-1}\left(\frac{\alpha\kappa'}{\alpha\kappa + m}\right)\right]. \tag{32}
\end{align*}$$

Keep in mind that for practical calculations of the values of the function $arg(E)$, equation (32) is used and its summation is carried out from $m = 1$ to $m = 100000$. When $a$ goes to zero in equation (32), equation (27) becomes

$$\begin{align*}
\kappa' + \tan^{-1}\left(\frac{\kappa'}{\kappa}\right) &= n\pi \quad (n = 0, \pm 1, \pm 2, \cdots), \tag{33}
\end{align*}$$

which is changed to

$$\begin{align*}
\kappa \tan \kappa' &= -\kappa'. \tag{34}
\end{align*}$$

This is the celebrated eigenvalue condition [6] of the 3-dimensional square-well potential (SQWP). From this it is shown explicitly that Ishidzu’s expression is a mathematical extension from the 3-dimensional square well potential to the Woods-Saxon potential.

Now we can plot $arg(E)$ and $h(n) (n = 1, 2, \cdots)$ against $E$ as in Figure 1, which shows us that the intersection points satisfy equations (27) and give the energy eigenvalues. When we want to obtain the exact eigenvalues numerically, we need only to apply Newton’s methods to the equation $f(E, n) = 0$, where $f(E, n)$ is defined by $f(E, n) = arg(E) - h(n)$. From Figure 1 we see the energies $E_n$ of the intersections for $n = 1, 2, 3,$ and 4 are approximately equal to $-40.0, -29.0, -15.0,$ and $-1.0$ MeV respectively. These values can be adopted as the starting values for Newton’s method.
Figure 1: The increasing curve with respect to $E$ represents $\arg(E)$ and horizontal lines correspond to $h(n)$ for each integer $n = 1, 2, 3,$ and $4$.

In what follows, using the Runge-Kutta method we solve equations (7) and (8) over an interval $[a,b]$ ($a < b$), where $a$ is very small and $b$ is sufficiently greater than $R$ (Nuclear radius). This time, at an intermediate point $r = c$ between $r = a$ and $r = b$ so that $a < c < b$, we split the interval $[a,b]$ into the two intervals $[a,c]$ and $[c,b]$. We solve numerically the equations over each interval using the Runge-Kutta method as stated in section 3. For the interval $[a,c]$ we solve forward from $r = a$ to $r = c$ with the initial conditions $u(E,a) = a^{l+1}$ and $v(E,a) = (l+1)a^l$ ($a \approx 0, l = 0$). For the interval $[c,b]$ we solve backward from $r = b$ to $r = c$ with the initial conditions $u(E,b) \approx \exp(-\frac{2m\sqrt{b}}{R}(-E))$ and $v(E,b) \approx -\frac{2m\sqrt{c}}{R}(-E)\exp(-\sqrt{\frac{2m}{R}}(-E))$. Then let $u_{in}(E,c)$ and $v_{in}(E,c)$ denote the numerical solutions at $r = c$ solved from $r = a$ to $r = c$ and let $u_{out}(E,c)$ and $v_{out}(E,c)$ denote the numerical solutions at $r = c$ solved from $r = b$ to $r = c$, and if we write the difference between their logarithmic derivatives as $f(E,c)$, then it is given by

$$f(E,c) = \frac{v_{out}(E,c)}{u_{out}(E,c)} - \frac{v_{in}(E,c)}{u_{in}(E,c)}$$ (35)

Now we can obtain an energy eigenvalue if we can determine a solution $E$ to $f(E,c) = 0$, the continuity of the logarithmic derivative of the wave function at $r = c$. This is an easy task for Newton’s method. We need to verify that the solution $E$ of $f(E,c) = 0$ is free of $c$.

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<th>Runge-Kutta</th>
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<td>SquareWell (MeV)</td>
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<td>no-solution</td>
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Table 1: The comparisons between Ishidzu formula and the Runge-Kutta (R-K) method. For the R-K method we adopt the parameters of the intervals explained in this section as $a = 0.0$ fm, $b = 25.0$ fm, $c = 6.0$ fm, and $N = 500$ for convenience. Each of the approximate energies are estimated from Fig. 1. The eigenvalues for the 3-dimensional square-well potential are calculated using equation (33) and also calculated from the R-K method using equation (35).† When the R-K method is applied, to avoid the singularity of the square-well potential at $r = R$, the following recipes are taken: The endpoint $c$ of the inner interval $[0,c]$ is shifted from $c = R$ to $c = R + 0.9999999$; the endpoint $c$ of the outer interval $[c,b]$ is shifted from $c = R$ to $c = R + 1.0000001$.  

†
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</table>

SQWP
-40.9937792 -31.9986175

Table 2: The energy eigenvalue dependence on the diffuseness parameter $d$. $r$ is defined as the diffuseness parameter $d$ divided by 0.67 fm ($d = r \cdot 0.67$ fm). The subscript numbers of $E$ correspond to the number $n$ in equation (27). $E_n(n = 1, 2, 3, 4)$ are the calculated values for $r$ using equation (27).

7 Concluding remarks

We have demonstrated that Newton’s method is a clearly powerful technique for solving eigenvalue problems of quantum mechanics and also have endorsed the validity of Ishizu’s analytical solution numerically using the Runge-Kutta method.

Although most of books on quantum mechanics are unfamiliar with Ishidzu’s analytic approximate expression explained in this paper in contrast to the eigenvalue problem for the 3-dimensional square-well potential, it should be noted that Ishidzu’s analytic approximate expression has a good accuracy and is very interesting from the viewpoint of mathematical physics.

In particular, we believe that most novice students beginning to learn practical uses of quantum mechanics can follow our calculations easily, which may have pedagogical merits for those students. Our approach may be of interest to those instructors who would like to introduce applications of Newton’s method to various fields into their courses.

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References


