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# Diffraction in the time of a confined particle and its Bohmian paths

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**Abstract**
Diffraction in the time of a particle confined in a box with its walls removed suddenly at $t = 0$ is studied. The solution of the time-dependent Schrödinger equation is discussed analytically and numerically for various initial wavefunctions. In each case Bohmian trajectories of the particles are computed and also the mean arrival time at a given location is studied as a function of the initial state.

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(Some figures in this article are in colour only in the electronic version)

## 1. Introduction

Several works have been done on time-dependent boundary conditions [1–7]. Diffraction in time was initially introduced by Moshinsky [1] by considering a situation involving a beam of particles impinging from the left on a totally absorbing shutter located at the origin which is suddenly turned off in an instant. The transient current has a close mathematical resemblance with the intensity of light in the Fresnel diffraction by a straight edge. An interesting feature of the solutions for cut-off initial waves, occurring both in the free case [18] and in the presence of a potential interaction [8], is that, if initially there is a zero probability for the particle to be at $x > 0$, as soon as $t = 0^+$, there is instantaneously a finite, though very small, probability of finding the particle at any point $x > 0$. This non-local behavior of the Schrödinger solution is due to its nonrelativistic nature and not as a result of the quantum shutter setup [9]. The application of the Klein–Gordon equation to the shutter problem [1] shows that the probability density is restricted to the accessible region $x < ct$ ($c$ is the speed of light). See [10] for a recent review. Gerasimov and Kazarnovskii [2] confined the initial wave in a finite region by introducing a second shutter at the point $x = L$. Godoy [11] pointed out the analogy with Fraunhoffer diffraction in the case of small box (compared to the de Broglie length), and Fresnel diffraction, for larger confinements. In this context, by considering the problem of a particle in a one-dimensional box potential with its walls suddenly removed at some time, the aim of the present paper is to probe some aspects of the time-dependent boundary condition for a particle confined in a square well focusing on Bohmian interpretation of quantum mechanics that have remained hitherto unnoticed. The computed Bohmian trajectories are instructive in revealing the conceptual ramifications of such an example.

Although the formalism of Bohmian mechanics does not give predictions going beyond those of QM whenever the predictions of the later are unambiguous, it should be favored because of its interpretational advantages stemming from the ontological continuity between the classical and the quantum domains [13]. Noting the Bohmian arrival time formulation by means of cut-off current, it has been argued that predictions of Bohmain mechanics are in contradiction to the standard quantum mechanical formalism [14]. In nonrelativistic Bohmian mechanics, the world is described by point-like particles which follow trajectories determined by a law of motion. The evolution of the positions of these particles are guided by a wavefunction which itself evolves according to the Schrödinger equation [15–19]. In this theory, in the absence of any measuring device, one finds [20–22] that for those particles that actually reach $x = X$, the arrival time distribution is given by the modulus of the probability current density, i.e. $|j(X,t)|$. We will proceed as follows. In section 2, the solution of the time-dependent Schrödinger equation is given for a particle which is initially confined in a box. Section 3 contains a very brief review of relevant parts of Bohm's interpretation of quantum mechanics. Section 4 gives numerical results. Finally, in section 5 we present the concluding remarks.

## 2. Free propagation of a particle initially confined in an square well

Consider a particle which is initially confined in an interval $[0, L]$ with wavefunction $\psi_0(x)$. If at time $t = 0$ it is free, then at any instant $t > 0$ its wavefunction is given by

$$\psi(x,t) = \int_{-\infty}^{\infty} G(x,t|x',0)\psi_0(x')\,\mathrm{d}x', \tag{1}$$

in which $G(x,t|x',0)$ is the free particle propagator and is determined by

$$G(x,t|x',0) = \sqrt{\frac{m}{2\pi\mathrm{i}\hbar t}}\mathrm{e}^{\frac{\mathrm{i}m}{2\hbar t}(x-x')^2}, \tag{2}$$

and $\psi_0(x')$ is the initial wavefunction. In this work we take initial wavefunction to be (a) a stationary state of a particle inside a well with hard (perfect reflective) walls at $x = 0$ and $x = L$ and (b) a motionless localized Gaussian wave-packet in that region with negligible overlap with the walls of the well. To avoid any problem concerning the boundary conditions, one can suppose in this case that the walls act as absorbers or the tails of the wave-packet have been cut by the walls of the well. In the first case, initial wavefunction is given by $\psi_0(x) = \phi_n(x) = \sqrt{2/L}\sin(k_n x)\chi_{[0,L]}(x)$, with $k_n = n\pi/L$. $\chi_{[0,L]}(x) = \Theta(L-x) - \Theta(-x)$ is the characteristic function in the interval $[0, L]$. By removing both walls at time $t = 0$, the wavefunction [11, 12, 18] at any instant $t$ is given by

$$\begin{aligned}\psi_n(x,t) &= \sqrt{\frac{m}{2\pi\mathrm{i}\hbar t}}\sqrt{\frac{2}{L}}\int_0^L \mathrm{e}^{\frac{\mathrm{i}m}{2\hbar t}(x-x')^2}\sin(k_n x')\,\mathrm{d}x',\\ &= \sqrt{\frac{m}{4\pi\mathrm{i}^3\hbar t L}}\int_0^L \mathrm{e}^{\frac{\mathrm{i}m}{2\hbar t}(x-x')^2}(\mathrm{e}^{\mathrm{i}k_n x'} - \mathrm{e}^{-\mathrm{i}k_n x'})\,\mathrm{d}x',\\ &\equiv \psi_{n,+}(x,t) + \psi_{n,-}(x,t),\end{aligned} \tag{3}$$

which is a superposition of a right and a left movement diffracted in time plane waves. After doing some simple algebra, one gets

$$\psi_{n,+}(x,t) = \frac{1}{\sqrt{4\mathrm{i}^3 L}}\,\mathrm{e}^{\mathrm{i}k_n x - \mathrm{i}E_n t/\hbar}[F_n(x-L,t) - F_n(x,t)], \tag{4}$$

$$\psi_{n,-}(x,t) = \frac{1}{\sqrt{4\mathrm{i}^3 L}}\,\mathrm{e}^{-\mathrm{i}k_n x - \mathrm{i}E_n t/\hbar}[F_n(L-x,t) - F_n(-x,t)], \tag{5}$$

with $E_n = \hbar^2 k_n^2 \big/ 2m$ and

$$F_n(x,t) = \int_0^{\xi_n(x,t)} \mathrm{d}u\,\mathrm{e}^{\mathrm{i}\pi u^2/2}, \tag{6}$$

with upper limit $\xi_n(x,t) = \sqrt{\frac{m}{\pi\hbar t}}\,(v_n t - x)$ in which $v_n = \hbar k_n/m$. Let us, for later use, compute the derivative of $\psi_n(x,t)$ with respect to $x$:

$$\frac{\partial\psi_{n,+}(x,t)}{\partial x} = \mathrm{i}k_n\psi_{n,+}(x,t) + \mathrm{e}^{\mathrm{i}k_n x - \mathrm{i}E_n t/\hbar}\left[\frac{\partial F_n(x-L,t)}{\partial x} - \frac{\partial F_n(x,t)}{\partial x}\right], \tag{7}$$

$$\frac{\partial\psi_{n,-}(x,t)}{\partial x} = -\mathrm{i}k_n\psi_{n,-}(x,t) + \mathrm{e}^{-\mathrm{i}k_n x - \mathrm{i}E_n t/\hbar}\left[\frac{\partial F_n(L-x,t)}{\partial x} - \frac{\partial F_n(-x,t)}{\partial x}\right], \tag{8}$$

in which

$$\frac{\partial F_n(x,t)}{\partial x} = -\sqrt{\frac{m}{\pi\hbar t}}\,\mathrm{e}^{\frac{\mathrm{i}\pi\xi_n^2(x,t)}{2}}. \tag{9}$$

Now, by some straightforward algebra, one can show that

$$\left.\frac{\partial\psi_n}{\partial x}\right|_{x=L/2} = 2\,\mathrm{e}^{-\mathrm{i}E_n t/\hbar}\cos(k_n L/2)\Bigg([F_n(-L/2,t) - F_n(L/2,t)] + \sqrt{\frac{m}{\pi\hbar t}}\big[\mathrm{e}^{\frac{\mathrm{i}\pi\xi_n^2(L/2,t)}{2}} - \mathrm{e}^{\frac{i\pi\xi_n^2(-L/2,t)}{2}}\big]\Bigg), \tag{10}$$

which is zero for odd $n$. Note that one can find this without doing any algebra. Wavefunction is an even (odd) function for odd (even) $n$ with respect to the point $x = L/2$, so its derivative is an odd (even) function for odd (even) $n$ with respect to that point.

In the second case $\psi_0(x) = \frac{1}{(2\pi\sigma_0^2)^{1/4}}\,\mathrm{e}^{-\frac{(x-x_0)^2}{4\sigma_0^2}}\,\chi_{[0,L]}(x)$, in which $x_0$ is the center of the packet and $\sigma_0$ is its rms width, $\sigma_0 = \langle x^2\rangle_0 - \langle x\rangle_0^2$. After simultaneous removal of both walls, wavefunction is given by

$$\psi(x,t) = \frac{1}{\left(2\pi\sigma_0^2\right)^{1/4}}\sqrt{\frac{m}{2\pi\mathrm{i}\hbar t}}\int_0^L \mathrm{d}x'\,\mathrm{e}^{-\frac{(x'-x_0)^2}{4\sigma_0^2} + \frac{\mathrm{i}m}{2\hbar t}(x-x')^2}. \tag{11}$$

## 3. Bohmian trajectories

In nonrelativistic Bohmian mechanics the world is described by point-like particles which follow trajectories determined by a law of motion. The evolution of the positions of these particles is guided by a wavefunction which itself evolves according to the Schrödinger equation. Given the initial position $x^{(0)} \equiv x(t=0)$ of a particle with the initial wavefunction $\psi_0(x)$, its subsequent trajectory $x(x^{(0)},t)$ is uniquely determined by simultaneous integration of the time-dependent Schrödinger equation, and the guidance equation $\frac{\mathrm{d}x(t)}{\mathrm{d}t} = v(x(t),t)$, in which $v = \frac{j}{\rho}$, where $j = \frac{\hbar}{m}\Im\left(\psi^*\frac{\partial\psi}{\partial x}\right)$ is the probability current density and $\rho = |\psi(x,t)|^2$

is the probability density. In the context of Bohmian mechanics arrival time distribution at a given location, say $x = X$, is given by [20–22]

$$\Pi_X(\tau) = \frac{|j(X,\tau)|}{\int_0^\infty \mathrm{d}t\,|j(X,t)|}. \tag{12}$$

So, mean arrival time at observation point $x = X$ is determined by

$$\tau(X) = \int_0^\infty \mathrm{d}t\, t\,\Pi_X(t). \tag{13}$$

A general formulation for Bohmian arrival times was given in [23] and a formula for the numerical calculation of such Bohmian arrival times in the case of 1D rigid inertial detectors (exactly the cases we have here) was presented in [24]. The derived formula in [24] does not require the explicit calculation of the Bohmian trajectories and the resulting 'cut-off current' can be considered to be a generalization of the arrival time probability density introduced by Leavens [20–22]. According to equation (12) of [24], the probability density $\Pi_X(\tau)$ of the arrival time distribution for a point detector at $x = X$ takes the form

$$\begin{aligned}\Pi_X(\tau) = \left(\lim_{t\to\infty} P(t)\right)^{-1} & j(X,\tau)[\Theta(f_X(\tau) - \max\{f_X(s)/0 \leqslant s \leqslant \tau\}) \\ & - \Theta(-f_X(\tau) - \max\{-f_X(s)/0 \leqslant s \leqslant \tau\})],\end{aligned} \tag{14}$$

in which $P$ is the detection probability,

$$P(t) = \max\{f_X(s)/0 \leqslant s \leqslant t\} + \max\{-f_X(s)/0 \leqslant s \leqslant t\}, \tag{15}$$

with

$$f_X(s) = \int_0^s j(X,t)\,\mathrm{d}t. \tag{16}$$

For the case of positive or negative $j(X,t)$ equation (14) reduces to equation (12).

## 4. Numerical results

For numerical calculation, the width of the well is chosen as $L = 1\ \mu$m. All of the calculations are presented for Rubidium atoms with mass $m = 1.42 \times 10^{-25}$ kg. Figure 1 shows probability density versus distance $x(\mu\mathrm{m})$ for state $n = 6$ at different times. At longer times there are two spatial packets placed about the box and moving apart. As pointed out by del Campo and Muga [12], this takes place after the semiclassical time $t_n = mL^2/2n\pi\hbar$ as a result of the mapping of the underlying momentum distribution to the density profile expected asymptotically. For our parameters $t_n = (0.214/n)$, hence, $t_7 = 0.031$ ms and $t_{500} = 4.28 \times 10^{-4}$ ms. Figure 2 shows probability current density as a function of time at observation point $x = 2\ \mu$m outside the box after removal of the walls for various stationary states. From equation (3) it is obvious that $x = L/2$ remains a node of the wavefunction for even $n$, i.e. $\psi_n(x = L/2, t) = 0$ for even $n$. Since the property of Bohmian paths is well-known, we know that the Bohmian particle cannot be initially located at $x = L/2$ or even pass through this point for even values of $n$. As mentioned above, right after equation (10), for odd $n$ the distance derivative of the wavefunction is zero at point $x = L/2$. Thus, the current probability density and consequently the Bohmian velocity are zero at this point all the time. Therefore, a Bohmian particle, which is initially at $x^{(0)} = L/2$, will remain at rest. Because of the noncrossing property of Bohmian path, particles with $x^{(0)} < L/2$ ($x^{(0)} > L/2$) will go backward (forward), see figure 3. We have used the Runge–Kutta method for the simultaneous integration of the time-dependent Schödinger equation and the guidance law to compute Bohmian trajectories. For $n = 7$, after

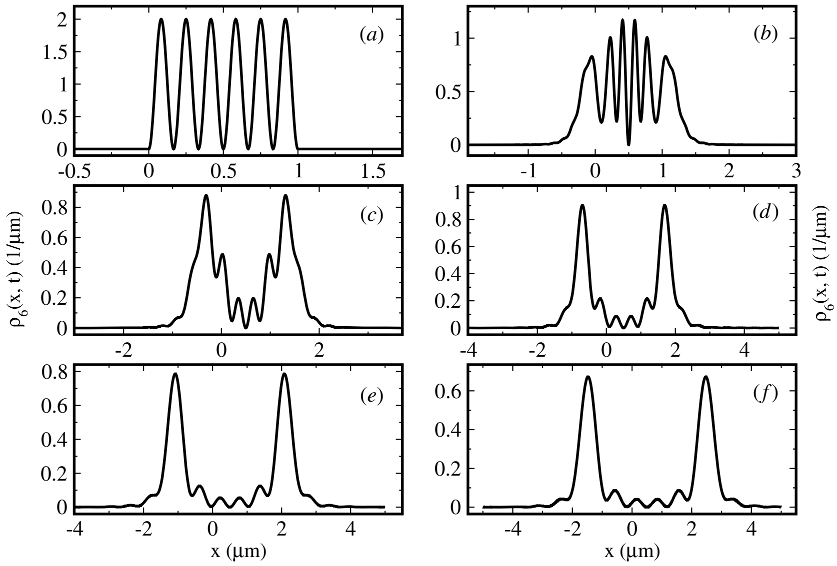


**Figure 1.** Probability density versus distance $x(\mu\text{m})$ for state $n = 6$ at times $(a)$ $t = 0$, $(b)$ $t = 0.03$ ms, $(c)$ $t = 0.06$ ms, $(d)$ $t = 0.09$ ms, $(e)$ $t = 0.12$ ms and $(f)$ $t = 0.15$ ms.

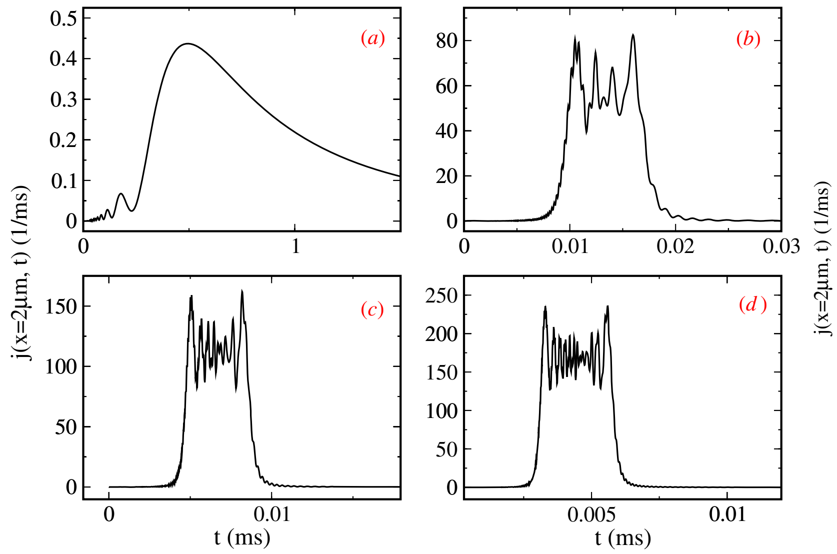


**Figure 2.** Probability current density (1 $\text{ms}^{-1}$) as a function of time $t$ (ms) at observation point $x = 2\,\mu$m for states $(a)$ $n = 1$, $(b)$ $n = 50$, $(c)$ $n = 100$ and $(d)$ $n = 150$.

$t = 0.03$ ms trajectories exhibit a bifurcation into two main branches while for $n = 500$ this takes place after $t = 0.0004$ ms. These values coincide very well with $t_7$ and $t_{500}$ in the above. Figure 4 shows the mean arrival time, in the context of Bohmian mechanics, as a function of quantum number $n$ at the observation point $x = 2\,\mu$m. It is clear that $\tau$ decreases with $n$ as one expects, because by growing $n$, semiclassical velocity increases.

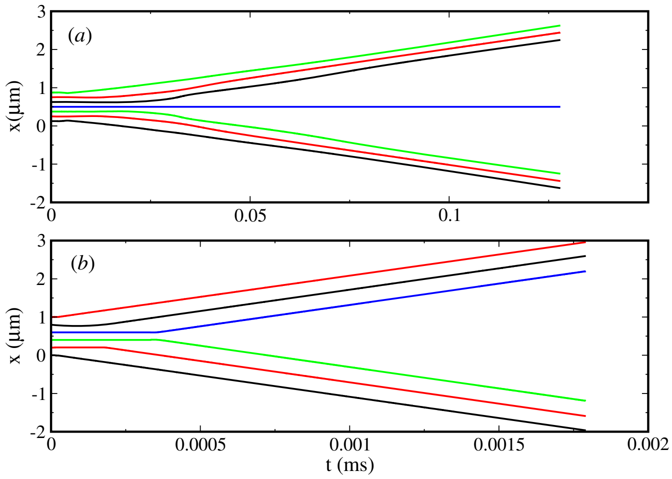


**Figure 3.** A selection of Bohmian paths for states (*a*) $n = 7$ and (*b*) $n = 500$.

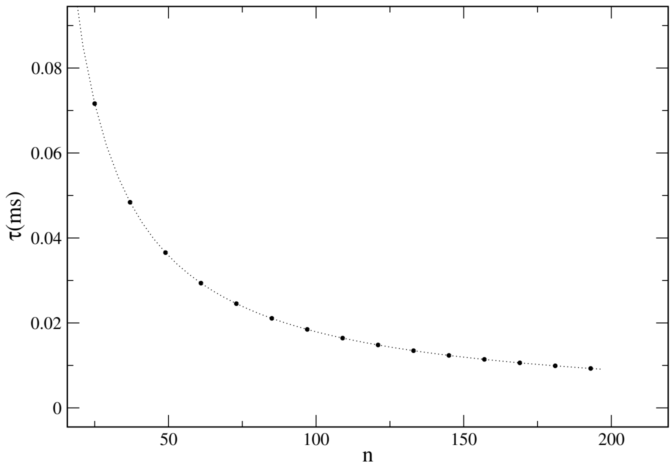


**Figure 4.** Mean arrival time at detector position $x = 2\,\mu$m for different states.

In the case of a Gaussian packet, parameters of the packet are chosen as $x_0 = 0.5\,\mu$m and $\sigma_0 = 0.25\,\mu$m. It should be noted that with these parameters, the initial Gaussian packet is not normalized to unity but to 0.954 543 (truncated Gaussian packet). If someone chooses the initial packet narrower than ours, in such a way that it locates totally inside the well, then after removing the walls its evolution will be the same as that of a free Gaussian packet which is not desired here. To show the differences we consider a free Gaussian packet with the same parameters as well. Figure 5 shows the probability density versus distance, 0.1 ms after removal of the walls and the probability current density at observation point $x = 2\,\mu$m as a function of time for a free and a confined truncated Gaussian packet. In the confined case one sees some oscillations in the plot of current density which are absent in the free case. Finally, figure 6 shows a selection of Bohmian paths for both cases. In the free case, trajectories are

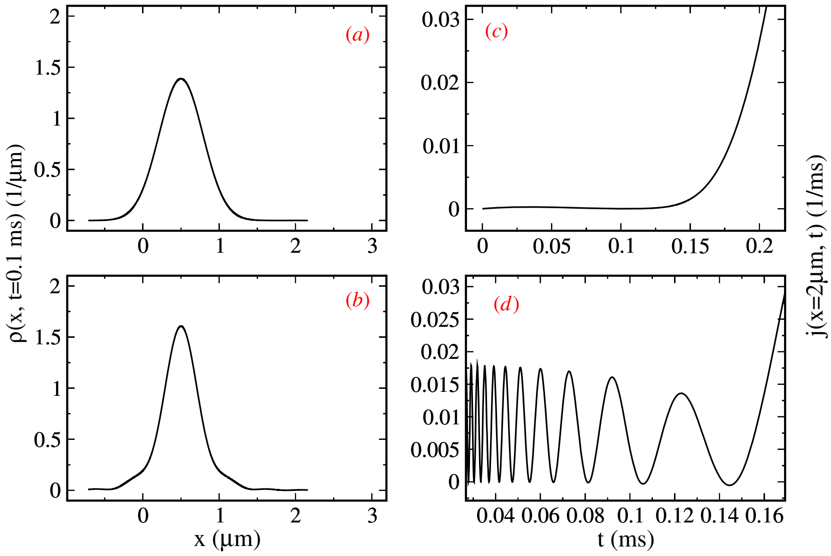


**Figure 5.** Probability density (1 $\mu$m$^{-1}$) versus distance $x(\mu\text{m})$ at time $t = 0.1$ ms for (*a*) a free motionless Gaussian wave-packet and (*c*) a motionless truncated Gaussian wave-packet initially confined in a box. Probability current density (1 ms$^{-1}$) versus time $t$ (ms) at observation point $x = 2\ \mu$m for (*b*) a free motionless Gaussian wave-packet and (*d*) a motionless truncated Gaussian wave-packet initially confined in a box.

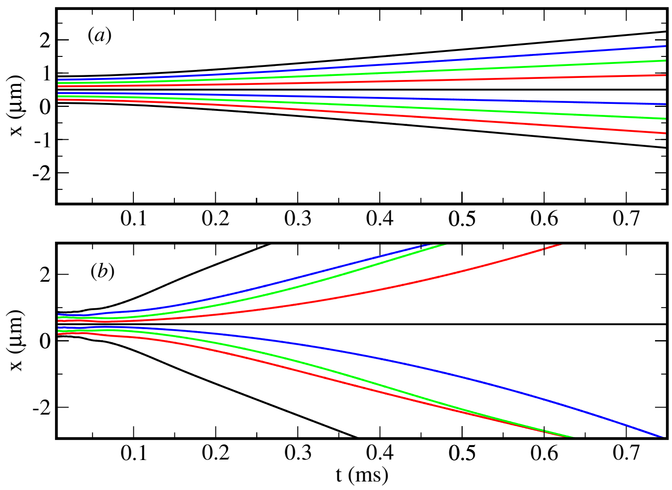


**Figure 6.** A selection of Bohmian paths for (*a*) a free motionless Gaussian wave-packet and (*b*) a motionless truncated Gaussian wave-packet initially confined in a box.

determined by $x(t) = x_0 + (x^{(0)} - x_0)\sqrt{1 + \left(\hbar t/2m\sigma_0^2\right)^2}$, where $x^{(0)}$ is the initial position of the particle [18]. From the figure it follows that the trajectory which starts at $x^{(0)} = x_0$ is the bifurcation trajectory in both cases and Bohmian velocity of a path in confined case is larger than the Bohmian velocity of the corresponding path in the free case.

## 5. Summary and conclusion

The dynamics of particles, with various initial wavefunction, released from a box has been studied. Different boundary conditions, the absorbing wall and the reflecting one, are considered. Such studies suggest that the time-varying boundary conditions can give rise to the interesting action-at-a-distance effects in quantum mechanics. Quantum temporal oscillations of matter waves released from a confinement region constitute the hallmark of the diffraction in time effect. The mean arrival time at an observation point outside the box has been considered for various initial states. Moreover, Bohmian paths of the particle are computed. Our calculated mean arrival time may have no relevance to the experiment. Within Bohm's causal theory of quantum mechanics if we try to measure properties other than *position* (the only intrinsic property), we find that the result is affected by the process of interaction in a way that depends, not only on the total wavefunction, but also on the details of the initial conditions of both the particle and the apparatus. Our calculations can be verified if mean arrival times can be experimentally measured in such a way that the experiment does not perturb the unmeasured quantity.

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