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Solutions of the Harmonic Oscillator Equation in a B-Polynomial Basis

Muhammad I. Bhatti

Department of Physics and Geology
University of Texas-Pan American
Edinburg, Texas 78539-2999, USA
Bhatti@utpa.edu

Abstract

A method to construct approximate solutions for a quantum mechanical system has been introduced in a Bernstein-polynomial (B-polynomial) basis. The B-polynomial-Galerkin method is applied to produce the energy spectrum of quantum mechanical system harmonic oscillator equation. The discrete eigenstates are reproduced after applying the initial condition to the generalized eigenvalue problem constructed from the exact analytic matrix elements. The numerical discrete eigenvalues and the corresponding eigenstates are in excellent agreement with the exact results of the harmonic oscillator. However, the accuracy of the results depends on the number of B-polynomials chosen to construct the approximate solutions. To check the quality of the spectrum, the resulting basis set is used to evaluate the Thomas-Reiche-Kuhn (TRK) sum rules. In addition, perturbations through 5^{th} order are calculated to first excited state of harmonic oscillator using a perturbation potential and excellent agreement is observed with exact results.

Keywords: Harmonic Oscillator, Quantum System, Perturbation Theory, Bernstein-Polynomials, Energy Spectrum

1 Introduction

Continuous piecewise polynomials are increasingly becoming useful mathematical tools in scientific and engineering computations for solving challenging problems. They are precisely defined, calculated rapidly on a modern PC and can represent a great deal of functions. They can be differentiated and integrated seemingly, and can be used to form spline curves that can approximate any function to a desired accuracy. Over the past few decades, the spectral

methods that involve such polynomials have been successfully used in solving physics related computations. In particular, the B-splines methods have been employed to predict atomic structure by several authors. In reference [5], a method was used for calculating the static Polarizabilities of the ground and excited states of the hydrogenic systems utilizing the n^{th} degree B-splines Galerkin method. The B-splines method created a complete set of basis functions that were used to approximate solutions to the differential equations depending on the degree n and number (N) of the B-splines defined by the recursive definition [5],

$$\begin{aligned} &B_i^0(r) = \begin{cases} 1 & \text{if } t_i \leq r < t_{i+1} \\ 0 & \text{otherwise} \end{cases} \\ &\text{and} \\ &B_i^n(r) = \left(\frac{r-t_i}{t_{i+n}-t_i}\right) B_i^{n-1}(r) + \left(\frac{t_{i+n+1}-r}{t_{i+n+1}-t_{i+1}}\right) B_{i+1}^{n-1}(r). \end{aligned} \tag{1.1}$$

The function $B_i^n(r)$ is a piecewise polynomial of degree n defined on a knot sequence $\{t_i\}$. The knots defining the grid have $(n+1)$-fold degeneracy at the endpoints of the interval.

It is discovered that when number of B-splines is set to $N = n+1$, the set of B-splines in Eq.(1.1) defined over a knot sequence collapses to a set of continuous B-polynomials over the entire range. This paper presents a method of how to construct solutions of harmonic oscillator equation and a spectrum over a finite interval [a, b] using finite set of B-polynomials. Since B-polynomials do not depend on the nature of any interior sub-interval points, also known as knots, the matrix elements are evaluated exactly on the entire region [a, b]. In the following sections, we explain the method for approximations; define B-polynomials basis and present general formulas ready to be applied to the harmonic oscillator problem.

2 Polynomial Basis and Explicit Formulas

Our aim is to present solutions of the harmonic oscillator equation on a closed interval [a,b] with continuous B-polynomials which require no interval grid points. The details of such polynomials have been provided in an enormous number of publications [5-10]. As mentioned earlier, a basis of B-polynomials may be obtained from Eq. (1.1) by setting number of B-splines equal to $n+1$, where n represents the degree of B-splines. The general form of the B-polynomials of n^{th} degree over an interval [a, b] is defined in ref.[6]

$$B_{i,n}(x) = \begin{pmatrix} n \\ i \end{pmatrix} \frac{(x-a)^i (b-x)^{n-i}}{(b-a)^n} \quad 0 \leq i \leq n, \tag{2.1}$$

where the binomial coefficients are given

$$\left(\begin{array}{c} n \\ r \end{array} \right) = \frac{n!}{r!\,(n-r)!}. \tag{2.2}$$

There are $n+1$ n^{th} degree polynomials. For convenience we set $B_{i,n}(x) = 0$, if $i < 0$ or $i > n$. A simple code written in Mathematica or Maple may be used to create all the non-zero polynomials of any degree n supported over an interval. The first and last polynomials are generally related to the Boundary Conditions of the problem under investigation. The dual basis function for the Bernstein polynomials basis is given in ref.[11],

$$D_{i,n}(x) = \sum_{j=0}^{n} \alpha_{i,j} B_{i,j}(x), \quad (i, j = 0, 1, ..., n). \tag{2.3}$$

Where the real coefficients $\alpha_{i,j}$ have explicit expression

$$\alpha_{i,j} = \frac{1}{(b-a)} \frac{(-1)^{i+j}}{\left(\begin{array}{c} n \\ i \end{array} \right) \left(\begin{array}{c} n \\ j \end{array} \right)} \sum_{q=0}^{\min(i,j)} (2q+1) \left(\begin{array}{c} n+q+1 \\ n-i \end{array} \right) \left(\begin{array}{c} n-q \\ n-i \end{array} \right) \left(\begin{array}{c} n+q+1 \\ n-j \end{array} \right) \left(\begin{array}{c} n-q \\ n-j \end{array} \right), \tag{2.4}$$

and the dual basis must satisfy the relationship,

$$(D_{i,n}(x),\, B_{j,n}(x)) = \int_a^b D_{i,n}(x)\, B_{j,n}(x)\, dx = \delta_{i,j} = \left\{ \begin{array}{l} 1,\ i = j \\ 0,\ \text{otherwise} \end{array} \right. . \tag{2.5}$$

Here we list a closed form explicit formulas involving inner products and derivatives of polynomials:

$$(B_{i,n}(x),\, B_{j,m}(x)) = \frac{(b-a) \left(\begin{array}{c} n \\ i \end{array} \right) \left(\begin{array}{c} m \\ j \end{array} \right)}{(n+m+1) \left(\begin{array}{c} n+m \\ i+j \end{array} \right)}, \tag{2.6}$$

$$x^m\, B_{i,n}(x) = \left(\begin{array}{c} n \\ i \end{array} \right) \sum_{k=0}^{m} \frac{a^{m-k} (b-a)^k \left(\begin{array}{c} m \\ k \end{array} \right)}{\left(\begin{array}{c} n+k \\ i+k \end{array} \right)} B_{i+k,n+k}(x), \tag{2.7}$$

$$(x^m\, B_{i,n}(x), B_{j,n}(x)) = (b-a) \left(\begin{array}{c} n \\ i \end{array} \right) \left(\begin{array}{c} n \\ j \end{array} \right) \sum_{k=0}^{m} \frac{a^{m-k} (b-a)^k \left(\begin{array}{c} m \\ k \end{array} \right)}{(2n+k+1) \left(\begin{array}{c} 2n+k \\ i+j+k \end{array} \right)}, \tag{2.8}$$

and the p^{th} derivative is given by

$$D^p B_{i,n}(x) = \sum_{k=0}^{p} \beta_k^{p,n} B_{i-k,n-p}(x), \tag{2.9}$$

$$(D^p B_{i,n}, D^p B_{j,n}) = \frac{(b-a)}{(2n-2p+1)} \sum_{k,l=0}^{p} \beta_k^{p,n} \beta_l^{p,n} \frac{\left(\begin{array}{c} n-p \\ i-k \end{array} \right) \left(\begin{array}{c} n-p \\ j-l \end{array} \right)}{\left(\begin{array}{c} 2n-2p \\ i+j-k-l \end{array} \right)}, \tag{2.10}$$

where the $\beta_l^{p,n}$ are expressed as

$$\beta_l^{p,n} = \frac{(-1)^{l+p}}{(b-a)} \frac{n!}{(n-p)!} \left(\begin{array}{c} p \\ l \end{array} \right). \tag{2.11}$$

It is also straight forward to work out similar expressions with dual functions to the B-polynomial basis. In the following section, we plan to apply the explicit formulas to the harmonic oscillator.

3 Method and Harmonic Oscillator

Consider the Harmonic Oscillator Equation,

$$-\frac{\hbar^2}{2m} \frac{d^2y}{dx^2} + \frac{1}{2} K\, x^2 y = E\, y. \tag{3.1}$$

We seek solutions of the equation (3.1) in the closed interval [a, b] with initial condition $y(a) = 0$. After Transformation of variables and making substitutions such as $z = \sqrt{\alpha}\, x$, $\alpha = \frac{m\,\omega}{\hbar}, \varepsilon = \frac{2\,E}{\hbar\omega}$, and $\omega = \sqrt{K/m}$, we obtain the following equation:

$$-\frac{d^2y}{dz^2} + z^2 y = \varepsilon\, y. \tag{3.2}$$

Approximating the function (y) with $y(z) = \sum_{i=0}^{N} c_i\, B_{i,n}(z)$ and substituting this solution in the Eq. (3.2), we take scalar product with B-polynomial $B_{j,n}(z)$to obtain,

$$-c_i(B''_{i,n}, B_{j,n}) + c_i(z^2\, B_{i,n}, B_{j,n}) = c_i\, \varepsilon\, (B_{i,n}, B_{j,n}) \tag{3.3}$$

Using the identity $-(B''_{i,n}, B_{j,n}) = (B'_{i,n}, B'_{j,n})$, we may rewrite the equation (3.3)

$$c_i(B'_{i,n}, B'_{j,n}) + c_i(z^2\, B_{i,n}, B_{j,n}) = c_i\, \varepsilon\, (B_{i,n}, B_{j,n}) \tag{3.4}$$

In Eq.(3.4), the matrix elements have closed forms which are evaluated using the formulas provided in the previous section:

$$\begin{aligned} a_{i,j} = (B'_{i,n}, B'_{j,n}) &= \sum_{k=0}^{1} \beta_k^n \sum_{l=0}^{1} \beta_l^n \, (B_{i-k,n-1}, B_{j-l,n-1}) \\ &= \tfrac{(b-a)}{(2n-1)} \sum_{k,l=0}^{1} \beta_k^n \, \beta_l^n \, \frac{\left(\begin{array}{c} n-1 \\ i-k \end{array} \right) \left(\begin{array}{c} n-1 \\ j-l \end{array} \right)}{\left(\begin{array}{c} 2n-2 \\ i+j-k-l \end{array} \right)}, \end{aligned} \tag{3.5}$$

$$b_{i,j} = (x^2 B_{i,n}, B_{j,n}) = (b-a) \left(\begin{array}{c} n \\ i \end{array} \right) \left(\begin{array}{c} n \\ j \end{array} \right) \sum_{k=0}^{2} \frac{a^{2-k} (b-a)^k \left(\begin{array}{c} 2 \\ k \end{array} \right)}{(2n+k+1) \left(\begin{array}{c} 2n-k \\ i+j-k \end{array} \right)}, \, and \tag{3.6}$$

$$d_{i,j} = (B_{i,n}, B_{j,n}) = \frac{(b-a) \left(\begin{array}{c} n \\ i \end{array} \right) \left(\begin{array}{c} n \\ j \end{array} \right)}{(2n+1) \left(\begin{array}{c} 2n \\ i+j \end{array} \right)}, \tag{3.7}$$

where,

$$\beta_k^n = \frac{(-1)^{k+1}}{(b-a)} \; n \left(\begin{array}{c} 1 \\ k \end{array} \right) \tag{3.8}$$

The Eq.(3.4) may be rewritten in the matrix form:

$$(A+B)\, C = \varepsilon \, D \, C. \tag{3.9}$$

Where in Eq. (3.9), the elements of each matrix A, B and D are given in equations (3.5), (3.6) and (3.7), respectively. The column matrix C represents expansion coefficients of the approximate solution to the Eq.(3.4) which are determined solving the generalized eigenvalue problem of Eq.(3.9). We choose the interval [-5, 5] to create a spectrum of the harmonic oscillator. The wave functions are expressed as a linear combination of B-polynomials of degree $n = 25$. Imposing the initial condition that the wave function must vanish at $y(a) = 0$ of interval effectively reduces the number of B-polynomials from $N = 26$ to $N = 25$. The command Eigensystem in Mathematica is called to compute the eigenvalue problem in Eq.(3.9). The results of eigenvalues are shown in Table 1. It is obvious from the Table 1, 25 of these eigenvalues grow from small positive values to large positive values since the potential energy term is positive. It is worth mentioning that the present calculations are not based on any particular type of grid; instead integrations are performed

analytically, and exactly, to evaluate the matrix elements in equations (3.5-3.7), which are expressed in terms of continuous B-polynomials over the entire length of the interval [-5, 5]. The low lying energy spectrum is also compared against exact eigenvalues $E_n = (n + 1/2)\ \hbar\omega$ of the harmonic oscillator.

Several tests can be performed to check the quality of the spectrum created in the B-polynomials basis. A stringent test of the basis is to calculate the Thomas-Reiche-Kuhn (TRK) sum rule. The TRK sum rule is given by

$$\frac{2\mu}{\hbar^2}\sum_{k}^{N}(E_k - E_0)|x_{k0}|^2 = 1. \tag{3.10}$$

The Eq.(3.10) may be written in terms of B-polynomial basis ($\hbar = \mu = 1$),

$$2\sum_{k}^{N}(E_k - E_0)|C_k \bullet M \bullet C_0|^2 = 1. \tag{3.11}$$

Where the column matrix C represents normalized eigenvectors and the element of Matrix M in Eq.(3.11) are given as

$$b_{i,j} = (x\,B_{i,n}, B_{j,n}) = (b-a)\begin{pmatrix} n \\ i \end{pmatrix}\begin{pmatrix} n \\ j \end{pmatrix}\sum_{k=0}^{1}\frac{a^{1-k}(b-a)^k\begin{pmatrix} 1 \\ k \end{pmatrix}}{(2n+k+1)\begin{pmatrix} 2n-k \\ i+j-k \end{pmatrix}}, \tag{3.12}$$

The basis set with $N = 25$ polynomials is generated by solving equation (3.9). The results of the TRK sum rule are shown in Table 2 and also compared with the exact result equal to 1. The accuracy of better than one part in 10^6 is observed by just summing over the first 8 terms.

Second test of the basis set may be considered to calculate the energy corrections to the first excited state. Suppose we consider harmonic oscillator in the first excited state $|\psi_1\rangle$with energy $E_1 = \frac{3}{2}\hbar\omega$. We calculate perturbations of the energy of this state by adding a small perturbation $V(x) = \beta\, x^4$to the potential$\frac{1}{2}K\,x^2$. All order iterative perturbation formula is used

$$T_E^{(n)} = \sum_{\alpha}\frac{|\alpha\rangle\,\langle\alpha|\,V(x)\left|T_E^{(n-1)}\right\rangle}{E_1 - E_\alpha} \tag{3.13}$$

to calculate energy corrections to the first excited state,

$$E^{(n)} = \langle\psi_1|\,V\left|T_E^{(n-1)}\right\rangle. \tag{3.14}$$

Where $\left|T_E^{(0)}\right\rangle = |\psi_1\rangle$. From equation (3.13), the corrections through 5^{th} order perturbations are calculated using the eigenvalues of Table 1 and eigenvectors solving equation (3.9). Table 3 represents the results of the perturbations using the basis set with $n = 25$ polynomials. For perturbation theory to be valid it is determined that the strength of perturbation must be $\beta = 0.01$ to converge as shown in Table 3. It is also seen that only 8 terms in the sum in Eq.(3.13) were enough to see convergence.

4 Results and Discussion

We have demonstrated a powerful method to solve harmonic oscillator problem in a B-polynomial basis. Table 1 shows the spectrum of eigenvalues obtained by the B-polynomials Galerkin method as discussed in sections 2 and 3. As can be readily seen, the method provides a very accurate approximation of the solutions of the Schrödinger equation with initial condition. Using closure form of matrix formalism, the symmetric generalized eigensystem Eq. (3.9) is solved to provide n eigenvalues and n eigen functions. The present method is for the first time applied to solve the harmonic oscillator and has been determined to be faster and more direct to implement.

It is also shown that the quality of the spectrum is superior when calculating the completeness property and TRK sum rules. The results of the TRK sum rule converge by just summing over 8 states in Eq.(3.11). The results of the TRK sum rule are provided in Table 2. In addition we have also carried out calculations of energies up to 5^{th} order in perturbation theory. A small perturbation potential is considered to see the effects of perturbation on the first excited state of the harmonic oscillator. The energy corrections are calculated using Eq.(3.14) and the results up to 5^{th} order of the perturbation are reported in Table 3. It is noticed that the perturbation expansion is valid if $\beta = 0.01$. In summary, we have shown that the B-polynomial Galerkin method returns valid results and is a powerful tool that we may utilize to overcome the difficulties associated with complex differential systems with much less computational efforts and cost. This method also provides confidence that it may be extended to evaluate many-body perturbation expressions for atomic properties in ref.[12]. All the present calculations are performed using Mathematica 6.0.

References

[1] [1] W. R. Johnson, M. Idrees, and J. Saperstein, *Phys. Rev. A*, **37**(2), 35, 3218-3226 (1987).
[2] W. R. Johnson, S. A. Blundell, and J. Saperstein, *Phys. Rev. A*, **37**(2), 307-315 (1988).
[3] C. F. Fischer and M. Idrees, *Computers in Physics* **23**, 53-58 (1989).
[4] C. F. Fischer and F. A. Parpia, *Phys. Lett. A* **179**, 198-204 (1993).
[5] M. I. Bhatti, K. D. Coleman, and W. F. Perger, *Phys. Rev. A*, **68**(4), 44503-1(2003).
[6] M. Bhatti, P. Bracken, *J. Comp. and Applied Math*, **205**, 7, 272-280 (2007).
[7] M. Bhatti and D. Bhatta, *Phys. Scr.*, **73**, 1-6 (2006).
[8] D. Bhatta and M. Bhatti, *Applied Mathematics and Computation*, **174**, 1255-1268 (2006).
[9] R. Farouki and V. T. Rajan, *Algorithms for polynomials in Berstein form, Comput. Aided Geom. Design*, **5**, 1-26 (1988).
[10] P. J. Barry and R. N. Goldman, *Three examples of dual properties of Bézier curves, in: Mathematical methods in Computer Aided Geometric Design*, (Academic Press, Boston, pp. 61-69), (1989).
[11] B. Jüttler, *Adv. Comput. Math.*, **8**, 345-352 (1998).
[12] W. F. Perger, M. Xia, K. Flurchick, and M. I. Bhatti, *Comput. Sci. Eng.*, **3**, 38 (2001).

Table 1. Eigenvalues are given of the symmetric generalized eigensystem equation (3.9). The B-polynomial Galerkin method is used to approximate the solutions of the harmonic oscillator in the interval [-5, 5] and energies, $E = \frac{\hbar\omega}{2}\,\varepsilon\,, \hbar = \omega = 1$, are calculated using $N = 25$ polynomials.

State	Eigenvalues (E)
1	0.50000000122
2	1.50000000962
3	2.50000061088
4	3.50000167756
5	4.50004454811
6	5.50007583261
7	6.50110361049
8	7.50130018043
9	8.51141522636
10	9.50754248041
11	10.54739424387
12	11.54326795956
13	12.75708173752
14	14.10879344646
15	15.89900809843
16	18.04430700029
17	20.88492827733
18	24.55756295402
19	29.70629164676
20	37.18044950948
21	49.16893966147
22	70.54629558195
23	116.05909100458
24	245.00571205703
25	939.71927997628

Table 2. The TRK sum rules equations (3.11) are evaluated using harmonic oscillator finite basis set. The basis is calculated in the interval [-5, 5] and ($\mu = \hbar = 1$).

No. of State	Exact	Calculated	Difference
1	-1.00000000	-1.00000005	0.00000005
2	-1.00000000	-1.00000005	0.00000005
3	0.99999999	1.00000138	0.00000138
4	0.99999999	1.00000138	0.00000138
5	0.99999999	1.00000138	0.00000138
6	0.99999999	1.00000138	0.00000138
7	0.99999999	1.00000138	0.00000138
8	0.99999999	1.00000138	0.00000138

Table 3. The energy corrections to the first excited state of harmonic oscillator are calculated using the equation (3.14) in the perturbation potential$V(x) = \beta\, x^4$. We used only 8 eigenvectors of the basis set to achieve this accuracy. The results are compared with exact results using exact eigen functions of the oscillator. $\mu = \hbar = m = \omega = 1$, $\beta = 0.01$

Order	Calculation	Exact
$E^{(0)}$	1.50000001	1.50000000
$E^{(1)}$	3.74999953 β	3.75000000
$E^{(2)}$	-20.6250037 β^2	-20.6250000β^2
$E^{(3)}$	281.6011632β^3	281.6015625β^3
$E^{(4)}$	-5127.69315β^4	-5127.37061β^4
$E^{(5)}$	108955.7617β^5	108906.8587β^5

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