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Symmetric Extended Wavelets and One Dimension Schrodinger Equation

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Abstract: In this research, we present a numerical solution for schrodinger equation. This method is based on generalized Legendre wavelets and generalized operational matrices. Generalized Legendre wavelets are a complete orthogonal set on the interval [-s, s] (s is a real large positive number.) The mother function of generalized Legendre wavelets are generalized legendre functions. Generalized Legendre functions are an orthogonal set on the interval [-s, s]. The schrodinger equation is equal to a variational problem and we convert the variational problem to a non linear algebraic equations. From the solving of algebraic equation to get the eigen-states of schrodinger equation. We applied this method to one dimension nonlinear oscillator ($V(x) = 1/2kx^n$, $-\infty < x < \infty$) and to get the eigen-states of oscillator for various n. For n = 2, the oscillator is linear and there is an exact solution for its. The results for n = 2 demonstrate the validity of this solution.

Key words: Schrodinger equation, wavelets, operational method, one dimension, symmetric extended

INTRODUCTION

Orthogonal functions and polynomial 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 (Chen and Hsiao, 1975), block pulse functions (Hwang and Shih, 1985), Laguerre polynomials (Hwang and Shih, 1985), Legendre polynomials (Chang and Wang, 1983), Chebyshev polynomials (Horng and Chou, 1985) and Fourier series (Razzaghi and Razzaghi, 1988). Legendre functions is an orthogonal set on the [-1, 1]. Legendre functions satisfy Legendre differential equation and it is covered in many textbooks of mathematical physics (Arfken, 1985). One of the most applications of Legendre functions is in differential calculus. The Legendre wavelets are defined over [0, 1]. Legendre wavelets can be used for variational problems (Razzaghi and Yyousefi, 2000, 2001a, b). Legendre wavelets can be used for two dimension variational problems (Parsia, 2005). In this study, we want to represent a generalized Legendre wavelets. Then, we get an operational matrix of integration and another operational matrices for them. In final to present a numerical solutions for time independent schrodinger equation.

GENERALIZED LEGENDRE FUNCTIONS

In recent years, wavelets have found their way in many different field of sciences and engineering. Wavelets constitute a family of functions that constructed from dilation and translation of a single function. Legendre wavelets is proposed by Razzaghi and Yousefi (2000, 2001a, b) for solving variational problems. The mother function of Legendre wavelets is Legendre functions. In this here, we define generalized Legendre wavelets by generalized Legendre functions. Generalized Legendre functions satisfied the differential equations below,

$$(s^2 - x\ )y''(x) - 2xy'(x) + n(n+1)y(x) = 0 \tag{1}$$

The solutions of late equation are an orthogonal set over [-s,s]. We choosing

$$y(x) = \sum c_l x^l$$

and substituting y(x) in (1), easily find

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

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Differential representation of generalized Legendre functions can be obtain from (2)

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

The generalized Legendre wavelets to be defined

$$\psi_{n.m}(s;x) = \begin{cases} \sqrt{\frac{2m+1}{2s^{2m+1}}}\, 2^{\frac{k}{2}} P_m(s; 2^k x - (2n-1)s) & \frac{2n-2}{2^k}s \le x < \frac{2n}{2^k}s \\ 0 & \text{otherwise} \end{cases} \tag{3}$$

In which we define $n = -2^{k-1}+1, -2^{k-1}+2, \ldots, 0, 1, \ldots, 2^{k-1}$ and $m = 0,1,2,\ldots M-1$. Generalized Legendre wavelets are an orthogonal set such that

$$\int_{-s}^{s} \psi_{n,m}(s;x)\psi_{n',m'}(s;x)dx = \delta_{n,n'}\delta_{m,m'} \tag{4}$$

We represent two operational matrices for Legendre wavelets such that

$$\int_{-s}^{t} \Psi(s;x)dx = P \cdot \Psi(s;x) \tag{5}$$

$$x\Psi(s;x) = \Gamma \cdot \Psi(s;x) \tag{6}$$

In which $\Psi(s;x)$, P and Γ are defined for generalized Legendre wavelets as below:
The matrix column $\Psi(s;x)$ is a $2^k M \times 1$ dimension that defined as

$$\Psi(s;x) = [\psi_{-2^{k-1}+1,0}(s;x), \psi_{-2^{k-1}+1,1}(s;x), \ldots, \psi_{-2^{k-1}+2,0}(s;x), \ldots, \psi_{2^{k-1},M-1}(s;x)]^T \tag{7}$$

The P matrix is a $2^k M \times 2^k M$ matrix as below

$$P = \frac{s}{2^k}\begin{pmatrix} L & F & F & \cdots & F \\ O & L & F & \cdots & F \\ O & O & L & \cdots & F \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ O & O & O & \cdots & L \end{pmatrix}$$

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

$$F = \begin{pmatrix} 2 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 0 \end{pmatrix} \tag{8}$$

And

$$L = \begin{pmatrix} 1 & \frac{1}{\sqrt{3}} & \cdots & 0 & 0 \\ -\frac{1}{\sqrt{3}} & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & 0 & 0 \\ 0 & 0 & \cdots & 0 & \frac{1}{\sqrt{2M-3}\sqrt{2M-1}} \\ 0 & 0 & \cdots & -\frac{1}{\sqrt{2M-3}\sqrt{2M-1}} & 0 \end{pmatrix} \tag{9}$$

The $2^k M \times 2^k M$ dimensions operational matrix Γ is

$$\Gamma = \frac{s}{2^k}\begin{pmatrix} U_{-2^k+1} & O & O & \cdots & O \\ O & U_{-2^k+2} & O & \cdots & O \\ O & O & U_{-2^k+3} & \cdots & O \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ O & O & O & \cdots & U_{2^k-1} \end{pmatrix} \tag{10}$$

While U_n is a $M \times M$ matrix given by

$$U_n = \begin{pmatrix} n & \frac{1}{\sqrt{3}} & \cdots & 0 & 0 \\ \frac{1}{\sqrt{3}} & n & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & n & \frac{M-1}{\sqrt{2M-3}\sqrt{2M-1}} \\ 0 & 0 & \cdots & \frac{M-1}{\sqrt{2M-3}\sqrt{2M-1}} & n \end{pmatrix} \tag{11}$$

NUMERICAL SOLUTION

The time independent schrodinger equation is a Fundamental equation of quantum mechanics (John and Powell, 1961). That is

$$H\psi_n(x) = E\psi_n(x) \tag{12}$$

subject to constraint $\Psi_n(\pm\infty) = 0$. In which $H = -\hbar^2/2m\, d^2/dx^2 + V(x)$ is a hamiltonian of system, $\Psi_n(x)$ and E_n are wave function and energy state of system.

This is equal to the variation problem. The extremum of quantity

Table 1: Energy states of various oscillator $V(x) = 1/2\,kx^n$, n = 2 for s = 6, k = 3, M = 3

Number of state	Energy state (n=2)	Energy state (n=4)	Energy state (n=6)	Energy state (n=8)
1	1.00194	1.058941	1.144552	1.232409
2	3.00384	3.829998	4.474100	5.031860
3	5.04701	7.798936	10.152840	12.480238
4	7.10115	12.625725	18.023182	25.217360
5	9.20016	19.019775	29.186824	45.072125

$$E_n = <\psi_n(x)|H|\psi_n''(x)> = \frac{\hbar^2}{2m} <\psi_n'(x)|\psi_n'(x)> + <\psi_n(x)|V(x)|\psi_n(x)> \quad (13)$$

subject to the constraint $<\Psi_n(x)|\Psi_n(x)> = 1$. For any nonsingular potentials we have

$$V(x) = \sum_{l=0}^{\infty} a_l x^l \quad (14)$$

From substituting the relation (14) in (13), choosing

$$a_l = \gamma_l \frac{m^{\frac{1}{2}} \omega^{\frac{l+2}{2}}}{\hbar^{\frac{l-2}{2}}}$$

and change the variable

$$y = \sqrt{\frac{m\omega}{\hbar}}\, x,$$

we have

$$\hat{E}_n = <\psi_n'(y)|\psi_n'(y)> + \sum_{l=0}^{\infty} \gamma_n <\psi_n(y)|y^l|\psi_n(y)> - \beta(<\psi_n(y)|\psi_n(y)> - \sqrt{\frac{m\omega}{\hbar}}) \quad (15)$$

In which $\beta = 2\lambda/\hbar\omega$ and is λ coefficient Lagrange multiplier. If we choose $\Psi'(y) = C^T.\ \Psi(s; y)$ we have $\Psi(y) = C^T.\ \Psi(s; y)$. From substituting $\Psi'(y)$ and $\Psi(y)$, $\hat{E}_n$ convert to matrix form as bellow

$$\hat{E}_n = C^T \cdot C + C^T \cdot P \cdot V \cdot P^T \cdot C - \beta\left(C^T \cdot P \cdot P^T \cdot C - \left(\frac{m\omega}{\hbar}\right)^{\frac{1}{2}}\right) \quad (16)$$

Where,

$$V = \sum_{l=0}^{\infty} \gamma_l \Gamma^l$$

The (16) is minimize provided that

$$\frac{\partial}{\partial C^T}\hat{E}_n = 0,\ \frac{\partial}{\partial \beta}\hat{E}_n = 0. \quad (17)$$

Table 2: Energy states of simple harmonic oscillator for s = 6, k = 3, M = 3

Number of state	Wavelet solution ($\hbar\omega/2$)	Exact solution ($\hbar\omega/2$)	Error (percent)
1	1.00194	1	0.00194
2	3.00384	3	0.00128
3	5.04701	5	0.00940
4	7.10115	7	0.01445

The Eq. 17 are a set of nonlinear algebraic equation. There are solution for its provided that the determinant of coefficient is been zero.

$$\mathrm{Det}[A] = 0 \quad (18)$$

The matrix A in (18) is defined as, $A = I + P.\ V.\ P^T - \beta P.\ P^T$, in which I is unit matrix.

NONLINEAR OSCILLATOR

We apply this method for quantum oscillator

$$V(x) = \frac{1}{2}kx^n, \quad n = 2,4,6,...$$

potential and the results is written in Table 1.

The result of this method for n = 2 is compared to exact solution in Table 2.

CONCLUSION

The wavelet method is a semi analytical approximate method for solution the schrodinger equation. This method is based on orthogonal set and in compare to perturbation theory has a simple algorithm. In perturbation theory we need to have two conditions:

- We must to have an exact solution of unperturbed Hamiltonian.
- The perturbation Hamiltonian is very small in compare to unperturbed Hamiltonian. While, we don't need any condition in applying wavelet methods.

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