

FEYNMAN PATHS IN THE QUANTUM MECHANICS OF A SIMPLE HARMONIC OSCILLATOR

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ABSTRACT

The propagator in path-integral quantum mechanics is as versatile as a wave function in Schroedinger's formulation. The main challenge in this work is in computing the quantum propagator, K_s , of a simple harmonic oscillator as it entails summation over infinite number of paths. Using Van Vleck's formula, the classical propagator, K_{cl} , is computed as the analytical result. The graphical display of the result with Feynman-Schullman's checkerboard model used to enumerate the paths, gives a reasonable comparison between K_s and K_{cl} . This work further shows that instead of infinite number of paths uniformly weighted, K_s , can be reasonably computed by windowing off a large number of the paths and then weighting the rest non-uniformly. The weights used are gaussian and velocity window functions: w_g and w_v respectively.

KEY WORDS: Path-integral, propagator, checkerboard model, windowing, weights

1.1 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 $\psi(q_0, t_0)$ by a convolution integral

$$\psi(q, t) = \int K(q, t, q_0, t_0) \psi(q_0, t_0) dq_0$$

The Kernel $K(q, t, q_0, t_0)$ of this integral denoted by $\langle q, t | q_0, t_0 \rangle$ is known as the propagator. In the path - integral formulation of quantum mechanics by Feynman,

$$K = \sum_j \exp[iR_j(q, t, q_0, t_0)/\hbar]$$

where R_j is the action on the j^{th} path connecting space-time (q_0, t_0) with (q, t) .

$$R_j \equiv \int_{t_0}^t L(q, q_0, \tau) d\tau$$

(j^{th} path)

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.

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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).

1.2 BACKGROUND

In geometrical optics, however, the propagation of light along definite paths, or rays, is considered. Let U be any of the field components in the electromagnetic wave. It can be written as $U = Ae^{i\phi}$ (which A and ϕ real) where A is called amplitude and ϕ the phase of the wave (called, in geometrical optics, the eikonal). The limiting case of geometrical optics corresponds to small wavelength expressed mathematically by saying ϕ varies by a large amount over short distances.

Similarly, to the limiting case of classical mechanics, there corresponds, in quantum mechanics, a wave function of the form

$$\psi = Ae^{i\phi} \quad 1.2.1$$

where ϕ takes large values. As is well known, the path of a particle can be determined in mechanics by means of the variational principle. According to this, the so called classical action, R , of a mechanical system must take its extremum value (Goldstein 1950, Landau and Lifshitz 1960). This principle is analogous to the Fermat's principle in geometrical optics according to which the optical length of the ray (i.e., difference between its phases at the beginning and at the end of the path) must take its extremum value. In particular from the transformation theory of Dirac, we deduce that $\phi = R/\hbar$. (Dirac, 1933, 1935, 1945). As such we can write 1.2.1 as

$$\psi = Ae^{iR/\hbar} \quad 1.2.2$$

It should be noted that equation (1.2.2) gives the wave function of a classical particle. By this we mean a particle moving in a definite path known as "trajectory" (because it is completely determined by equations of motion) with R having its extremum value. For a quantum system, there is no such deterministic path. So for any motion, all paths are possible, that is, infinitely many probable paths are involved. In such cases

$$\psi = \sum_{j=1}^N A_j e^{iR_j/\hbar} \quad 1.2.3$$

where r_j is the action on the j^{th} path

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

1.4 BASIS OF WINDOWING

Geometrically, Feynman's quantum paths are like rays of optics. As such 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 stepwise 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. 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

$$\left(F_j\right)^2 = \left(\frac{1}{1 + (r_j/a)^2}\right)^{n/2+1} \quad (1.4.1)$$

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 thus

screening them out which 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. 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

$$\text{Number of paths} = (N_q)^{N_t} \quad 1.4.4$$

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

$$0 < (q_1 - q_3)/(l_1 - l_3) < c \quad 1.4.5$$

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.

Figure 1. 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).

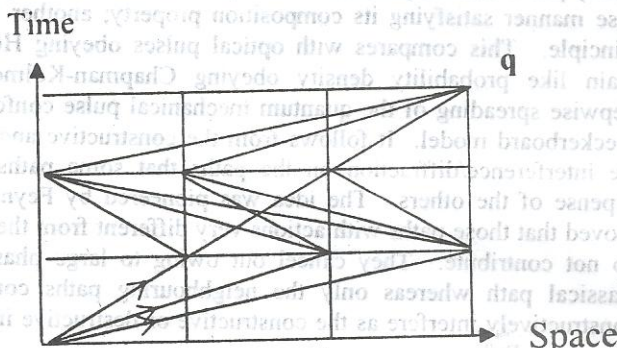


Fig. 1. A set-up like an infinite potential well with paths bouncing away from the walls.

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. 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

matrix diagonalisation methods. In such methods too, there is always the cutting-off of some "wild" paths.

2. RESULTS

2.1 THE PROPAGATOR OF A SIMPLE HARMONIC OSCILLATOR

A simple harmonic oscillator is a point mass attracted to a fixed centre by a force that is proportional to the displacement from that centre. Its study is important because more complicated systems can always be analysed in terms of normal modes of motion whenever the interparticle forces are linear functions of the relative displacements and these normal modes are formally equivalent harmonic oscillators [Schiff (1968)]. Thus the system forms the corner-stone of quantum theory of radiation. According to Merzbacher (1970), all modern field theories take their origin from this simple system.

The Lagrangian in this case is given by

$$L = \frac{m}{2} (\dot{q}^2 - \omega_o^2 q^2) \quad 2.1.1$$

and the corresponding propagator has been known to be (Feynman et al 1965).

$$K_{ci} = \left(\frac{m\omega_o}{2\pi i\hbar \sin \omega_o(t-t_o)} \right)^{1/2} \exp \left\{ \frac{im\omega_o}{2\hbar \sin \omega_o(t-t_o)} \left[(q^2 + q_o^2) \cos \omega_o(t-t_o) - 2qq_o \right] \right\} \quad 2.1.2$$

The results follow in the graphs of Figure 2 as in Ituen(1997). K_{ci} is the analytical formula while K_s 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 $|K_{ci}|^2$ gives a constant. This is in agreement with the work of Feynman et al (1965) and Scher et al (1980).

2.2 WINDOW EFFECTS ON QUANTUM PROPAGATORS

With the chosen region of contributing paths as a type of infinite potential well and the checkerboard space-time model, we can conveniently study the effects of the various window functions on the propagator, K , of the simple harmonic oscillator. That is, it now becomes possible to enumerate the paths as follows.

In the case study, we specify the number of vertical segments, N_v , to be 7 and that of horizontal segment, N_h , 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 simple harmonic oscillator, we compute the quantum propagator, K_s for N ,

$$K(q, q_0, t) = \sum_{j=1}^N \exp i R_j(q, q_0, t) \quad 2.2.1$$

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

$$K_w(q, q_0, t) = \frac{\sum_{j=1}^N [W_j \exp i R_j(q, q_0, t)]}{M} \quad n \leq N \quad 2.2.2$$

Note that the choice of $N_w < N$ 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

$$M = \sqrt{\sum_{j=1}^N |W_j|^2} \quad 2.2.3$$

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 according to Ituen(1997).

2.3 GAUSSIAN WINDOW FUNCTION, W_g

This is expressed as

$$W_g = \exp - \left(\frac{(R_j - R_{\min})^2}{R_{\min}} \right)$$

i.e. Gaussian on the action itself. W_g , like W_e , is meant to enhance paths with actions close to R_{\min} at the expense of the wild paths. In addition, the effect of W_g should be more pronounced than that of W_e owing to the sketch shown in figure 2.3.1.

• The non-uniform propagator is K_{wg} . The values of W_g for the free particle are generally small and mostly zero. As such we cannot reduce the number of weighted path beyond $N_w = 1000$, as seen in Figures 2.3.1

$$W_g = \exp - [(R_j - R_{\min})/R_{\min}]^2$$

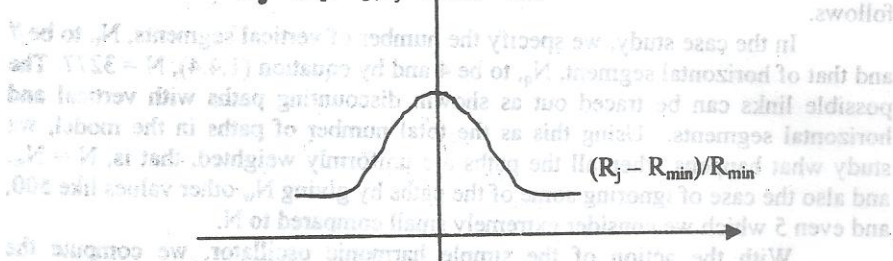


Fig. 2.3.1 Gaussian window function

2.4 VELOCITY WINDOW FUNCTION, W_v

We chose ϵ_j such that the speed, v_j is given by

$$v_j = \frac{|X_j - X_{j-1}|}{\epsilon_j} < c \quad 2.4.1$$

(c is the velocity of light).

This implies boundedness as required in fundamental physics. Then the window function,

$$W_v = \begin{cases} 1 & \text{if no physical violation} \\ 0 & \text{if physical violation} \end{cases} \quad 2.4.2$$

i.e. for any path, we calculate

$$I_k = \sum_{j=1}^N |X_j - X_{j-1}| \quad 2.4.3$$

with $t = I_k/v$ on condition, $v_j = I_k/t < v_c$ where v_c is a chosen values. Then

$$R_K = \frac{m}{2} \sum_i \frac{(X_j - X_{j-1})^2}{\epsilon_j} \quad 2.4.4$$

otherwise, when condition is not met

$$R_k = 0 \quad 2.4.5$$

N_w is determined by v_c given by

$$v_c = IN_q/N_t = I \left(\frac{\text{Total space division}}{\text{Total time division}} \right) \quad 2.4.6$$

$I = 2,4,5$ and the possible values are $N_w = 2457, 1638, 819$ as seen in Figures 2.4.1-2.4.2

3.1 DISCUSSION

From the series of graphs in figures 2.1 - 2.4 which compares K_{cl} with $K_{theoretical}$, we notice reasonable agreement between the analytical and theoretical computations. This is a logical evidence that the model used for the work is reliable. Actually, the plot of the real part of K_{cl} for a simple harmonic oscillator 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 $1/\sqrt{(\sin t)}$, tends to prevail which appears in the Van Vleck's determinant of the simple harmonic oscillator. The explanation for this observation is clear, and is the fact that the values of t has to be appreciably large to avoid clumsy structures.

Consequently, the phase takes small values for fixed positions and as such its contribution to the waveform is negligible.

The first set of graphs shows the effect with variation in time while the second set has to do with variation of position in space. The arrangement is such that we can see at glance the role played by the number of weighted paths N_w compared to N . In all cases, the departure of the waveform of $|K_w|^2$ from $|K|^2$ becomes significant as N_w gets small like $N_w = 5$. This distortion tends 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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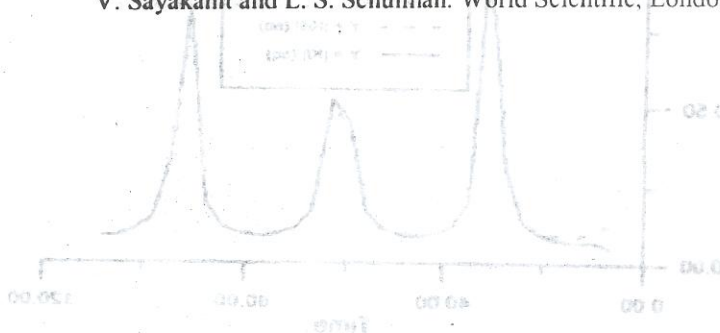


Fig. 2 Comparing propagator of simple harmonic oscillator with analytical result. (a) with time (N = 100)

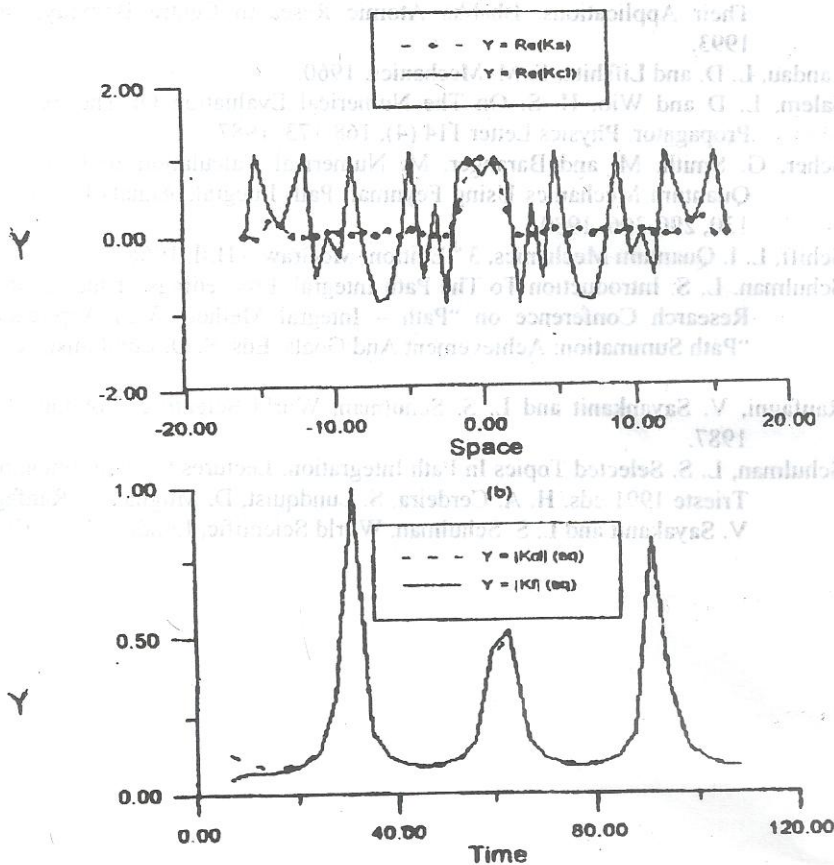


Fig.2 Comparing propagator of simple harmonic oscillator with analytical result: (a) with space, (b) with time ($N = 3277$)

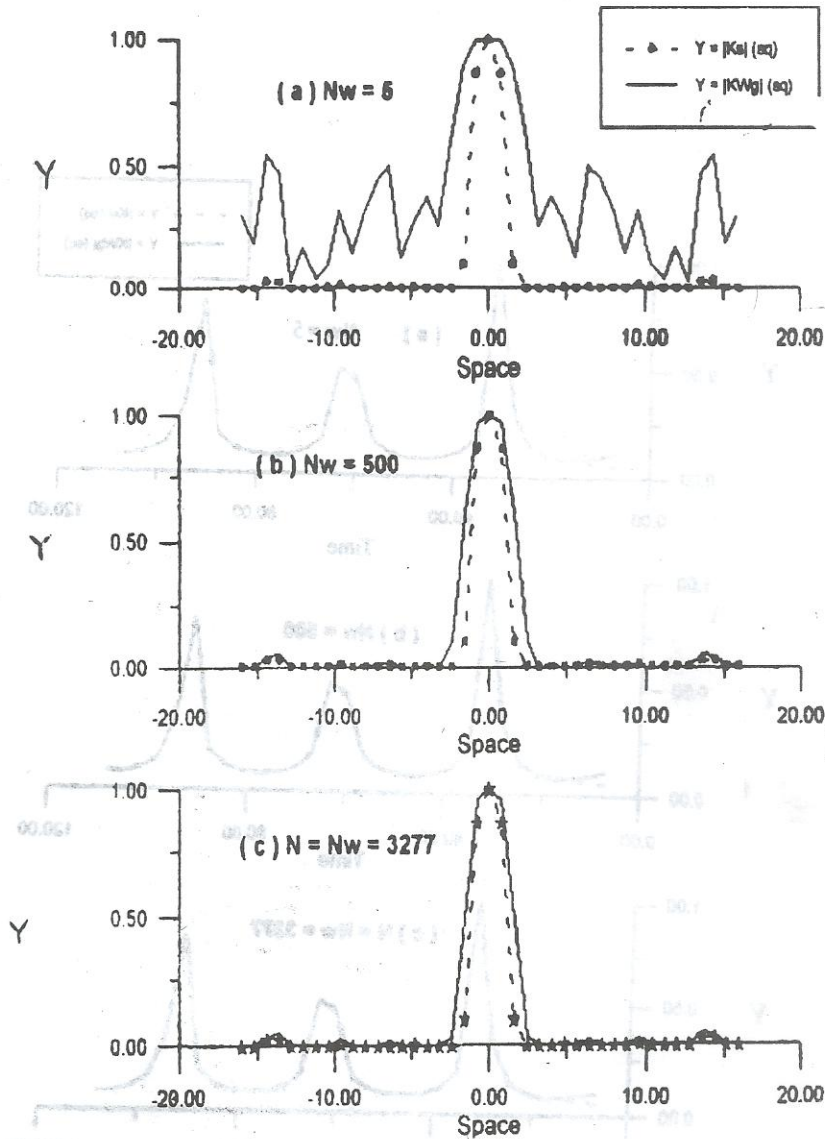


Fig 2.3.1

Gaussian window of simple harmonic oscillator (Vs Space):

 (a) $Nw = 5$; (b) $Nw = 3277$

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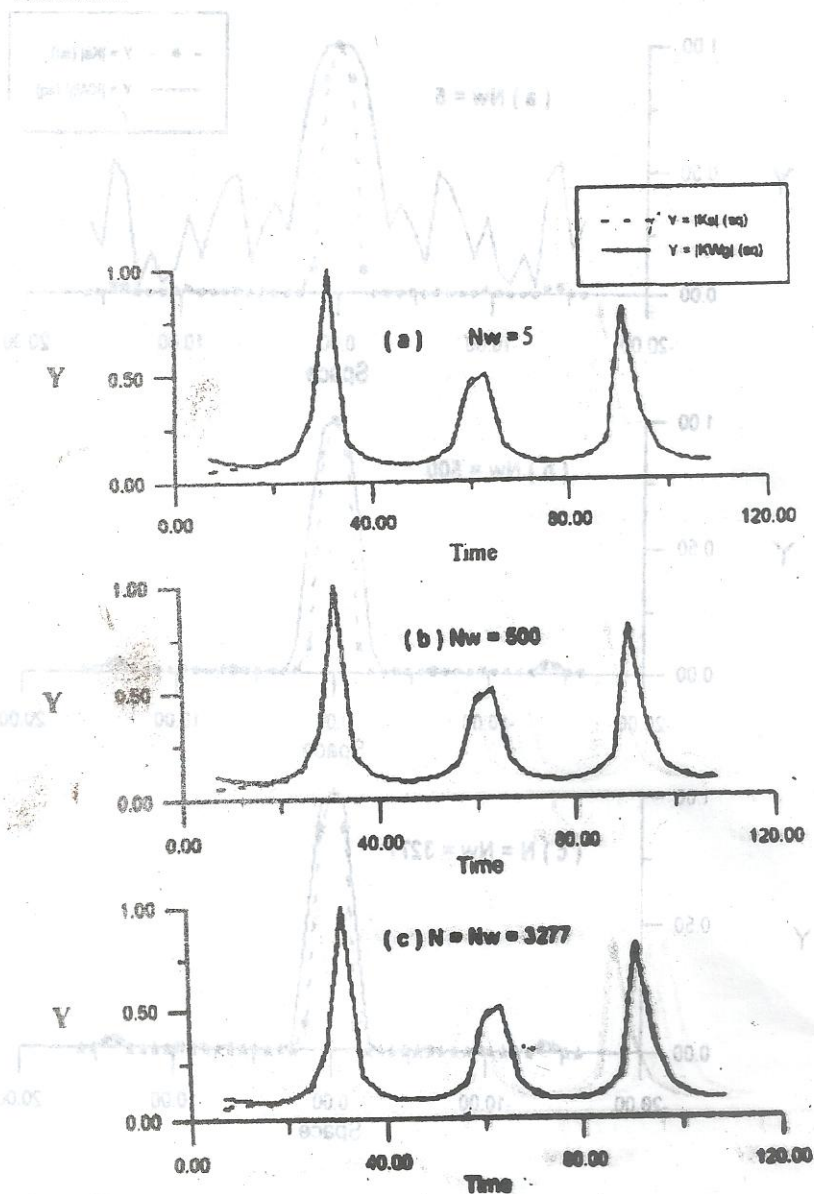


Fig. 2.3.2 Velocity window of simple harmonic oscillator (V vs Time):
 (a) $Nw = 819$; (b) $Nw = 1638$; (c) $N = 3277$; $Nw = 2457$

Fig. 2.4.2 Velocity widow of a simple harmonic oscillator (Vs Time):
 (a) $Nw = 819$; (b) $Nw = 1638$; (c) $N = 2457$

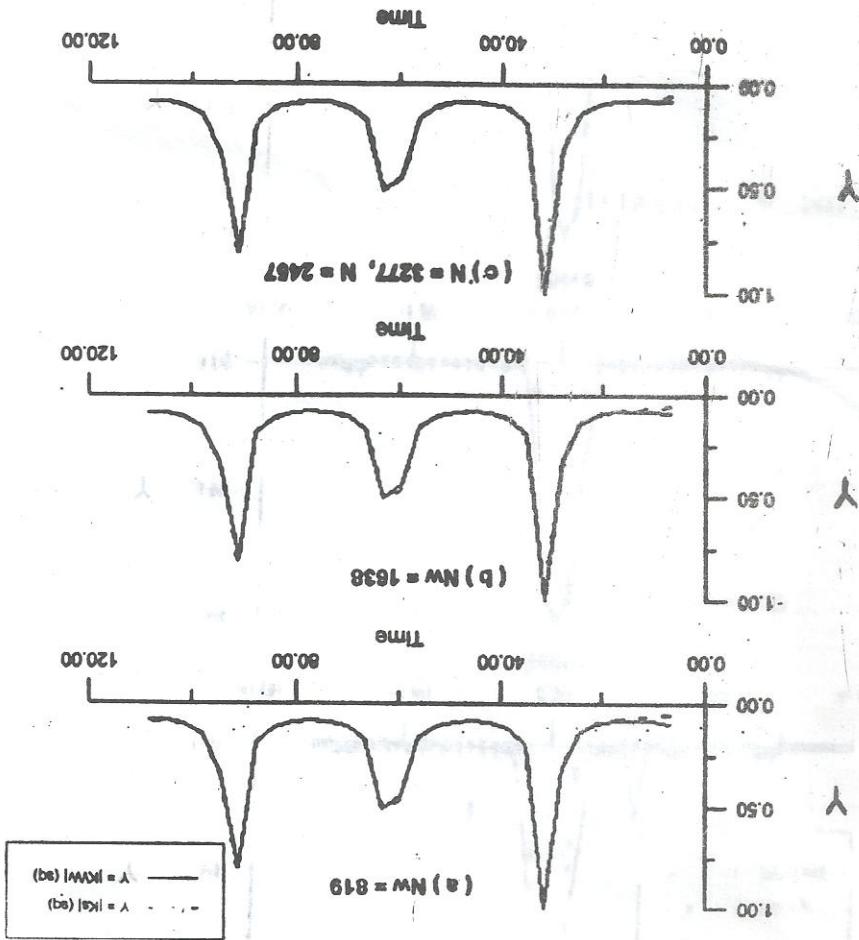


Fig. 2.4.1 Velocity window of a simple harmonic oscillator (Vs Space):
 (a) $Nw = 819$; (b) $Nw = 1638$; (c) $N = 3277$; $Nw = 2457$

