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Numerical study of radial Schrödinger Equation for free particle, using Legender wavelet

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Abstract

This paper deals with the Legendre wavelet (LW) collocation method for the numerical solution of the radial Schrödinger Equation for free particle (electron) in spherical coordinate. Approximately analytical also numerical results of the ground state mode $l = 0$, of wave function or probability density function $R(r)$, has been presented and compared with the exact solution.

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1. Introduction

One of the most important eigenvalue equations in physics is the Schrödinger's wave equation. For a particle mass m in the potential $V(r)$ is:

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) + V(\mathbf{r}) = E\psi(\mathbf{r}) \tag{1}$$

In which $\psi(\mathbf{r})$ is the particle wave function and E is an energy eigenvalues [1]. For one-dimensional potential $V(x)$, equation (1) is as follow;

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

The Schrödinger's wave function, must be convergent as $x \to \infty$, because:

$$\int_{-\infty}^{+\infty} \psi(x)\psi^*(x)dx = 1, \tag{3}$$

which means that the particle must be somewhere in the x axes [1]. The first derivative of the wave function also must be continuous as if, it's second derivative which is appearing in the equation (2), could be exist.

The numerical solution of the above equation is the subject of many research in the last two decades. This equation has the analytical answers for the few potential energy

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$V(r)$. For many potentials, in physics and chemistry, it cannot be solved analytically. So in quantum mechanics, the numerical or approximately analytical solution of the Schrödinger's wave equation is a real need. The aim of this paper is to study and obtain the results of the new approach of, Legendre wavelet expansion of the solution of Eq. (1). comparison will be made whit the other well known numerical solution's methods.

2. Schrödinger equation for free particle

In the spherical coordinate, Radial Schrödinger equation for the central potential V(r) as follows:

$$\left[\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right]R(r)+\frac{2\mu}{\hbar^2}\left[E+V(r)-\frac{l(l+1)\hbar^2}{2\mu r^2}\right]R(r)=0 \tag{4}$$

μ is the reduced mass of system, l is the orbital quantum number and $R(r)$ is the radial wave function. In free space, particle moves without any potential energy $V(r)=0$, thus:

$$\left[\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right]R(r)+\frac{2\mu}{\hbar^2}\left[E-\frac{l(l+1)\hbar^2}{2\mu r^2}\right]R(r)=0. \tag{5}$$

For simplicity, rewrite Eq. (5) in dimensionless form as [1]:

$$\frac{d^2R(\rho)}{d\rho^2}+\frac{2}{\rho}\frac{dR(\rho)}{d\rho}-\frac{l(l+1)}{\rho^2}R(\rho)+R(\rho)=0 \tag{6}$$

where:

$$\rho=\sqrt{\frac{2\mu|E|}{\hbar^2}}\ r. \tag{7}$$

With assumuming that particle is electron, we have:

$$\frac{2\mu}{\hbar^2}=\frac{2m_ec^2}{\hbar^2c^2}\simeq\frac{2\times0.511\times10^6(\text{eV})}{(1973)^2(eV.A^\circ)^2}\simeq0.26246\,(\frac{1}{eV.A^{\circ2}}). \tag{8}$$

From quantum mechanics it is known that, $r^2|R(r)|^2$ represents the probability density of finding the particle in place of r from the center of coordinate. State which particle have it's minimum energy, called the ground state. In this state $l=0$ and the initial conditions $R(r)|_{r=0}=1$ and $\frac{dR}{dr}\big|_{r=0}=0$, is imposed maximum presence of particle at the origin.

3. Method of solution

Consider the the Schrödinger equation (5). First, we approximate $R(t)$ in terms of the LWs [2, 3] as follows

$$R(r)\simeq C^T\Psi(r)=\Psi^T(r)C, \tag{9}$$

where C is the LWs coefficient vector. By using the approximate $R(t) \simeq C^T\Psi(t)$ and operational matrix of derivative D, the residual function for the Schrödinger equation in the ground state $l = 0$, can be written as

$$\mathbf{Res}(r) = C^T\left[D^2 + \frac{2}{r}D\right]\Psi(r) + \frac{2\mu}{\hbar^2}C^T\,[E-0]\,\Psi(r), \tag{10}$$

Hereafter, in order to approximate solution of the Schrödinger equation (5) with initial conditions, as in the typical collocation method, we generate $2^k(M+1)-2$ equations by applying

$$\mathbf{Res}(r_i) = 0, \quad i = 1, 2..., 2^kM - r. \tag{11}$$

Moreover, by using following initial condition:

$$C^T\Psi(10^{-4}) = 1, \tag{12}$$

$$C^TD\Psi(10^{-4}) = 0, \tag{13}$$

Eqs. (11) together with (12) and (13) generate a system of $2^k(M+1)$ algebraic equations for $2^k(M+1)$ unknown elements of the unknown vector C. This system can be solved for unknown coefficient vector C and unknown function $R(r)$ can be obtained by substituting the obtained vector C in Eq. (9).

With the above considerations, approximate analytical LW expansion of wave function, $R(r)$, with $M = 8, k = 0$ is obtained as follow:

$$R(r) \simeq \begin{cases} 0.0000000 & r < 0 \\ -0.00018597601r^8 + 0.00083651506r^7 - \\ -0.0015816998r^6 + 0.0016209070r^5 - \\ -0.00041023806r^4 + 0.00035908484r^3 - & 0 \le r < 1 \\ -0.043819796r^2 + 0.00000875837r + \\ +1.0000001 \\ 0.0000000 & 1 < r. \end{cases} \tag{14}$$

Numerical results for the solution of the radial Schrödinger Eq. (5) in the case of $l = 0$, is shown in Table 1, for various methods.

4. Conclusion

In this paper a new approach, Legendre wavelet (LW) is used and an approximate analytic expansion is derived for radial wave function of free electron in its ground state. Numerical results obtained from LW expansion, compared with exact and other well known numeric methods in Table 1. Runge Kutta Fehlberg and LW expansion methods, are shown accurate results. Forth order Runge Kutta method and Modified Euiler method (Heun) both with step size 0.1, are shown less accurate results than others.

Table 1. Comparison of the numerical solution for the radial Schrödinger equation in the ground state of the free electron $R(r)$

r	Exact solution	RKF45	RK4 $h = 0.1$	HUEN $h = 0.1$	LW expansion
0.1	0.99956	0.99956	0.99869	0.99869	0.99956
0.2	0.99825	0.99825	0.99777	0.99738	0.99825
0.3	0.99607	0.99607	0.99574	0.99541	0.99607
0.4	0.99302	0.99302	0.99277	0.99251	0.99302
0.5	0.98910	0.98910	0.98891	0.98869	0.98910
0.6	0.98433	0.98433	0.98417	0.98398	0.98433
0.7	0.97870	0.97870	0.97857	0.97841	0.97870
0.8	0.97224	0.97224	0.97212	0.97198	0.97224
0.9	0.96494	0.96494	0.96484	0.96472	0.96494
1.0	0.95683	0.95683	0.95674	0.95662	0.95683

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