The Himalayan Physics *Vol. 6 & 7, April 2017* (54-57) ISSN 2542-2545

Construction of Dirac Delta Function from the Discrete Orthonormal Basis of the Function Space

Hari Prasad Lamichhane
Central Department of Physics, Tribhuvan University, Kirtipur
Email: hlamichhane1@gmail.com

Abstract: *Orthonormal basis of the function space can be used to construct Dirac delta function. In particular, set of eigenfunctions of the Hamiltonian operator of a particle in one dimensional infinite potential well forms a non-degenerate discrete orthonormal basis of the function space. Such a simple basis set is suitable to study closure property of the basis and various properties of Dirac delta function in Physics graduate lab.*

Key Words: Dirac Delta Function, Closure Relation, Orthogonal Basis, Generator of Dirac Delta Function

1. INTRODUCTION

Graduate course on quantum mechanics stems on observables, orthonomal basis functions or vectors, Dirac delta function and Schrodinger equation [1-8]. These basic quantum mechanical terms generally shocks the physics graduate students in the beginning of the semester. One of the most striking problems is understanding what the closure property of orthonormal basis functions is. Closure property of orthonormal basis functions is not only important for testing completeness of the basis functions but also for constructing and studying various properties of Dirac delta function. Such type of work takes enormous effort so that it is better to design a numerical experiment which will digout various properties of Dirac delta function and the basis functions and finally the students will be able to better understand quantum mechanics.

2. THEORY

State of a quantum particle is described using a wavefunction. The wavefunction of a particle can be expanded in terms of the complete set of orthonormal basis functions. Set of eigen functions of an observable forms an orthonormal basis in the wave function space. Orthonormal basis of the function space satisfies the following properties:

a) The scalar product of two basis functions is equal to Kroncker delta function.

b) The set of basis functions should be complete. In other words, any function of the wave function space can uniquely be expanded in terms of the orthonormal basis. This property can be tested by studying closure property of the basis functions. Closure property is very important because it can be used to construct a Dirac delta function.

Among various options of observables we can consider Hamiltonian oparator of a particle bounded in one dimensional potential well defined as:

$$H = \frac{-\hbar^2 d^2}{2mdx^2} + V(x) \text{ --------------(1)}$$

Where V(x) = 0 for 0≤ x ≤ L;

= ∞ otherwise.

Graphical representation of the potential energy V(x) is shown in Figure 1.

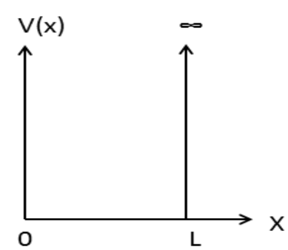


Figure 1. Infinite Well Potential Energy [2]

Time independent energy eigen functions of the Hamiltonian operator can be obtained by solving Schrodinger wave equation:

H u(x) = E u(x) -----------------(2)

where E is the energy eigenvalue and u(x) is the energy eigen function.

The normalized wavefunctions of the Schrodinger wave equation (2) for a particle whose Hamiltonian operator is given by equation 1 are

$$u_n(x) = \sqrt{\frac{2}{L}}\text{Sin}\left(\frac{n\pi x}{L}\right) \text{ -------------------(3) for } 0 \le x \le L. \text{ [2]}$$

Otherwise equal to 0. Values of n are positive integers 1, 2, 3, …… The energy eigenvalues are

$$E_n = \frac{\hbar^2 n^2 \pi^2}{2mL^2}.$$

The scalar product of two eigenfunctions of a Hermitian operator is defined as

$$\left(u_n(x), u_m(x)\right) = \int_0^L u_n^*(x) u_m(x) dx = \delta_{nm} \quad \text{---------------(4)}$$

The closure relation is

$$\sum_n u_n^*(x) u_n(x') = \delta(x - x') \quad \text{---------------------(5)}$$

where δ(x-x') is the Dirac delta function and the sum runs upto n equals to infinity.

Basic Properties of Dirac Delta Function [3-4, 9] are as follows:

1) $\delta(x-x') = \infty$ when $x = x'$;

2) $\delta(x-x') = 0$ when $x \neq x'$;

3) $\int_{-\infty}^{\infty} \delta(x - x') dx = 1$

Third property of Dirac delta function can be simplified as

$$1 = \int_{-\infty}^{\infty} \delta(x - x') dx = \int_0^L \sum_n u_n^*(x) u_n(x') dx = \sum_n \frac{4}{(2n-1)\pi} \text{Sin}\{\frac{(2n-1)\pi x'}{L}\} \quad \text{--(6)}$$

where n can take positive integer values and $u_n(x)$ is given in equation 3.

The sum on the left hand side term of equation 4 for finite n can be defined as a generator of Dirac delta function as

$$F(x, x', n) = \sum_n u_n^*(x) u_n(x') \ \text{……………….(7).}$$

Integration of the generator function defined in equation 7 in the interval $x = x_1$ to x_2 for $u_n(x)$ given by equation 3 can be calculated as

$$\int_{x_1}^{x_2} \sum_n u_n^*(x) u_n(x') dx = \sum_n \left(\frac{2}{n\pi}\right) Sin\left(\frac{n\pi x'}{L}\right) [Cos\left(\frac{n\pi x_1}{L}\right) - Cos\left(\frac{n\pi x_2}{L}\right)] \quad \text{-- (8)}$$

Students can use computer programs such as excel, origin, matlab, etc. to study the properties of the generator of Dirac delta function in the lab. One of the noteworthy properties of the generator will be its dependance on n. By changing n for given values of x and x' students will understand how the generator of the Dirac delta function will actually be attained the Dirac delta function and hence, proved the closure relation of discrete orthonormal basis functions.

3. RESULT AND DISCUSSION

The generator function F(x, x', n) defined in equation 7 is plotted in Figure 2 for L = 1, n = 100 and x' = 0.1 against x. The generator function is almost zero everywhere except at x = x' = 0.1. This generator function clearly shows the nature of Dirac delta function except the finite height at x equal to x'.

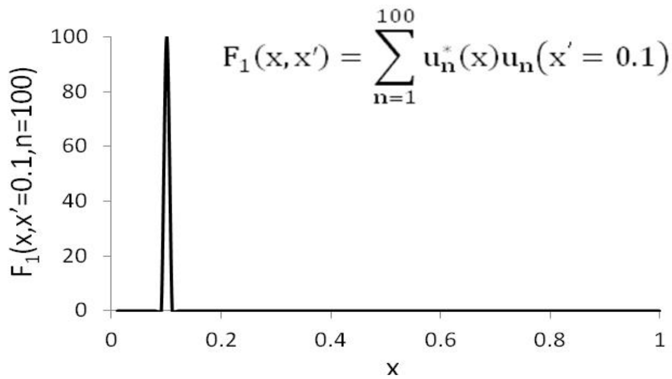


Figure 2. Generator of Dirac delta function as a function of x for n = 100, x'= 0.1 and L = 1. $u_n(x)$ is given by equation 3 [6].

The height variation of the generator function on the value of n at x = x' = 0.1 and L =1 is shown in Figure 3. Figure 3 shows that the height of the generator function almost linearly increases on increasing n with average slope 1 and period n = 10.

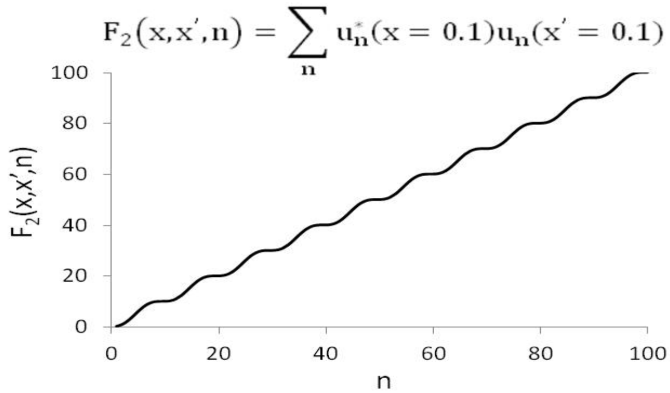
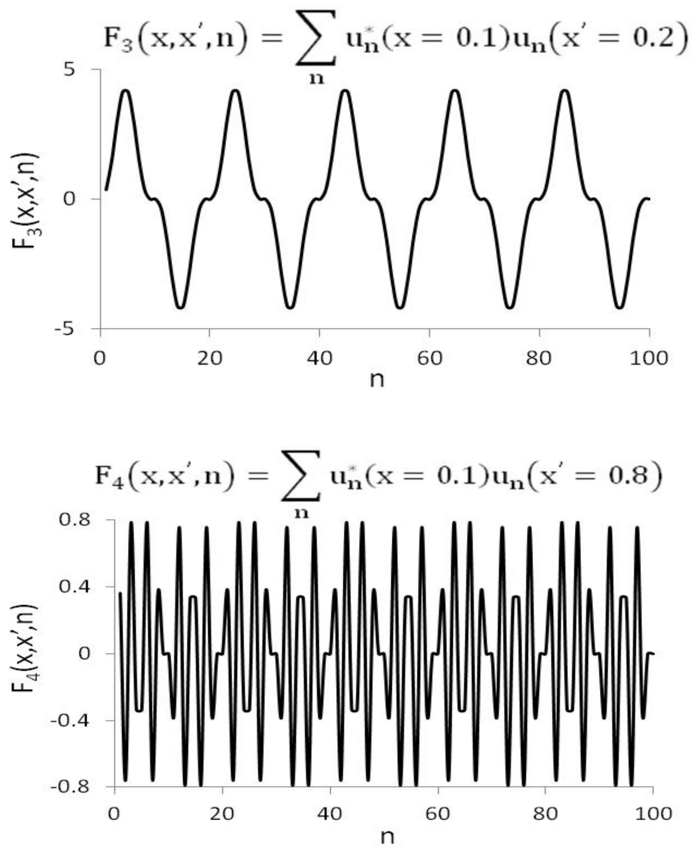


Figure 3. Generator of Dirac delta function as a function of n for x = x'= 0.1 and L = 1. $u_n(x)$ is given by equation 3.

The nature of generator function is also studied for different values of x and x'. The generator functions F_3 and F_4 as defined in Figure 4 are not zero for x not equal to x' as implied in Figure 2 but show periodic nature on n. The amplitude and the period of the generator function depend on the values of x and x'. Figure 4 A shows that the generator F_3 has amplitude 4.14 and period 20 for x = 0.1 and x' = 0.2. On the otherhand Figure 4 B shows that the generator function F_4 has amplitude 0.78 and many oscillations within the period 20. However, the average values of both functions are equal to zero.



A B

Figure 4. Generator of Dirac delta function as a function of n for A) x = 0.1, x'= 0.2 and L = 1; B) x = 0.1, x'= 0.8 and L = 1. $u_n(x)$ is given by equation 3.

Generator of Dirac delta function (F_5) is plotted against x at x' equal to 0.1 and n equal to 14 and 94 in Figure 5. As can be seen in Figure 5, the function F_5 is oscillating more rapidly at n = 94 as compared to at n = 14. The function F_5 is also larger and narrower at n = 94 than at n = 14. We can concluded from this result that the generator of Dirac delta function will be much larger as well as much narrower at x = x'. The generator of Dirac delta function will oscillate at very high frequency with mean value 0 in the region where x is not eqal to x'. Generally, an ordinary function (a sufficiently regular function) does not rapidly vary in any short interval of x and hence can be taken as constant in that interval of x but over the same region of x the Dirac Delta function oscillates many times. That is why one should take an average value of Dirac delta function in an infinitesimal interval of x in order to expand an ordinary function.

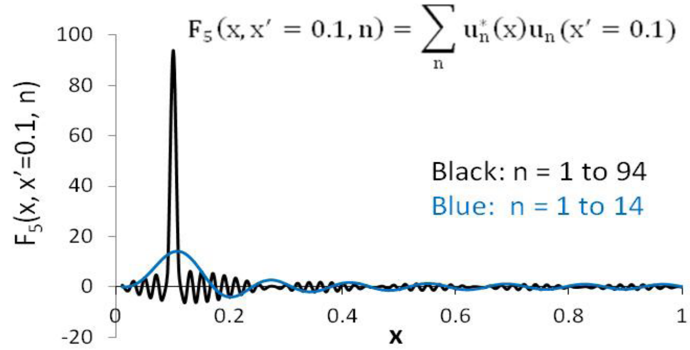


Figure 5. Generator of Dirac delta function as a function of x for x'= 0.1, L = 1, n = 14 and 94.

The integration of the generator of Dirac delta function as a function of n for x'= 0.1 in the interval x = 0 to 1 is shown in Figure 6. The x integration of the generator function also shows periodic nature on n. The amplitude of oscillation decreases on increasing the value of n and the function finally attained value 1 as demanded by the property of Dirac delta function.

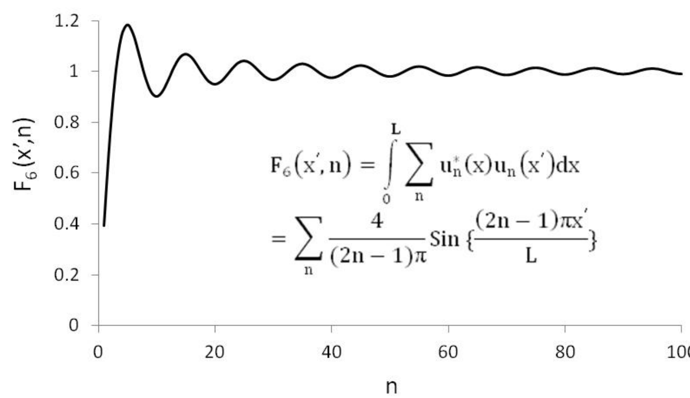


Figure 6. Integration in the interval x = 0 to 1 of the generator of Dirac delta function as a function of n for x'= 0.1. $u_n(x)$ is given by equation 3.

Piecewise integration of the generator of the Dirac delta function as given by equation 8 is shown in Figure 7. As shown in Figure 7, the integration of the generator of the delta function converges to zero for large n whenever the range of integration does not include point x'. However, if the range of integration interval encloses the point x', the integral converges to 1 for large value of n.

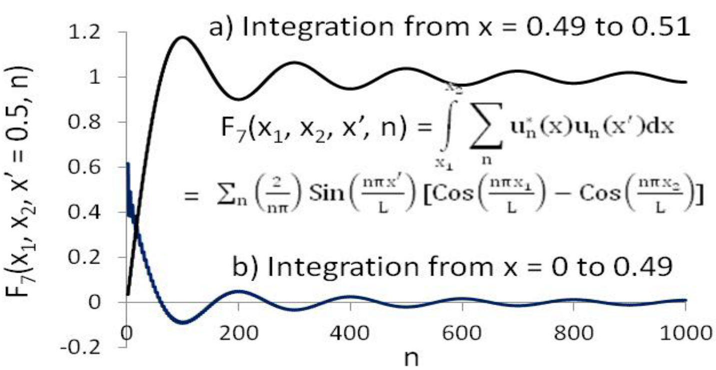


Figure 7. Integration of the generator of the Dirac delta function in the interval of x a) from 0.49 to 0.51, b) from 0 to 0.49 for x' = 0.5 and L = 1 as a function of n. The function is given in equation 8.

4. CONCLUSIONS

Generator function of Dirac delta function can be constructed using closure relation of the discrete orthonormal basis functions. The orthonormal basis functions are set of eigenfunctions of some Hermitian operators. On playing with the generator of the Dirac delta function i. e., by changing the values of variables x, x' or n, students will be able to get knowledge about orthonormal basis functions of quantum particles and also explore various properties of Dirac delta function. Most importantly, students will know how the ideal property of Dirac delta function can be obtained from the closure relation of orthonormal basis functions.

REFERENCES

1. Cohen-Tannoudji, C., Diu, D., and Laloe, F., (1977). Quantum Mechanics, Volume I, page 99, John Wiley and Sons, Inc., New York.
2. Cohen-Tannoudji, C., Diu, D., and Laloe, F., (1977). Quantum Mechanics, Volume I, page 270, John Wiley and Sons, Inc., New York.
3. Cohen-Tannoudji, C., Diu, D., and Laloe, F., (1977). Quantum Mechanics, Volume II, page 1465, John Wiley and Sons, Inc., New York.
4. Schiff, L. I., (1968), Quantum Mechanics, page 55, McGraw-Hill McGraw-Hill Book Company, Singapore.
5. Pipes, L. A. and Harvill, L. R., (1977), Applied Mathematics for Engineers and Physicists (3rd ed.), page 166. McGraw-Hill Book Company, Singapore.
6. Arfken, G. B., Weber, H. J. and Harris, F. E., (2013), Mathematical Methods for Physicists (7th ed.), page 263. Elsevier Inc., MA, USA.
7. Mathews, J. and Walker, R. L. (1970), Mathematical Methods of Physicists (2nd ed.), page 114, Pearson Education, Inc., CA, USA.
8. Powell, J.L. and Crasemann, B. (1988), Quantum Mechanics (9th reprint) page 482, Narosa Publishing House, New Delhi.
9. Li, Y. T.; Wong, R. (2008), "Integral and series representations of the Dirac delta function", Commun. Pure Appl. Anal., **7** (2): 229–247, *doi*:*10.3934/cpaa.2008.7.229*, *MR* *2373214*.