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QUANTUM MECHANICS OF A FREE PARTICLE BEYOND DIFFERENTIAL EQUATIONS

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ABSTRACT

With Feynman's path- integral method we can obtain the quantum mechanics of a quantum system like a free particle outside Schroedinger's method of differential equations and Heisenberg's method of algebra. The work involves obtaining the quantum propagator K_f, of the system which leads to summation over infinite number of paths. With Van Vleck's formula in one dimension, the classical propagator K_{cl} for a free particle is computed as the analytical result. This then serves as a yardstick for justifying the theoretical method used to compute the quantum propagator, k_f, by direct path summation. The graphical display of the results shows that the Feynman – Schulman's checkerboard model used to enumerate the paths is reliable. Furthermore, this work shows that by windowing off a large number of paths and weighting the rest non uniformly we can compute the required propagator. The weights used in this case are the random and exponential window functions, w_r and w_e respectively, which yield kw_r and kw_e to compare with k_f.

Key words: Propagator, action, path - integral, window function, free particle.

INTRODUCTION

Path Integral Quantum Mechanics

In quantum mechanics, the probability amplitude $\psi(q, t)$ of finding a particle near position q at time t is related to $\psi(q_o, t_o)$ by a convolution integral (Ituen, 1997)

$$\psi(q, t) = \int K(q, t, q_o, t_o)\, \psi(q_o, t_o) dq_o \qquad 1.1.1$$

The Kernel $K(q, t, q_o, t_o)$ of this integral denoted by $< q, t \mid q_o, t_o >$ is known as the propagator. In the path – integral formulation of quantum mechanics by Feynman,

$$K = \sum_j \exp [iR_j (q, t, q_o t_o)/ \hbar] \qquad 1.1.2$$

where R_j is the action on the j^{th} path connecting space-time (q_o, t_o) with (q, t).

$$R_j \equiv \int_{t_o}^{t}_{(jth\ path)} L (q', q, \tau) d\tau \qquad 1.1.3$$

and where L is the Lagrangian of the system under consideration. In principle, K is the sum of equally weighted $\exp(iR_j/ \hbar)$ over all the infinitely many possible paths, including the classical trajectory. (Ituen, 1997)

The concept of path integral was first introduced to physicists by Feynman as a third formulation of quantum mechanics equivalent to that of Schroedinger, as well as the one of Heisenberg and Dirac. While the Heisenberg-Dirac method relies on algebra, Schroedinger's approach is based on differential equations and hence uses analysis. Feynman's innovation is mainly a "geometrical" way of expressing the quantum superposition principle. It is intuitive since it allows us to visualize directly, the constructive or destructive interference arising from many different paths (Khandekar, Lawande and Bhagwat 1993).

The "Checkerboard" Model

Whenever we have a solution of a Schroedinger equation we may look at it as analytic continuation of a situation of the diffusion equation. This was remarked by Marc Kac who, in 1950, was the first to link Feynman's path integral with Wiener functional integral used in Brownian motion. That is, evolution of a Schroedinger or quantum particle is like diffusion, which is an example of Brownian motion or random walk. As a random walk, the particle suffers displacement along the coordinate axis in the form of a series of steps of same length each being taken in either direction within a certain period of time as being discretised. The model is the same as Schulman's "Checkerboard" model with the motion of each point particle representing a Feynman's path in one space, one time direction. Feynman et al (1965) referred to the same picture when he noted that the path is a zig-zag of straight segments with slope differing only in sign from zig to zag. It is the case of very short-time scale as Schulman (1987, 1991) explained, otherwise

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(i.e., at a wide interval) many reversals would have occurred unaccounted for. This would lead to uncorrelated successive steps.

Basis of Windowing

Geometrically, Feynman's quantum paths are like rays of optics. They undergo diffraction and interference as they move through the discretised space-time; a prototype of diffraction grating. Gutzwiller (1990) had rightly put it that the propagator is a quantum-mechanical pulse spreads in a step-wise manner satisfying its composition property; another form of superposition principle. This compares with optical pulses obeying Huygen's principle and again like probability density obeying Chapman-Kolmogorov's rule. This stepwise spreading of the quantum mechanical pulse conforms with the adopted checkerboard model. It follows from the constructive and destructive effects of the interference/diffraction on the paths that some paths are enhanced at the expense of the others. The idea was pioneered by Feynman himself when he proved that those paths with actions very different from the classical action really do not contribute. (Ituen. 1997) They cancel out owing to large phase difference with the classical path whereas only the neighbouring paths contribute in phase and constructively interfere as the constructive or destructive interference depends on the phases R_j/h.

Using F_j as a measure of the contribution of action R_j to the expected value of the propagator, K, Akin-Ojo (1996) has shown that

$$(F_j)^2 = \left(\frac{1}{1 + (r_j/a)^2}\right)^{n/2+1} \qquad 1.3.1$$

where $r_j = (R_j - R_{min})/h$; R_{min} being the classical action, and a is a set of n constants such that the Hamiltonian of the system can be expressed as H (q, a). The deductions from equation (1.4.1) consolidates that fact that R_{min} is the most important action while other actions decrease in influence as R_j departs from R_{min}.

It is clear from the foregoing discussions that one can "filter off" some of the paths with no significant error. This is the main idea of "Windowing" in path-integral quantum mechanics. It is a case of non-uniform weighting of the paths. The window functions are expected to give zero weight to some of the paths and thus screening them out. This is a great relief to the predicament of having to handle infinite number of paths.

Another aspect of window effects include the following:

(i) From the picture originally given by Schulman (1987), we limit the region of contributing paths to a particular rectangle as shown in Fig. 1.3. For the illustrative results required in this work, we had to stipulate the number of time slices, N_t as well as that of space N_q, say. These numbers determine the number of paths involved as

Number of paths = $(N_q)^{N_t}$ 1.3.2

In addition, we need to observe a further precaution namely that of avoiding any vertical or horizontal motion because

$0 < (q_1 - q_3)/(l_1 - l_3) < c$ 1.3.3

is a very important requirement physically; c being the velocity of light. Hence for $N_t = N_q = 3$ the picture is as in Figure 1.3

Figure 1.3 resembles an infinite potential well with the paths bouncing away from the walls. By concentrating only on such prescribed set-up we have cut-off several paths.This is a type of windowing.

(ii).

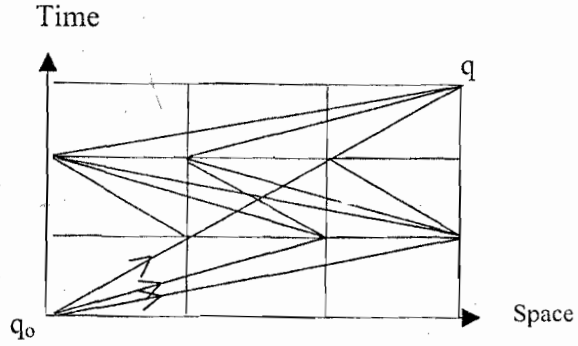


Fig. 1.3: A set-up like an infinite potential well with paths bouncing away from the walls.

Generally, anyone embarking on this direct path summation is confronted with trying to devise a means of handling infinite number of quantum paths. So far, many have resorted to Monte Carlo method especially for the case of imaginary time, which is closer to a Wiener process. (Scher et al, 1980) This method involves random sampling of the paths which is also a way of leaving out some paths. Actually, only very few have ventured into the real time case namely Scher et al (1980) as well as Salem and Wio (1986) using, respectively, numerical matrix multiplication and matirx diagonalisation methods. In such methods too, there is always the cutting-off of some "wild" paths.

RESULTS

The Propagator of Free Particle

The most fundamental and elementary application of quantum mechanics is to the system consisting of a free-particle, or particle in a constant potential field. That is, its velocity and consequently momentum and kinetic energy are constant. As such its Lagrangian is given by

$$L = \frac{m}{2}\dot{q}^2 \qquad 2.1.1$$

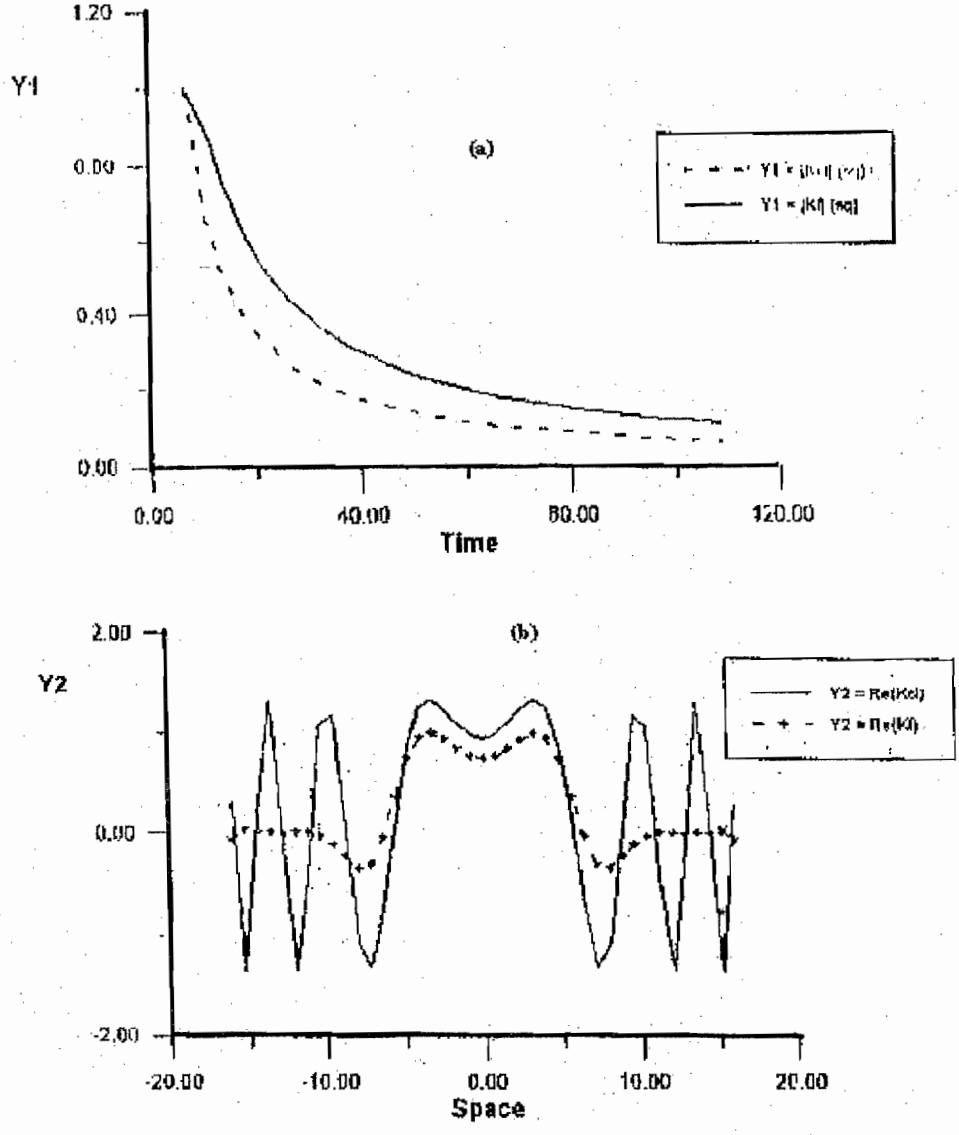


Fig 2: Comparing the propagator of free particle with analytical result: (a) With space. (b) With time (N=3277)

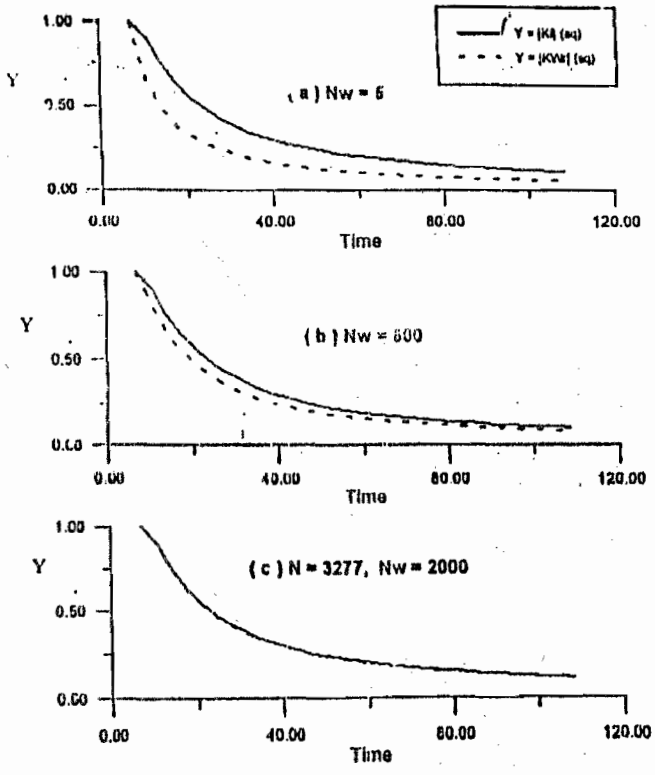


Fig 1.3.1 Random window of a free particle (Vs Time): (a) Nw = 5; (b) Nw = 500; (c) N = 3277, Nw = 2000

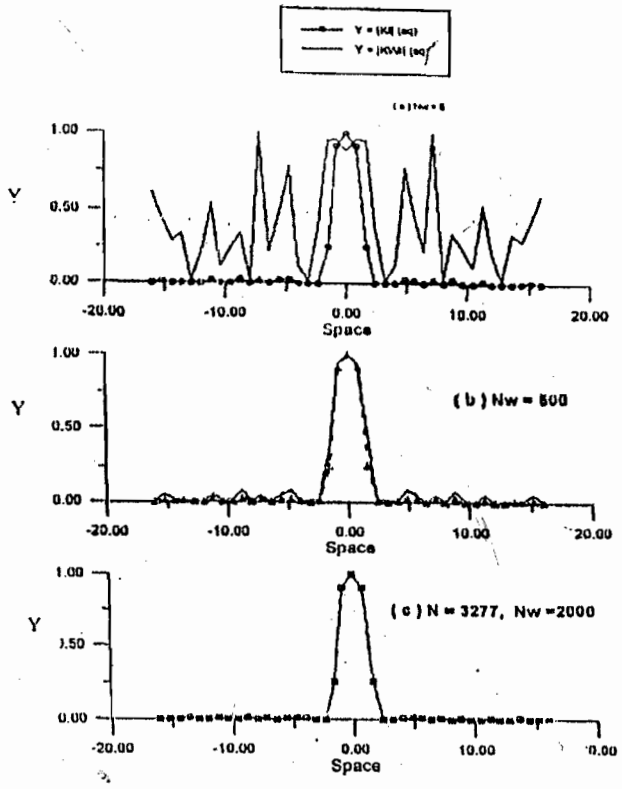


Fig 1.3.1 Random window of a free particle (Vs Space): (a) Nw = 5: (b) Nw = 500: (c) N = 3277, Nw = 2000

The expression for the classical propagator is already known (Feynman et al 1965) as

$$K_{cl}(q,t;q_o,t_o) = \left[\frac{2\pi i\, h\,(t-t_o)}{m}\right]^{-\frac{1}{2}} \exp i \left\{\frac{m(q-q_o)^2}{2\,h\,(t-t_o)}\right\} \qquad 2.1.2$$

The results follow in the graphs of Figures 2.1, (a and b) as in Ituen (1997). K_{cl} is the analytical formula while K_f is from the model used for the theoretical computations as displayed. For the variation with space, we plot the real part of the propagator because $|K_{cl}|^2$ gives a constant. This is in agreement with the work of Feynman et al (1965) and Scher et al (1980).

Window Effects on Quantum Propagators

For the study, we specify the number of vertical segments, N_t, to be 7 and that of horizontal segment, N_q, to be 4 and by equation (1.4.4), N = 3277. The possible links can be traced out as shown; discounting paths with vertical and horizontal segments. Using this as the total number of paths in the model, we study what happens when all the paths are uniformly weighted, that is, $N = N_w$, and also the case of ignoring some of the paths by giving N_w other values like 500, and even 5 which we consider extremely small compared to N.

With the action of the free particle, we compute the quantum propagator, K_f for N,

$$K(q, q_o, t) = \sum_{j=1}^{N} \exp i\, R_j\,(q, q_o\, t)/\, h \qquad 2.2.1$$

We then compare the results to that of using the window functions to weight each term in the expression

$$K_w\,(q,q_o,\, t) = \sum_{j=1}^{n} \frac{[W_j \exp i\, R_j\,(q,\, q_o,\, t)/\, h]}{M}\;;\quad n \le N \qquad 2.2.2$$

Note that the choice of Nw < N for further results, implies that $W_j = 0$ for some paths; thus cutting down on the infinite number. This produces the desired window effects, where M is a normalization factor given by

$$M = \sqrt{\sum_{j=1}^{n} |W_j|^2} \qquad 2.2.3$$

The results for each of the window functions involve the display of the uniformly weighted propagator, K and the corresponding weighted or non-uniform propagator, K_w versus time and versus space as in Figures 2.3 – 2.4 from Ituen (1997).

Random Window Function, w_r

It is so called because it is randomly generated and it windows out paths at random. Besides, unlike other cases, the weights were generated as complex numbers. The results are shown in Figures 2.3.1 – 2.3.2; as in Ituen (1997). Kw_r is the non-uniform propagator to compare with K. For this window function W_r, the available facilities for computations did not permit weighting all the 3277 paths. The reason is that W_r being complex has two sets of values. In this case the value of N_w is restricted to $N_w <$ 3000.

Exponential window function w_e

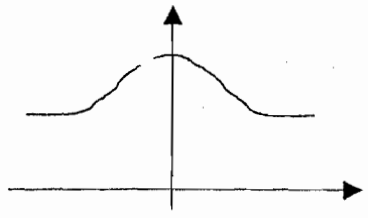
This is a type of Gibb's weight and is expressed as follows:

$W_e = \exp - (R_j - R_{min})/R_{min}$ 2.4.1

Where R_{min} is the classical action for the system. By the sketch shown in Figure 2.4, the aim is to eliminate paths with large action. Such paths may be termed as wild paths referred to by Feynman et al (1965).

The results are presented in Figures 2.4.1 – 2.4.2; as in Ituen (1997). Kw_r represents the non-uniform propagator. There is no restraint on the choice of N_w in this case. So we choose N_w = 3277, 500, 5

$\omega_e = \exp - (R_j - R_{min})/R_{min}$



$(R_j - R_{min})/R_{min}$

Fig. 2.4: Exponential window function

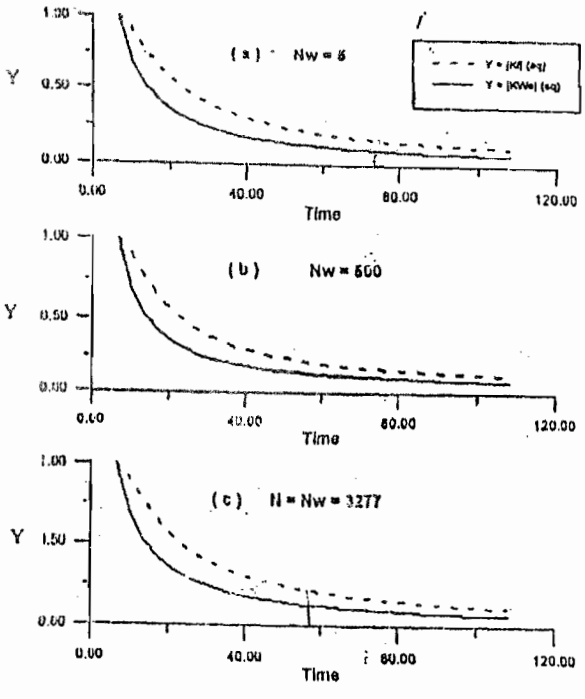


Fig 2.4.1 Exponential window of free particle (Vs Time): (a) Nw = 5; (b) Nw = 500; N = Nw = 3277

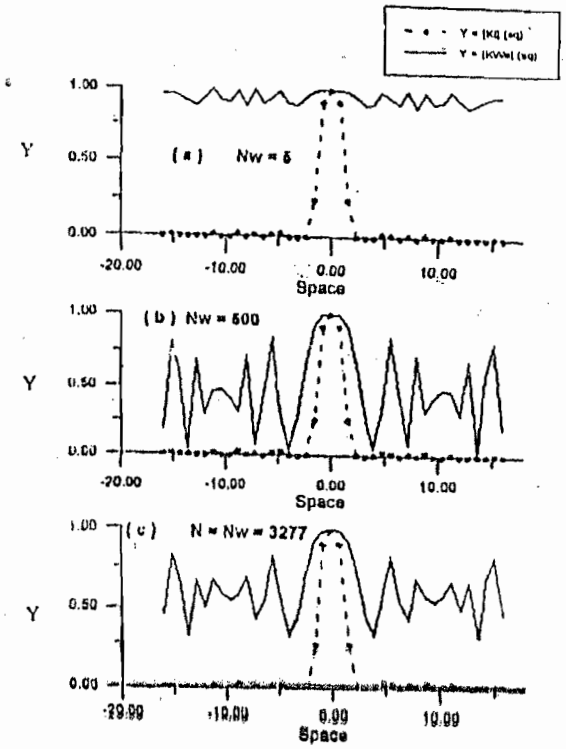


Fig 2.4.2 Exponential window of a free particle (Vs Space): (a) Nw = 5; (b) Nw = 500; N = Nw = 3277

DISCUSSION

From the series of graphs in figures 2.1 – 2.4 which compares K_{cl} with $K_{theoretical}$, we notice a reasonable agreement between the analytical and theoretical computations. This is a logical evidence that the model used for this work is reliable. Actually, the plot of the real part of K_{cl} for a free particle tallies with those of Feynman et al (1965) and Scher et al (1980).

In general, for the variation of the propagator with time, the factor, $t^{-1/2}$, tends to prevail which appears in the Van Vleck"s determinant of the free particle. The explanation for this observation is clear, namely, that the values of t must be appreciably large to avoid clumsy structures. Whereas, the phase takes small values for fixed positions and thus its contribution to the waveform is negligible.

The arrangement is such that we can see at a glance the role played by the number of weighted paths N_w compared to the total number, N. In all cases, the departure of the waveform of $|K_w|^2$ from $|K|^2$ becomes significant as N_w gets as small as $N_w = 5$. This distortion tends to disappear as N_w gets large and becomes minimum when $N_w = N$. In the aspect of variation with time, owing to the large values of the time, the effects of the window functions are hardly observable graphically.

CONCLUSION

From the various results obtained in this work, we see that windowing is a useful tool in path integral quantum mechanics. We have seen that with the extreme case of $N_w = 5$ compared with $N = 3277$, there is still a reasonable harmony between K and K_w. This conforms to the idea that we can filter off some paths with no significant error. It is a direct step out of the quantum mechanical doctrine of existence of infinitely many paths during an event; since all paths are probable

It follows that $N_w = 5$ is not too small compared to $N = 3277$ to get the same information for a required quantum mechanical analysis. Similarly, in the usual case of N tending to infinity, one can work with a countable N_w using a suitable window function for excellent results.

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