GRAM-SCHMIDT ORTHOGONALIZATION PROCEDURE AND CONSTRUCTION OF TWO-BODY BOUND STATE WAVE FUNCTIONS

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Abstract

Gram-Schmidt procedure for orthogonalizing vectors or functions is well known. But it is not straight forward to orthogonalize a large set of vectors or functions. We show how this can be accomplished by starting with a set of non-orthogonal set of basis functions. Once orthogonalized, they are normalized so that we have an ortho-normal set of functions. In order to test our functions, they are used as the basis set in expanding the wavefunction of a bound state Schrodinger equation with a specific potential. For test potentials, we use the harmonic oscillator potential and linear potential. The eigen energies and wavefunctions obtained are compared with analytical results for harmonic oscillator potential. For the linear potential, we compare with the standard numerical results. We also compare with the results obtained by using some known ortho-normal basis set of functions.

Keywords: Orthogonalization, basis functions, bound state, wavefunctions

Introduction

Orthogonal set of functions are very useful in many situations. In solving quantum mechanical equations for eigen-energies and eigen-functions, either in position space or in momentum space, basis function expansion methods is commonly applied. If the basis set of functions do not form an orthogonal set, the basis function expansion does not render the eigen-equation into a simple matrix eigen-equation. There are many well known orthogonal set of functions, such as the harmonic oscillator basis, Gauss-Lagauree basis, Jacobi polynomial basis and others, but computational time becomes prohibitively large when we do calculations in three or four body systems. Therefore, in this paper, we study a few simple functions which can be orthogonalized by using Gram-Schmidt orthogonalization procedure.

Gram-Schmidt Orthogonalization Procedure

In this section, we outline the Gram-Schmidt orthogonalization method. We first start with a set of vectors $\{|g_1>, |g_2>, \ldots, |g_N>\}$. These vectors do not form an orthogonal set, but they are normalized. i.e $< g_i| g_i > = 1$. Next we want to construct an orthonormal set $\{|f_1>, |f_2>, \ldots, |f_N>\}$ with the property that $< f_i| f_j > = \delta_{ij}$.

We first start by setting $|f_1> = N_1|g_1>$. Where $N_1 = 1$. Then we define

$$|f_2> = N_2 (\ |g_2> - C_1 |f_1>)$$

Where C_1 is the constant to be found. We accomplish this by requiring that $|f_2>$is orthogonal to $|f_1>$.

This gives

$$0 =< f_1|f_2> = N_2(< f_1|g_2> - C_1 < f_1|f_1>$$

$$C_1 =< f_1|g_2>$$

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Next we find the normalization constant N_2 by using the normalization condition

$$1 =< f_2|\, f_2 > = (N_2)^2(\, < g_2| - < g_2|f_1 >< f_1|)(|g_2 > \, - |f_1 >< f_1|g_2 >)$$

This gives

$$N_2 = \frac{1}{\sqrt{1 - < g_2|f_1 >< f_1|g_2 >}}$$

Continuing in this manner, we obtain

$$|f_N > = N_N(\, |g_N > \, - \sum_{i=1}^{N-1} |f_i >< f_i|g_N >)$$

$$N_n = \{\ \ 1 - \sum_{i}^{\{n-1\}} < g_n|f_i >< f_i|g_n > \ \ \}^{-\frac{1}{2}}$$

Now by using the last two equations, we can construct a new ortho-normal set $\{|f_i >\}$.

For practical calculations, it is convenient to derive a recursion relation for

$t_{jn} =< g_j|f_n > = < f_n|g_j >$. By projecting with $< g_j|$ on $|f_n >$ we obtain,

$$< g_j|\, f_n > = N_n(< g_j|g_n > \, - \sum_{i}^{n-1} < g_j|f_i >< f_i|g_n >)$$

or, in terms of t_{jn}

$$t_{jn} = N_n(\, S_{jn} - \sum_{i=1}^{n-1} t_{ji}t_{in})$$

And the normalization constants are given by

$$N_n = \{\ \ 1 - \sum_{i}^{\{n-1\}} t_{in}t_{in} \qquad \}^{-\frac{1}{2}}$$

Note that, here $S_{jn} =< g_j|\, g_n >$ the overlaps among the original set of vectors $|g_j >$'s. And also note that $j > n > i$ must hold. Now the procedure is clear. First we generate all the overlaps S_{jn} of the non-orthogonal vectors $|g_i >$'s. Then we generate the t_{jn} 's and the normalization constants N_n 's starting with $N_1 = 1$. Then we can generate all the vectors in new orthonormal set $\{\ \ |f_i >\}$.

Orthogonalzing functions

Indefining or thogonality of functions, one usually define it with respect to a chosen weight. Let us first define the relation between our vectors and functions on the real line R^1. We will consider the case where both domain and the range of our functions is R^1 . We define our functions by

$$g_n(x) =< x \mid g_n >$$

$$f_n(x) =< x \mid f_n >$$

We demand that our $g_n(x)$ are normalized and our $f_n(x)$ are orthonormal. i.e

$$\int_0^\infty f_n(x) f_m(x)\, w\, dx = \delta_{nm}$$

Here w is the weight function and we choose $w = x^2$. In many physics applications, where the domain of the function is the three dimensional space, the weight function w is x^2 which is part of the volume element in 3-dimensional case. For one-dimensional case, w is usually taken to be unity..i.e w=1.

Example set of functions

The set of functions that we choose to test our Gram-Schmidt procedure is a set of non-orthogonal Gaussian functions which are already normalized. They are given by

$$g_i(x) = \frac{2}{(\pi)^{\frac{1}{4}}}(2A)^{\frac{3}{4}}\exp(-n_i x^2)$$

Where $A = i^2 b$. Here we choose $n_i = i\, b$, where b is a parameter to be chosen. For example b=0.01 . The index iruns from 1 to N, where N is the number of functions to be orthogonalized.

The overlap of these functions $g_i(x)$are

$$S_{ij} = \int_0^\infty g_i(x) g_j(x) x^2 dx = \frac{\sqrt{\pi}}{4}\, 1/(A+B)^{\frac{3}{2}}$$

With $B = j^2 b$. Note that here we are using $w = x^2$ which will be suitable for realistic 3-dimensional quantum mechanical calculations. We can also use w=1 for 1-dimensional problems such as 1-dimensional harmonic oscillator.

Application

We consider two applications. The first one is the 1-dimensional harmonic oscillator problem. The solution is well known and is given as a half-integer multiple of $\hbar\omega$. Since the exact ground state wave function of the harmonic oscillator problem is a simple Gaussian, our calculations yield the exact results with even a few number of basis functions. The interesting one is the Schrodinger equation with linear potential. i.e. $V(r) = Ar$ where A is the strength of the potential. This potential is usually used as the confining potential for the bound states of quarks or in meson spectra where meson are described as bound states of a quark and an anti-quark. Here we choose to solve in momentum space. The Schrodinger equation in momentum space for l^{th} state can be written as

$$\frac{p^2}{2m}\phi_l(p) + \int_0^\infty V_l(p,p')\phi_l(p') p'^2\, dp' \; = E\phi_l(p)$$

Here $V_l(p,p')$ is the l^{th} partial wave component of $< p|\, V|p' >$ which is the Fourier transform of the position space potential $V(r)$. i.e

$$< p|V|p' > = \frac{1}{2\pi^2 q}\int_0^\infty V(r) Sin(qr) r\, dr$$

$$V_l(p,p') = 2\pi \int_{-1}^{1} < p|V|p' > P_l(x)dx$$

For l=0

$$V_{l=0}(p,p') = \frac{1}{\pi pp'}\frac{1}{2}\log(\quad |(y+1)/(y-1)|\,)$$

Where $y = \frac{p+p'}{p-p'}$

Fourier was done by first introducing a damping factor in the potential i.e$V(r) = A\,r\,exp(-\eta r)$ where η is the damping factor which was taken to be zero later. To take care of the singularity in the potential, the substraction procedure of Maung et al .In order to solve this equation we expand the wave function in our ortho-normalized basis set

$$\phi_l(p) = \sum_i C_i f_i(p)$$

After this expansion, and by projection with $f_j(p)p^2$ and integrating over p we obtain a matrix eigen value equation

$$\sum D_{ji}C_i = EC_j$$

Where the matrix D_{ji} is given by

$$D_{ji} = \int_0^\infty \frac{p^2}{2m} f_i(p)f_j(p)p^2dp \;+\; \int\int V_l(p,p')f_j(p)f_i(p')p'^2dp'p^2dp$$

Now after the matrix D_{ji} is calculated, we can solve the matrix eigenvalue equation. The usual eigen-routines provides us with the energy eigen-values and eigen-vectors whose components are the expansion coefficients $C_i's$. With the strength of the linear potential A=1GeV^2,mass m=1 GeV the exact energies of this eigen-equation are the roots of the Airy's functions. The wave-functions can be constructed once the expansion coefficients $C_i's$ are found.

We present our results in the following table. Here we use b=0.2 Note that b is the variational parameter which is chosen to minimize the eigen energy. As the number of basis function used is increased, the value of b becomes unimportant.

	N=4	**N=10**	**N=18**	**Exact answer [2] Ref. [3,4] 20 functions**
Ground State	2.3506473	2.33810741	2.33810741	2.33810741
1st excited state	4.6909371	4.08794945	4.08794944	4.08794944
2nd excited state	9.8607089	5.52056779	5.52055983	5.52055983
3rd excited state	28.625702	6.79152313	6.78670809	6.78670809
4th excited state		8.09869283	7.94413359	7.94413359

Conclusion

We have presented Gram-Schmidt orthogonalization procedure which is useful in quantum mechanical calculations. We derive a recursion relation for the overlap functions $< g_i|f_j >$which is useful in the calculation. We constructed an orthonormal basis set of functions from a previously defined set of functions which are not mutually orthogonal. We used these orthonormal set of functions in solving the Schrodinger equation in momentum space with linear potential. We obtained very satisfactory results.

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