Relative Deviation between a Uniformly Weighted Propagator and a Windowed Propagator of a Simple Harmonic Oscillator

Eno Etim Ituen
Department Of Physics, University Of Uyo, Nigeria

Abstract

The paper elaborates more on the process of windowing in the computation of the quantum propagator, k_s, for a simple harmonic oscillator as a follow up of Ituen 2002b. More window functions are analysed in this case, namely, random, W_r exponential, W_e, gaussian, W_g and velocity, W_v window functions. The values of the propagator as Kw_r, Kw_e, Kw_g, Kw_v compares reasonably with K_s and hence with the analytical result K_{cl}. The slight deviations are measured as relative deviation α_r, α_e, α_g, α_v depending on the window functions, which gives a measure of their suitability. Measurements were done with variations in time only; variations with space being reserved as a further work.

Key Words: Action, propagator, window function, relative deviation.
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1 0 Introduction

1.1 Basis of Windowing

As stated already in Ituen (2002b), Feynman's quantum paths are like rays of optics, geometrically. Thus 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. 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 $\frac{R_j}{\hbar}$.

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

$$\left(F_j\right)^2 = \left(\frac{1}{1+\left(\frac{r_j}{a}\right)^2}\right)^{\frac{n}{2+1}} \tag{1.1}$$

where $r_j = \frac{R_{j} - R_{\min}}{\hbar}$; $R_{\min}$ 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 (1.1) consolidate 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.

This can be illustrated as follows with the idea of young's double slit interference experiment in Optics. Feynman's paths are considered as "interfering alternatives" to a moving particle from an initial point to the final. Those paths are a counterpart of the two holes of Young's experiment, $S_2P = S_1P + \Delta = r + d\sin\theta$. Let r be the displacement in the direction of the wave ϕ (P) then

$$\psi = e^{ikr} + e^{ik(r+\sin\theta)} \tag{1.2}$$

where k is the propagation constant or wave number (vector).

With non-uniform weights W_1 and W_2, equation (1.2) becomes

$$\psi = W_1 e^{ikr} + W_2 e^{ik(r+\sin\theta)} \tag{1.3}$$

By taking the magnitude of each, the interference term in the latter is $\omega_1\omega_2 e^{ikd\sin\theta}$ instead of $e^{ikd\sin\theta}$ in the former. Thus by introducing the weights the constructive or destructive interference becomes modified. Hence the window functions actually amplify the window effects to facilitate the study. In this work the window functions are in the form of weights as discussed later.

Another aspect of window effects includes the following:

(i) From the picture originally given by Schulman (1987), we limit the region of contributing paths to a particular rectangle as shown above. 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

$$\text{Number of paths } (N_q)^{N_t} \tag{1.4}$$

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

$$0 < (q_1 - q_3)/(l_1 - l_3) < c \tag{1.5}$$

is a very important requirement physically; c being the velocity of light. Hence for $N_t = 3$ and $N_q = 3$ 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.

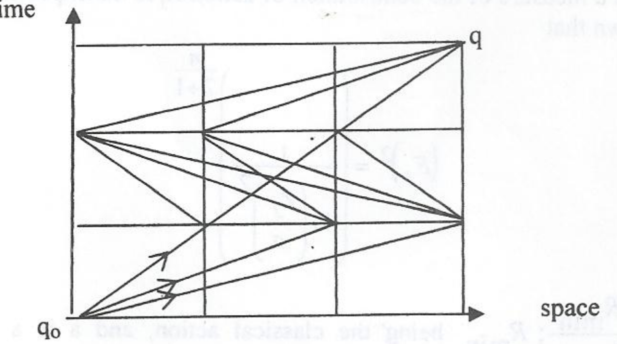

Figure 1: A set-up like an infinite potential well with paths bouncing away from the walls.

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) and 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. (Ituen 2002b)

1.2 The Propagator of a Simple Harmonic Oscillator

According to Merzbacher (1970), all modern field theories take their origin from this simple system. The Lagrangian in this case is given by

$$L = \frac{m}{2}\left(\dot{q}^2 - w_0^2 q^2\right) \tag{1.6}$$

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

$$K_{el} = \left(\frac{m\varpi_0}{2\pi i \sin\varpi_0 (t - t_0)}\right)^{\frac{1}{2}} \exp\left\{\frac{im\varpi_0}{2\sin\varpi_0 (t - t_0)}\left[\left(q^2 + q_0^2\right)\cos\varpi_0 (t - t_0) - 2qq_0\right]\right\} \tag{1.7}$$

Recall that Figures 7(a and b) show the comparison between K_{cl}, analytical propagator, and K_s, computed propagator. Again we plot the real parts of the quantity versus space because $|K_{cl}|^2$ constant at all points. By Ituen, (2002b), the result is in agreement with Feynman et al (1965) and Scher et al (1980).

2.0 Window Effects on Quantum Propagators

As in Ituen (2002b) the same model is used with N = 3277. Hence the result of the last section above. We compute the quantum propagator, K, for N, with the original expression

$$K(q, q_0, t) = \sum_{j=1}^{N\to\infty} \exp iR_j \frac{(q, q_0, t)}{h} \tag{2.1}$$

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

$$K_0(q, q_0, t) = \sum_{j=1}^{Nw} \frac{\left[W_j \exp iR_j\left(\frac{q, q_0, t}{h}\right)\right]}{M} \qquad N_w \le N \tag{2.2}$$

Note that the choice of $N_w < N$ for further results, is to make $W_j = 0$ for some paths since there are infinite number of them. This is again an enhancement to the desired window effects, where M is a normalization factor given by

$$M = \sqrt{\sum_{j=1}^{N_w} |W_j|^2} \tag{2.3}$$

The results for each of the window functions involve the display of the uniformly weighted propagator, K_s, and the corresponding weighted or non-uniform propagator, K_w versus time as in Figures 8 - 11. The relative deviation, α, defined between K_s (or $K_{theoretical}$) and K_w are calculated as.

$$\alpha = \frac{\sum\left(|K_w|^2 - |K_{theoretical}|^2\right)}{\sum |K_{theoretical}|^2} \tag{2.4}$$

This is contained in Table 1.

Table 1: Displaying α of the four window functions for Simple Harmonic Oscillator Vs Time

N_w	α_r	α_c	α_g	α_v
2457	0.00028	0.00098	0.00220	0.00199
1638	0.00006	0.00176	0.00216	0.00200
819	0.16100	0.13800	0.32600	0.40300

2.1 Illustration of the Model

Case i:

If the minimum number of divisions in the model is one, only one path is possible as in Figure 2.

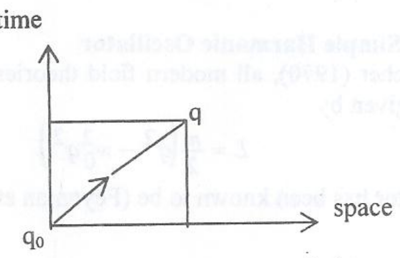

Figure 2: The only possible path in one division

Then $$K \approx \exp[iR_1(q,q_0,t)], \ |K| = 1 \tag{2.5}$$

Case ii:

If that minimum is two, only one path is also possible since we have to discount paths with any vertical or horizontal segment because,

Speed $\neq 0$, and speed $\neq \infty$

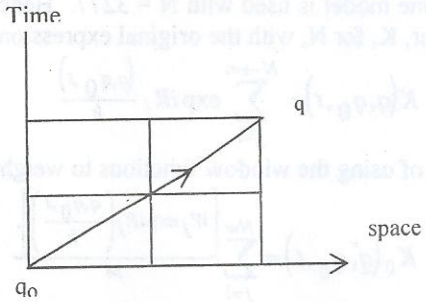

Figure 3:The only path in two division

This is also unsuitable from figure 2.

Case iii:

Consider when the minimum is three divisions. There are at least three possible paths from figure 4. Then from equation (2.1)

$$K \approx \exp i[R_1 + R_2 + R_3] = \exp iR_1 + 2\exp iR_2 \tag{2.6}$$

From equation (2.2),

$$K_W = W_1 \exp i R_1 + 2W_2 \exp i R_2 \tag{2.7}$$

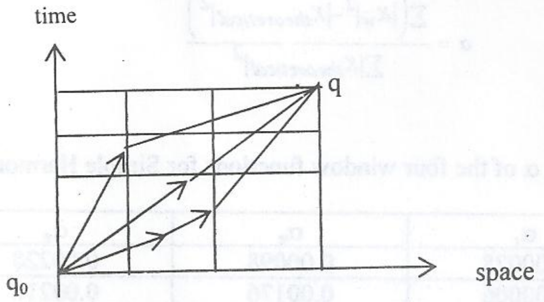

Figure 4: At least three paths possible in three divisions

This case gives a more reasonable picture and how the windowing applies which is required to illustrate the queer Quantum Mechanics condition of infinite number of paths. Hence the larger the number of paths, N, the better the model in demonstrating this Quantum Mechanics condition. In the work, N = 3277, while different values of $N_W \leq N$ were taken as in the previous work.

3.0 Results

3.1 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 Figure 8. Kw_r is the non-uniform propagator to compare with K_s. 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 $N_w < 3000$.

3.2 Exponential Window Function W_e

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

$$W_e = \exp - (R_j - R_{min})/R_{min} \tag{3.1}$$

where R_{min} is the classical action for the system. By the sketch shown in Figure 3.2 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 Figure 9. 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.

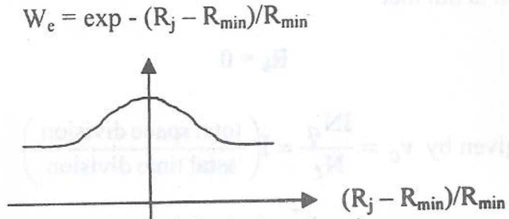

Figure 5: Exponential window function

3.3 Gaussian Window Function, W_g

This is expressed as

$$W_g = \exp - \left(\frac{R_j - R_{min}}{R_{min}}\right)^2 \tag{3.2}$$

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 6. Figure 10 show the corresponding results. The non-uniform propagator is Kw_g.

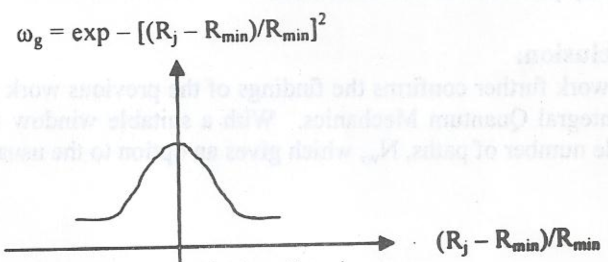

Figure 6: Guassian window function

3.4 Velocity Window Function, W_v

We choose ε, such that the speed, v_j is given by

$$V_j = \frac{x_j - x_{j-1}}{\varepsilon_j} \prec c \qquad (3.3)$$

(c is the velocity of light).
This implies boundedness as required in fundamental physics. Then the window function,

$$W_v = \begin{cases} 1, \text{if no physical violation} \\ 0, \text{ if physical violation} \end{cases} \qquad (3.4)$$

i.e. for any path, we calculate

$$I_k = \sum_{j=1}^{N} \left| x_j - x_{j-1} \right| \qquad (3.5)$$

with $t = \frac{I_k}{v}$ on condition $v_j = \frac{I_k}{t} \prec v_c$ where v_c is chosen values. Then

$$R_k = \frac{m}{2} \sum_{J} \frac{\left(x_j - x_{j-1}\right)^2}{\varepsilon_j} \qquad (3.6)$$

otherwise when condition is not met

$$R_k = 0 \qquad (3.7)$$

N_w is determined by v_c given by $v_c = \frac{IN_q}{N_t} = I\left(\frac{\text{total space division}}{\text{total time division}}\right)$

I = 2,4,5 and the possible values are N_w = 2457, 1638, 819 as seen in Figure 11

4.0 Discussion

Table 1 contains computed values of the relative deviation α of the 4 window functions for the various systems with different N_w. α provides reasonable quantitative details about the measure of suitability of the window functions. Besides, it gives more elaborate information about the effects of the window functions, which is not obvious from the waveforms of K_s and K_w; as the two appear to coincide almost completely when plotted on the same page.

Since the values of α_r, α_e, α_g, α_v are consistently minute, it confirms the closeness of K_s and K_w. As expected also, the more N_w approaches N, the smaller the value of α, thus supporting the Quantum Mechanical doctrine of infinitely many paths involved in an event.

5.0 Conclusion:

This work further confirms the findings of the previous work Ituen 2002b about windowing as a useful tool in Path Integral Quantum Mechanics. With a suitable window functions, one can have excellent results using countable number of paths, N_w, which gives an option to the usual infinitely many paths condition.

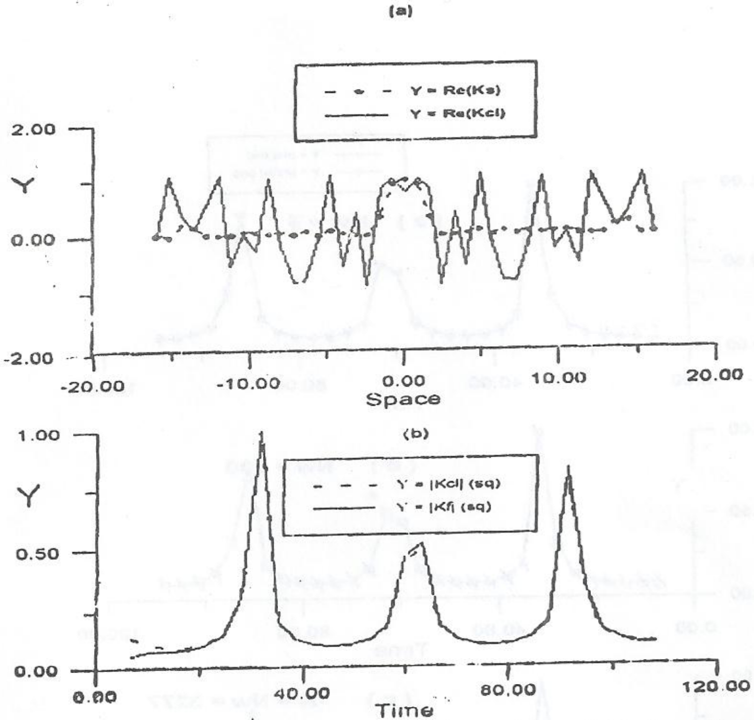

Figure 7: Comparing propagator of simple harmonic oscillator with analytical result: (a) with space, (b) with time N = 3277).

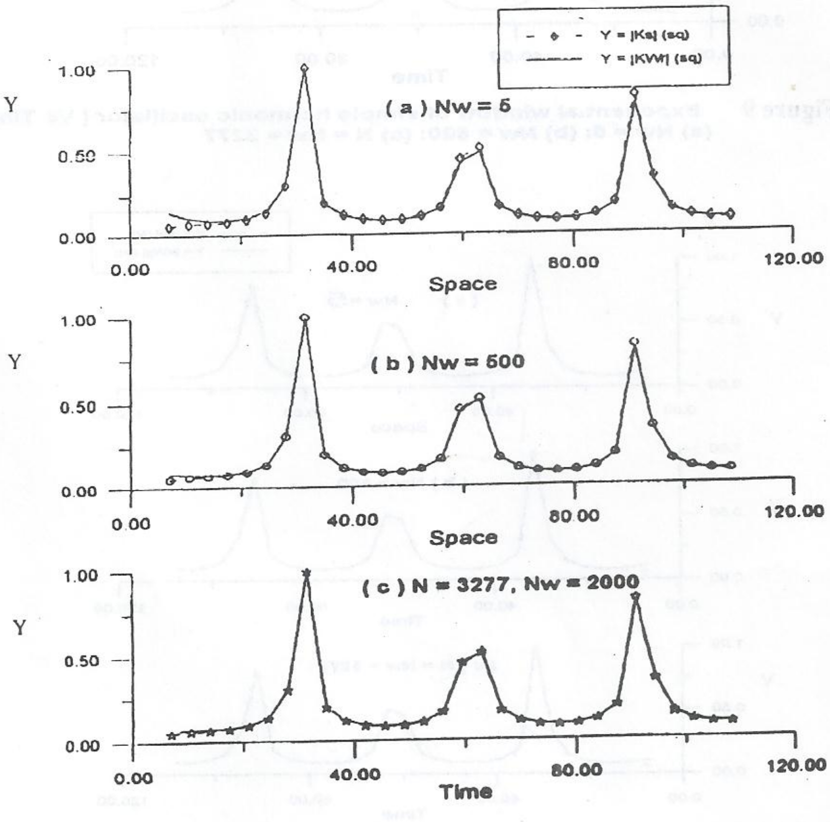

Figure 8 **Random window of a simple harmonic oscillator (Vs Time): (a) Nw = 5: (b) Nw = 500: (c) N = 3277, Nw = 2000**

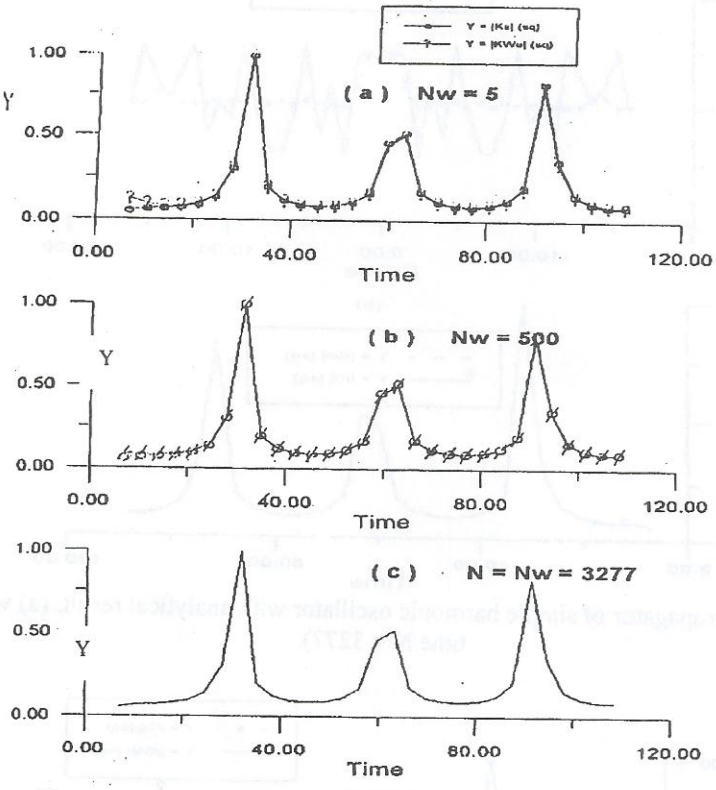

Figure 9 Exponential window of simple harmonic oscillator (Vs Time): (a) Nw = 5: (b) Nw = 500: (c) N = Nw = 3277

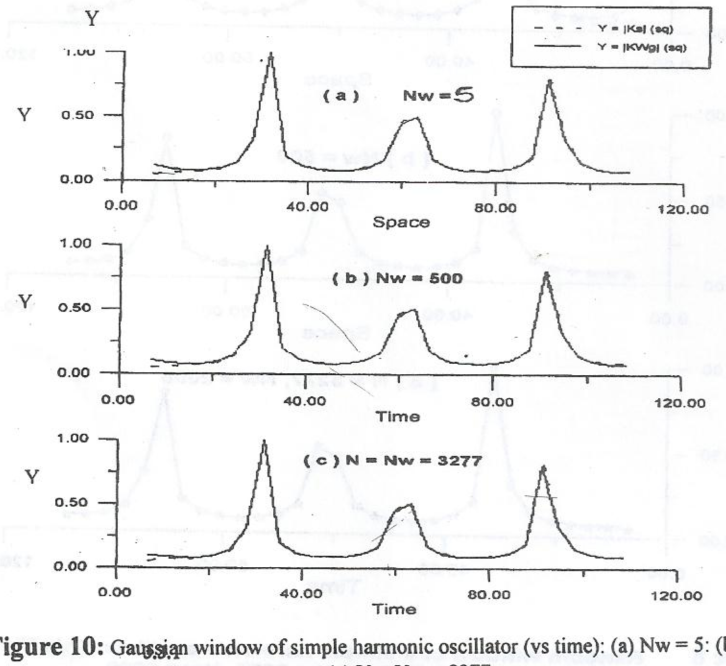

Figure 10: Gaussian window of simple harmonic oscillator (vs time): (a) Nw = 5: (b) Nw = 500 (c) N = Nw = 3277

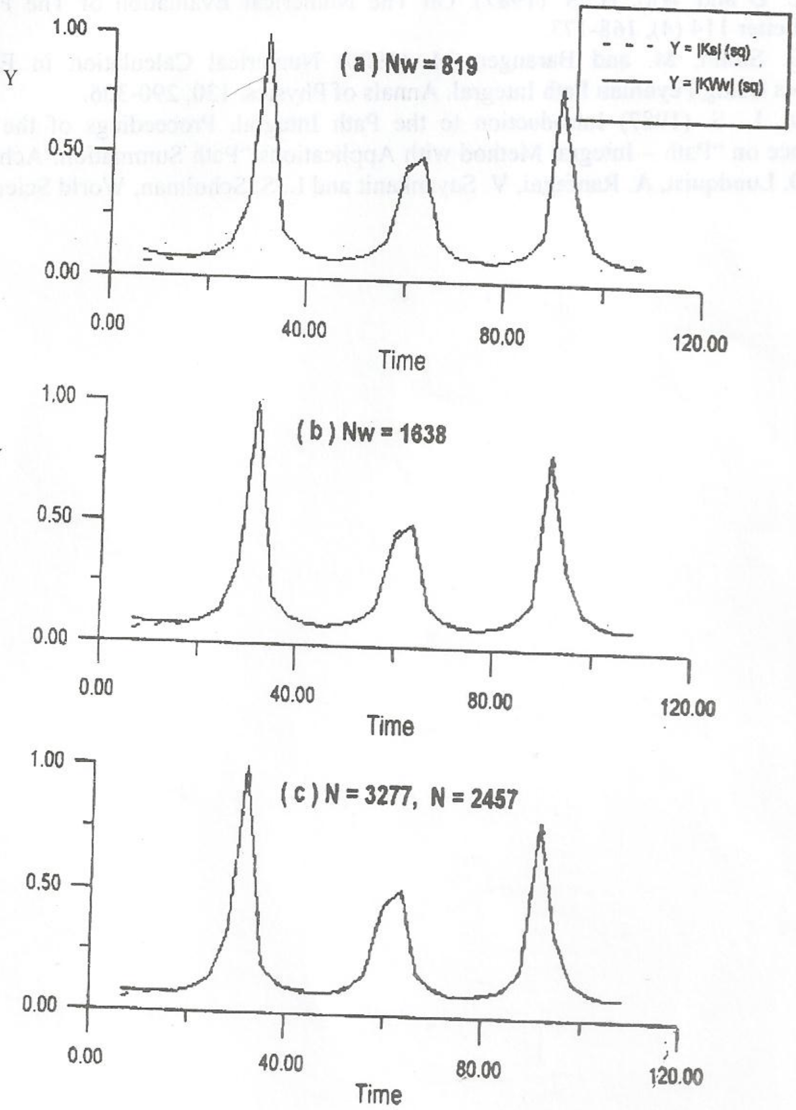

Figure 11: Velocity window of a simple harmonic oscillator (vs time): (a) Nw = 819; (b) Nw = 1638; (c) N= 3277; Nw = 2457

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