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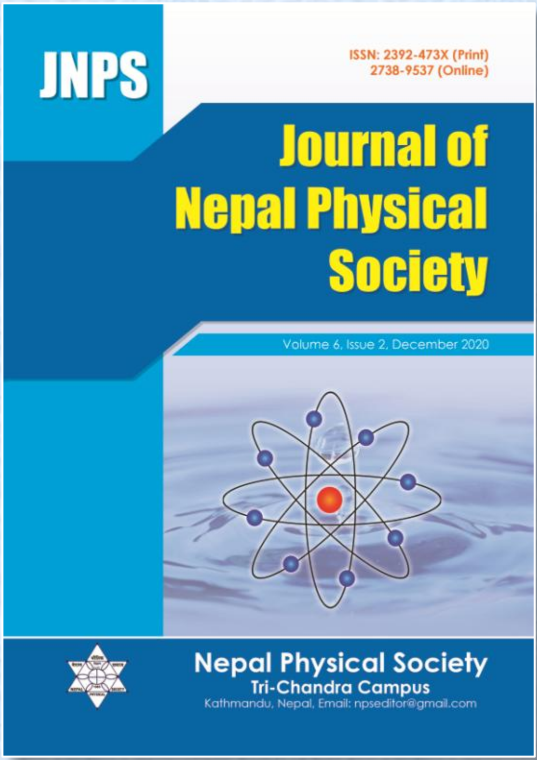

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Dirac Delta Function from Closure Relation of Orthonormal Basis and its Use in Expanding Analytic Functions

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Abstract

One of revealing and widely used concepts in Physics and mathematics is the Dirac delta function. The Dirac delta function is a distribution on real lines which is zero everywhere except at a single point, where it is infinite. Dirac delta function has vital role in solving inhomogeneous differential equations. In addition, the Dirac delta functions can be used to explore harmonic information's imbedded in the physical signals, various forms of Dirac delta function and can be constructed from the closure relation of orthonormal basis functions of functional space. Among many special functions, we have chosen the set of eigen functions of the Hamiltonian operator of harmonic oscillator and angular momentum operators for orthonormal basis. The closure relation of orthonormal functions then used to construct the generator of Dirac delta function which is used to expand analytic functions $log(x+2), exp(-x^2)\ and\ x$ within the valid region of arguments.

Key Word: Dirac Delta function, Closure relation, Orthonormal basis, Generator of Dirac delta function, Analytic functions.

1. INTRODUCTION

The process of creation and advance developments of science needs theoretical basis and mathematical formulations [1]. One of the achievements of modern mathematics and Physics is the generalized function particularly "The Dirac Delta functions" [1, 2]. The delta function is sometimes thought of as an infinitely high, infinitely thin spike at a certain origin, with its total area one under the spike, and physically represents the density of an idealized point mass or point charge. In 1930, for the solution of problems of theoretical Physics great British theoretical physicist, Dirac, one of the founders of quantum mechanics, introduced an object, called delta function [2, 3]. The completeness of basis set in the function space is a significant tool to obtain the Dirac delta function. The orthonormal basis means that scalar product of any two functions of this basis is the Kronecker delta function can be expanded in their linear combination [1, 4, 5], Thus, wave function $\psi(\vec{r})$ as;

$$\psi(\vec{r}) = \sum_i C_i\, u_i(\vec{r}) = \sum_i (u_{i,}\psi)\, u_i(\vec{r}) \ldots\ldots\ldots [1.1]$$

$$= \sum_i \left[\int d^3{}' u_i^*\left(\vec{r'}\right)\psi\left(\vec{r'}\right)\right] u_i(\vec{r})$$

$$\psi\left(\vec{r'}\right) = \int d^3r'\,\psi(\vec{\ }')\left[\sum_i u_i(\vec{r})u_i^*\left(\vec{r'}\right)\right] \ldots\ldots\ldots [1.2]$$

Equation (1.2) will be valid if the sum satisfies the closure relation [6, 7].

$$\sum_i^{\infty}\left[u_i(\vec{r})u_i^*\left(\vec{r'}\right)\right] = \delta\left(\vec{r}-\vec{r'}\right) \ldots\ldots\ldots\ldots\ldots [1.3]$$

Where $\delta\left(\vec{r}-\vec{r'}\right)$ Dirac is delta function and sum over I runs from 1 to infinity.

For an illustration of Dirac delta function one can defined a function $\xi^{\epsilon}(x)$ as;

$$\xi^{\epsilon} = \frac{1}{\epsilon}\ \ for\ \left(x_0 - \frac{\epsilon}{2} < x < x_0 + \frac{\epsilon}{2}\right)\ \epsilon > 0$$

$$= 0, \text{ otherwise.}$$

The function $\xi^{\epsilon}(x)$ satisfies basic properties of Dirac delta function in the limit $\epsilon \to 0$ [8, 9].

Not only the wave function but also any analytic function $g(\vec{r})$can be explained with Dirac delta function as;

$$g(\vec{r}) = \int d^3r' g\left(\vec{r'}\right) \delta\left(\vec{r} - \vec{r'}\right) \text{....[1.4], [7].}$$

The Hermite polynomial is defined as

$$H_n(x) = \sum_s^{\frac{n}{2}} \frac{(-1)^s n!}{(n-2s)!s!} (2x)^{n-2s} \text{ .... [1.5]}$$

For n even and for n odd, the sum goes to $\frac{n-1}{2}$.

The harmonic oscillator wave function which is defined as;

$$\psi(x) = N_n exp\left(\frac{-x^2}{2}\right) H_n(x)$$
$$= \sqrt{\frac{1}{2^n\sqrt{\pi}n!}} H_n(x) e^{\frac{-x^2}{2}} \text{.......[1.6]}$$

Using equation (1.3) we can obtain the Dirac delta function can be constructed for the harmonic oscillator wave function as;

$$\delta(x-t) = \sum_{n=0}^{\infty} \frac{H_n^*(x) exp\left(\frac{-x^2}{2}\right) H_n(t) exp\left(\frac{-t^2}{2}\right)}{2^n\sqrt{\pi}n!} \text{.......[1.7]}$$

The sum in equation (1.7) converges in many practical cases for finite n. Therefore, let us defined the generator of Dirac delta function $F(n, x, t)$ as;

$$F(N, x, t) = \sum_{n=0}^{N} \frac{H_n^*(x) exp\left(\frac{-x^2}{2}\right) H_n(t) exp\left(\frac{-t^2}{2}\right)}{2^n\sqrt{\pi}n!} \text{......[1.8]}$$

Expansion of an analytic function $f(x)$ with the generator of Dirac delta function (1.8) is written by using the equation (1.3) as;

$$f(N, x) = \int_{-\infty}^{\infty} f(t) \left[\sum_{n=0}^{N} \frac{H_n^*(x) exp\left(\frac{-x^2 - t^2}{2}\right) H_n(t)}{2^n\sqrt{\pi}n!}\right] dt$$

...[1.9], [9, 10]

The Legendre polynomial is defined as;

$$P_n(x) = \sum_{k=0}^{N} (-1)^k \frac{(2n-2k)!}{2^n k!(n-k)!(n-2k)!} x^{n-2k}$$

...[1.10]

Where, $N = \frac{n}{2}$ for n even and $N = \frac{(n-1)}{2}$ for n odd [11].

Therefore the closure relation for this basis function is given by

$$\delta(x-t) = \sum_{n=0}^{\infty} \frac{2n+1}{2} P_n^*(x) P_n(t) \text{ .... [1.11]}$$

Where the term $\frac{2n+1}{2}$ is normalizing constant. The generator of the Dirac delta function with Legendre polynomial basis is

$$F(N, x, t) = \sum_{n=0}^{N} \frac{2n+1}{2} P_n^*(x) P_n(t) \text{ .... [1.12]}$$

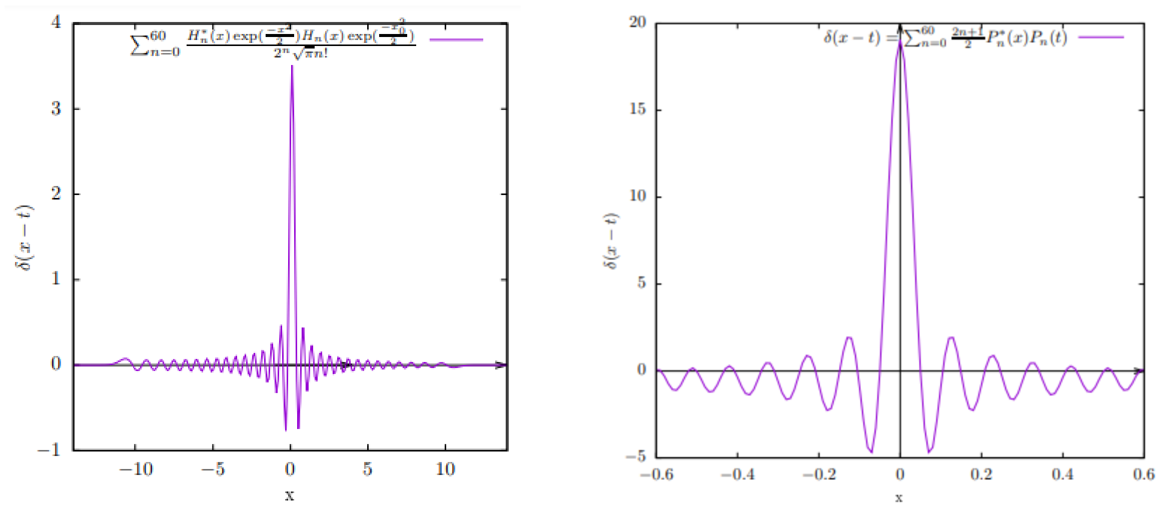
In this work we considered analytic functions to the expanded with Dirac delta functions are. $log(x + 2), exp(-x^2)\ and\ x$. Effect of truncation of the series sum of the generator of Dirac delta function, limits of integration, and choice of orthonormal basis in the expansion of analytical functions will be studied [12, 13].

2. NUMERICAL METHOD

Machine-language used in this work is C programming. First of all Hermite polynomials are generated using relation (1.5) then, expansion of a function $f(x)$ is performed using relation (1.9). Convergence of the series is assured by the exponential factor $e^{-\frac{x^2}{2}}$ and the finite value of n. Similarly, Legendre polynomials are generated using relation (1.10) and the expression of the function $f(x)$ is carried out using the formula (1.12). Convergence of the series is guaranteed by the finite values of x_1 and x_2 which lies in the range of -1 to 1. The variables x and t are floating numbers and variables n, s and k are integers. The sum is performed iteratively.

3. RESULT AND DISCUSSION

Closure relation of orthonormal basis of the function space is used to test the completeness of the basis and also to generate Dirac delta function. The graphs of the generators of Dirac delta function with respect to the arguments for N equal to 60 using harmonic oscillator basis functions and Legendre basis functions are shown in Figures 1(a) and 1(b) respectively. As can be seen in the Figures 1(a) and 1(b), both generators of the Dirac delta function peak at x_0 equal to zero. The generators oscillate on both sides of the main peak and the amplitudes of oscillations decrease as the arguments deviate from zero. Magnitudes of generators become negligible for most of the regions of arguments away from the region of the main peak and thus removed from the plot. These generators differ from the ideal nature of the Dirac delta function which has infinite peak at x_0 and zero elsewhere. Generator of Dirac delta function never resembles the ideal Dirac delta function even if the number of terms N in the sum goes to infinity. Magnitude of the main peak of the generator goes to infinity as N goes to infinity, however, the oscillating nature of the function never ceases. On the other hand, the period of oscillation decreases as N increases. In the real physical observation one should take piecewise averages of the function if the period of oscillation is smaller than the least count of the measuring device. In this sense the least count of the measuring device will be used to locally average the sum to get a realistic generator of Dirac delta function which looks like ideal Dirac delta function for sufficiently large value of N.

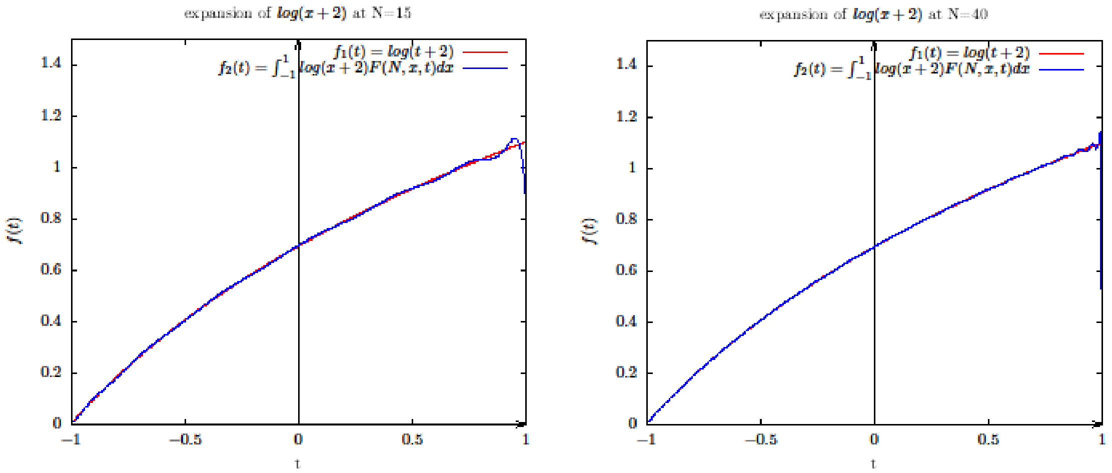


(a) (b)

Fig. 1: Generators of the Dirac delta function (a) Harmonic oscillator wave function as a basis with N = 60 and (b) Legendre functions as a basis with N = 60.

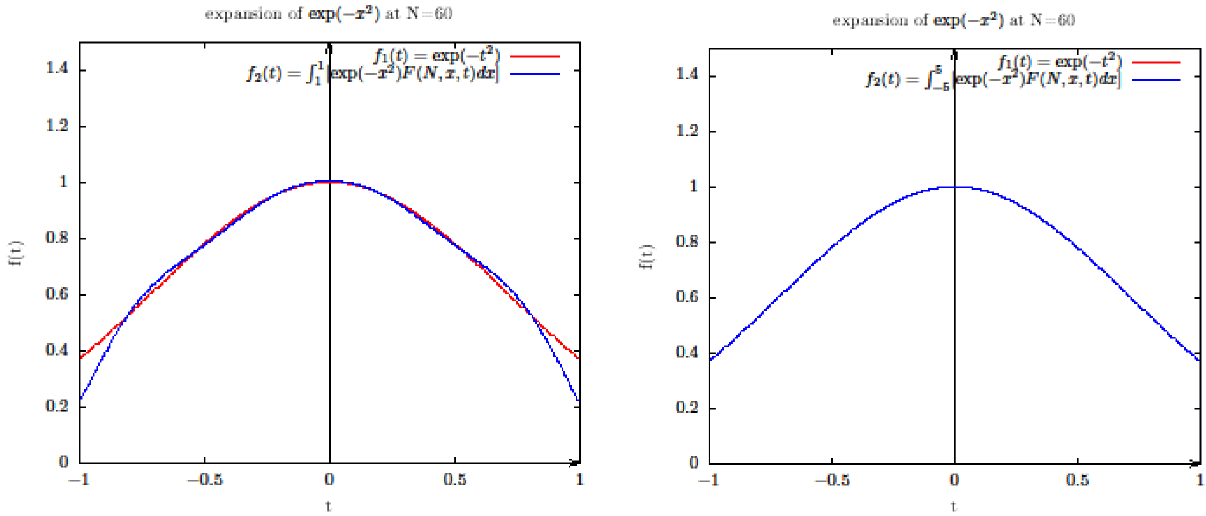
To explore the potentiality and the limitations of the generator of the Dirac delta function three functions $\log(x+2)$, $\exp(-x^2)$ *and* x are expanded in terms of the generator of the Dirac delta function. Effects of the value of N, the maximum value of the quantum number n, limit of integration and selection of basis in the expansion of the analytical functions are the focus of this study. The effect of the variation of the value of N is tested by expanding $\log(x+2)$ in terms of the generator of the Dirac delta function constructed using Legendre basis functions in the whole range (-1, 1) of the argument for N equal to 15 and 40. Corresponding plots of the generated functions are shown in Figures 2 (a) and (b). Both of the generated functions follow the pattern of the actual log function. However, as can be seen in Figure 2, the generated functions contain small oscillatory nature in the main region of the argument and more deviation from the actual log function at the range edge around x equal 1. The deviation of the generated log function from the actual log function reduces as the value of N increases from 15 to 40. This observation shows that the realistic generated function can be obtained using maximum possible value of N.

Likewise, the effect of choice of the integration limit in the expansion of the analytical functions is studied on the expansion of the Gaussian function by fixing the value of N at 60 and the harmonic oscillator basis. Though the range of Gaussian function covers the whole region of the real axis from - ∞ to ∞, only two sets of limits (-1, 1) and (-5, 5) of the integration are used in this work. The generated Gaussian functions are plotted in the interval (-1, 1) of the argument and compared with the actual Gaussian function and the graphs are shown in Figures 3 (a) and (b). Figure 3 shows that both generated Gaussian functions follow the nature of the actual Gaussian function. However, the Gaussian function generated using narrower range of integration, see Figure 3 (a), is more deviated from the actual function as compared to that of the function generated using wider range of integration. The generated function using smaller range of integration has more deviations at the edge of the integration limits and the function also has noticeable amplitudes of oscillations in the main range of the plot. The amplitudes of oscillations and the deviation at the end points -1 and 1 of the argument are greatly reduce when the limit of integration is increased from (-1, 1) to (-5, 5). Thus, one can express a function more realistically in terms of the generator of the Dirac delta function using wider range of permissible range of integration.



(a) (b)

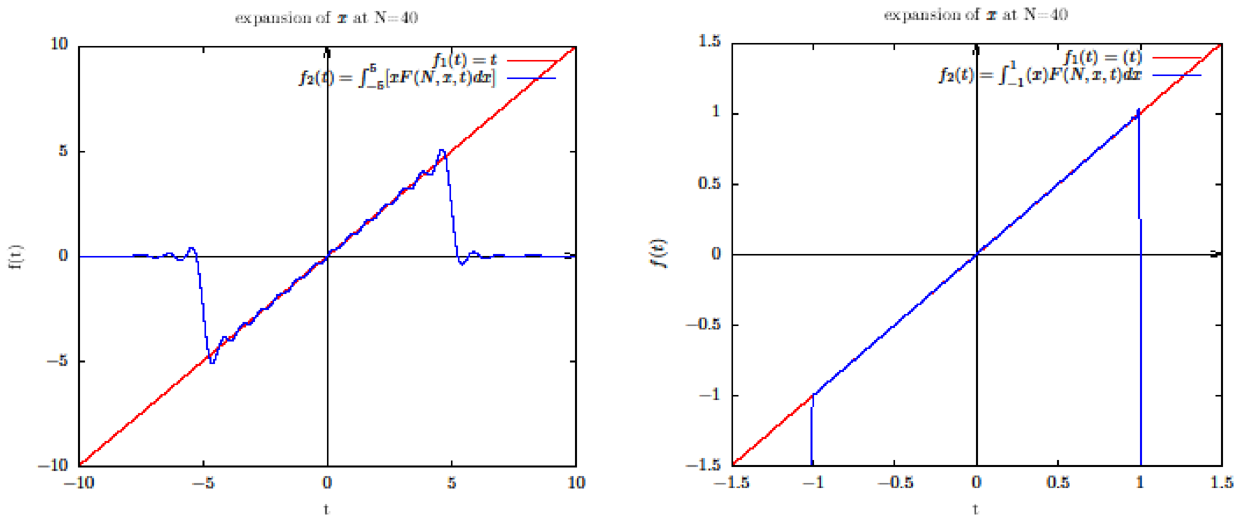
Fig. 2: Graphs of log(x+2) in terms of the generator of the Dirac delta function obtained using Legendre functions with (a) N = 15 and (b) N = 40. (Actual function is red colour and generated function is purple colour).



(a) (b)

Fig. 3: Plots of exp(-x^2) in terms of the generator of the Dirac delta function obtained using harmonic oscillator wave functions with N = 60 and the limits of integrations (a) (-1, 1) and (b) (-5, 5). (Actual function is red colour and generated function is purple colour).

Finally, the versatility of the choosing a basis for construction of the generator of Dirac delta function along with the convergence nature series while expanding an analytic function in terms of the generator of Dirac delta function is studied using two orthonormal basis: the harmonic oscillator wave functions and Legendre functions. A function $f(x) = x$ is expanded in terms of the generator of Dirac delta functions using harmonic oscillator wave function with N = 40 and range of integration (-5, 5), and Legendre functions with N = 40 and range of integration (-1, 1). Corresponding plots of the generated functions are shown in Figures 4 (a) and (b) respectively. As can be seen in Figure 4, both of the generated functions show the characteristics of the linear function x in the region of the argument used in the integration. However, there are some variations between the generated functions and the actual plot of the function x. For the same value of N, the function generated using the Legendre basis more resembles to the actual function than the function generated using harmonic oscillator basis. One of the main reasons of differences is that the range of argument used in the integration. In generating the function using Legendre basis its whole permissible range (-1, 1) of the argument is used in the integration. While, covering whole permissible range (-∞, ∞) of integration is computationally not possible. It suggests that in expanding an analytical function it is wise to use a basis whose whole permissible range of argument is finite and computationally accessible.



(a) (b)

Fig. 4: Plots of the function x in terms of the generator of the Dirac delta function obtained using (a) the harmonic oscillator wave functions with the limits of integrations (-5, 5) and (b) the Legendre functions with the limits of integrations (-1, 1) both for N = 40. (Actual function is red colour and generated function is purple colour).

4. CONCLUSION

Properties of the Dirac delta function constructed using the closure relation of the orthonormal basis functions of the function space have been studied. Nature of the Dirac delta function can be seen while summing the terms in the closure relation starting from discrete quantum number n equals zero onwards. Due to the computation limit of the computer one cannot sum the terms up to very large value of the quantum number n and thus the series in the closure relation should be truncated at some sufficiently large number N of n. The truncated series is defined as the generator of the Dirac delta function.

Generators of Dirac delta functions constructed using harmonic oscillator wave functions and Legendre polynomials have shown fundamental peak at x_0 and the function oscillates with small amplitudes on both sides of the fundamental peak. The height of the fundamental peak increases and its width decreases as the value of quantum number n increases. The frequency of oscillations of side lobes also increases with increase of the value of n.

On expanding various analytical functions in terms of generator of Dirac delta function in the valid region of the argument we have observed that the generated functions resembles the original function at sufficiently large value of N, the maximum value of the quantum number n used in the series. The truncation of the series mostly affects at the regions near the boundaries of the range of arguments. Thus, we can conclude that the generated function at the boundaries of the arguments mostly depends on the higher frequency components of the basis that we have truncated in the closure relation.

We have also observed that the generated function using generator of Dirac delta function depends on the limit of integration. The generated function looks more realistic when the limit of integration is increased in the valid region of the argument. The artifacts observed in the regions outside the region of integration has no meaning. Finally, we have expanded the same function in terms of two types of the basis with sufficiently large value of N and the limits of integrations and come to the conclusion that using different basis does not bring significant difference in the nature of the generated function.

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