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Relative deviation between a uniformly weighted propagator and windowed propagator of a simple Harmonic Oscillator–2

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Abstract

A further processing of windowing in the computation of the quantum propagator, k_s, for a simple harmonic oscillator is performed with variation in space; instead of time as in Ituen (2003b). All the four window functions are analysed as before, namely, random, W_r, exponential, W_e, gaussian, W_g and velocity, W_v window functions. Again the values of the propagator as Kw_r, Kw_e, Kw_g, Kw_v, in space, compare reasonably with K_s and hence K_{cl}. The quantities σ_r, σ_e, σ_g, σ_v are the respective slight relative deviations measured with variation in space as expected in this case.

Keywords: Action, propagator, window function, relative deviation.

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1.0 Introduction

The basis of windowing is the same as given in [7, 8]. It is based on [5]'s definition of propagator as a quantum-mechanical pulse spreading in a step-wise manner and this satisfies its composition property; another form of superposition principle. The idea was pioneered by [3] by proving that those paths with actions very different from the classical action really do not contribute. Some paths cancel out owing to large phase difference with the classical path whereas only the neighbouring paths contribute in phase and constructively interfere; since constructive or destructive interference depends on the phases $\frac{R_j}{\eta}$

Again using F_j as a measure of the contribution of action R_j to the expected value of the propagator, K, [1] had 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 $r_j = \frac{\left(R_j - R_{\min}\right)}{\eta}$ $R_{\min}$ 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 the fact that $R_{\min}$ is the most important action while other actions decrease in influence as R_j departs from $R_{\min}$.

The foregoing discussions are supportive of the fact that one can "filter off" some of the paths with no significant error and this is the doctrine of windowing.

The idea of Young's double slit interference experiment in Optics can be used as a further illustration by considering [3] paths as "interfering alternatives" to a moving particle from an initial point to the final. Those paths are a counterpart of the two paths S_1P and S_2P of Young's experiment.

$$S_2P = S_1P + \Delta = r + d \sin \theta$$

Let r be the displacement in the direction of the wave ψ (P) then

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

where k is the propagation constant or wave number (vector). With non-uniform weights W_1 and W_2, equation (1.2) becomes

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

By taking the magnitude of each, the interference term in the latter is $W_1W_2e^{ikd\sin\theta}$ instead of $e^{ikd\sin\theta}$ in the former. By introducing the weights the constructive or destructive interference becomes modified; thus amplifying the window effects to facilitate the study. In the work the weights represent window functions.

Another aspect of window effects is in the model which the same as in the listed previous works. The picture was originally given by [12] to be a limited region of contributing paths just like a particular rectangle. 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

$$Number\ \ of\ \ paths = (Nq)^{N_t - 1} \tag{1.4}$$

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

$$0 < (q_1 - q_3)/(t_1 - t_3) < c \tag{1.5}$$

is a very important requirement physically; c being the velocity of light. Figure 1.1 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.

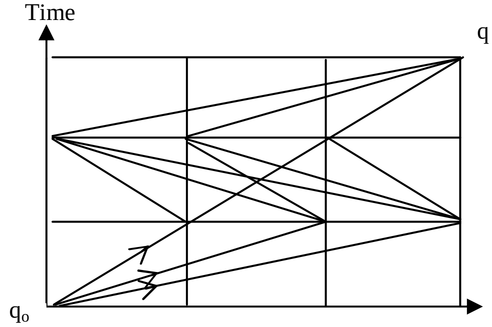


Figure 1.1: A set-up like an infinite potential well with paths bouncing away from the walls.

Remark:

Generally, anyone embarking on this direct path summation is confronted with devising 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 [10, 11] using respectively numerical matrix multiplication and matirx diagonalisation methods. In such methods too, there is always the cutting-off of some “wild” paths [6].

2.0 The propagator of a simple harmonic oscillator

It is important to remember that the Lagrangian of this system as

$$L = \frac{m}{2}\left(\dot{q}^2 - \omega_0^2 q^2\right) \tag{2.1}$$

[9] and the corresponding propagator has been known to be:

$$K_{cl} = \left[\frac{m\omega_0}{2\pi i\hbar \sin\omega_0(t-t_0)}\right]^{\frac{1}{2}} exp\left[\frac{im\omega_0}{2\hbar \sin\omega_0(t-t_0)}\left\{\left(q^2+q_0^2\right)\cos\omega_0(t-t_0) - 2qq_0\right\}\right] \tag{2.2}$$

as in [3]. Recall that Figures 2.2 (a and b) show the comparison between K_{cl}, analytical propagator, and K_s, computed propagator. As already pointed out in [6], [7], [8] the result is in agreement with [3], [11].

3.0 Window effects on quantum propagators

The main point distinction between this work and [8] is that computation is done with variation in space throughout. So, using the usual model with $N = 3277$, we repeat the whole process as in [8], namely;

The quantum propagator, K, for N, is obtained from the original expression

$$\mathrm{K}_w\left(q, q_{0,} r\right) = \sum_{j=1}^{N\to\infty} \frac{\exp iR_j\left(q, q_0, t\right)}{\eta} \tag{3.1}$$

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

$$K_w\left(q, q_0, t\right) = \sum_{j=1}^{N_W} \frac{\left\lfloor W_j \; exp\; iR_j\left(q, q_0, t\right) / \eta \right\rfloor}{M}; \qquad N_w \leq N \tag{3.2}$$

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

$$M = \sqrt{\sum_{j=1}^{N_W} \left| W_j \right|^2} \tag{3.3}$$

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 3.1 - 3.4. The relative deviation, σ, defined between K_s (or $K_{theoretical}$) and K_w are calculated as.

$$\sigma = \frac{\sum \left(\left| K_w \right|^2 - \left| K_{theoretical} \right|^2 \right)}{\sum \left| K_{theoretical} \right|^2} \tag{3.4}$$

This is contained in Table 1.

4.0 Results

4.1 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 Figures 3.1. 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 $N_w < 3000$.

4.2 Exponential window function, W_e

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

$$W_e = \frac{\exp - \left(R_j - R_{\min}\right)}{R_{\min}} \tag{4.1}$$

Where R_{min} is the classical action for the system. By the sketch shown in Figure 4.1 the aim is to eliminate paths with large action. Such paths may be termed as wild paths referred to by [3].

The results are presented in Figures 3.2. Kw_r represents the non-uniform propagator. There is no restraint on the choice of N_w in this case. So we choose $N_w = 3277, 500, 5$.

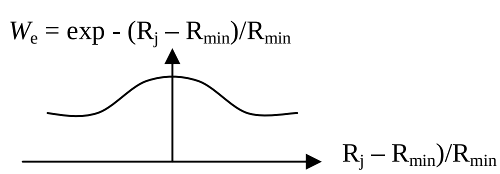


Figure 4.1: Exponential window function

4.3 Gaussian window function, W_g

This is expressed as

$$W_g = \exp - \left[\frac{\left(R_j - R_{\min}\right)}{R_{\min}} \right]^2 \tag{4.2}$$

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.4.3. Figure 3.3 show the corresponding results. The non-uniform propagator is Kw_g.

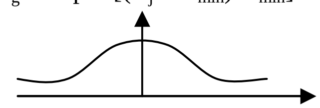


Figure 4.2: Guassian window function

5.0 Velocity window function, W_v

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

$$V_j = \frac{x_j - x_{j-1}}{\varepsilon_j} \pi c \tag{5.1}$$

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

function,
$$W_v = \begin{cases} 1, \text{if no physical violation} \\ \\ 0, \text{if physical violation} \end{cases} \tag{5.2}$$

i.e. for any path, we calculate
$$1_k = \sum_{j=1}^{N} \left| x_j - x_{j-1} \right| \tag{5.3}$$

with $t = l_k/v$ on condition $v_j = \underline{l_k}/t < v_c$ where v_c is a chosen values. Then

$$R_k = \frac{m}{2} \sum_j \frac{\left(x_j - x_{j-1}\right)^2}{\varepsilon_j} \tag{5.4}$$

otherwise when condition is not met
$$R_k = 0 \tag{5.5}$$

N_w is determined by v_c given by

$$v_c = \frac{IN_q}{N_t} = I\left(\frac{total\ space\ division}{total\ time\ division}\right)$$

I = 2,4,5 and the possible values are N_w = 2457, 1638, 819 as seen in Figure 3.5

6.0 Discussion

As in [8], Table 1 contains computed values of the relative deviation σ of the 4 window functions for the various systems with different N_w. σ 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.

Table 1: Displaying σ of the four window functions for Simple Harmonic Oscillator vs. Space

N_w	σ_r	σ_e	σ_g	σ_v
2457	0.0326	0.0241	0.2718	0.0920
1638	0.0775	0.0685	0.2815	0.1920
819	0.0009	0.0022	0.0021	0.0021

Since the values of σ_r, σ_e, σ_g, σ_v are small throughout, it again confirms the closeness of K_s and K_w. This is in consistent with [8].

7.0 Conclusion

The work further consolidates the findings of its counterpart work [8]. The constant smallness of the values of σ is indicative of the suitability of the window functions.

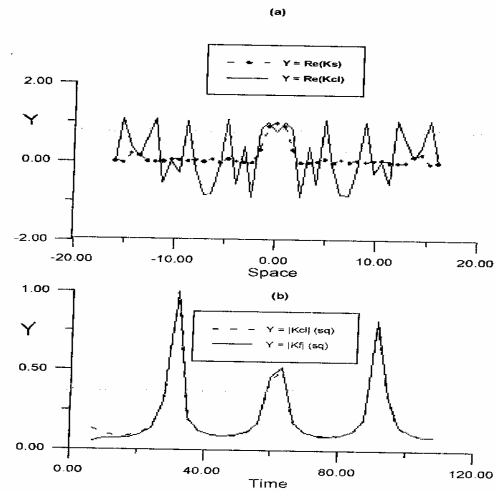


Fig. 3.3 Comparing propagator of simple harmonic oscillator with analytical result: (a) with Space, (b) with time (N= 3277)

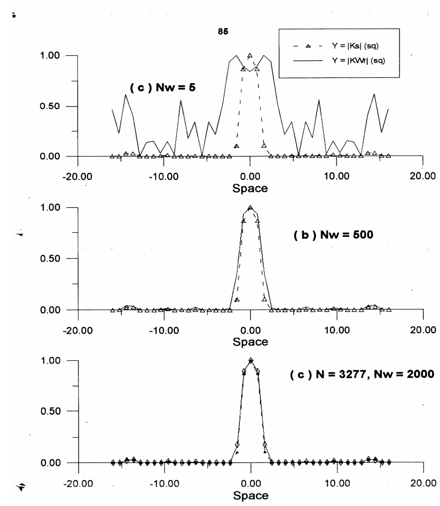
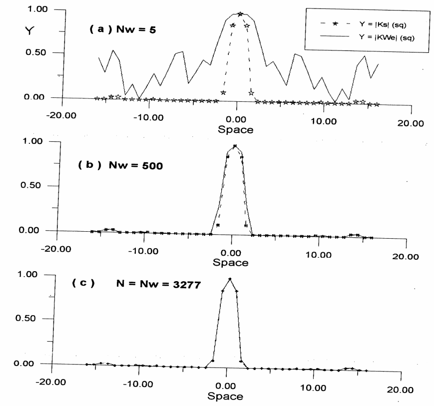


Fig 4.13 Random window of a simple harmonic oscillator (Vs Space): (a) Nw = 5: (b) Nw = 500: (c) N = 3277, Nw = 2000



g. 4.23 Exponential window of simple harmonic oscillator (Vs Space):
(a) Nw = 5: (b) Nw = 500: N = Nw = 3277

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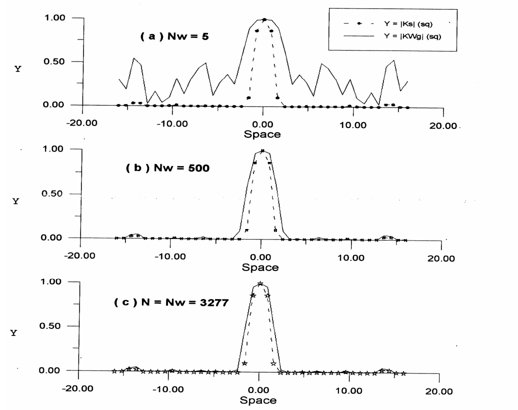

Fig.4.35 Gaussian window of simple harmonic oscillator (Vs Space):
(a) Nw = 5: (b) Nw = 500: (c) N = Nw = 3277

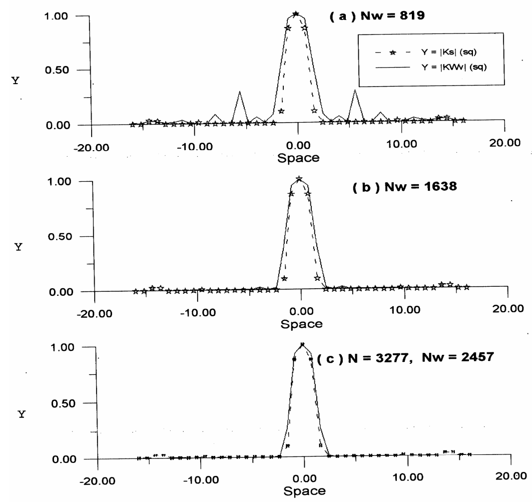

Fig4.43 Velocity window of a simple harmonic oscillator (Vs Space):
(a) Nw = 819; (b) Nw = 1638; (c) N = 3277; Nw = 2457

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