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A Numerical Solution for Hydrogen Atoms Like

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Abstract: Wavelets constitute a family of functions that constructed from dilation and translation of a single function. They are suitable tools for solving variational problems. In this study, we want to extremum the Hamiltonian of hydrogen atom using Legendre wavelets. Legendre wavelets are defined on the domain [0,1]. For solving this problem, we represent a generalized Legendre functions and generalized Legendre wavelets on the [-s, s] and [0, s], respectively. We start from the radial equations of hydrogen atom like and represent the wave function in term of generalized Legendre function and then convert the redial equation of hydrogen atom like to a polynomial in term of coefficients of wave function. The eigenstate will be minimize provided that, the derivative of it respect to the all of coefficients of wave function to be equal zero. The last equation is a algebraic equation and the solutions are the energy states of hydrogen atom like.

Key words: Hydrogen atoms, hamiltonian, wawe function

INTRODUCTION

Orthogonal functions and polynomials series have received attention in dealing with various problems of dynamic systems. The orthogonal functions and polynomial series reduce these problems to those of solving a system of algebraic equations. For example, Special attention has been given to applications of Walsh functions[1], block pulse functions[2], Laguerre polynomials[3], Legendre polynomials[4], Chebyshev polynomials[5] and Fourier series[6]. Legendre functions is an orthogonal set on the [-1,1]. Legendre functions satisfy Legendre differential equation and it is covered in many text Books of mathematical physics[7]. One of the most applications of Legendre functions is Legendre Wavelets in differential calculus. The Legendre wavelets are defined over [0,1]. Legendre wavelets can be used for variational problems[8-10]. Legendre wavelet scan be used for two dimension variational problems[11]. In this study we want to represent a generalized Legendre wavelets that is an orthogonal set over the interval [0,s]. Then, We get an operational matrix of integration and another operational matrices for them. In final, we present a numerical solution for Hydrogen atoms like.

Generalized Legendre functions: Generalized Legendre Differential Equation (GLDE). It is obviously that the following differential equation is GLDE.

$$(s^2 - x)y''(x) - 2y'(x) + n(n+1)y(x) = 0 \qquad (1)$$

The solutions of late equation are an orthogonal set over [-s,s]. We choosing $y(x) = \Sigma c_l x^l$ and substituting y (x) in (1), easily find

$$\begin{aligned} P_0(s;x) &= 1 \\ P_1(s;x) &= x \\ P_2(s;x) &= \frac{1}{2}(3x^2 - s^2) \\ P_3(s;x) &= \frac{1}{2}(5x^3 - 3s^2x) \\ P_4(s;x) &= \frac{1}{8}(35x^4 - 30s^2x^2 + 3s^4) \\ P_5(s;x) &= \frac{1}{8}(63x^5 - 70s^2x^3 + 15s^4x) \\ P_6(s;x) &= \frac{1}{16}(231x^6 - 315s^2x^4 + 105s^4x^2 - 5s^6) \end{aligned} \qquad (2)$$

It is obviously that the polynomials in (2) reduce to Legendre polynomials for s = 1 or in general

$$P_n(s;x) = s^n P_n(x/s) \qquad (3)$$

We can easily find the generating functions for generalized Legendre functions.

$$\frac{1}{\sqrt{1-2xt+{}^2t^2}} = \sum_{n=}^{\infty} P_n(s;x)t^n \qquad (4)$$

Recurrence relations for generalized Legendre functions can be find from (4).

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$$xP_m(s;x)=\frac{m+1}{2m+1}P_{m+1}(s;x)+\frac{m}{2m+1}s^2P_{m-1}(s;x)$$

$$(2m+1)P_m(s;x)P'_{m+1}(s;x)-s^2P'_{m-1}(s;x) \qquad (5)$$

Differential representation of generalized Legendre functions can be obtain from (3)

$$P_n(s;x)=\frac{1}{2^n n!dx^n}(x^2-s^2)^n \qquad (6)$$

Legendre functions are an orthogonal set on the [-1,1] respect to the weight function ω(x) = 1. Then, generalized Legendre functions are an orthogonal set on the [-s, s] . Respect to the weight function ω(x) = 1.

$$\int_S^S P_n(s;x)P_m(s;x)dx=\frac{2}{2n+1}s^{2n+1}\delta_{n,m} \qquad (7)$$

Generalized legendre wavelets: We define generalized Legendre wavelets from generalized Legendre functions.

$$\psi_{n,m}(s;x)=\begin{cases}\sqrt{\frac{2m+1}{2s^2m+1}}2^{\frac{k}{2}}P_m(s;2^kx-(2n-1)s) & \frac{2n-2}{2^k}S\le x<\frac{2n}{2^k}S\\ 0 & \text{Otherwise}\end{cases} \qquad (8)$$

We represent some of them with details in below.

$$\psi_{1,0}(s;x)=\begin{cases}\sqrt{\frac{1}{2s}}2^{\frac{k}{2}} & 0\le x<\frac{2n}{2^k}S\\ 0 & \text{Otherwise}\end{cases}$$

$$\psi_{1,1}(s;x)=\begin{cases}\sqrt{\frac{3}{2s^3}}2^{\frac{k}{2}}(2^kx-s) & 0\le x<\frac{2n}{2^k}S\\ 0 & \text{Otherwise}\end{cases}$$

$$\psi_{1,2}(s;x)=\begin{cases}\sqrt{\frac{5}{2s^5}}2^{\frac{k}{2}}(\frac{3}{2}(2^kx-s)^2-\frac{s^2}{2}) & 0\le x<\frac{2n}{2^k}S\\ 0 & \text{Otherwise}\end{cases}$$

Generalized Legendre wavelets are an orthonormal set such that

$$\int_0^s\psi_{n,m}(s;x)\psi_{n',m'}(s;x)dx=\delta_{n,n'}\delta_{m,m'} \qquad (9)$$

OPERATIONAL MATRICES

In this study we want to compute two operational matrices such that

$$\int_0^t\psi(s;x)dx=P.\psi(s;x) \qquad (10)$$

And

$$x^m\psi(s;x)=\Gamma^m.\psi(s;x) \qquad (11)$$

In which m is a positive integer and) ; (x s Ø defined as below

$$\Psi(s;x)=[\psi_{1,0}(s;x),\psi_{1,1}(s;x),...,\psi_{2,0}(s;x),\psi_{2,1}(s;x),...,\psi_{2^{k-1},1}(s;x),\psi_{2^{k-1},M-1}(s;x)]^T$$

For computation the operational matrix P, we have

$$\int_0^1\psi_{1,0}(s;x)dx=\begin{cases}\sqrt{\frac{2}{s}}t & 0\le t<\frac{s}{2}\\ \sqrt{\frac{2}{s}} & \frac{s}{2}\le t<s\end{cases}$$

$$\int_0^t\psi_{1,0}(s;x)dx=\frac{s}{4}\psi_{1,0}(s;t)+\frac{s}{\sqrt[4]{3}}\psi_{1,1}(s;t)\frac{s}{2}\psi_{2,0}(s;t)$$

$$\int_0^t\psi_{1,1}(s;x)dx=-\frac{s}{\sqrt[4]{3}}\psi_{1,0}(s;t)\frac{s}{\sqrt[4]{3}\sqrt{5}}\psi_{1,2}(s;t) \qquad (12)$$

$$\int_0^t\psi_{1,2}(s;x)dx=-\frac{s}{\sqrt[4]{3}\sqrt{5}}\psi_{1,1}(s;t)+\frac{s}{\sqrt[4]{3}\sqrt{5}}\psi_{1,3}(s;t)$$

$$\int_0^t\psi_{2,0}(s;x)dx=-\frac{s}{4}\psi_{2,0}(s;t)+\frac{s}{\sqrt[4]{3}}\psi_{2,1}(s;t)$$

$$\int_0^t\psi_{2,1}(s;x)dx=-\frac{s}{\sqrt[4]{3}}\psi_{2,0}(s;t)+\frac{s}{\sqrt[4]{3}\sqrt{5}}\psi_{2,2}(s;t)$$

If we represent the results in matrix form, We have

$$P_{6\times6}=\frac{s}{2^2}\begin{bmatrix}1 & \frac{1}{\sqrt{3}} & 0 & 2 & 0 & 0\\ -\frac{1}{\sqrt{3}} & 0 & \frac{1}{\sqrt{3}\sqrt{5}} & 0 & 0 & 0\\ 0 & -\frac{1}{\sqrt{3}\sqrt{5}} & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 1 & \frac{1}{\sqrt{3}} & 0\\ 0 & 0 & 0 & -\frac{1}{\sqrt{3}} & 0 & \frac{1}{\sqrt{3}\sqrt{5}}\\ 0 & 0 & 0 & 0 & -\frac{1}{\sqrt{3}\sqrt{5}} & 0\end{bmatrix}$$

And in general

$$P=\frac{s}{2^k}\begin{bmatrix} L & F & F & \dots & F \\ O & L & F & \dots & F \\ O & O & L & \dots & F \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ O & O & O & \dots & L \end{bmatrix} \qquad (13)$$

in which O, F and L are M M .matrices. The O is null matrix and F and L defined as

$$F=\begin{bmatrix} 2 & 0 & 0 & \dots & 0 \\ 0 & 0 & 0 & \dots & 0 \\ 0 & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 0 \end{bmatrix} \qquad (14)$$

And

$$L=\begin{pmatrix} 1 & \frac{1}{\sqrt{3}} & \cdots & 0 & 0 \\ -\frac{1}{\sqrt{3}} & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & 0 & 0 \\ 0 & 0 & \cdots & 0 & \frac{1}{\sqrt{2M-3}\sqrt{2M-1}} \\ 0 & 0 & \cdots & \frac{1}{\sqrt{2M-3}\sqrt{2M-1}} & 0 \end{pmatrix} \qquad (15)$$

For computation the operational matrix Γ, we use the recurrence relations (5) and easily find

$$p=\frac{s}{2^k}\begin{pmatrix} U_1 & O & O & \dots & O \\ O & U_3 & O & \dots & O \\ O & O & U_5 & \dots & O \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ O & O & O & \dots & U_{2^K-2} \end{pmatrix} \qquad (16)$$

while U_n is a M×M matrix given by

$$p=\frac{s}{2^k}\begin{pmatrix} n & \frac{1}{\sqrt{3}} & \dots & 0 & 0 \\ \frac{1}{\sqrt{3}} & n & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & n & \frac{M-1}{\sqrt{2M-3}\sqrt{2M-1}} \\ 0 & 0 & \dots & \frac{M-1}{\sqrt{2M-3}\sqrt{2M-1}} & n \end{pmatrix} \qquad (17)$$

Hydrogen atom like: Consider the radial equation of time independent schrodinger equation in spherical coordinate[12].

$$-\frac{\hbar^2}{2\mu}\frac{d}{dr}\left(r^2 R'(r)\right)-ze^2 rR(r)+\frac{\hbar}{2\mu}l(l+1)=Er^2 R(r) \qquad (18)$$

Determine the energy state of Hydrogen atom like, E, provided that

$$\int_0^\infty R^*(r)R(r)r^2\,dr-1=0$$

If we do the changing of variable $\rho=\sqrt{\frac{8\mu E}{\hbar^2}}\,r$ the (18) reduce to

$$\frac{d}{d\rho}\left(\rho^2 R'(\rho)\right)-\frac{\rho^2}{4}R(\rho)-l(l+1)R(\rho)=-\varepsilon\rho R(\rho) \qquad (19)$$

in which, $\varepsilon=\frac{ze^2}{\hbar}\sqrt{\frac{\mu}{2|E|}}$ We have

$$\int_0^\infty \rho R^*(\rho)\frac{d}{d\rho}\left(\rho^2 R'(\rho)\right)d\rho-l(l+1)\int_0^\infty \rho R^*(\rho)R(\rho)d\rho$$
$$-\int_0^\infty \frac{\rho^3}{4}R^*(\rho)R(\rho)d\rho=-\varepsilon\left(\frac{8\mu|E|}{\hbar^2}\right)^{\frac{3}{2}} \qquad (20)$$

And use the multiplier lagrange technique

$$\hat{J}=\int_0^\infty \rho R^*(\rho)\frac{d}{d\rho}\left(\rho^2 R'(\rho)\right)d\rho+l(l+1)\int_0^\infty \rho R^*(\rho)R(\rho)d\rho$$

$$+\int_0^\infty \frac{\rho^3}{4} R^*(\rho)R(\rho)d\rho - \lambda\left(\int_0^\infty R^*(\rho)R(\rho)\rho^2 d\rho - \varepsilon\left(\frac{8\mu|E|}{\hbar^2}\right)^{\frac{3}{2}}\right)$$

If we choose $R'(\rho) = C^T.\Psi(s; x)$ (In which C is column matrix of coefficient and ^{T}indicate the transpose of matrix) we have $R(\rho) = C^T. P .\Psi(s; x)$

$$\hat{J} = C^T.P.\Gamma^2.C + C^T.\Gamma^3.C + l(l+1)$$

$$C^T.P.\Gamma.P^T.C + \frac{1}{4}C^T.P.\Gamma^3.P^T.C$$

$$-\lambda\left(CT.P.\Gamma 2.PT.C - \left(\frac{8\mu|E|}{\hbar^2}\right)^{\frac{3}{2}}\right) \quad (22)$$

The (22) is minimize provided that

$$\frac{\partial}{\partial C}\hat{J} = 0, \qquad \frac{\partial}{\partial \lambda}\hat{J} = 0 \quad (23)$$

The (23) have solutions provided that

$$\text{Det (A)} = 0 \quad (24)$$

In which

$$A = P.\Gamma^2 + \Gamma^3 + l(l+1)P.\Gamma.P^T + \frac{1}{4}P.\Gamma^3 P^T - \lambda P.\Gamma^2.P^T$$

From solving (24) find the energy state of hydrogen atom. Tables 1, 2 and 3 shows the results for various l and s = 15, k = 4, M = 3. Parameter λ is first quantum number of Hydrogen atom like n . As you know $n \geq l+1$.

Table 1: Exact solution and Legendre wavelet solution Hydrogen atom for l = 0 and s = 15, k = 4, M = 3

No	Exact solution λ	Estimate solution λ
1	1	1.00094
2	2	1.88885
3	3	2.78469
4	4	3.66495

Table 2: Exact solution and Legendre wavelet solution Hydrogen atom for l = 1 and s = 15, k = 4, M = 3

No	Exact solution λ	Estimate solution λ
1	2	2.00138
2	3	2.92433
3	4	3.66456
4	5	4.38912

Table 3: Exact solution and Legendre wavelet solution Hydrogen atom for l = 2 and s = 15, k = 4, M = 3

No	Exact solution λ	Estimate solution λ
1	3	2.96964
2	4	3.77261
3	5	4.85850
4	6	6.49375

CONCLUSION

In this study, we present a numerical method for Hydrogen atoms like. This method is based on orthogonal sets. This method is suitable perturb Hydrogen atoms like.

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