

# ARRIVAL TIMES OF QUANTUM WAVE PACKETS

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## CERTIFICATE FROM THE SUPERVISOR

This is to certify that the thesis entitled **Arrival Times of Quantum Wave Packets** submitted by **Md. Manirul Ali**, who got his name registered on **June 25, 2004** for the award of **Ph.D. (Science) degree** of **Jadavpur University**, is absolutely based upon his own work under the supervision of **Dr. Archan S. Majumdar** at **S. N. Bose National Centre For Basic Sciences, Kolkata, India** and that neither this thesis nor any part of it has been submitted for any degree/diploma or any other academic award anywhere before.

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## Chapter 1

### Introduction

#### 1.1 Time in Quantum Theory

In his famous 1913 paper Bohr [1] suggested that the interaction of radiation and atoms occurred by means of instantaneous transitions, “quantum jumps”, among the allowed atomic orbits. The jumps were accompanied by the absorption or emission of radiation, whose frequency corresponded to the energy difference of the stationary orbits,  $\nu = \Delta E/h$ . However, no mechanism for the *timing* of these transitions was provided. Soon Rutherford pointed out to Bohr that this was a “grave difficulty” of his theory, and Slater noted a contradiction between the assumed instantaneous character of the jumps and the observed narrow widths of the spectral lines. Heisenberg tried to solve the problems of the old quantum theory by creating a discontinuous matrix mechanics, in which visualizable models based on a space-time continuum, in particular the orbits, would be eliminated. However, the timing of events did not quite fit in this scheme, as evidenced by a letter from Pauli [2] to Bohr in 1925

*“In the new theory, all physically observable quantities still don’t really occur. Absent, namely, are the time instants of transition processes, which are certainly in principle observable (as for example, are the instants of the emission of photoelectrons)”*.

He also speculated that perhaps time could be defined through the concept of energy, and asked the meaning of a time duration. Heisenberg<sup>1</sup> answered a few days later [4]:

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<sup>1</sup>Heisenberg, in a letter to Einstein, wondered if the times of transition should be regarded as observable or not [3].

*“Your problem of “durarion” plays a fundamental role,...When, as in the new theory, a point in space has no longer a fixed place, or when this place is still only defined formally and symbolically, then the same is true also of the time-point of an event. But there is always given a rough duration, as also a rough place in space: with our geometric picture we shall still be able to achieve a rough picture of the phenomena”.*<sup>2</sup>

Heisenberg’s words reflect some aspects of his uncertainty paper. However, things were not quite matured at that stage. The original agenda of matrix theorists was quite radical; they doubted that the “position of the electron in time” could be given any meaning. However, reacting to the success of the visualizable and continuous wave mechanics of *Schrödinger*, matrix theorists retreated eventually from the extreme original program. Even though *Schrödinger* had shown the formal equivalence between matrix and wave mechanics for bound systems, an interpretational war began, and the two approaches were for a while competing, each claiming a superior or more fundamental status. Born’s aim in his two 1926 collision papers was to harmonize the jumps and the wave picture [6, 7]. For an electron-atom collision he interpreted the squared modulus of the stationary wave function coefficients at infinite distances as probabilities for the electron “to be thrown” into a given direction for a given atomic state. The theory would therefore not provide the actual state of the atom after the collision, but rather the probability of a certain event, identified by Born as a quantum jump. In this description, however, the wave function considered was stationary, so the question of the timing of the event was not really addressed. Pauli expressed his doubts about the role of time in his first Encyclopedia article [8] and emphasized that Einstein’s probabilistic treatment of absorption and emission was mute about the times of transition. Did this fact indicate a fundamental restriction, or was it due to the incompleteness of the theory? *“This is very much debated, yet still an unsolved issue”*, he concluded. He also insisted on the problem of the duration of the jump, suggesting that perhaps the precision limit of the time of transition was of the same order of magnitude as the period of the light emitted, but admitted that he could not offer a more precise analysis. Heisenberg [9] in his famous 1927 paper mentioned *“...the time of transitions or “quantum jump” must be as concrete and determinable by measurement as,*

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<sup>2</sup>The main source for this section is a recent book edited by J.G. Muga, I.L. Egusquiza and R. Sala Mayato [5].

say, *energies in stationary states.*” The duration question is still being studied nowadays [10].

An important landmark in the history of time in quantum mechanics is a footnote of Pauli’s second Encyclopedia article of 1933 [11], re-edited with minor changes in 1958 [12], in which the argument runs as follows: If there existed a self-adjoint time operator  $\hat{T}$  canonically conjugate to the Hamiltonian,  $[\hat{H}, \hat{T}] = i\hbar$ , the application of the unitary operator  $\exp(-iE_1\hat{T}/\hbar)$  to the energy eigenstate  $|E\rangle$  would produce a new energy eigenstate with energy eigenvalue  $E - E_1$ , so that the spectrum of  $E$  would necessarily extend continuously over the range  $[-\infty, \infty]$ . In principle this precludes the existence of a self-adjoint time operator for systems where the spectrum of the Hamiltonian is bounded, semibounded, i.e., for most of the systems of physical interest [11]-[17]. Pauli’s conclusion was that “...*the introduction of an operator  $\hat{T}$  must fundamentally be abandoned...*”. One year before Pauli’s article, von Neumann had published his “Mathematical Foundations of Quantum Mechanics” [18] where he pinpoints as the “chief weakness of quantum mechanics” its non-relativistic character, which distinguishes  $t$  (without a corresponding operator) from the three space coordinates  $x, y, z$  represented by operators. Until the fifties there had been no substantial change in the foundations of quantum theory, and the Copenhagen interpretation was rather well founded and accepted according to which events, or facts, within quantum theory would occur through discontinuous jumps which are *not* contained in the quantum equations and obviously, if they are not contained in the quantum equations, how can we predict the time distributions for these events? This lack of an explicit description of events has been considered by some physicists as a major problem of the theory. Some have tried to modify or re-interpret quantum mechanics to include events and/or discontinuous jumps explicitly. The Bohmian model of quantum mechanics [19] in terms of the causal trajectories of individual particles was a major step along that direction.

## 1.2 Time as an observable

One of the first lessons of quantum mechanics was that a property of a system does not correspond to an element of reality until it is measured. It makes no sense to talk about

the position of a particle or the momentum of the particle, in and of itself. It is only when we measure a physical quantity that we can actually say that a system possesses it. The particle does not have a position until its position is actually measured.

Ordinarily in quantum mechanics, one is interested in measuring properties of a system at a particular time  $t$ . One might want to know a particle's position, momentum, or spin and the measurement of this quantity occurs at a certain time. For experiments at a fixed time, quantum mechanics provides us with a useful formalism to describe reality. Observables are represented by self-adjoint operators, and in the Heisenberg representation they evolve in time. The possible results of any measurement and expectation values at any instant of time  $t$  can be found by applying these operators to the wave function of the system at that time. This immediately raises the question of what the parameter time  $t$  represents in the Heisenberg equations of motion. Since  $t$  is a number and not a self-adjoint operator, it does not appear to be an observable in the usual sense. For any measurement of an observable  $\mathbf{A}(t)$  of a system, one can imagine a measurement, where one attempts to measure the time  $t_A$  at which the system attains a particular value of  $\mathbf{A}$ . In other words this measurement determines the time at which a certain event occurs, where the event in question is the system attaining a particular value (or values) of an observable. For example, instead of measuring the position of a particle at a certain time, one can consider the measurement where the roles of  $x$  and  $t$  are interchanged. Instead of measuring where the particle is at time  $t$ , one measures the time that a particle is found at a particular location  $x_A$ . In this kind of measurement, the position  $x_A$  is the parameter while the time becomes the observable one. This kind of measurements are quite common in modern laboratory experiments. However, surprisingly, this kind of time measurements are not easily dealt with using the conventional tools of quantum mechanics. In contrast to the difficulties found for a consistent theoretical treatment of the arrival time, many experimental techniques measure "arrival time" or "times of flight". In particle physics one often wants to know the time at which certain collisions or decays occurred. The standard interpretation of these "times of flight" experiments is purely classical.

### 1.3 Nonexistence of a time operator in quantum mechanics

In spite of the emphasis of quantum mechanics on the concept of “observable”, formalization of time observables is still an open and challenging fundamental question. The role that time plays in quantum mechanics has always been controversial. This is in part a consequence of the rather singular status that time exhibits in nonrelativistic physics. In particular, time enters the Schrödinger equation as an external parameter and, accordingly, the quantum formalism is usually concerned with probability distributions of measurable quantities at a definite instant of time. However, one may also ask for the instant of time at which a certain property of a quantum system takes a given value. In this case time has the character of a dynamical variable: It depends on the initial state of the system and on its dynamical evolution, and appears as an intrinsic property of the physical system under study. Since such an instant of time is, in principle, a perfectly measurable quantity it seems natural to try to incorporate the concept of a time observable into the quantum formalism.

However, this is not an easy task. The standard quantum formalism associates measurable quantities with self-adjoint operators acting on the Hilbert space of physical states, and postulates that the probability distribution of the outcomes of any well-designed measuring apparatus can be obtained in terms of the orthogonal spectral decomposition of the corresponding self-adjoint operator, with no explicit dependence on the particular properties of the measuring device. Let us concentrate on the problem of finding a suitable time operator which is usually accomplished via the correspondence principle, starting from the corresponding classical expressions and quantizing by using certain specific quantization rules.

Given the Hamiltonian  $H(q, p)$  of a conservative classical system, expressed in terms of canonical variables  $(q, p)$ , one can always make a canonical transformation to new canonical variables  $(H, T)$ , where  $H$  is the Hamiltonian of the system and  $T$  its conjugate variable, which satisfies Hamilton’s equation[20, 21]

$$\frac{dT}{dt} = \{H, T\} = 1 \quad (1.1)$$

$\{H, T\}$  denoting the Poisson bracket of  $H$  and  $T$ . The important point is that the above equation clearly reflects that the canonical variable  $T$  is nothing but the interval of time.

Thus the next step would be to take advantage of this desirable fact and translate the above formulation to the quantum framework. This can be easily accomplished by means of the *canonical quantization method* [22], which basically states that the classical formulation remains formally valid in the quantum domain with the substitution of Poisson brackets by commutators,  $\{H, T\} \rightarrow 1/i\hbar[\hat{H}, \hat{T}]$ , and interpreting the dynamical variables as self-adjoint operators in the Heisenberg picture. Then, based on the correspondence principle and the canonical quantization method, one is led to look for a self-adjoint time operator conjugate to the Hamiltonian,

$$[\hat{H}, \hat{T}] = i\hbar \quad (1.2)$$

As can be easily verified, this commutation relation also holds true in the Schrödinger picture, and has the additional desirable consequence that it implies the uncertainty relation

$$\Delta H \Delta T \geq 1/2|[\hat{H}, \hat{T}]| \quad (1.3)$$

with  $\Delta H$  and  $\Delta T$  being the usual root-mean-square deviations of the corresponding dynamical variables. Unfortunately no such time operator exists. As remarked by Pauli, the existence of a self-adjoint operator satisfying the above commutation relation is incompatible with the semibounded character of the Hamiltonian spectrum [11, 12].

The lack of a proper time observable has a number of consequences [23]. In particular, the time-energy uncertainty relation has remained unclear over the years. This is so basically because, contrary to what happens with the well-known position-momentum uncertainty relation, there exists no unique way to put in a quantitative setting what is really meant by the time spread  $\Delta T$ . In fact the consequences derived from incorrect application of the time-energy uncertainty relation have led to a great deal of confusion.

As stated earlier, according to Pauli's argument, because of the semibounded character of the energy spectrum, there exists no self-adjoint operator conjugate to the Hamiltonian, *i.e.*, satisfying the commutation relation (1.2). The same negative conclusion was found by Allcock [13] using a somewhat different argument based on the time-translation property of the arrival time concept.

If  $\{|T\rangle\}$  denotes a set of measurement eigenstates for the arrival time at a given spatial point of a particle in the quantum state  $|\psi\rangle$ , then, according to the standard quantum

formalism, the probability amplitude for the arrival time at the instant  $t = T$  would be given by  $\psi(T) = \langle T|\psi\rangle$ . If one translates the state of the system forward through time by an amount  $\tau$ , *i.e.*,  $|\psi\rangle \rightarrow |\psi'\rangle = \exp(-i\hat{H}\tau/\hbar)|\psi\rangle$ , then it seems natural to expect the probability amplitude to transform according to  $\psi(T) \rightarrow \psi'(T) = \psi(T + \tau)$ . That is,

$$\langle T|\psi'\rangle = \langle T + \tau|\psi\rangle \quad \text{or} \quad (1.4)$$

$$\langle T|\exp(-i\hat{H}\tau/\hbar)|\psi\rangle = \langle T + \tau|\psi\rangle \quad (1.5)$$

Since this transformation property must be true for any state vector  $|\psi\rangle$ , it follows that the measurement eigenstates  $\{|T\rangle\}$  must satisfy

$$|T + \tau\rangle = e^{i\hat{H}\tau/\hbar}|T\rangle \quad (1.6)$$

which reflects the fact that, under a translation backward in time by an amount  $\tau$ , any measurement eigenstate corresponding to arrival time at the instant  $t = T$  transforms into another measurement eigenstate, corresponding to an arrival time  $t = T + \tau$ . Based on general grounds, Allcock showed that measurement eigenstates with such a desirable property cannot be orthogonal, which implies that it is not possible to construct the corresponding self-adjoint arrival-time operator. It is not difficult to see that this negative conclusion can be traced back again to the semi-infinite nature of the Hamiltonian spectrum. To this end one can consider the following three statements [15].

(i) There exists a self-adjoint operator  $\hat{T}$  conjugate to the Hamiltonian  $\hat{H}$ , *i.e.*, satisfying  $[\hat{H}, \hat{T}] = i\hbar$ .

(ii) There exists a self-adjoint operator  $\hat{T}$ , whose (orthonormal and complete) set of eigenstates  $\{|T\rangle\}$  transforms under time-translations as  $e^{i\hat{H}\tau/\hbar}|T\rangle = |T + \tau\rangle$ .

(iii) There exists a self-adjoint operator  $\hat{T}$  which generates unitary energy translations, *i.e.*, such that for any energy eigenstate  $|E\rangle$  and any parameter  $\varepsilon$  with dimensions of energy, it holds that

$$e^{i\hat{T}\varepsilon/\hbar}|E\rangle = |E - \varepsilon\rangle, \quad (1.7)$$

where the operator  $\hat{T}$  is assumed to be defined onto the whole Hilbert space spanned by the Hamiltonian eigenstates. It is not difficult to see that these statements are in fact equivalent. Indeed, if (i) is true, then, by induction, one has

$$[\hat{H}^n, \hat{T}] = in\hbar\hat{H}^{n-1}, \quad n \geq 1, \quad (1.8)$$

where  $\hat{H}^0 \equiv \mathbf{1}$ . Of course the validity of Eq.(1.8) rests on the reasonable assumption that the Hamiltonian is well behaved enough so as to guarantee the existence of all its higher integer powers. Since it also holds that  $[\hat{H}^n, \hat{T}] = 0$  for  $n = 0$ , then, multiplying Eq.(1.8) by  $(i\tau/\hbar)^n/n!$  ( $\tau$  being an arbitrary parameter with dimension of time) and summing from  $n = 0$  to  $n = \infty$ , one finds

$$[e^{i\hat{H}\tau/\hbar}, \hat{T}] = -\tau e^{i\hat{H}\tau/\hbar}. \quad (1.9)$$

If  $\{|T\rangle\}$  denotes a complete and orthonormal set of eigenstates of  $\hat{T}$ , then, according to Eq.(1.9), it holds that

$$\hat{T}e^{i\hat{H}\tau/\hbar}|T\rangle = (T + \tau)e^{i\hat{H}\tau/\hbar}|T\rangle, \quad (1.10)$$

which after suitable choice of normalization and phase leads to statement (ii). Conversely, if (ii) is true for any eigenstate  $|T\rangle$  and any parameter  $\tau$ , then one can repeat the same steps backward to reach (i). On the other hand, it can be readily seen that statement (i) also implies statement (iii). Indeed, if (i) holds, one has by induction that

$$[\hat{H}, \hat{T}^n] = in\hbar\hat{T}^{n-1}, \quad n \geq 0, \quad (1.11)$$

where  $\hat{T}^0 \equiv \mathbf{1}$ , which implies that, for any parameter  $\varepsilon$  with dimensions of energy,

$$[\hat{H}, e^{i\hat{T}\varepsilon/\hbar}] = -\varepsilon e^{i\hat{T}\varepsilon/\hbar}. \quad (1.12)$$

Therefore, according to Eq.(1.12) any energy eigenstate  $|E\rangle$  will satisfy

$$\hat{H}e^{i\hat{T}\varepsilon/\hbar}|E\rangle = (E - \varepsilon)e^{i\hat{T}\varepsilon/\hbar}|E\rangle, \quad (1.13)$$

from which after proper normalization follows (iii). An analogous reasoning can be repeated from (iii) to (i), which shows the equivalence among the above three statements. Now, since (iii) is obviously incompatible with a semibounded Hamiltonian spectrum, it follows that it is not possible to find a self-adjoint arrival time operator satisfying the desirable conditions (i) or (ii).

## 1.4 Towards a probability distribution of arrival time

In recent years there has been an upsurge of interest in understanding theoretically the concept of tunneling times, decay times, dwell times, delay times, arrival times or jump times and also in measuring these time quantities in quantum theory. The simplest problem involving time as a dynamical variable is that concerned with the time of arrival of a free particle at a given spatial point. Consider the following experimental arrangement. A particle moves in one dimension, along the  $x$  axis. A detector is placed in the position  $x = X$ . Let  $T$  be the time at which the particle is detected, which we denote as the “time of arrival” of the particle at  $X$ . Can we predict  $T$  from the knowledge of the initial state of the particle ?

In classical mechanics, the answer is simple. Let  $x(t; x_0, p_0)$  be the general solution of the equations of motion corresponding to initial position and momentum  $x_0$  and  $p_0$  at  $t = 0$ . We obtain the time of arrival  $T$  as follows. We invert the function  $x = x(t; x_0, p_0)$  with respect to  $t$ , obtaining the function  $t(x; x_0, p_0)$ . The time of arrival  $T$  at  $X$  of a particle with initial data  $x_0$  and  $p_0$  is then  $T = t(X; x_0, p_0)$

In quantum mechanics, the problem is harder where the state of the centre of mass-motion of an elementary particle (say, a neutron, or of a composite atom) does not in general specify its position precisely but rather a probability distribution for finding it at any particular point in space. In the same vein, one might expect from theory not a prediction of a precise arrival time but rather a distribution of measured arrival times given only the state in which the particle was prepared. More precisely, let  $\Pi(T)dT$  be the probability that the particle is detected at detector location  $X$  within the time interval  $T$  and  $T + dT$ . Thus  $\int_{T_1}^{T_2} \Pi(T)dT$  is the probability that the particle is detected between the time  $T_1$  and the time  $T_2$ . How can we compute  $\Pi(T)$  from the quantum state, e.g., from the particle’s wave function  $\psi(x)$  at  $t = 0$  ? This is not just an academic question because the arrival time is a perfectly measurable quantity whose probability distribution can, in principle, be experimentally measured by simply placing a detector at a fixed position and noting the time at which it “clicks”. Nevertheless, the objective to find a proper arrival time distribution  $\Pi(T)$  within the framework of quantum mechanics has been carried out only partially since the different distributions proposed are still subject

to discussion, interpretation, and controversy, even for this simplest one dimensional, free motion case.

There are claims that the arrival time of a quantum particle cannot be precisely measured and that theory is unable to define consistently such a quantity. One of the first objections was obviously due to Pauli, who stated that there cannot be a self-adjoint time operator conjugate to a Hamiltonian bounded from below. Despite this, many researchers have evidently not been discouraged from seeking an expression for the arrival time distribution within a consistent theoretical framework. Transit, passage, or arrival times have been invoked sporadically, usually in vague terms, since the early days of quantum mechanics (e.g. by Bohr in his discussion in Como in 1927 of the time-energy uncertainty principle [24]). An important milestone in the theoretical investigation of the time of arrival in quantum mechanics was the publication of three thorough papers by Allcock in 1969 [13]. He was apparently the first to pay specific attention to the arrival time rather than the more abstract question of finding time operators conjugate to the Hamiltonian, which had already been discussed in earlier works, in particular in [11, 12, 23], frequently in connection with the uncertainty principle. Although Allcock managed to elude Pauli's theorem by considering a quantum particle emitted by a source and hence described by positive and negative energy components, he ultimately concluded that wave mechanics cannot accommodate an exact and ideal (apparatus independent) arrival time concept. After the publication of Allcock's papers Razavi attempted to circumvent the difficulties by looking at self-adjoint functions of time rather than the time operator itself [25], and Wigner stated without detailed discussions, in a footnote of a paper on time-energy uncertainty [26], that he did not share Allcock's pessimism. A key result was due to Kijowski [27] in 1974, who, instead of starting with the time operator, introduced an arrival-time distribution by imposing a number of conditions motivated by the classical mechanical case. This work was re-examined by Werner [28] in the light of a theory of "ideal screen observables" that emphasizes the covariance of the distribution under time translations and overcomes Pauli's objection by admitting non-self-adjoint operators in the framework of positive operator valued measures (POVMs). One of the earlier attempts to define a time-of-arrival operator was due to Aharonov and Bohm [23] from which one can derive the Kijowski's distribution. The relation to time observables and

POVMs was also discussed by Holevo [29]. On the other hand, the discussion of Misra and Sudarshan of the quantum Zeno effect [30], and the “consistent histories” analyses of Yamada and Takaji [31] supported the pessimistic conclusion of Allcock. In the last ten years there has been considerable increase of activity that can be divided into theories based on renewal equations [32], trajectory models [33, 34], measurement models (toy models [14, 35], absorber models [36, 37], models of decoherence [38]), and construction of time operators or POVMs [15, 16, 39] related with Kijowski’s distribution. A common theme is that classical mechanics, deterministic or stochastic, is always a fundamental reference on which all of these approaches are based.

What are the difficulties and why is there such a variety of approaches ? First, a closer look at time variables reveals that they do not share all the properties of ordinary observables, even in classical mechanics [40]. For example, if at time ‘ $t$ ’ a particle is detected at location  $X$ , then we can say with certainty that at the same time ‘ $t$ ’, the particle was not at any other location  $X'$ . However, if we turn on a detector located at position ‘ $x$ ’, and detect a particle at time  $T$ , then it is quite possible that this particle might also have been detected at any number of other times  $T'$ . In classical deterministic dynamics, the continuous trajectory of a point particle moving in 1D intersects a given point either from one side or the other. This implies being instantaneously at a definite point with momentum of definite sign. But the quantum operators associated with these two concepts do not commute. Similarly, the probability to find a particle at  $t=T$  is generally not independent of the probability to find the particle at some other time  $t=T'$ , *i.e.*, the projectors for being in a region of space at different times do not commute [40, 41]. Actually these difficulties make the problem of arrival time more, not less interesting. The variety of approaches may reflect different quantum versions of the same classical question and it is of course important to determine which are relevant, and in what circumstances.

Having discussed the general status of time within the framework of quantum mechanics, and the difficulties encountered in treating time as an observable, we will henceforth concentrate on a particular approach towards studying the arrival time problem. There is no unique prescription to calculate the arrival time probability distribution in standard quantum theory. In this thesis we shall proceed by adopting the “probability current den-

sity approach” [33, 36, 42, 43]. An important goal of this thesis will be to throw some light on possible experimental manifestations of our investigations. This thesis contains mainly the theoretical study of the arrival time distribution and the time-dependent probability of arrival at particular locations for quantum wave packets evolving under different kinds of potentials. The important implications obtained from the dynamical evolution of the wave packets under these potentials are discussed.

The thesis is organised as follows. In Chapter2, we discuss the probability current density approach in calculating the arrival time distribution for free particles. The probability current is interpreted as the streamlines of conserved flux and has been used in the quantum mechanical predictions of arrival/transit time distributions. It can be shown that in the non-relativistic quantum mechanics the form of the probability current is *not unique* which leads an ambiguity [34] in the arrival time distribution. The probability current can be uniquely fixed if one starts from a relativistic quantum wave equation and finally this *uniqueness* will also be preserved in the non-relativistic limit of the relevant relativistic equation [43]. A novel spin dependent effect on the arrival time distribution for free particles is shown by demonstrating the uniqueness of the conserved probability current in the non-relativistic limit of Dirac equation. The mean arrival time is computed using the modulus of the unique (spin-dependent) probability current density for spin-1/2 free particles associated with a propagating Gaussian wave packet. This spin-dependent effect highlights the feature that the spin of a particle is an *intrinsic* property and is *not* contingent on the presence of an external field. We also discuss the possibility of an experimentally realizable scheme which can test any postulated quantum mechanical approach for calculating the arrival time distribution.

In Chapter3, we investigate the classical limit of arrival time defined through the probability current in the context of *classical limit problem* of quantum mechanics. Here for the purpose of illustration we consider the evolution of a quantum *free* particle represented by a Gaussian wave packet. We formulate the classical analogue of the arrival time distribution for an ensemble of *free* particles represented by a phase space distribution function evolving under the classical Liouville’s equation. The expression for classical probability current constructed by us matches exactly with the quantum probability current density *only* when the position and momentum spread of the classical phase space

distribution satisfy the minimum uncertainty condition. We note that the uncertainty condition is not a stringent requirement for the case of the initial classical distribution. Thus the classical arrival time distribution  $J_C(X, t)$  will in general be different from the quantum distribution  $J_Q(X, t)$  if we do not impose the minimum uncertainty restriction on the initial distribution. In the present example that we construct, the quantum results for the probability current and through it the arrival time distribution, approaches smoothly to the classical result in the large mass limit. Our outlook is concerned about an approach to test the quantitative equivalence between the classical statistical prediction and the prediction obtained in the macroscopic limit of quantum mechanics. What we see is that the *mean time* of arrival of a freely moving quantum particle computed through the probability current depends on the mass of the particle even if its group velocity is fixed. The predicted mass dependence of mean arrival time is, in principle, amenable for experimental verification, and is a clear signature of the probability current approach to time in quantum mechanics [33, 36, 42, 43].

In Chapter 4, we study the free fall of quantum *wave packets* under the gravitational potential. A gedanken quantum analogue of Galileo's leaning tower experiment is revisited. The position probability density and the arrival time distribution for the particle calculated through probability current density exhibits mass dependence. The observable position probability and the *mean time* (computed through the quantum probability current) taken by the freely falling particle to arrive at a particular location are also shown to be mass dependent. Our results of mass-dependence of these observable quantities indicate the manifest violation of a particular form of the quantum analogue of the weak equivalence principle [44]. The variation of the detection probability with mass disappears in the limit of large mass of the freely falling particles, as is expected for classical objects. This saturation of the detection probability is also reflected in the mean arrival time distribution defined through the quantum probability current, which approaches the classical result in a continuous manner with the increase of mass. We show that the compatibility of the weak equivalence principle with quantum mechanics can be achieved in the classical limit within this framework for particles falling freely under gravity. Our results re-emphasize that the probability current approach for computation of the mean arrival time of a quantum ensemble not only provides an unambiguous definition of ar-

rival time at the quantum mechanical level, but also addresses the issue of obtaining the proper classical limit of the time of flight of massive quantum particles. Subsequently, we discuss a classical statistical analogue of the same problem where we see a similar mass dependence in the position and arrival time distribution for a classical ensemble of particles described by a phase space distribution function which evolves according to the classical Liouville's equation.

In Chapter5 we discuss a new quantum mechanical effect which occurs in the time dependent reflection/transmission probabilities for a propagating Gaussian wave packet which encounters localised time-dependent rectangular potential barriers. We analyze the counter intuitive enhancement of probabilities that takes place as a result of barrier perturbation. By reducing the height of the barrier to zero in a short span of time during which there is a significant overlap of it with the wave packet, one sees that the reflection probability is larger compared to the case of reflection from a static barrier for a small but finite interval of time. Other cases of time dependent barriers with oscillating height and width can be considered to lead to superarrivals in the reflected as well as transmitted probabilities. We further show that in superarrivals for both the reflection and transmission case the wave function plays the role of a field or carrier through which information is transmitted. Information about barrier perturbation, or change in the boundary conditions, propagates across the wave function and then reaches the detector with a finite speed (signal velocity,  $v_e$ ) which is also proportional to the rate at which the barrier height is reduced. We find the magnitude of superarrivals to be proportional to the rate of reduction of the potential barrier. Next, we present a new manifestation of wave-particle duality in the context of the phenomenon of superarrivals where we argue that both classical wave-like and classical particle-like properties can be exhibited in the same gadenken experimental set-up for obtaining superarrivals through Schrödinger dynamics.

Up to Chapter5 we discuss several novel and interesting quantum effects. Two such effects that could be highlighted are the spin dependent contribution to the arrival time distribution of free particles, and the phenomenon of quantum superarrivals manifested in the reflection and transmission probabilities of wave packets scattered from time dependent potential barriers. The purpose of the Chapter6 is to obtain a clearer physical insight into these results by invoking the Bohmian interpretation of quantum theory [19].

It should be emphasized that though all our previous results are obtained within the standard framework of quantum mechanics, here we strive towards a sounder pedagogical footing in the context of Bohmian mechanics. This is especially true regarding the use of the probability current density in calculating the arrival time distribution, as we argue in section 6.2. Further, we see in section 6.3 that a clear understanding as to how superarrivals originate is obtained with the help of the quantum potential of the Bohm model. We compute the “particle trajectories” and derive a quantitative estimate of the magnitude of superarrivals using the Bohmian interpretation of quantum mechanics to have a deeper insight into the nature of superarrivals. A final summary of our work is presented in Chapter 7. Here we discuss the implications of our key results leading to insights for future directions of study.

## Chapter 2

# Probability current density as the arrival time distribution

We know from Born interpretation that the squared modulus of the wave functions  $|\psi(\mathbf{x}, t_1)|^2, |\psi(\mathbf{x}, t_2)|^2 \dots$  give the position probability distributions at different instants  $t_1, t_2 \dots$ . Now, the question that immediately arises is that if we fix the positions at  $\mathbf{x} = \mathbf{X}_1, \mathbf{X}_2 \dots$ , can the functions  $|\psi(\mathbf{X}_1, t)|^2, |\psi(\mathbf{X}_2, t)|^2 \dots$  give the time probability distributions at different positions  $\mathbf{X}_1, \mathbf{X}_2 \dots$ ? It is well known that if at any instant  $t = t_i$ ,  $\int_{-\infty}^{+\infty} |\psi(\mathbf{x}, t = t_i)|^2 d^3x = 1$ , the probability of finding the particle anywhere at that instant is unity. But if we fix the position at, say,  $\mathbf{x} = \mathbf{X}_1$  and  $t$  is varied, the value of the integral  $\int_0^{\infty} |\psi(\mathbf{x} = \mathbf{X}_1, t)|^2 dt \neq 1$ . In this case what may be pictured is that at a given point, say,  $\mathbf{X}_1$  the relevant probability changes with time and this change of probability is governed by the following continuity equation which suggests a “flow of probability”

$$\frac{\partial}{\partial t} |\psi(\mathbf{x}, t)|^2 + \nabla \cdot \mathbf{J}(\mathbf{x}, t) = 0 \quad (2.1)$$

where is the probability current density given by

$$\mathbf{J}(\mathbf{x}, t) = \frac{i\hbar}{2m} (\psi \nabla \psi^* - \psi^* \nabla \psi) \quad (2.2)$$

Here we adopt the definition of arrival time distribution in terms of the quantum probability current density  $\mathbf{J}(\mathbf{x} = \mathbf{X}, t)$ . Interpreting the equation of continuity in terms of the flow of physical probability, the Born interpretation for the squared modulus of the wave function and its time derivative suggest that the mean arrival time of the particles

reaching a detector located at  $\mathbf{X}$  may be written as

$$\bar{\tau} = \frac{\int_0^\infty |\mathbf{J}(\mathbf{x} = \mathbf{X}, t)| dt}{\int_0^\infty |\mathbf{J}(\mathbf{x} = \mathbf{X}, t)| dt} \quad (2.3)$$

However, we emphasize that the definition of the mean arrival time used in Eq.(2.3) is *not* a uniquely derivable result within standard quantum mechanics. It should also be noted that  $\mathbf{J}(\mathbf{x}, t)$  can be negative, hence one needs to take the modulus sign in order to use the above definition.

## 2.1 Ambiguity of arrival time distribution in quantum mechanics

Although the probability current density is interpreted as the streamlines of a conserved flux and has been used in the quantum mechanical predictions of time distributions [33, 36, 42, 43, 45] such as the arrival time, tunneling and reflection times, it is easily seen that in non-relativistic quantum mechanics the form of the probability current density is *not unique*, a point which has been explored by a number of authors [34, 46, 47]. If we replace  $\mathbf{J}$  by  $\mathbf{J}'$  in Eq.(2.1) where  $\mathbf{J}' = \mathbf{J} + \delta\mathbf{J}$ , with  $\nabla \cdot \delta\mathbf{J} = 0$ ,  $\mathbf{J}'$  satisfies the same probability conservation as given by Eq.(2.1). Then this new current density  $\mathbf{J}'$  will lead to a different distribution function for the arrival time [34]. Hence the arrival time distribution in Schrödinger dynamics is *not unique* and the question arises *how* one can uniquely fix the arrival time distribution via the quantum probability current in the regime of non-relativistic quantum mechanics ?

In order to address the above question, we take a vital clue from the interesting result Holland [48, 49] showed in the context of analysing the uniqueness of the Bohmian model of quantum mechanics, viz. that the Dirac equation implies a *unique* expression for the probability current density for spin 1/2 particles in the non-relativistic regime. In Section–2.2 we highlight the feature that the uniqueness of the probability current density is a *generic* consequence of *any* relativistic equation of quantum dynamics. In Section–2.3, the particular case of the spin dependent probability current density as derived from the Dirac equation is discussed. Subsequently, using the non-relativistic limit of the Dirac current density, we compute the effect of spin on the arrival time distribution of free

particles for an initial Gaussian wave packet.

## 2.2 Uniqueness of the probability current density for any relativistic wave equation

The probability current density obtained from *any* consistent relativistic quantum mechanical equation needs to satisfy a covariant form of the continuity equation of  $j^\mu$  where the zeroth component ( $j^0$ ) of  $j^\mu$  is associated with the position probability density. If one replaces  $j^\mu$  by  $\bar{j}^\mu$  which is also conserved, i.e.,  $\partial_\mu \bar{j}^\mu = 0$  where  $\bar{j}^\mu = j^\mu + a^\mu$  ( $a^\mu$  is an arbitrary divergenceless 4-vector), then the zeroth component ( $\bar{j}^0$ ) of  $\bar{j}^\mu$  will have to be the *same* as the position probability density given by  $j^0$ . Hence it follows that  $a^0 = 0$ . Next, we consider this current as seen from another Lorentz frame. This is given by  $\bar{j}^{\mu'} = j^{\mu'} + a^{\mu'}$ . Hence in this frame  $\bar{j}^{0'} = j^0 + a^{0'}$ , and again if the position probability density has to remain *unchanged*, then one must have  $a^{0'} = 0$ . But we know that the *only* 4-vector whose fourth component vanishes in *all* frames is the *null vector*. Thus  $a^\mu = 0$ . It therefore follows that for any consistent relativistic quantum mechanical equation satisfying the covariant form of the continuity equation, the relativistic current is *uniquely fixed*. Unique expressions for the conserved currents have been explicitly derived by Holland [48, 49] for the Dirac equation, the Klein-Gordon equation, and also for the coupled Maxwell-Dirac equations.

This uniqueness will *also* be preserved in the non-relativistic limit of the relevant relativistic equation. Hence starting from *any* relativistic wave equation, one can calculate the unique form of the current which can be used in the non-relativistic regime. Then using the (normalized) modulus of the probability current density as the arrival time distribution, if one calculates the mean arrival time, it can be used to empirically test *any* relativistic wave equation, such as the relativistic Kemmer equation [50] for the massive spin 0 and spin 1 bosons. Of late, a unique form of the probability current density expression has been derived in the non-relativistic limit of the relativistic Kemmer equation for spin-0 and spin-1 particles [51]. Although the general scheme we outline for testing a relativistic quantum wave equation in terms of the arrival time distribution is not contingent on any specific form of the relativistic wave equation, in the following

detailed study we specifically use the Dirac equation for spin-1/2 particles.

### 2.3 A novel spin dependent effect on the arrival time distribution for free particles

The Dirac equation for a *free particle* is

$$i\hbar \frac{\partial \Psi}{\partial t} = \left( \frac{\hbar c}{i} \alpha_i \frac{\partial}{\partial x_i} + \beta m_0 c^2 \right) \Psi \quad (2.4)$$

where

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}, \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \Psi = \begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix}$$

$\Psi$  is a four component column matrix and  $\sigma_i$  are the Pauli matrices. Choosing a representation where  $\Psi_1$  and  $\Psi_2$  are two component spinors, one gets two coupled equations

$$\frac{\partial \Psi_1}{\partial t} = -c \sigma_i \frac{\partial \Psi_2}{\partial x^i} - \frac{i m_0 c^2}{\hbar} \Psi_1 \quad (2.5)$$

$$\frac{\partial \Psi_2}{\partial t} = -c \sigma_i \frac{\partial \Psi_1}{\partial x^i} + \frac{i m_0 c^2}{\hbar} \Psi_2 \quad (2.6)$$

Multiplying Eq.(2.5) by  $\Psi_1^\dagger$  from the left and multiplying again the hermitian conjugate of Eq.(2.5) by  $\Psi_1$  from the right, then adding them one gets

$$\frac{\partial}{\partial t} (\Psi_1^\dagger \Psi_1) = -c \Psi_1^\dagger \sigma_i \frac{\partial \Psi_2}{\partial x^i} - c \frac{\partial \Psi_2^\dagger}{\partial x^i} \sigma_i \Psi_1 \quad (2.7)$$

For positive energies, one can take  $\Psi_2 \propto \exp(-iEt/\hbar)$ , where  $E$  is the total energy. In the non-relativistic limit,  $E \cong m_0 c^2$  and then we have  $E + m_0 c^2 \cong 2m_0 c^2$ . Using this with Eq.(2.6) one can write

$$\Psi_2 = -\frac{i\hbar c}{(E + m_0 c^2)} \sigma_i \frac{\partial \Psi_1}{\partial x^i} = -\frac{i\hbar}{2m_0 c} \sigma_i \frac{\partial \Psi_1}{\partial x^i} \quad (2.8)$$

Putting this value of  $\Psi_2$  in Eq.(2.7), one gets

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J} = 0 \quad (2.9)$$

where  $\mathbf{J}$  is the Dirac current in the non-relativistic limit that can be decomposed [48, 52] into two terms as,

$$\begin{aligned}\mathbf{J} &= -\frac{i\hbar}{2m} \left[ \Psi_1^\dagger \boldsymbol{\sigma} (\boldsymbol{\sigma} \cdot \nabla) \Psi_1 - (\nabla \Psi_1^\dagger \cdot \boldsymbol{\sigma}) \boldsymbol{\sigma} \Psi_1 \right] \\ &= -\frac{i\hbar}{2m} \left[ \Psi_1^\dagger (\nabla \Psi_1) - (\nabla \Psi_1^\dagger) \Psi_1 \right] + \frac{\hbar}{2m} \nabla \times (\Psi_1^\dagger \boldsymbol{\sigma} \Psi_1)\end{aligned}\quad (2.10)$$

and  $\rho = \Psi_1^\dagger \Psi_1$ .  $\Psi_1$  is a two component spinor which can be written for a particle in a spin eigenstate as

$$\Psi_1 = \psi(x, t) \chi \equiv \left[ R(x, t) \exp\left(\frac{iS(x, t)}{\hbar}\right) \right] \chi \quad (2.11)$$

Here  $\psi(x, t)$  is the Schrödinger wavefunction and  $\chi$  is a spin eigenstate. Putting this form of  $\Psi_1$  in the expression for current in Eq.(2.10) one gets

$$\mathbf{J} = \frac{1}{m} \rho \nabla S + \frac{1}{m} (\nabla \rho \times \mathbf{s}) = \mathbf{J}_i + \mathbf{J}_s \quad (2.12)$$

with  $\mathbf{s} = (\hbar/2) \chi^\dagger \boldsymbol{\sigma} \chi$ ,  $\rho = R^2$  and  $\chi^\dagger \chi = 1$ . The first term ( $\mathbf{J}_i$ ) in Eq.(2.12) is independent of spin, while the second term ( $\mathbf{J}_s$ ) contains the contribution of the spin of a free particle to the unique conserved vector current in the non-relativistic limit. Now, since the mean arrival time given by Eq.(2.3) can be computed by using the unique expression for  $\mathbf{J}$  in Eq.(2.12), one can thus obtain a spin-dependent contribution to the expression for the mean time of arrival for free particles. This could be experimentally measurable. On the other hand, if one ignores the spin-dependent term one would obtain the mean arrival time given by

$$\bar{\tau}_i = \frac{\int_0^\infty |\mathbf{J}_i| t dt}{\int_0^\infty |\mathbf{J}_i| dt} \quad (2.13)$$

Now we will study the situations where the difference between the magnitudes of  $\bar{\tau}$  and  $\bar{\tau}_i$  is significant, thereby enhancing the feasibility of detecting the predicted spin-dependent effect. To see the computed effects on the arrival time distribution we consider a freely evolving Gaussian wave packet in the two separate cases corresponding to an initially *symmetric* and an *asymmetric* wave packet respectively.

**Case A:** *Symmetric wave packet*

Let us consider a Gaussian wave packet for a free spin 1/2 particle of mass  $m$  centered at the point  $x = 0$ ,  $y = 0$ , and  $z = 0$ . We choose the spin to be directed along the  $z$ -axis, i.e., ( $\mathbf{s} = \frac{1}{2}\hat{z}$ ).

$$\psi(\mathbf{x}, t = 0) = \frac{1}{(2\pi\sigma_0^2)^{3/4}} \exp(i\mathbf{k}\cdot\mathbf{x}) \exp\left(-\frac{\mathbf{x}^2}{4\sigma_0^2}\right) \quad (2.14)$$

The time evolved wave function can be written as

$$\psi(\mathbf{x}, t) = R(\mathbf{x}, t) \exp\left[\frac{iS(\mathbf{x}, t)}{\hbar}\right] \quad (2.15)$$

where  $R(\mathbf{x}, t)$  and  $S(\mathbf{x}, t)$  are respectively given by

$$R(\mathbf{x}, t) = (2\pi\sigma^2)^{-3/4} \exp\left[-\frac{(\mathbf{x} - \mathbf{u}t)^2}{4\sigma^2}\right] \quad (2.16)$$

$$S(\mathbf{x}, t) = -\frac{3\hbar}{2} \tan^{-1}\left(\frac{\hbar t}{2m\sigma_0^2}\right) + m\mathbf{u}\cdot(\mathbf{x} - \frac{1}{2}\mathbf{u}t) + \frac{(\mathbf{x} - \mathbf{u}t)^2 \hbar^2 t}{8m\sigma_0^2\sigma^2} \quad (2.17)$$

with ( $\mathbf{u} = \hbar\mathbf{k}/m$ ) the initial group velocity taken along the  $x$ -axis, and

$$\sigma = \sigma_0 \left[1 + \frac{\hbar^2 t^2}{4m^2\sigma_0^4}\right]^{1/2} \quad (2.18)$$

The total current density can be calculated using Eq.(2.12) to be (we set  $m = 1$ ,  $\hbar=1$ )

$$\begin{aligned} \mathbf{J} &= \rho \left[ \left( u + \frac{(x-ut)t}{4\sigma_0^2\sigma^2} \right) \hat{\mathbf{x}} + \left( \frac{yt}{4\sigma_0^2\sigma^2} \right) \hat{\mathbf{y}} + \left( \frac{zt}{4\sigma_0^2\sigma^2} \right) \hat{\mathbf{z}} \right] \\ &+ \rho \left[ -\left( \frac{y}{2\sigma^2} \right) \hat{\mathbf{x}} + \frac{(x-ut)}{2\sigma^2} \hat{\mathbf{y}} \right] = \mathbf{J}_i + \mathbf{J}_s \end{aligned} \quad (2.19)$$

where the contribution of spin is contained in the second term only. We can now compute  $\bar{\tau}$  and  $\bar{\tau}_i$  numerically by substituting Eq.(2.19) in Eqs.(2.3) and (2.13) respectively. It is instructive to examine the behaviour of the contribution of spin-dependent term towards the mean arrival time. For this purpose, we define a quantity

$$\bar{\tau}_s = \frac{\int_0^\infty |\mathbf{J}_s| t dt}{\int_0^\infty |\mathbf{J}_s| dt} \quad (2.20)$$

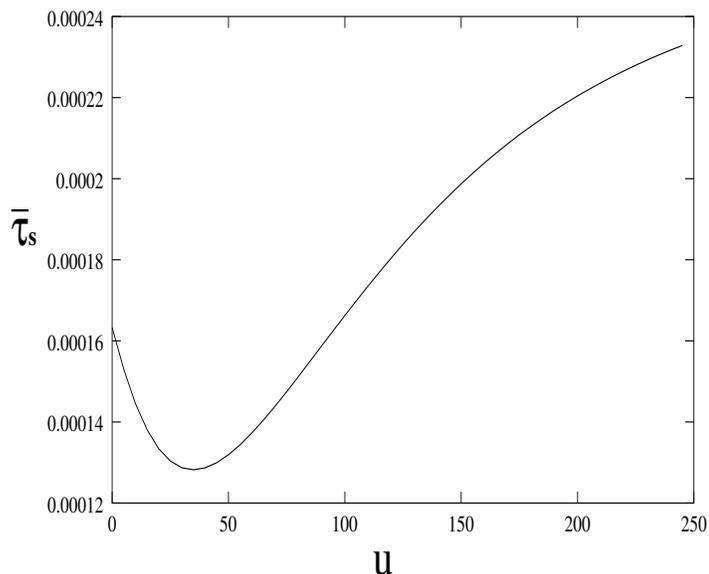


Figure 2.1: The spin-dependent contribution to the mean arrival time computed at the point  $x=1, y=1, z=1$  is plotted against the initial group velocity of the packet along the  $x$ -axis.

We first compute  $\bar{\tau}_s$  for a range of the initial velocity  $u$  in units of  $m=1$ , and  $\hbar=1$ . We find that the spin of a free particle contributes towards altering its mean arrival time for a wide range of initial velocities. This feature holds generally, except for very small magnitudes of velocity where the spin-dependent contribution may be negligible depending on the location of the detector vis-a-vis the direction of the initial group velocity  $\mathbf{u}$ . This feature is shown in Figure 2.1 where we plot the variation of  $\bar{\tau}_s$  with  $u$ . The initial wave packet is peaked at the origin with  $\sigma_0 = 0.01$ . The detector position is chosen at  $(x = 1, y = 1, z = 1)$ . We find that the difference of magnitude between  $\bar{\tau}$  and  $\bar{\tau}_i$  can be increased by choosing asymmetric detector positions as well as asymmetric spread for the initial wave packet, an example of which we will now discuss.

### Case B: *Asymmetric wave packet*

We consider an initial free particle wave packet in three dimensions which is centered

at the point  $x = -x_1, y = 0, z = 0$ .

$$\begin{aligned} \psi(x, y, z, t = 0) &= \left( \frac{1}{\pi^3 a^2 b^2 c^2} \right)^{1/4} \exp(ikx) \exp \left[ -\frac{(x + x_1)^2}{2a^2} \right] \\ &\quad \exp \left[ -\frac{(y)^2}{2b^2} \right] \exp \left[ -\frac{(z)^2}{2c^2} \right] \end{aligned} \quad (2.21)$$

where  $a, b, c$  are positive constants. (Such a form for the wave function was considered by Finkelstein [34] in the context of arrival time distributions.) The particle is given an initial velocity in the  $x$  direction represented by  $u = \hbar k/m$ . The time evolved wave function is given by

$$\begin{aligned} \psi(x, y, z, t) &= \left( \frac{a^2 b^2 c^2}{\pi^3} \right)^{1/4} \frac{\exp[i(kx - k^2 t/2)]}{\alpha \beta \gamma} \exp \left[ -\frac{(x + x_1 - kt)^2}{2\alpha^2} \right] \\ &\quad \exp \left[ -\frac{y^2}{2\beta^2} \right] \exp \left[ -\frac{z^2}{2\gamma^2} \right] \end{aligned} \quad (2.22)$$

where  $\alpha = (a^2 + it)^{1/2}$ ;  $\beta = (b^2 + it)^{1/2}$ ;  $\gamma = (c^2 + it)^{1/2}$ . Now writing the wave function as  $\psi(x, y, z, t) = R(x, y, z, t) \exp[iS(x, y, z, t)/\hbar]$  one obtains

$$\begin{aligned} R(x, y, z, t) &= \left( \frac{a^2 b^2 c^2}{\pi^3} \right)^{1/4} \frac{1}{(p^2 + q^2)^{1/4}} \exp \left[ -\frac{a^2(x + x_1 - kt)^2}{2(a^4 + t^2)} \right] \\ &\quad \exp \left[ -\frac{b^2 y^2}{2(b^4 + t^2)} \right] \exp \left[ -\frac{c^2 z^2}{2(c^4 + t^2)} \right] \end{aligned} \quad (2.23)$$

and

$$\begin{aligned} S(x, y, z, t) &= \hbar kx - \frac{\hbar k^2 t}{2} - \frac{\hbar}{2} \tan^{-1}(q/p) + \frac{\hbar t(x + x_1 - kt)^2}{2(a^4 + t^2)} \\ &\quad + \frac{\hbar t y^2}{2(b^4 + t^2)} + \frac{\hbar t z^2}{2(c^4 + t^2)} \end{aligned} \quad (2.24)$$

with  $p = (a^2 b^2 c^2 - a^2 t^2 - b^2 t^2 - c^2 t^2)$  and  $q = (a^2 b^2 t + a^2 c^2 t + b^2 c^2 t - t^3)$ . Considering again a spin-1/2 particle with spin directed along z-axis ( $\mathbf{s} = \frac{1}{2} \hat{z}$ ), the total current density defined in Eq.(2.12) is given by (in units of  $\hbar = 1 = m$ )

$$\begin{aligned} \mathbf{J} &= \rho \left[ \left( u + \frac{(x + x_1 - ut)t}{(a^4 + t^2)} \right) \hat{\mathbf{x}} + \frac{yt}{(b^4 + t^2)} \hat{\mathbf{y}} + \frac{zt}{(c^4 + t^2)} \hat{\mathbf{z}} \right] \\ &\quad + \rho \left[ -\frac{b^2 y}{(b^4 + t^2)} \hat{\mathbf{x}} + \frac{a^2(x + x_1 - ut)}{(a^4 + t^2)} \hat{\mathbf{y}} \right] = \mathbf{J}_i + \mathbf{J}_s \end{aligned} \quad (2.25)$$

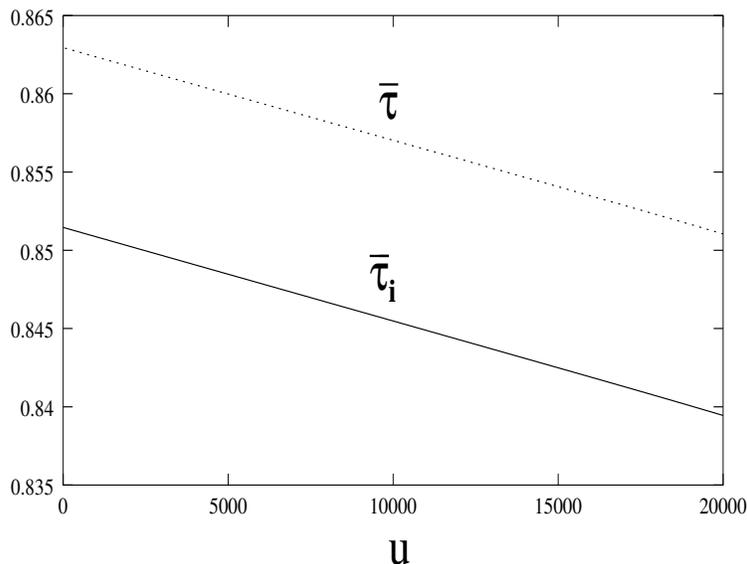


Figure 2.2: The mean arrival times  $\bar{\tau}$  (upper curve) and  $\bar{\tau}_i$  (lower curve) computed at the point  $x = 1, y = 2, z = 1$  are plotted against the initial group velocity of the packet along the  $x$ -axis. and  $a = 0.001, b = 0.4, c = 0.01, x_1 = 0$ .

where the second term represents the spin-dependent contribution to the current. We now compute numerically the mean arrival times  $\bar{\tau}$  and  $\bar{\tau}_i$ . Figure 2.2 shows the variation of  $\bar{\tau}$  and  $\bar{\tau}_i$  with the initial group velocities ( $u$ ) of the wave packet. Here we choose the parameters as  $x_1 = 0, a = 0.001, b = 0.4, c = 0.01$ . Accordingly the mean arrival time is computed at the position  $x = 1.0, y = 2.0, z = 1.0$ . One sees that the difference in the magnitudes of  $\bar{\tau}$  and  $\bar{\tau}_i$  can suitably be enhanced by a judicious choice of asymmetric initial spreads and detector positions.

Before concluding this chapter let us discuss about the possibility of an experimentally realizable scheme [53] which can test any postulated quantum mechanical approach for calculating the arrival time distribution. It is important to mention here that the usual experimental analysis for measuring the “arrival time” or “time of flight” are usually done semi-classically or classically [54]. Although a number of authors [13, 14] have pointed out various conceptual and mathematical problematic aspects of time measurement, several specific toy models [55] have also been proposed to investigate the feasibility of *how*

actually the measurement of a time distribution can be performed in a way consistent with the basic principles of quantum mechanics.

Since there are debates arising essentially if one considers *how to directly measure* time in quantum mechanics, here we bypass this vexed issue by adopting the following strategy. We consider a spin-rotator (SR) as a “*quantum clock*” where the basic quantity which determines the actually observable results is the probability density function  $\Pi(\phi)$  which corresponds to the probability distribution of spin orientations along different directions for the particles emerging from the SR,  $\phi$  being the angle by which the spin orientation of a spin-1/2 neutral particle (say, a neutron) is rotated from its initial spin polarised direction. Note that this angle  $\phi$  is determined by the transit time ( $t$ ) within the SR. Hence the probability density function  $\Pi(\phi)$  stems from  $\Pi(t)$  which represents the distribution of times over which the particles interact with the constant magnetic field while passing through the SR. It is the evaluation of this quantity  $\Pi(t)$  which critically depends on what quantum mechanical approach one adopts for calculating such a time distribution.

Let us consider an ensemble of spin 1/2 neutral particles, say, neutrons having magnetic moment  $\mu$  (with all their spins oriented along  $+\hat{\mathbf{x}}$  -axis) passing through a spin-rotator (SR) containing a constant magnetic field  $\mathbf{B}$  directed along the  $+\hat{\mathbf{z}}$  -axis. Next, we recall that when a spin-polarised particle (say, a neutron) passes through the constant magnetic field within a SR, its spin orientation is rotated by an angle  $\phi$  with respect to the initial spin polarised direction along  $+\hat{\mathbf{x}}$  axis. This angle is fixed by the time ( $t$ ) spent by the particle within the SR, given by the well known quantum mechanical relation  $\phi = 2\omega t$  where  $\omega = \mu B/\hbar$  [56]. Now, if we consider a wavepacket associated with the neutron beam passing through the spin-rotator then we should expect an arrival *time distribution*  $\Pi(t)$  or a transit time distribution for the particles at the exit point of the spin-rotator. This *time distribution*  $\Pi(t)$  is not uniquely defined in standard quantum mechanics and one can adopt different approaches to calculate this time distribution. Based on this time distribution  $\Pi(t)$  the particles emerging from the SR will have a distribution  $\Pi(\phi)$  of their spins oriented along different directions since the spin rotation is proportional to the transit time.

Thus the emergent spin states get polarised along different directions and consequently the final ensemble of particles emerging from the SR (at *any* time which is large enough

so that by which all the particles of the ensemble, i.e., the total wave packet have passed through the spin-rotator) is in a *mixed state* of spin states polarised along various directions ( $\phi$ ) with different respective probabilities  $\Pi(\phi)$ . Now, for testing the scheme we have outlined for calculating the probability density function  $\Pi(\phi)$ , one may consider the measurement of a spin variable (on the particles emerging from the spin-rotator), say  $\hat{\sigma}_\theta$ , by a Stern-Gerlach device in which the inhomogeneous magnetic field is oriented along a direction  $\hat{n}(\theta)$  in the xy-plane making an angle  $\theta$  with the initial spin-polarised direction ( $+\hat{x}$  axis). Then the *probabilities* of finding the spin components (along  $+\hat{n}(\theta)$  and its opposite direction) can be calculated. The estimations of these *probabilities* crucially depend on *how* one calculates the quantity  $\Pi(\phi)$  whose evaluation, in turn, is contingent on the procedure adopted for calculating the relevant time distribution  $\Pi(t)$  specifically, which might be taken to be represented by the modulus of the probability current density  $|\mathbf{J}(\mathbf{x}, t)|$  (suitably normalised) evaluated at the exit point of the spin-rotator.

## 2.4 Summary

To summarize, in this chapter we have elaborated the probability current density approach in calculating the arrival time distribution for *free* particles. Although the probability current is interpreted as the streamlines of conserved flux and has been used in the quantum mechanical predictions of arrival/tunneling time distributions, it can be easily seen that in the non-relativistic quantum mechanics the form of the probability current is *not unique* which leads an ambiguity in the arrival time distribution. The probability current can be uniquely fixed if one starts from a relativistic quantum wave equation and finally this *uniqueness* will also be preserved in the non-relativistic limit of the relevant relativistic equation. A novel spin dependent effect on the arrival time distribution for *free* particles was shown by demonstrating the uniqueness of the conserved probability current in the non-relativistic limit of Dirac equation. The mean arrival time was computed using the modulus of the unique (spin-dependent) probability current density for spin-1/2 free particles associated with a propagating Gaussian wave packet. This spin-dependent effect highlights the feature that the spin of a particle is an *intrinsic* property and is *not* contingent on the presence of an external field.

One may also perceive the significance of such an effect as follows. Although the dynamical properties of free particles like position, momentum, and energy are measurable, one cannot measure the *static* or *innate* particle properties such as charge without using any external field. Nevertheless, the scheme we have discussed shows that the magnitude of total spin can be measured *without* subjecting the particle to an external field. Another implication of measuring the spin-dependent arrival times for free particles could be to view this as implying an interesting difference between the magnitude of the total spin of a particle and its other static properties such as mass and charge. This is because the measurability of the property of spin of a free particle arises from the relativistic nature of the dynamical evolution of the wave function where the relevant wave function is fundamentally 4-component (or, 2-component), even in the *non relativistic limit*. Now, since the spin-dependent term which contributes significantly to the arrival time distribution has been computed in the nonrelativistic regime by starting from the relativistic Dirac equation, this provides a rather rare example of an empirically detectable manifestation of a relativistic dynamical equation in the *non relativistic regime*. This effect *cannot* be derived *uniquely* from the Schrödinger dynamics. A future line of investigation as an offshoot of this analysis could be to explore the possibilities of using the relativistic quantum mechanical wave equations of particles with spins other than spin 1/2 (such as using the relativistic Kemmer equation for spin 0 and spin 1 bosons) in order to compute the spin-dependent terms in the probability current densities and their effects on the arrival time distribution. Such a study seems worthwhile because then the arrival time distribution may provide a means of checking the validity of the various suggested relativistic quantum mechanical equations which have otherwise eluded any empirical verification. Finally, we have discussed the possibility of an experimentally realizable scheme which can test any postulated quantum mechanical approach for calculating the arrival time distribution.

## Chapter 3

# Classical limit of arrival time

### 3.1 Outlook

It is generally believed that a necessary requirement for the universal validity of quantum mechanics is that its results in the macroscopic limit must agree with those of classical mechanics, because the latter is well verified in the macroscopic domain. However, there exist vexed problems regarding the connection between classical and quantum mechanics; the question whether quantum mechanics in the macroscopic limit is completely equivalent to classical mechanics remains the focal point of diverging view points. This is sharply reflected in the various controversies persisting in the relevant literature [57]-[65]. The traditional opinion against the observation of *quantum effects* for macroscopic objects is that even if quantum mechanics was valid in the macroscopic world, it would be impossible in practice to detect it. However, since there is no definite boundary between the microscopic and the macroscopic worlds, one can always speculate the universal validity of quantum mechanics. The nonobservability of quantum superposition of macroscopic apparatus states is at the heart of the quantum measurement problem/the Schrödinger cat paradox which presupposes universal validity of quantum mechanics even in the macroscopic world. Recently, quantum interference experiments [66] with large molecules have gained importance to test whether there are limits to quantum physics and how far one can push the experimental techniques to visualize quantum effects in the mesoscopic world for objects of increasing size, mass, and complexity [67]. A general argument has been recently given against the universal validity of the superposition principle [68].

A widely discussed approach of the classical limit, which is followed in many text books

of quantum mechanics, is to derive the classical equations of motion from the Schrödinger equation in the limit  $\hbar \rightarrow 0$ . But the problem in this approach is that since  $\hbar$  is a dimensional quantity one can not set it equal to zero and the notion that  $\hbar$  is “small” has no absolute meaning because its value depends on the system of units. In the widely studied WKB approximation method, a quantum mechanical wave function is expanded in power series of  $\hbar$  around  $\hbar = 0$ . Then the series is truncated by neglecting higher powers of  $\hbar$ - subsequent calculations are based on this truncated series. This procedure can be considered a semiclassical (but essentially nonclassical) computing procedure, useful in many problems but should be considered distinct from the classical limit problem because wave functions are, in general, highly non analytic in the neighbourhood of the limit point  $\hbar = 0$ . Moreover, there are examples where the quantum mechanically predicted results are independent of  $\hbar$ . It is therefore not legitimate to make naïve statements like “every classical system is essentially the  $\hbar = 0$  limit of a quantum one”.

Another frequently discussed classical limit approach of quantum mechanics is that to examine whether in the large principle quantum number limit ( $n \rightarrow \infty$ ) the quantum mechanical ensemble represented by an energy eigenfunction is equivalent with the corresponding classical ensemble. It is generally believed that if a wave function belongs to the “classical domain” (in such a domain wave functions correspond to those energy eigenvalues which are much greater than the energy difference between successive discrete eigenstates, *i.e.*,  $Lt_{n \rightarrow \infty}(E_{n+1} - E_n)/E_n \rightarrow 0$  so that in this domain the classical continuum of energies is attained), the quantum probability density should approach its classical counterpart. The important point to be emphasized is that even if the individual energy eigenstates lead to the required classical results in the limit  $n \rightarrow \infty$ , their superpositions do not necessarily satisfy this requirement [69]. Hence it is also not a universal criterion that the classical dynamical behaviours emerges from an arbitrary quantum mechanical wave function in the high-energy or  $n \rightarrow \infty$  limit. Further, it has been demonstrated that quantum nonlocality exhibited through the violation of Bell-type inequalities, persists, in general, in the limit of a large number of constituents, or large quantum number [70].

Discussions of the classical limit of quantum mechanics [71] are often based on Ehrenfest’s theorem [72], according to which under certain conditions (when the spread in position of the wave packet is sufficiently small) the mean quantum evolution resembles

classical dynamical behavior. It needs to be noted is that even if Ehrenfest's theorem holds good in a given situation, it does not suffice to guarantee complete equivalence with classical mechanics. The fact that averages of the observed values of the dynamical quantities pertaining to an ensemble of particles satisfy classical equations does not imply that the behavior of an individual member of the ensemble conforms to classical dynamics—vastly different ensembles can give rise to the same mean behavior. Ehrenfest's theorem is *neither necessary nor sufficient* to define the classical regime. Lack of sufficiency—that a system may obey Ehrenfest's theorem but not behave classically is proved by the example of the harmonic oscillator where the quantum mechanical averages of the dynamical variables obey the classical equations of motion. Yet a quantum oscillator has discrete energy levels, which make its thermodynamic properties quite different from those of the classical oscillator. Lack of necessity—the system may behave classically even when Ehrenfest's theorem does not apply. The centroid of a classical ensemble (the probability distribution in phase space for a classical ensemble which satisfies the Liouville's equation) need *not* follow a classical trajectory if the width of the probability distribution is not negligible. But the statistical ensemble description of classical dynamics does not pertain only to a localized probability distribution.

Einstein [59] and Pauli [60] strongly advocated the tenet that in the macroscopic limit, not only the localised wave functions but all physically admissible solutions of the *Schrödinger* equation must lead to predictions equivalent to those obtainable from classical mechanics; this is known as Einstein-Pauli tenet which has been the focal point of vigorous debates. Such comparison between the two mechanics can be meaningful only within the framework of the ensemble interpretation. Thus the classical limit problem boils down to probing whether there is complete equivalence, in the macroscopic limit, between the empirical predictions of classical and quantum mechanics with respect to the properties of the same initial ensemble. This is the spirit which motivates the present investigation. Therefore we should not expect to recover an individual classical trajectory when we take the classical limit of quantum mechanics. Rather, we should expect the probability distributions of quantum mechanics to become equivalent to the probability distributions of an ensemble of classical trajectories.

For complete equivalence between classical mechanics and the macroscopic limit of

quantum mechanics it is necessary that, in the classical limit, all the measurable properties of a quantum mechanical ensemble corresponding to any normalizable wave function  $\psi(x, t)$  should be equally reproduced by the classical phase space formalism using a distribution function  $D(x, p, t)$  such that the following necessary conditions are satisfied in the classical limit:

A. The time-development of  $D(x, p, t)$  is in accordance with the classical Liouville's equation:

$$\frac{\partial D}{\partial t} + [D, H] = 0 \quad (3.1)$$

B. The *expectation value* of an arbitrary operator  $\hat{A}(\hat{x}, \hat{p})$  representing a certain quantum mechanical observable should be equal to the mean value of the function  $A(x, p)$  which is evaluated through phase space integration using  $D(x, p, t)$ ;  $A(x, p)$  is obtained by replacing the operators  $\hat{x}$  and  $\hat{p}$  in the expression for  $\hat{A}(\hat{x}, \hat{p})$  with scalar variables  $x$  and  $p$ :

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx dp A(x, p) D(x, p, t) = \int_{-\infty}^{\infty} \psi^* \hat{A}(\hat{x}, \hat{p}) \psi \quad (3.2)$$

C. The classical phase space distribution function  $D(x, p, t)$  must be positive definite.

It is well known that the uncertainty principle makes the concept of phase space in quantum mechanics problematic. Because a particle cannot simultaneously have a well defined position and momentum, one cannot define a probability that a particle has a position  $x$  and a momentum  $p$ , i.e., one cannot define a true phase space probability distribution for a quantum mechanical particle. Nevertheless, efforts have been made to construct quantum mechanical analogues of a phase space density or the “phase space formulation of quantum mechanics” as a mathematical tool to investigate the quantum dynamics of various systems e.g. Wigner distribution function, Husimi distribution function, Glauber-Sudarshan distribution function, etc [73].

## 3.2 Motivation

The current investigation [74] is concerned about a *new approach* to test the quantitative equivalence between classical mechanical prediction and the prediction obtained in the macroscopic limit of quantum mechanics. Here we formulate the classical phase space

distribution in a way which is completely classical unlike the one that is called the *quantum phase space distribution function* such as the Wigner distribution function. The latter is essentially a quantum entity obtained by directly using the expression of the wave function, and is constructed to reproduce the results of quantum mechanics, but it does not satisfy the classical Liouville's equation. So, the Wigner distribution function, not being a positive definite quantity in general, does not provide the results of a classical phase space evolution. In contrast we formulate a phase space distribution function  $D(x, p, t)$  that is positive definite and also satisfies the classical Liouville's equation. The motivation for this work is to study the comparison between quantum mechanical results and those obtained from a purely classical phase space description by formulating a proper classical counterpart of the quantum ensemble. Here our focus is on the *arrival time* of the *free particles* but one can also investigate the quantum-classical comparison for other dynamical variables for particles in various types of potentials using the same approach.

We have seen from the discussion of first two chapters that there exists an extensive literature on the treatment of *arrival time distribution* in quantum mechanics. A key issue for any definition of time of arrival in quantum mechanics is to secure an acceptable classical limit of the arrival time formulation. Here we will investigate aspects of the quantum-to-classical transition of the arrival time for an ensemble of particles. Such a study, if undertaken extensively, is not only expected to throw light on the comparative merits of different arrival time formulations, but also to be of relevance to the behaviour of mesoscopic systems where a great deal of experimental activity is presently underway [75]. To this end we formulate a classical analogue of the arrival time distribution for free particles obtained via the quantum probability current. We consider an ensemble of particles represented by a phase space density function which evolves freely under classical Liouville's equation. Our approach brings out the correspondence between the quantum arrival time distribution defined through the probability current density and its classical counterpart that we formulate. We will see that using the explicit *mass-dependence* of the mean arrival time within this framework, it is possible to demonstrate the smooth transition from the quantum to classical behaviour of the mean arrival time by continuously increasing the mass of the particles.

As we discussed in Chapter 2, a consistent approach of formulating a definition for

arrival time distribution is through the quantum probability current. A logically consistent and unambiguous definition of the quantum probability current contains the spin of a particle [48]. However, for the case of massive spin-0 particles it has been shown recently by taking the non-relativistic limit of relativistic Kemmer equation that the unique probability current is given by the Schrödinger current, and hence, the Schrödinger current gives the unique probability current density or the unique arrival time distribution for spin-0 particles. In the present analysis we restrict our attention to massive spin-0 particles only and for the current investigation we use the Schrödinger current ( $\mathbf{J}(\mathbf{x}, t) = \frac{i\hbar}{2m}(\Psi\nabla\Psi^* - \Psi^*\nabla\Psi)$ ) to define the arrival time distribution for free particles and the mean arrival time of the particles reaching a detector located at  $\mathbf{x} = \mathbf{X}$  may be written as

$$\bar{\tau} = \frac{\int_0^\infty |\mathbf{J}(\mathbf{x} = \mathbf{X}, t)| dt}{\int_0^\infty |\mathbf{J}(\mathbf{x} = \mathbf{X}, t)| dt} \quad (3.3)$$

Henceforth, for simplicity we shall restrict ourselves to only one spatial dimension. One should keep in mind that the definition of the mean arrival time used in Eq.(3.3) is not a uniquely derivable result within standard quantum mechanics. However, the Bohmian interpretation [19] of quantum mechanics in terms of the causal trajectories of individual particles implies the above expression for the mean arrival time in a unique and rigorous way. It should also be noted that in certain situations  $\mathbf{J}(\mathbf{X}, t)$  can be negative over some time interval provided the initial flux  $\mathbf{J}(\mathbf{X}, t = 0)$  is negative [76]. In order to account for the back flow effect in such cases, the decomposition of  $J(X, t)$  into right and left moving parts could be undertaken. However, our present analysis is carried out using a simple example that is free from such complications.

### 3.3 Quantum-classical correspondence

Let us now consider a Gaussian wave packet representing a quantum free particle moving in 1-D whose initial wave function  $\Psi(x, 0)$  and its Fourier transform  $\Phi(p, 0)$  are respectively given by

$$\Psi(x, 0) = \frac{1}{(2\pi\sigma_0^2)^{1/4}\sqrt{1+iC}} e^{\left\{ikx - \frac{x^2}{4\sigma_0^2(1+iC)}\right\}} \quad (3.4)$$

$$\Phi(p, 0) = \left( \frac{2\sigma_0^2}{\pi\hbar^2} \right)^{1/4} e^{-\left\{ \frac{\sigma_0^2(p-\bar{p})^2}{\hbar^2} (1+iC) \right\}} \quad (3.5)$$

where the group velocity of the wave packet  $u = \hbar k/m = \bar{p}/m$ . For generality we have taken the initial Gaussian wave function  $\Psi(x, 0)$  which is not a minimum uncertainty state ( $\Delta x \Delta p = (\hbar/2)\sqrt{1+C^2} > \hbar/2$ ), but which could represent a squeezed state [77] with parameter  $C$ . The Schrödinger time evolved wave function  $\Psi(x, t)$ , the quantum position probability density  $\rho_Q(x, t)$  and the probability current density  $J_Q(x, t)$  at a particular location  $x$  are then respectively given by

$$\Psi(x, t) = \frac{1}{(2\pi\sigma_0^2)^{1/4} \sqrt{1 + i(C + \frac{\hbar t}{2m\sigma_0^2})}} e^{ik(x - \frac{1}{2}ut)} \exp \left\{ -\frac{(x - ut)^2}{4\sigma_0^2 \left[ 1 + i(C + \frac{\hbar t}{2m\sigma_0^2}) \right]} \right\} \quad (3.6)$$

$$\rho_Q(x, t) = |\Psi(x, t)|^2 = \frac{1}{(2\pi\sigma_0^2)^{1/2} \sqrt{1 + (C + \frac{\hbar t}{2m\sigma_0^2})^2}} \exp \left\{ -\frac{(x - ut)^2}{2\sigma_0^2 \left[ 1 + (C + \frac{\hbar t}{2m\sigma_0^2})^2 \right]} \right\} \quad (3.7)$$

$$J_Q(x, t) = \rho_Q(x, t) \left\{ u + \frac{\hbar(C + \frac{\hbar t}{2m\sigma_0^2})(x - ut)}{2m\sigma_0^2 \left[ 1 + (C + \frac{\hbar t}{2m\sigma_0^2})^2 \right]} \right\} \quad (3.8)$$

In order to elucidate the classical counterpart of the quantum probability current, we now construct a classical formulation of arrival time for an ensemble of free particles. We take the initial phase space distribution function for the ensemble of particles as a product of two Gaussian functions matching with the initial quantum position and momentum distributions from Eqs.(3.4) and (3.5) as

$$D_0(x_0, p_0, 0) = |\Psi(x_0, 0)|^2 |\Phi(p_0, 0)|^2 = \frac{1}{\pi\hbar\sqrt{1+C^2}} \exp \left\{ -\frac{x_0^2}{2\sigma_0^2(1+C^2)} - \frac{2\sigma_0^2(p_0 - \bar{p})^2}{\hbar^2} \right\} \quad (3.9)$$

where the variables  $x_0$  and  $p_0$  are the initial positions and momenta of the particles. Note that our approach to compare the quantum and classical predictions is not contingent to any particular initial form of the wave function. The key point of this scheme is to choose the initial classical ensemble in such a way that it reproduces the initial quantum

position and momentum distributions. Classically of course, there are other choices for  $D_0(x_0, p_0, 0)$ . But in quantum mechanics, due to the uncertainty principle, given a wave function  $\psi(x, t)$ , the momentum space wave function  $\phi(p, t)$  is automatically fixed by the Fourier transform of  $\psi(x, t)$ . In this way the position probability density  $|\psi|^2$  and the momentum probability density  $|\phi|^2$  are *correlated* in quantum mechanics. There is no such restriction for the position and momentum densities in classical statistical mechanics. But it is quite reasonable to take the initial classical phase space distribution exactly matching with the initial quantum position and momentum probability densities in order to compare the results obtained from the dynamical evolutions of classical and quantum mechanics. This is precisely the motivation to take the initial phase space distribution  $D_0(x_0, p_0, 0)$  in a way given by Eq.(3.9). Now to obtain the final time evolved density function  $D(x, p, t)$  we focus on the classical dynamics of a freely moving particle. The Hamiltonian is  $H = p^2/2m$  and the Hamilton's equations are  $x = pt/m + x_0$  and  $p = p_0$  where the variables  $x_0$  and  $p_0$  are the initial position and momentum of the particle which are respectively given by  $x_0 = x - pt/m$  and  $p_0 = p$ . Substituting these values of  $x_0$  and  $p_0$  in the expression of  $D_0(x_0, p_0, 0)$  we obtain the final time evolved distribution function  $D(x, p, t)$ . This is because here we are considering the free evolution of an ensemble of particles whose initial positions ( $x_0$ ) and momenta ( $p_0$ ) are distributed according to the initial density function  $D_0(x_0, p_0, 0)$ . The time evolved phase space distribution satisfying the Liouville's equation under free evolution [65] is then given by

$$D(x, p, t) = \frac{1}{\pi\hbar\sqrt{1+C^2}} \exp\left\{-\frac{(x - \frac{pt}{m})^2}{2\sigma_0^2(1+C^2)} - \frac{2\sigma_0^2(p - \bar{p})^2}{\hbar^2}\right\} \quad (3.10)$$

It is instructive to write down the the Wigner distribution function which is calculated from the time evolved wave function ( $\Psi(x, t)$ ), and is given by

$$D_W(x, p, t) = \frac{1}{\pi\hbar} \int_{-\infty}^{\infty} \Psi^*(x+y, t)\Psi(x-y, t) \exp\{2ipy/\hbar\} dy \quad (3.11)$$

By substituting the value of  $\Psi(x+y, t)$  and  $\Psi(x-y, t)$  using Eq.(3.6) we obtain

$$D_W(x, p, t) = \frac{1}{\pi\hbar} \exp\left\{\frac{-2(p - \bar{p})^2\sigma_0^2}{\hbar^2}\right\} \exp\left\{-\frac{[x - pt/m - 2C(p - \bar{p})\sigma_0^2/\hbar]^2}{2\sigma_0^2}\right\} \quad (3.12)$$

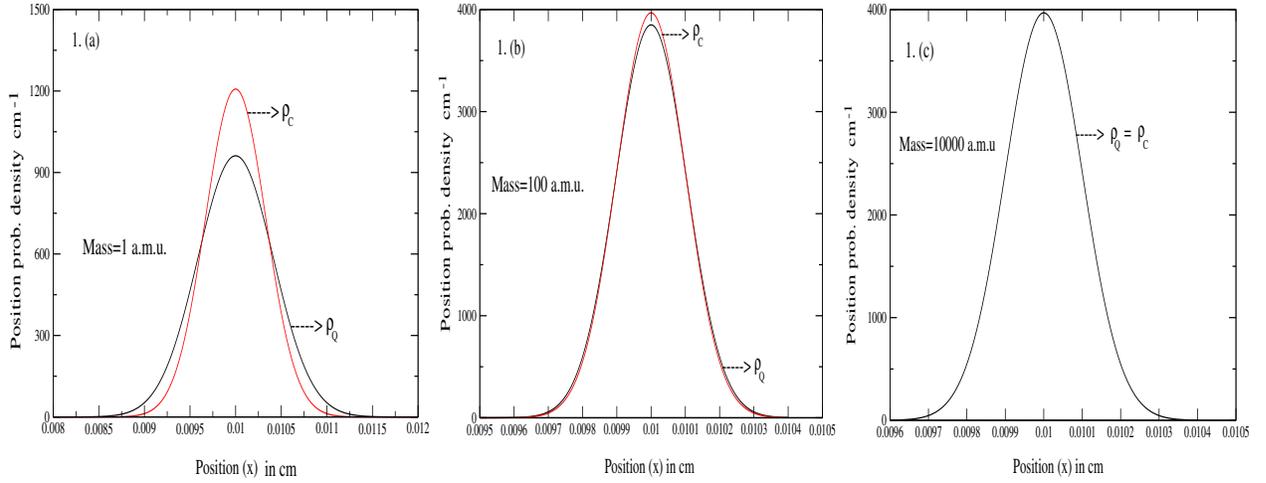


Figure 3.1: The position probability densities  $\rho_Q(x, t)$  and  $\rho_C(x, t)$  are plotted for varying mass of the particles (in atomic mass units) with  $\sigma_0 = 10^{-5}$  cm,  $u = 10^3$  cm/sec,  $C=10$  and  $t=10^{-5}$  sec.

Note here that the Wigner function  $D_W(x, p, t)$  is not identical with our classical phase space distribution  $D(x, p, t)$ . So, our formulated classical phase space distribution is completely classical unlike Wigner distribution function [73] which is essentially a quantum entity obtained directly by using the expression of the wave function, and is constructed in a way to reproduce the results of quantum mechanics. The Wigner distribution function, not being a positive definite quantity in general, does not provide the results of a classical phase space evolution because it does not satisfy the classical Liouville's equation.

Here we consider a classical statistical ensemble of particles defined by the phase space density function  $D(x, p, t)$  in *one dimension*. Then the position and momentum distribution functions are respectively  $\rho_C(x, t) = \int D(x, p, t) dp$  and  $\rho_C(p, t) = \int D(x, p, t) dx$ . The classical position probability distribution for this ensemble is given by

$$\rho_C(x, t) = \int D(x, p, t) dp = \frac{1}{(2\pi\sigma_0^2)^{1/2} \sqrt{1 + C^2 + \frac{\hbar^2 t^2}{4m^2\sigma_0^4}}} \exp \left\{ -\frac{(x - ut)^2}{2\sigma_0^2(1 + C^2 + \frac{\hbar^2 t^2}{4m^2\sigma_0^4})} \right\} \quad (3.13)$$

All the density functions are assumed to be normalized and  $D(x, p, t)$  satisfies the

classical Liouville's equation given by

$$\frac{\partial D(x, p, t)}{\partial t} + \dot{x} \frac{\partial D(x, p, t)}{\partial x} + \dot{p} \frac{\partial D(x, p, t)}{\partial p} = 0 \quad (3.14)$$

Since for free particles  $\dot{p} = 0$  and  $\dot{x} = p/m$ , we have

$$\frac{\partial D(x, p, t)}{\partial t} + \frac{p}{m} \frac{\partial D(x, p, t)}{\partial x} = 0 \quad (3.15)$$

Integrating the above equation with respect to  $p$  one gets

$$\frac{\partial \rho_C(x, t)}{\partial t} + \frac{\partial}{\partial x} \left[ \frac{1}{m} \bar{p}(x, t) \rho_C(x, t) \right] = 0 \quad (3.16)$$

where  $\bar{p} = \int p D(x, p, t) dp / \int D(x, p, t) dp$  is the ensemble average of the momentum. Defining  $\bar{v}(x, t) = \bar{p}(x, t)/m$  as the average velocity, one obtains

$$\frac{\partial \rho_C(x, t)}{\partial t} + \frac{\partial}{\partial x} J_C(x, t) = 0 \quad (3.17)$$

where  $J_C(x, t)$  and  $\bar{v}(x, t)$  represent the mean motion of the continuum matter at  $(x, t)$ . Eq.(3.17) is the equation of continuity for the continuous density function  $\rho_C(x, t)$  of a statistical ensemble of particles. The expression for the classical probability current is given by

$$J_C(x, t) = \frac{1}{m} \int p D(x, p, t) dp \quad (3.18)$$

and is related to the mean velocity by  $J_C(x, t) = \rho_C(x, t) \bar{v}(x, t)$ .

Now substituting the expression for the time evolved phase space distribution function  $D(x, p, t)$  from Eq.(3.10) in Eq.(3.18) we get the expression for the current density or the arrival time distribution at a particular detector location  $x=X$  for this classical ensemble of free particles given by

$$J_C(x, t) = \rho_C(x, t) \left\{ u + \frac{(x - ut) \hbar^2 t}{[\hbar^2 t^2 + 4m^2 \sigma_0^4 (1 + C^2)]} \right\} \quad (3.19)$$

If we impose here the minimum uncertainty condition *viz.*,  $C = 0$  then one can check from Eqs.(3.7), (3.8), (3.13) and (3.19) that both  $\rho_Q(x, t) = \rho_C(x, t)$  and  $J_Q(X, t) = J_C(X, t)$  hold, i.e., the classical and quantum probability currents are similar. Thus, if we take the initial phase space distribution function for the classical ensemble of particles as

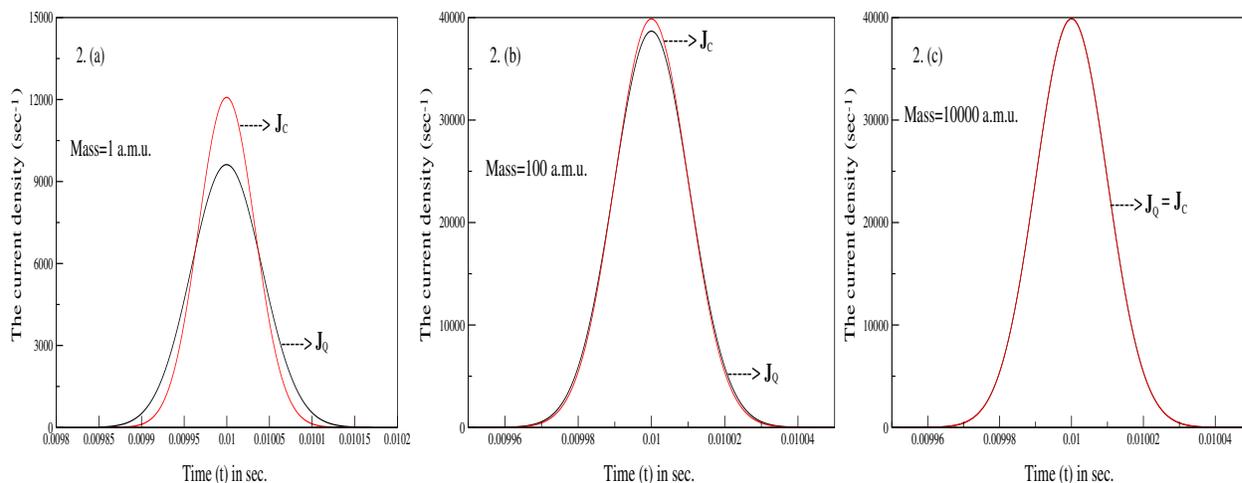


Figure 3.2: The probability current densities  $J_Q(x, t)$  and  $J_C(x, t)$  are plotted for varying mass of the particles (in atomic mass units) at a detector location  $X=10$  cm with  $\sigma_0 = 10^{-4}$  cm,  $u = 10^3$  cm/sec,  $C=100$ .

a product of two Gaussian functions matching with the initial *quantum* position and momentum distributions then the classical arrival time distribution exactly matches with the quantum one provided the minimum uncertainty relation is satisfied. But in general the quantum and classical distribution functions are different when the minimum uncertainty condition is not satisfied ( $C \neq 0$ ).

Though  $J_Q(X, t)$  and  $J_C(X, t)$  are in general not equal for  $C \neq 0$ , the large mass limits of both are the same. This is seen from Figures 3.1 and 3.2 where the probability distributions and the currents are plotted respectively for different masses. It is apparent that in the large mass limit quantum distributions reduce to the classical distributions. The mass dependence in the arrival time distributions and also in the position probability densities (for both the quantum and classical case) arises from the spreading of the wave packet.

We now compute the mean arrival time  $\bar{\tau}$  by substituting the expressions for the quantum current in Eq.(3.3). [One should note that though the integral in the numerator of Eq.(3.3) formally diverges logarithmically, several techniques have been employed in the literature [78] ensuring rapid fall off for the probability distributions asymptotically, so that convergent results are obtained for the integrated arrival time. Here we have

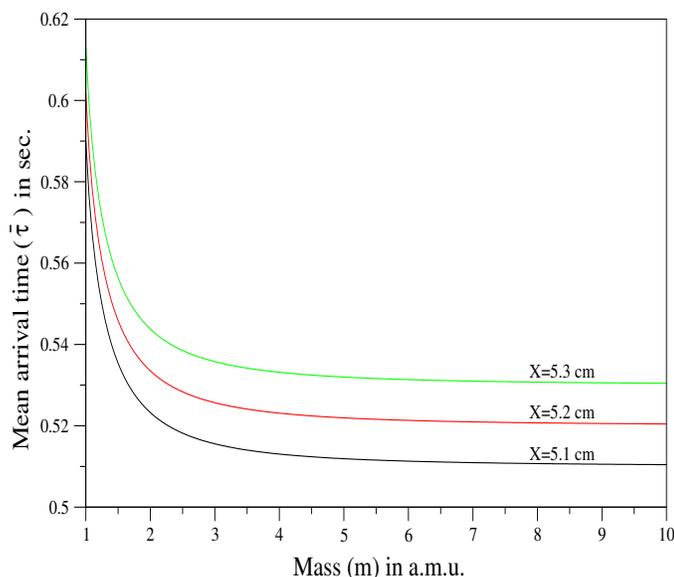


Figure 3.3: The mean arrival time  $\bar{\tau}$  is plotted against the mass of the particles (in atomic mass unit) at different detector locations  $X = 5.1$  cm,  $X = 5.2$  cm, and  $X = 5.3$  cm. for  $C=10$ ,  $\sigma_0 = 0.0001$  cm,  $u = 10$  cm/sec.

employed a simple strategy of taking a cut-off ( $t = T$ ) in the upper limit of the time integral with  $T = (X + 3\sigma_T)/u$  where  $\sigma_T$  is the width of the wave packet at time  $T$ . In other words, our computations of the arrival time are valid up to the  $3\sigma$  level of spread in the wave function.] It is instructive to examine the variation of mean arrival time with the different parameters of the wave packet. In Figure 3 we have plotted the variation of  $\bar{\tau}$  with mass at different detector locations, keeping the group velocity  $u$  and initial width  $\sigma_0$  fixed. One sees that the mean arrival time calculated by using the quantum current  $J_Q(X, t)$  as the arrival time distribution asymptotically approaches the classical result in the limit of large mass.

### 3.4 Summary

To summarise, in this chapter we have investigated the classical limit of arrival time defined through the probability current. Here for the purpose of illustration we have considered the evolution of a quantum *free* particle represented by a Gaussian wave packet.

We have formulated the classical analogue of the arrival time distribution for an ensemble of *free* particles represented by a phase space distribution function evolving under the classical Liouville's equation. The expression for classical probability current constructed by us matches exactly with the quantum probability current density *only* when the position and momentum spread of the classical phase space distribution satisfy the minimum uncertainty condition. We have noted that the uncertainty condition is not a stringent requirement for the case of the initial classical distribution. Thus the classical arrival time distribution  $J_C(X, t)$  will in general be different from the quantum distribution  $J_Q(X, t)$  if we do not impose the minimum uncertainty restriction on the initial distribution. We have pointed out that this issue needs to be explored further in order to have a deeper understanding of the quantum-classical comparison of arrival time. However, in the example that we have constructed, the quantum results for the probability current and through it the arrival time distribution, approaches smoothly to the classical result in the large mass limit. Also, we emphasize that it is worthwhile to investigate the classical limit of arrival time distribution calculated from different theoretical approaches that have been suggested in the literature [31]-[43]. Such studies, if undertaken extensively, are not only expected to throw light on the comparative merits of different arrival time formulations, but could also be of relevance to the behaviour of mesoscopic systems where a great deal of experimental activity is presently underway [75].

In the discussion of classical limit of quantum mechanics it is usually assumed that the peak mean position of the wave packet moves according to the classical trajectory derived from the Ehrenfest theorem. It could be argued though that one should not expect to recover an individual classical trajectory when one takes the classical limit of quantum mechanics. Rather, one should expect the probability distributions of quantum mechanics to become equivalent to the probability distributions of an ensemble of classical trajectories. Our outlook is concerned about an approach to test the quantitative equivalence between the classical statistical prediction and the prediction obtained in the macroscopic limit of quantum mechanics. What we see is that the *mean time* of arrival of a freely moving quantum particle computed through the probability current depends on the mass of the particle even if its group velocity is fixed. Classically we know that a point particle with uniform motion will reach a particular location at a time which is

independent of the mass of the particle and depends only on its uniform velocity. So it turns out that the characteristic of *mean time* in this framework is different from that of mean position. The predicted mass dependence of mean arrival time is, in principle, amenable for experimental verification, and is a clear signature of the probability current approach to time in quantum mechanics.

## Chapter 4

### Wave packets under free fall

In this chapter we shall study the arrival time of quantum wave packets in free fall under gravitational potential. The status of the gravitational equivalence principle for quantum entities in the context of the classical limit of arrival time will be investigated by revisiting a quantum analogue of Galileo's leaning tower experiment [79]. We will see that the arrival time distribution for the particle calculated through probability current density approach and also the position probability density turn out to be mass dependent. The mean arrival time of the freely falling particle computed through the quantum probability current also exhibits mass dependence which vanishes in the limit of large mass. Though this indicates a manifest violation of the weak equivalence principle at the quantum level, the compatibility between the weak equivalence principle and quantum mechanics is recovered in the classical limit of the latter within this framework. We shall also discuss a classical statistical analogue of the same problem where we see a similar mass dependence on the position and arrival time distribution for a classical ensemble of particles described by a phase space distribution function which evolves according to the classical Liouville's equation. There seems to be curious parallelism between classical and quantum prediction. Before going into the details let us have a closer look at the role of equivalence principle in quantum mechanics.

#### 4.1 Quantum mechanics and the equivalence principle

As a consequence of the equality of gravitational and inertial mass, all classical test bodies fall with an equal acceleration independently of their mass or constituent in a

gravitational field. Historically, the first experimental study to probe this feature was conceived by Galileo with test bodies in free fall from the leaning tower of Pisa [80]. In modern times several tests have been performed with pendula or torsion balances leading to extremely accurate confirmations of the equality of gravitational and inertial masses [81]. Though most of these schemes consider only classical test bodies, there exist indications about the validity of the equality of gravitational and inertial masses even for quantum mechanical particles using the gravity-induced interference experiments [82, 83]. The universal character of the law of gravitation, however, has a much richer structure than the above equality, as embodied in the principle of equivalence in its various versions.

There are three statements of the equivalence principle which are equivalent according to classical physics but are logically distinct. Holland [44] emphasized the importance of separating them clearly in order to discuss their quantum analogues: (i) *Inertial mass is equal to Gravitational mass;  $m_i = m_g = m$ .* (ii) *With respect to the mechanical motion of particles, a state of rest in a sufficiently weak, homogeneous gravitational field is physically indistinguishable from a state of uniform acceleration in a gravity-free space.* A natural quantum analogue of this statement is [84]: “The laws of physics are the same in a frame with gravitational potential  $V = -mgz$  as in a corresponding frame lacking this potential but having a uniform acceleration  $g$  instead”. This is also true [85] in quantum mechanics because if  $\psi(z, t)$  be the wavefunction in the unaccelerated frame, obeying the free particle Schrödinger equation then under the coordinate transformation  $z' = z + \frac{1}{2}gt^2$ ,  $t' = t$ , the transformed wave function  $\phi(z', t')$  satisfies the same Schrödinger equation with an extra gravitational potential  $V = -mgz'$ . The old and the new wavefunctions are related by the following unitary transformation  $\phi(z', t') = e^{i\xi} \psi(z, t)$ ,  $\xi = (m/\hbar)(gt'z' - g^2t'^3/6)$ . Predictions of the Schrödinger equation in a noninertial frame have been shown to be experimentally observed [84]. (iii) *All sufficiently small test bodies fall freely with an equal acceleration independently of their mass or constituent in a gravitational field.* To obtain its quantum analogue this statement might be replaced by some principle such as the following [44]: “The results of experiments in an external potential comprising just a (sufficiently weak, homogeneous) gravitational field, as determined by the wavefunction, are independent of the mass of the system”. The status of this last version of the equivalence principle for quantum mechanical entities is the subject of investigation of

the present chapter. We shall henceforth call this version (iii) as the weak equivalence principle of quantum mechanics (*WEQ*).

The compatibility between the equivalence principle and quantum mechanics is an interesting issue which is yet to be completely settled. This issue was first elaborated in detail by Greenberger [86]. Evidence supporting the violation of *WEQ* already exists in interference phenomena associated with the gravitational potential in neutron and atomic interferometry experiments [82, 83] where the observable interference patterns are mass dependent. Further, at the theoretical level, on applying quantum mechanics to the problem of a particle bound in an external gravitational potential it is seen that the radii, frequencies and binding energy depend on the mass of the bound particle [85, 86, 87]. The possibility of quantum violation of the equivalence principle is also discussed in a number of other papers, for instance using neutrino mass oscillations in a gravitational potential [88].

Recently, Davies [89] has provided a particular quantum mechanical treatment of the violation of the equivalence principle for a quantum particle whose time of flight is proposed to be measured by a model quantum clock [90]. This model quantum clock actually measures the phase change of the wave function during the particle's transit of a specified spatial region. In this treatment Davies considered a variant of the simple Galileo experiment, where particles of different mass are projected vertically in a uniform gravitational field. Quantum particles are able to tunnel into the classically forbidden region beyond the classical turning point and the tunneling depth depends on the mass. One might therefore expect a small but significant mass-dependent "quantum delay" in the return time. Such a delay would represent a violation of *WEQ*. Using the concept of the Peres clock [90] the time of flight is calculated from the *stationary state* wave function for the quantum particle moving in a gravitational potential. However, this violation is *not* found far away from the classical turning point of the particle trajectory. Within a distance of roughly one de Broglie wave length from the classical turning point there were significant quantum corrections to the turn-around time, including the possibility of a mass-dependent delay due to the penetration of the classically forbidden region by the evanescent part of the wavefunction. Hence this quantum "smearing" of the equivalence principle is restricted to distances within the normal position uncertainty of a quantum

particle.

In a similar gedanken experimental scheme Viola and Onofrio [91] have studied the free fall of a quantum test particle in a uniform gravitational field. Using Ehrenfest's theorem for obtaining the average time of flight for a test mass, they have shown that if one takes gravitational mass to be equal to the inertial mass then the mean time taken by the particle to traverse a distance  $H$  under free fall is  $\langle t \rangle = \sqrt{2H/g}$  which is exactly equal to the classical result. A rough estimate of the fluctuations around this mean value was estimated using a semiclassical approach with the initial wave function taken as a Schrödinger cat state. This fluctuation around the mean time of flight was shown to be dependent on the mass of the particle.

In the present chapter, we study the issue of violation of *WEQ* from a somewhat different perspective. We consider an ensemble of identical quantum particles represented by a Gaussian wave packet which evolves under the gravitational potential. We first compute the *position detection probability* for the particles projected upwards against gravity around two different points; one around the classical turning point and another around a region of the initial projection point after it returns back. We show an explicit *mass dependence* of the position probability computed at both these points, thus indicating violation of the weak equivalence principle (*WEQ*) not only at the *turning point* of the classical trajectory, but also *far away* from it at the initial projection point. We then make use of the quantum probability current in computing the mean arrival time for a wave packet under free fall. We observe an explicit *mass dependence* of the *mean arrival time* at an arbitrary detector location indicating again the manifest violation of *WEQ*. Another issue of interest as discussed by Greenberger [87] is to understand whether compatibility with the weak equivalence principle (*WEQ*) is recovered in the macroscopic limit of quantum mechanics. We show that the quantum probability current approach of obtaining the mean arrival time [33, 36, 42, 43] addresses this issue in a manner such that the compatibility emerges smoothly in the limit of large mass of the wave packet.

In the next section we consider a Gaussian wave packet that is projected upwards against gravity with a certain mean velocity from a point of projection. We compute the position detection probabilities for atomic and molecular mass particles at the classical turning point of the gravitational potential, and also at the return to the point of

projection. The mass dependence of the position probabilities resulting from the spread of the wave packet is clearly exhibited. In Section 4.3 we consider the case when the particles are dropped from a height with zero initial velocity. We obtain the mean arrival time through the quantum probability current for an ensemble of such particles in free fall reaching an arbitrary detector location. The observed mass dependence of the mean arrival time vanishes smoothly in the limit of large mass giving the classical value of arrival time. Compatibility with the weak equivalence principle is seen to be restored in the macroscopic limit. In section 4.4 we study the classical statistical analogue of the wave packet under free fall. We conclude with a brief summary of our results in Section 4.5 highlighting the key differences emanating from our approach compared to earlier works.

## 4.2 Mass dependence of position detection probabilities

A beam of quantum particles with an initial Gaussian distribution is considered to be projected upwards against gravity. Subsequently, the position probability distribution is calculated within an arbitrary region either around the classical turning point of the potential  $V = m_g g z$  or away from the turning point around the region from where the particles were projected. Such an observable quantity turns out to be mass dependent, as seen below.

Let us consider particles of different inertial masses that are thrown upward against gravity with the same initial mean position and mean velocity. The initial states of the quantum particles can be represented by the Gaussian wave functions given by

$$\psi^j(z, t = 0) = (2\pi\sigma_0^2)^{-1/4} \exp(ik^j z) \exp\left(-\frac{z^2}{4\sigma_0^2}\right) \quad (4.1)$$

peaked at  $z = 0$  with the initial group velocity  $u = \hbar k^j / m_i^j$  where  $m_i^j$  is the inertial mass of the  $j^{\text{th}}$  particle. The momentum space wave function  $\phi^j(p, t = 0)$  is the Fourier transform of  $\psi^j(z, t = 0)$  and is given by

$$\phi^j(p, t = 0) = (2\pi\sigma_p^2)^{-1/4} \exp\left\{-\frac{(p - \bar{p})^2}{4\sigma_p^2}\right\} \quad (4.2)$$

where  $\sigma_p = \hbar/2\sigma_0^2$  and  $\bar{p} = m_i^j u$ . In order to perform an ideal free fall experiment for quantum particles having different inertial masses  $m_i^1, m_i^2, \dots$  etc. (with suffix  $i$  representing

the inertial mass, and with  $m_i^1 \neq m_i^2$  etc.), we have to specify a proper initial preparation in such a way that any difference in the motion during the free fall must be ascribed to the effect of gravity. Now, within the classical Hamilton picture the Galileian prescription for initial positions and velocities fixes the ratio between the initial momenta in a well-defined way, i.e.,  $p_0^1/p_0^2 = m_i^1/m_i^2$ , etc. Following Ref.[91], we extend such a prescription to the quantum case, of course keeping in mind that the Heisenberg uncertainty principle forbids the simultaneous definition of the initial position and momentum for each particle. If  $\psi_1$  and  $\psi_2$  denote the initial wave functions for particles 1 and 2 in the *Schrödinger* picture, the quantum analogue of the situation can be achieved by stipulating the conditions

$$\langle \hat{z} \rangle_{\psi_1} = \langle \hat{z} \rangle_{\psi_2} = 0, \quad \frac{\langle \hat{p}_z \rangle_{\psi_1}}{m_i^1} = \frac{\langle \hat{p}_z \rangle_{\psi_2}}{m_i^2} \equiv u \quad (4.3)$$

where  $\langle \hat{z} \rangle_{\psi}$  and  $\langle \hat{p}_z \rangle_{\psi}$  denote the expectation values for position and momentum operators, respectively (confining to a one dimensional representation along the vertical  $z$  direction). The probabilistic interpretation underlying quantum mechanics allows us only to speak of probability distributions, for instance, characterized by *mean* initial conditions such as Eq.(4.3), as opposed to the sharply-defined values for the relevant classical observables.

With the above prescription one can consider the time evolution of the initial state under the potential  $V = m_g^j g z$ , where  $V = m_g^j$  is the gravitational mass of the  $j$ -th particle. At any subsequent time  $t$  the *Schrödinger* time evolved wave function  $\psi^j(z, t)$  is given by

$$\begin{aligned} \psi^j(z, t) &= (2\pi s_t^2)^{-1/4} \exp \left[ \frac{\left( z - ut + (m_g^j/m_i^j) \frac{1}{2} g t^2 \right)^2}{4s_t \sigma_0} \right] \\ &\times \exp \left[ i(m_i^j/\hbar) \left\{ \left( u - (m_g^j/m_i^j) g t \right) (z - ut/2) \right\} \right] \\ &\times \exp \left[ i(m_i^j/\hbar) \left\{ - (m_g^j/m_i^j)^2 \frac{1}{6} g^2 t^3 \right\} \right] \end{aligned} \quad (4.4)$$

where  $s_t = \sigma_0 \left( 1 + i\hbar t / 2m_i^j \sigma_0^2 \right)$ . We see even if one takes  $m_i^j = m_g^j$ , i.e., equates the inertial mass with the gravitational mass, the observable position probability density  $|\psi^j(z, t)|^2$  will have an explicit mass dependence

$$|\psi^j(z, t)|^2 = (2\pi\sigma^2)^{-1/2} \exp \left[ - \frac{\left( z - ut + \frac{1}{2} g t^2 \right)^2}{2\sigma^2} \right] \quad (4.5)$$

coming from the spread of the wave packet given by  $\sigma = \sigma_0 \left(1 + \hbar^2 t^2 / 4m_i^j \sigma_0^4\right)^{1/2}$  which is mass dependent.

The peak of the wave packet follows the classical trajectory and it has a turning point at the time  $t = t_1 = u/g$  at  $z = z_c = ut_1$ . At a later time  $t = t_2 = 2u/g$ , when the peak of the wave packet comes back to its initial position  $z = 0$ , if we compute the probability of finding particles  $P_1(m_i^j)$  within a very narrow region  $(-\epsilon$  to  $+\epsilon)$  around the initial mean projection point  $z = 0$  then that probability is found to be a *function of mass* and is given by

$$P_1(m_i^j) = \int_{-\epsilon}^{+\epsilon} |\psi(z, t_2)|^2 dz \quad (4.6)$$

This effect of the *mass dependence* of the probability occurs essentially because the spreading of the wave packet under gravitational potential is different for particles of different masses. We explicitly calculate below this effect for different masses. A different set of mass dependent probability  $P_1(m_i^j)$  may be obtained by taking a different value of the initial width  $\sigma_0$  of the initial wave packet. In the table 4.1 it is shown numerically how the “probability of finding the particles”  $P_1(m_i^j)$  around the mean initial projection point ( $z=0$ ) changes with the variation of mass for an initial Gaussian position distribution. We note that for further increase in mass of the particle beyond that of a protein molecule, the change in the probability  $P_1(m_i^j)$  gets negligibly small, or in other words the mass dependence of the probability gets saturated.

We then compute the probability of finding particles  $P_2(m_i^j)$  at  $t = t_1 = u/g$  within a very narrow detector region  $(-\epsilon$  to  $+\epsilon)$  around a point which is the classical turning point  $z = z_c = ut_1$  for the particle.  $P_2(m_i^j)$  will also be a function of mass and is given by

$$P_2(m_i^j) = \int_{-\epsilon}^{+\epsilon} |\psi(z, t_1)|^2 dx \quad (4.7)$$

In the table 4.2 it is shown numerically how the “probability of finding the particles”  $P_2(m_i^j)$  around the classical turning point changes with the variation of mass for a initial Gaussian position distribution. As in the previous case, we again find that the mass-dependence of the probability  $P_2(m_i^j)$  for finding the particle gets saturated in the limit of large mass.

Table 4.1: Mass dependence of the probability at the initial projection point. We take  $u = 10^3$  cm/sec,  $\sigma_0 = 10^{-3}$  cm,  $\epsilon = \sigma_0$ ,  $t = t_2 = 2u/g$  sec.

<i>System</i>	<i>Mass(<math>m_i^j</math>)</i> <i>in(a.m.u)</i>	<i>Probability</i> $P_1(m_i^j)$
<i>H</i>	1.00	0.0012
<i>H</i> <sub>2</sub>	2.00	0.0024
<i>Li</i>	6.94	0.0085
<i>Be</i>	9.01	0.0111
<i>C</i>	12.01	0.0148
<i>Ag</i>	107.87	0.1305
<i>C</i> <sub>60</sub>	720.00	0.5428
protein molecule	$7.2 \times 10^4$	0.6826
heavier molecule	$7.2 \times 10^7$	0.6826

Table 4.2: Mass dependence of the probability at the turning point. We take  $u = 10^3$  cm/sec,  $\sigma_0 = 10^{-3}$  cm,  $\epsilon = \sigma_0$ ,  $t = t_1 = u/g$  sec.

<i>System</i>	<i>Mass(<math>m_i^j</math>)</i> <i>in(a.m.u)</i>	<i>Probability</i> $P_2(m_i^j)$
<i>H</i>	1.00	0.0024
<i>H</i> <sub>2</sub>	2.00	0.0049
<i>Li</i>	6.94	0.0171
<i>Be</i>	9.01	0.0222
<i>C</i>	12.01	0.0296
<i>Ag</i>	107.87	0.2522
<i>C</i> <sub>60</sub>	720.00	0.7277
protein molecule	$7.2 \times 10^4$	0.7978
heavier molecule	$7.2 \times 10^7$	0.7978

### 4.3 Mass dependence of mean arrival time and the classical limit

Now let us pose the problem in a different way. We consider the quantum particle prepared in the initial state given by Eq.(4.1) satisfying Eq.(4.3) and with  $u = 0$ . The particle is subjected to free fall under gravity. We then ask the question as to when does the quantum particle reach a detector located at  $z = Z$ . In classical mechanics, a particle follows a definite trajectory; hence the time at which a particle reaches a given location is a well defined concept. On the other hand, in standard quantum mechanics, the meaning of arrival time has remained rather obscure. As discussed in Chapter 1 there exists an extensive literature on the treatment of arrival time distribution in quantum mechanics. A consistent approach of formulating a definition for the arrival time distribution that we have adopted throughout this thesis is through the quantum probability current [33, 36, 42, 43]. The quantum probability current if defined in an unambiguous manner contains the spin of a particle, as was pointed out by Holland [48]. As shown in Chapter 2 using the explicit example of a Gaussian wave packet, the spin-dependence of the probability current leads to the spin-dependence of the mean arrival time for free particles [43]. However, for the case of massive spin-0 particles it has been shown recently by taking the non-relativistic limit of Kemmer equation [50] that the unique probability current is given by the Schrödinger current [51]. Hence, the Schrödinger probability current density can be used to define an unambiguous arrival time distribution for spin-0 particles that are relevant for the present analysis.

The expression for the Schrödinger probability current density  $J(Z, t)$  at the detector location  $z = Z$  for the time evolved state is calculated using the initial state prepared in the Gaussian form given by Eq.(4.1) and satisfying Eq.(4.3). The particle falls freely under gravity along  $-\hat{z}$  direction from the initial peak position at  $z = 0$  with  $u = 0$  and  $J(Z, t)$  is given by

$$J(Z, t) = \rho(Z, t) v(Z, t) \quad (4.8)$$

where

$$\rho(Z, t) = (2\pi\sigma^2)^{-1/2} \exp\left[-\frac{(Z - \frac{1}{2}gt^2)^2}{2\sigma^2}\right] \quad (4.9)$$

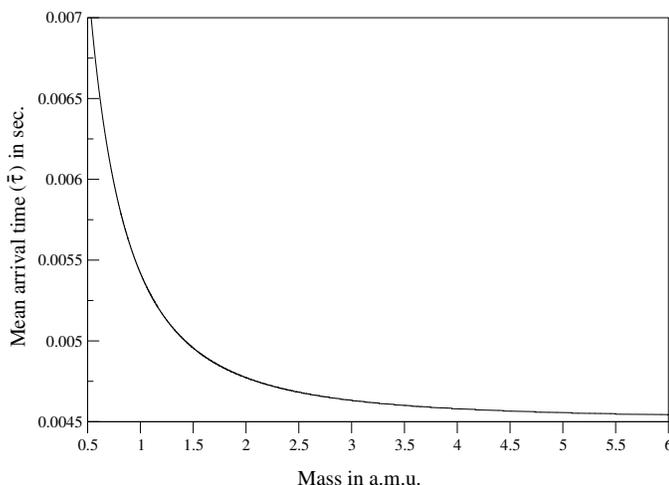


Figure 4.1: The variation of mean arrival time with mass (in atomic mass unit) at a detector location  $Z$  for an initial Gaussian position distribution. We take  $\sigma_0 = 10^{-4}$  cm,  $Z = 10^{-2}$  cm.

and

$$v(Z, t) = \left[ gt + \frac{\hbar^2 t}{4m_i^{j2} \sigma_0^2 \sigma^2} (Z - gt^2/2) \right] \quad (4.10)$$

Taking the modulus of the probability current density as determining the arrival time distribution, the mean arrival time  $\bar{\tau}$  at a particular detector location is computed for an ensemble of particles with an initial Gaussian position distribution *falling freely* under gravity. Then this observable quantity  $\bar{\tau}$  is given by

$$\bar{\tau}(m_i^j) = \frac{\int_0^\infty |J(Z, t)| t dt}{\int_0^\infty |J(Z, t)| dt} \quad (4.11)$$

Since  $\sigma = |s_t| = \sigma_0 \left(1 + \hbar^2 t^2 / 4m_i^{j2} \sigma_0^4\right)^{1/2}$  is mass dependent, it is seen from Eqs.(4.8–4.10) that  $J(Z, t)$  is mass-dependent. Hence the mean arrival time  $\bar{\tau}$  calculated by using Eq.(4.11) for the Gaussian wave packets corresponding to different masses falling freely under gravity is also mass dependent.

In Figure 4.1 we depict the variation with mass of the mean arrival time at a particular detector location for an ensemble of particles under free fall. The initial conditions are taken as  $\langle z \rangle_0 = 0$  and  $\langle p \rangle_0 = 0$ , where  $\langle z \rangle_0$  and  $\langle p \rangle_0$  are the position and momentum expectation values at  $t = 0$ . Note again that though the integral in the numerator of

Eq.(4.11) formally diverges, as in the case of Eq.(3.3) of Chapter 3 here also we employ the strategy of taking a cut-off ( $t = T$ ) in the upper limit of the time integral with  $T = \sqrt{2(Z + 3\sigma_T)/g}$  where  $\sigma_T$  is the width of the wave packet at time  $T$ . Thus, our computations of the arrival time are valid up to the  $3\sigma$  level of spread in the wave function. One can also see from Figure 4.1 that the mean arrival time  $\bar{\tau}$  asymptotically approaches the classical result (mass independent) in the limit of large mass.

#### 4.4 Classical statistical analogue of a wave packet under free fall

Now we discuss the behaviour of a classical ensemble of particles which evolves under a homogeneous gravitational potential. Here we adopt the same strategy that was used in discussing the classical limit problem of the arrival time of wave packets of free particles in Chapter 3. To calculate classical propagation we choose an expression for the initial phase space distribution (at time  $t=0$ ) for the ensemble of particles as a product of two Gaussian functions matching with the initial quantum position and momentum distributions from Eq.(4.1) and (4.2) which is given by

$$\begin{aligned} D_0(z_0, p_0, 0) &= |\psi^j(z, 0)|^2 |\phi^j(p, 0)|^2 \\ &= \frac{1}{(2\pi\sigma_0^2)^{1/2}} \exp\left\{-\frac{z_0^2}{2\sigma_0^2}\right\} \frac{1}{(2\pi\sigma_p^2)^{1/2}} \exp\left\{-\frac{(p_0 - \bar{p})^2}{2\sigma_p^2}\right\} \end{aligned} \quad (4.12)$$

where  $\sigma_0\sigma_p = \hbar/2$  and the variables  $z_0$  and  $p_0$  are the initial positions and momenta of the particles. Classically of course, there are other choices for  $D_0(z_0, p_0, 0)$ . But in quantum mechanics, due to the uncertainty principle, given a wave function  $\psi^j(z, 0)$ , the momentum space wave function  $\phi^j(p, 0)$  is automatically fixed by the Fourier transform of  $\psi^j(x, 0)$ . There is no such restriction for the position and momentum densities in classical statistical mechanics. But it is quite reasonable to take the initial classical phase space distribution exactly matching with the initial quantum position and momentum probability densities in order to compare the results obtained from the dynamical evolutions of classical and quantum mechanics. This is precisely the motivation to take the initial phase space distribution  $D_0(z_0, p_0, 0)$  in a way given by Eq.(4.12). Now to obtain the final time evolved density function  $D(z, p, t)$  we focus on the classical dynamics of a single particle moving in a gravitational potential  $V = mgz$ . We take the inertial mass equal to the

gravitational mass from the outset. The Hamiltonian is given by  $H = \frac{p^2}{2m} + mgz$ . The Hamilton's equations are  $z = z_0 + \frac{p_0 t}{m} - \frac{1}{2}gt^2$  and  $p = p_0 - mgt$  where the variables  $z_0$  and  $p_0$  are the initial position and momentum of the particle which are respectively given by  $z_0 = z - \frac{pt}{m} - \frac{1}{2}gt^2$  and  $p_0 = p + mgt$ . Substituting these values of  $z_0$  and  $p_0$  in the expression of  $D_0(z_0, p_0, 0)$  we obtain the final time evolved distribution function  $D(z, p, t)$ . This is because here we are considering the evolution of an ensemble of particles (under gravity) whose initial positions ( $z_0$ ) and momenta ( $p_0$ ) are distributed according to the initial density function  $D_0(z_0, p_0, 0)$ . The time evolved phase space distribution satisfying the Liouville's equation under  $V = mgz$  potential is then given by

$$D(z, p, t) = \frac{1}{(2\pi\sigma_0^2)^{1/2}} \exp\left\{-\frac{(z - \frac{pt}{m} - \frac{1}{2}gt^2)^2}{2\sigma_0^2}\right\} \frac{1}{(2\pi\sigma_p^2)^{1/2}} \exp\left\{-\frac{(p + mgt - \bar{p})^2}{2\sigma_p^2}\right\}$$

which satisfies the classical Liouville's equation given by

$$\frac{\partial D}{\partial t} = -\left\{\frac{\partial D}{\partial z} \frac{\partial H}{\partial p} - \frac{\partial D}{\partial p} \frac{\partial H}{\partial z}\right\} \quad (4.13)$$

The time evolved position probability density  $\rho_C(z, t)$  is given by

$$\begin{aligned} \rho_C(z, t) &= \int_{-\infty}^{\infty} D(z, p, t) dp \\ &= \frac{1}{(2\pi\sigma_c^2)^{1/2}} \exp\left\{-\frac{(z - \frac{\bar{p}t}{m} + \frac{1}{2}gt^2)^2}{2\sigma_c^2}\right\} \end{aligned} \quad (4.14)$$

where  $\sigma_c^2 = (\sigma_0^2 + \sigma_p^2 t^2 / m^2)$ . If we take  $\sigma_0 \sigma_p = \hbar/2$  from the outset, *i.e.* the minimum uncertainty condition then the above classical position probability density for the ensemble will be the same as that obtained for a quantum particle moving in a uniform gravitational potential. One can check that the classical current also matches with the quantum current in this particular choice of the initial phase space distribution. It is curious to see the parallelism between classical and quantum prediction although the two formalisms are so different. It appears from the classical phase space description that the mass dependence of the probability distributions comes from the uncertainty in position and momentum because in single particle classical dynamics this mass dependence does not occur due to the equivalence principle.

## 4.5 Summary

To summarise, we have studied the free fall of quantum *wave packets* under gravitational potential in the context of the equivalence principle by revisiting a gedanken quantum analogue of Galileo's leaning tower experiment. The position probability density and the arrival time distribution for the particle calculated through probability current density exhibits mass dependence. The observable position probability and the *mean time* (computed through the quantum probability current) taken by the freely falling particle to arrive at a particular location are also shown to be mass dependent. Our results of mass-dependence of these observable quantities indicate the manifest violation of a particular form of the quantum analogue of the weak equivalence principle. The variation of the detection probability with mass disappears in the limit of large mass of the freely falling particles, as is expected for classical objects. This saturation of the detection probability is also reflected in the mean arrival time distribution defined through the quantum probability current, which approaches the classical result in a continuous manner with the increase of mass.

We have seen that the compatibility of the weak equivalence principle (*WEQ*) with quantum mechanics can be achieved in the classical limit within this framework for particles falling freely under gravity. The probability current approach for computation of the mean arrival time of a quantum ensemble not only provides an unambiguous definition of arrival time at the quantum mechanical level, but also addresses the issue of obtaining the proper classical limit of the time of flight of massive quantum particles. Finally, we have discussed a classical statistical analogue of the same problem where we see a similar mass dependence in the position and arrival time distribution for a classical ensemble of particles described by a phase space distribution function which evolves according to the classical Liouville's equation.

## Chapter 5

# Quantum superarrivals

### 5.1 Overview

In recent years a number of interesting investigations have been reported on the wave-packet dynamics [92, 93]. Schrödinger and others [94]-[97] discussed the connections between the quantum and classical descriptions of nature by exhibiting explicit wave packet evolutions to many familiar problems, including the cases of the free-particle, uniform acceleration (constant electric or gravitational field), and under harmonic oscillator (forerunner of coherent and squeezed states) potential. The importance of the study of localized, time-dependent solutions to bound state problems in quantum mechanics, specially the various interesting aspects of wave packet propagation in an infinite potential well has been reviewed by Robinett [98]. The development of modern experimental techniques, involving the laser-induced excitation of atomic Rydberg wave packets, including the use of the “pump-probe” [99] or “phase modulation” [100] techniques to produce, and then monitor the subsequent time-development of such highly excited states of atoms and molecules led to widespread interest [98, 101] in the physics of wave packet dynamics including the phenomenon of quantum wave packet revivals [102], fractional revivals [103] and superrevivals [104] *etc.*

In the next section we shall elaborately discuss a curious effect on the reflection/transmission probabilities (or the probabilities of arrival at the left and right of a barrier) for a propagating wave packet which encounters a *time-dependent* rectangular potential barrier, named as the phenomenon of superarrivals. A detailed description of superarrivals will be provided by showing that if the barrier height is reduced while the wave packet

is being scattered, the time-evolving probability of reflection is larger during a specific interval of time in comparison to the reflection probability for a static barrier. It will also be shown that this counterintuitive effect also occurs in the transmitted probability provided a barrier is raised in the path of a freely propagating wave packet. The genesis of the work of superarrivals is from the effect of a time-dependent boundary on a wave packet associated with a particle in one dimensional infinite well where the particle is considered to be localized within the interior of the box, far away from the walls (which means that the wave function at the walls can be considered to be effectively zero) as was first proposed by Greenberger [93]. We shall now discuss it in detail in order to motivate our study in the next sections. For simplicity, we consider the walls of the box to be infinitely high. If now, one wall of the box is moved, so that the box grows wider, or narrower, the eigenfunctions of the Hamiltonian will grow or shrink accordingly, since the wave function must vanish at the walls. The particle wave function must be expandable in terms of these functions, and this will have two effects on the subsequent behaviour of the particle.

First, as the walls expand, the eigenvalues of the Hamiltonian will change, and so the term corresponding to  $\exp(\int E dt/\hbar)$  will produce a “dynamical” phase shift. But also, because the centre of mass of each eigenfunction will shift, as it will still be in the middle of the well, the wave function will acquire a phase representing the added momentum, and this will be reflected in what Berry calls a “geometrical” phase shift [105]. These two effects will affect the wave function of the particle, and even if the motion of the wall is then reversed, to bring it back to its original position, the overall motion will leave its imprint upon the wave function of the particle (it will experience a phase shift), even though the particle has never been in the vicinity of the wall, nor felt any force. This is a true non-local effect, utterly foreign to classical physics. Let us now see how this actually occurs. For a particle in an infinite square well, whose width is  $L_0$ , the Schrödinger equation is

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\left(\frac{x}{L_0}\right) \psi = i\hbar \frac{\partial \psi}{\partial t}, \quad (5.1)$$

where the wave function is subject to the boundary condition

$$\psi(x=0) = \psi(x=L_0) = 0 \quad (5.2)$$

Then the normalized solutions are

$$\psi_n = \sqrt{\frac{2}{L_0}} \text{Sin} \frac{n\pi x}{L_0}, \quad E_n = \frac{\hbar^2 n^2 \pi^2}{2mL_0^2} \quad (5.3)$$

If now the width of the box is variable, so that  $L_0 \rightarrow L = L(t)$ , then the Schrödinger equation is unchanged, but the boundary condition, Eq.(5.2) becomes

$$\psi(x=0) = \psi(x=L(t)) = 0 \quad (5.4)$$

and so one must solve the same equation, subject to this new condition. Introducing in place of the variables  $x, t$ , the new set of variables  $y, t'$ , where  $y = x/L(t)$ ,  $t' = t$ , so that

$$\frac{\partial}{\partial x} = \frac{1}{L} \frac{\partial}{\partial y} \quad \text{and} \quad (5.5)$$

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial t'} - \frac{\dot{L}}{L} y \frac{\partial}{\partial y}. \quad (5.6)$$

In terms of these new variables, the Schrödinger equation becomes

$$-\frac{\hbar^2}{2mL^2} \frac{\partial^2 \psi}{\partial y^2} + i\hbar \frac{\dot{L}}{L} y \frac{\partial \psi}{\partial y} + V(y)\psi = i\hbar \frac{\partial \psi}{\partial t}, \quad (5.7)$$

where we have set  $t' = t$ . Substituting

$$\psi = \frac{1}{\sqrt{L}} e^{i(m/2\hbar)L\dot{L}y^2} u(y, t), \quad (5.8)$$

the equation for  $u(y, t)$  becomes

$$-\frac{\hbar^2}{2m} \frac{\partial^2 u}{\partial y^2} + \left[ L^2 V(y) + \frac{m}{2} L^3 \ddot{L} y^2 \right] u = i\hbar \dot{L} L^2 \quad (5.9)$$

For simplicity, we restrict ourselves to the case of an infinite square well,

$$V(y) = \begin{cases} 0, & 0 \leq y \leq 1; \\ \infty, & \text{elsewhere.} \end{cases}$$

where the walls are expanded linearly (we choose the simplest case),  $L = L_0 + \alpha t$ , and where  $\alpha$  can be positive or negative. In this case, the term in brackets of Eq.(5.9) vanishes, and the exact solutions, subject to the boundary condition, Eq.(5.4), are

$$\psi_n(x, t) = \phi_n(y, t) e^{-i \int E_n dt / \hbar}, \quad \text{where} \quad (5.10)$$

$$\phi_n(y, t) = \sqrt{\frac{2}{L}} \exp\left(\frac{im\alpha Ly^2}{2\hbar}\right) \text{Sin}(n\pi y), \quad E_n = \frac{\hbar^2 n^2 \pi^2}{2mL^2} \quad (5.11)$$

The purpose of the “geometric” phase factor in this wave function is to keep track of the momentum. If one wall is expanding at the rate  $\dot{L}$ , then the average momentum of the eigenfunction wave packet is  $m\alpha/2$ , and the packet will have acquired an average velocity  $\alpha/2$ . One can calculate this directly, since

$$\langle p \rangle = \int \psi_n^* \left( -i\hbar \frac{\partial}{\partial x} \right) \psi_n dx = \frac{m\alpha}{2} = \frac{m\dot{L}}{2} \quad (5.12)$$

These wave functions possess a sort of orthogonality in the sense that

$$\int_0^L \psi_n(x, t)^* \psi_m(x, t) dx = \delta_{nm}, \quad (5.13)$$

for any  $t$ , and so one may make an expansion,

$$\psi(x, 0) = \sum a_n \psi_n(x, 0) \quad \text{and} \quad a_n = \int_0^{L_0} \psi_n(x, 0)^* \psi(x, 0) \quad (5.14)$$

and at arbitrary times one has

$$\psi(x, t) = \sum a_n \psi_n(x, t) \quad (5.15)$$

even though the functions  $\psi_n$  are not “stationary” in the usual sense, since  $L = L(t)$ . As an example, Greenberger [93] took a Gaussian wave packet associated with the particle as  $\psi_0 = A e^{-(x-b)^2/\gamma^2}$  where  $L_0 \geq b \geq \gamma$ , so that the packet is much smaller than the width of the well, and is located well away from the walls. Then one lets the wall expand linearly, so that  $L = L_0 + \alpha t$  until time  $t_1$ ; then contracts it until time  $t_2 = 2t_1$ , so that  $L = L_1 - \alpha(t - t_1)$ , then the wall will end up at the same width it started at. If one calculates the final wave function  $\psi(x, t_2)$  then it will be seen that the overall motion of the walls leave its imprint upon the wavefunction of the particle even though the particle has never been in the vicinity of the wall, nor felt any force. In the context of the above theoretical study an experiment was done [106] using neutron interferometry

to measure the phase shift arising from lateral confinement of a neutron beam passing through a narrow slit system. The phase shift arises mainly from neutrons whose classical trajectories do not touch the walls of the slits. In this respect, the non-locality of quantum physics is apparent.

## 5.2 Wave packet dynamics under time-varying potential barriers

Let us now discuss a curious effect on the reflection/transmission probabilities for a propagating wave packet which encounters a time-dependent rectangular potential barrier. The reflection/transmission probabilities for the scattering of wave packets by various obstacles are usually considered from static or unperturbed potential barriers. Generally, the time-independent (asymptotic) values of the reflection/transmission probabilities attained *after* a complete time evolution are calculated. Here we discuss an interesting effect that occurs *during* the time evolution of the wave packet. The dynamics of the wave packet is studied in detail when the packet is scattered from a barrier whose height is increased/decreased. It is seen that the time-dependent reflection/transmission probabilities gradually increases with time and finally the time-independent asymptotic values are reached after a sufficiently large time. An intermediate time interval is found during which this time-evolving probability of reflection/transmission is enhanced compared to the unperturbed case. To understand this counterintuitive phenomenon called superarrivals [107] (which is quantum mechanical in origin) let us first sketch the general description of the problem.

A time evolving gaussian wave packet strikes a potential barrier of height  $V_0$  and width  $\omega$ , a part of it is transmitted and a part is reflected. Now, when the Gaussian packet is coming towards the barrier, once it overlaps sufficiently with the barrier, we perturb the barrier in various ways and see what happens to the incident packet. The reflected particles are registered by a detector placed either to the left (for reflection) or to the right (for transmission) of the barrier. We first study the case of reflection. We place the detector in the left at  $x = x'$ . Here we perturb the barrier by reducing its height

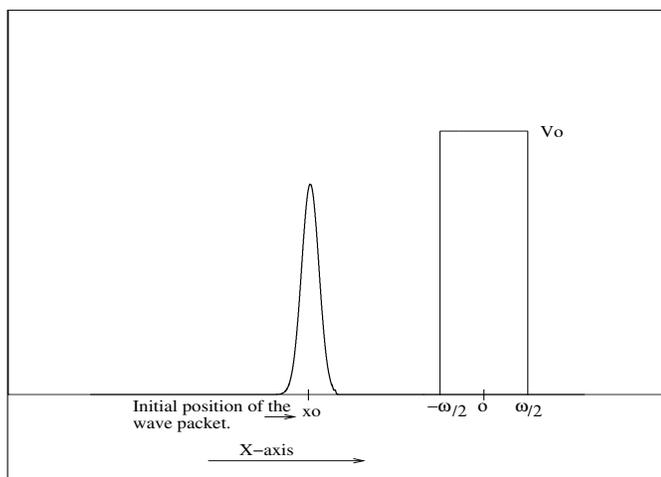


Figure 5.1: Description of the problem

from  $V_0$  to 0 within a very short interval of time. We reduce the barrier height linearly with time. The parameters of the barrier and the incident wave packet are so chosen such that the reflection probability is very close to one for the unperturbed barrier. For an unperturbed barrier the reflection probability for an initially localized wave packet  $\psi(x, t = 0)$  is calculated by considering the wave packet as a superposition of plane waves and by writing

$$|R_0|^2 = \int |\phi(p)|^2 |R(p)|^2 dp \quad (5.16)$$

where  $|R(p)|^2$  is the reflection probability corresponding to the plane wave component  $\exp(ipx)$  and  $\phi(p)$  is the Fourier transform of the initial wave packet  $\psi(x, t = 0)$ . Since a wave packet evolves in time,  $|R_0|^2$  defined by Eq.(5.16) denotes the time-independent value of reflection probability pertaining to a wave packet, this value being attained in the asymptotic limit ( $t_\infty$ ) of the time evolution. Thus  $|R_0|^2$  can be expressed in the following form:

$$|R_0|^2 = \int_{-\infty}^{x'} |\psi(x, t_\infty)|^2 dx \quad (5.17)$$

where  $\psi(x, t_\infty)$  is an asymptotic form of the wave packet attained by evolving from  $\psi(x, t = 0)$  and by being scattered from a rectangular potential barrier of finite height and width.

Note that  $x'$  lies at the left of the initial profile of the wave packet such that  $\int_{-\infty}^{x'} |\psi(x, t = 0)|^2 dx$  is negligible. Equivalence between the expressions (5.16) and (5.17) in the limit of large (compared to the time taken by the packet to get reflected from the barrier)  $t$  has been checked numerically. At any instant *before* the constant value  $|R_0|^2$  is attained, the time evolving reflection probability in the region  $-\infty < x \leq x'$  is thus given by

$$|R(t)|^2 = \int_{-\infty}^{x'} |\psi(x, t)|^2 dx \quad (5.18)$$

Now, suppose that *during* the time evolution of this wave packet, the barrier is perturbed by reducing its height to zero within a very short interval of time that is small compared to the time taken by the reflection probability to attain its asymptotic value  $|R_0|^2$ . The effects of this “sudden” perturbation on  $|R(t)|^2$  are computed. The salient features are as follows: (a) A finite time interval is found during which  $|R(t)|^2$  shows an *enhancement* (“superarrivals”) in the perturbed case even though the barrier height is reduced. This time interval and the amount of enhancement depend on the *rate* at which the barrier height is made zero. (b) It can be shown that the phenomenon of superarrivals is inherently quantum mechanical by demonstrating that superarrivals *disappear* in the classical treatment of the problem. (c) The *origin* of superarrivals may be understood by considering the wave function to act as a “field” through which a disturbance from the “kick” provided by perturbing the barrier travels with a definite speed.

In order to demonstrate the above features we begin by writing the initial wave packet (in the units of  $\hbar = 1$  and  $m = 1/2$ )

$$\psi(x, t = 0) = \frac{1}{[2\pi(\sigma_0)^2]^{1/4}} \exp\left[-\frac{(x - x_0)^2}{4\sigma_0^2} + ip_0x\right] \quad (5.19)$$

which describes a packet of width  $\sigma_0$  centered around  $x = x_0$  with its peak moving with a group velocity  $v_g = 2p_0 = \frac{\langle p \rangle}{m}$  towards a rectangular potential barrier. The point  $x_0$  is chosen such that  $\psi(x, t = 0)$  has a negligible overlap with the barrier. For computing  $|R(t)|^2$  given by Eq.(5.18) the time dependent Schrodinger equation is solved by using the numerical methods developed by Goldberg, Schey and Schwartz [108]. As a specific example, the parameters can be chosen as  $x_0 = -0.4$ ,  $\sigma_0 = 0.05/\sqrt{2}$  and  $p_0 = 50\pi$ . The barrier is centered around  $x_c = 0$  with a width  $\omega$  taken to be 0.016. For such a

width, height of the barrier ( $V$ ) before perturbation is chosen to be  $V = 2E$ , where  $E$  is the expectation value of the energy of the wave packet given by  $p_0^2 + \frac{1}{4}\sigma_0^{-2}$ . This choice ensures that: (1) The reflection probability is close to 1 since we are interested only in the reflection probability. (2) At the same time  $V$  is not too large. This ensures that the reduction of the barrier height is not too fast.

$|R(t)|^2$  is computed according to Eq.(5.18) by taking various values of  $x'$  satisfying the condition  $x' \leq x_0 - 3\sigma_0/\sqrt{2}$ . The computed evolution of  $|R(t)|^2$  corresponds to the building up of reflected particles with time. More precisely, it means that a detector located within the region  $-\infty < x < x'$  measures  $|R(t)|^2$  by registering the reflected particles arriving in that region up to various instants. First, we compute  $|R(t)|^2$  for the wave packet scattered from a static barrier  $V = 2E$ . The relevant curve is shown in Figure 5.2 which tends towards a time-independent value which is the stationary state reflection probability  $|R_0|^2$  given by Eq.(5.16), or equivalently by Eq.(5.17). Next, we proceed to study the consequence of reducing the barrier height from  $V = 2E$  to  $V = 0$ . The time evolution of  $|R(t)|^2$  in this case is studied by varying the ways in which the barrier height is reduced. If  $t_p$  be the instant around which we start to reduce the barrier height, then

$$\begin{aligned} V &= V_0 && \text{for } t < t_p \\ V &= \frac{(t_p + \epsilon - t)}{\epsilon} V_0 && \text{for } t_p < t < t_p + \epsilon \\ V &= 0 && \text{for } t > t_p + \epsilon \end{aligned}$$

In the specific cases studied, the potential  $V$  goes to zero linearly within a switching off time  $\epsilon$  starting at time  $t = t_p$  chosen to be  $8 \times 10^{-4}$  (note that numbers denoting the various instants are in terms of time steps; for example,  $t = 8 \times 10^{-4}$  corresponds to 400 time steps). Here  $\epsilon \ll t_0$ ,  $t_0$  being the time required for  $|R(t)|^2$  to attain the asymptotic value  $|R_0|^2$ . The short time span  $\epsilon$  over which the perturbation takes place is given by  $[t_p, t_p + \epsilon]$ .  $t_p$  is chosen such that at that instant the overlap of the wave packet with the barrier is significant. Figure 5.3 shows the evolution of  $|R(t)|^2$  for various values of  $\epsilon$ . Varying  $\epsilon$  signifies changing the time span over which the barrier height goes to zero which in turn means different rates of reduction. Figure 5.2 reveals that

$$|R_p(t)|^2 = |R_s(t)|^2 \quad t \leq t_d \quad (5.20)$$

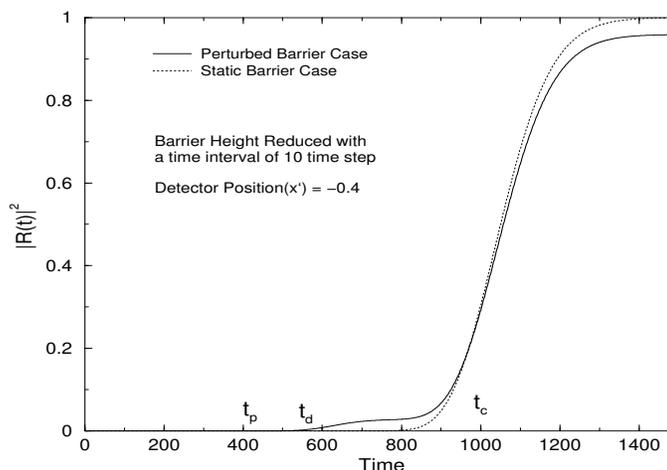


Figure 5.2: The reflection probability for particles reflected from a perturbed barrier is plotted against time (solid line). The corresponding reflection probability for the static barrier is shown by the dotted line.

$$|R_p(t)|^2 > |R_s(t)|^2 \quad t_d < t \leq t_c \quad (5.21)$$

$$|R_p(t)|^2 < |R_s(t)|^2 \quad t > t_c \quad (5.22)$$

where  $t_c$  is the instant when the two curves cross each other, and  $t_d$  is the time from which the curve corresponding to the perturbed case starts deviating from that in the unperturbed case. Here  $t_c > t_d > t_p$ .

As the barrier height is made zero, one does not expect at any time an increase in the reflected particle flux compared to that in the unperturbed case. Nevertheless, the inequality (5.21) shows that there is a finite time interval  $\Delta t \equiv t_c - t_d$  during which the probability of finding reflected particles is *more* (superarrivals) in the perturbed case than when the barrier is left unperturbed (see Figure 5.2). A detector placed in the region  $x < x'$  would therefore register *more* counts during this time interval  $\Delta t$  even though the barrier height had been *reduced* to zero *prior* to that.

In order to have a *quantitative measure* of superarrivals one can define the parameter  $\eta$  given by

$$\eta = \frac{I_p - I_s}{I_s} \quad (5.23)$$

where the quantities  $I_p$  and  $I_s$  are defined with respect to  $\Delta t$  during which superarrivals

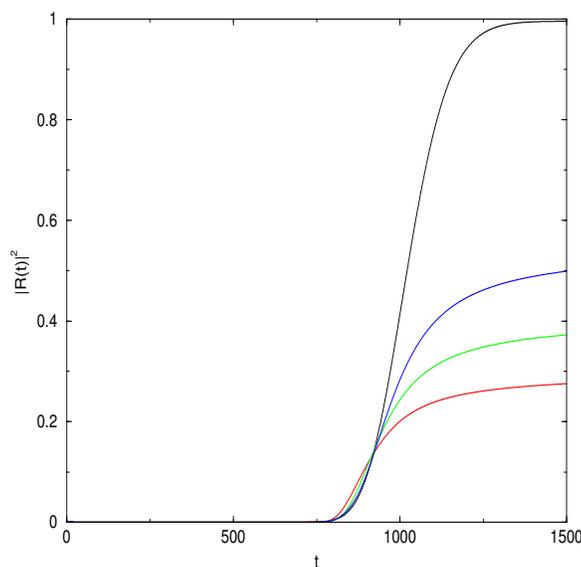


Figure 5.3: The top curve corresponds to the static case and reaches value 1 asymptotically.  $|R(t)|^2$  for other curves correspond to various values of  $\epsilon$ . The curve with the lowest asymptotic value corresponds to the smallest value of  $\epsilon$  chosen for this set. As one increases  $\epsilon$ , superarrivals are slowly wiped off.

occur

$$I_p = \int_{\Delta t} |R_p(t)|^2 dt \quad (5.24)$$

$$I_s = \int_{\Delta t} |R_s(t)|^2 dt \quad (5.25)$$

We plot the variation of  $\eta$  with respect to  $\epsilon$  for three different detector positions in Figure 5.4. The results obtained from Figures 5.2–5.4 can be summarized as follows: (a) There exists a finite time interval  $\Delta t$  during which an *increase* in the reflection probability (superarrivals) occurs for the perturbed cases compared to the unperturbed situation. (b) Superarrivals are inherently *nonclassical*. (c) The magnitude of superarrivals  $\eta$  is appreciable only in cases where the wave packet has some *significant overlap* with the barrier during its switching off. Both  $\eta$  and  $\Delta t$  (duration of superarrivals) *fall off* with *increasing*  $\epsilon$ . (d) Superarrivals given by  $\eta$  gradually reduce to *zero* upon *decreasing* the barrier width, while keeping the initial barrier height  $V_0$  fixed.

The above example of superarrivals in the reflection probability when the barrier height is brought down is not the only example of superarrivals with time dependent barriers.

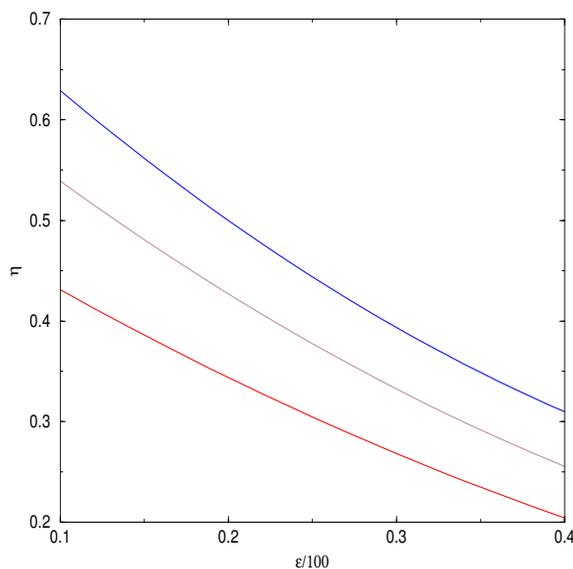


Figure 5.4: The magnitude of superarrivals  $\eta$  diminish with an increase in  $\epsilon$ , the time taken for barrier height reduction. This behaviour is seen for three different detector positions  $x' = -0.4, -0.5$  and  $-0.6$  respectively.

Indeed, other cases of time dependent barriers with oscillating height and width can be considered to lead to superarrivals in the reflected as well as transmitted probabilities. Let us now consider the case when initially there is no barrier, and the wave packet is allowed to propagate freely towards the right. A second detector placed far away at  $x''$  records the time-dependent transmission probability  $T_s(t)$  (counting the transmitted particles up to various instants of time). If a barrier is raised in the path of the wave packet, a portion of it will be reflected back. We denote by  $T_p(t)$  the transmitted probability in this case. At any instant *before* the asymptotic value of the transmission probability ( $= 1$  since there is no absorption) is attained, the time evolving transmission probability in the region  $x'' \geq x \geq \infty$  is given by

$$|T(t)|^2 = \int_{x''}^{\infty} |\psi(x, t)|^2 dx \quad (5.26)$$

one can compute the values of  $T_s(t)$  and  $T_p(t)$  using the same method of numerically solving the time dependent Schrödinger equation as used in [107], which was first developed in [108]. An example with the following values for the parameters has been studied [109] (in units of  $\hbar = 1$  and  $m = 1/2$ ):  $x_0 = -0.3$ ,  $\sigma_0 = 0.05/\sqrt{2}$ ,  $x_c = 0$ ,  $w = 0.016$ ,  $x'' = 0.5$  and  $t_p = 8 \times 10^{-4}$ . It should be emphasized that the observation of the phenomenon of

superarrivals does *not* hinge upon the choice of these particular values of the parameters. Indeed, the quantitative dependence of superarrivals on the parameter values were shown in the previous section. We choose one particular set of values here for the present example. The potential barrier is raised from  $V = 0$  to  $V = 2E$  (where  $E$  is the average energy of the incident wave packet) linearly in time. If  $t_p$  be the instant around which we start to rise the barrier height, then the change of barrier height with time is given as follows (here for the case of transmission),

$$\begin{aligned} V &= 0 && \text{for } t < t_p \\ V &= \frac{(t - t_p)}{\epsilon} V_0 && \text{for } t_p < t < t_p + \epsilon \\ V &= V_0 && \text{for } t > t_p + \epsilon \end{aligned}$$

In Figure 5.5 we plot the computed values of  $T_s(t)$  and  $T_p(t)$  for different values of  $\epsilon$ , the time taken for raising the barrier from 0 to  $V_0$ . It is seen that superarrivals are also exhibited in the transmitted wave packet. Superarrivals can be quantitatively defined here in the case of transmission by a parameter  $\eta'$  (which has been plotted against  $\epsilon$  in Figure 5.6) given by

$$\eta' = \frac{I'_p - I'_s}{I'_s} \quad (5.27)$$

where the quantities  $I'_p$  and  $I'_s$  are defined with respect to  $\Delta t = (t_c - t_d)$  during which superarrivals occur for the case of transmitted wave packet

$$I'_p = \int_{\Delta t} |T_p(t)|^2 dt \quad (5.28)$$

$$I'_s = \int_{\Delta t} |T_s(t)|^2 dt \quad (5.29)$$

Next, we consider the question as to *how fast* the influence of barrier perturbation travels across the wave packet (signal velocity  $v_e$ ). Note that even in a classical theory the information content of a wave packet does *not* always propagate with the group velocity  $v_g$  of a wave packet which is usually identified with the velocity of the peak of a wave packet [110]. Profiles of the quantum wave packet are plotted at various instants in Figure 5.7. An incident packet gets distorted upon hitting the time-varying barrier. It

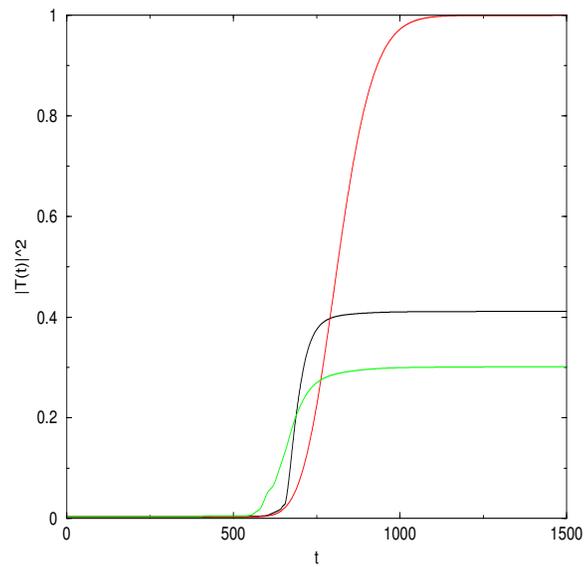


Figure 5.5: The transmission probability  $|T(t)|^2$  is plotted for various values of  $\epsilon$ . The top curve reaches value 1 asymptotically and corresponds to the zero barrier case. The next two curves with ( $\epsilon = 10$ ) and ( $\epsilon = 40$ ) respectively, represent the transmission probabilities for the rising barriers.

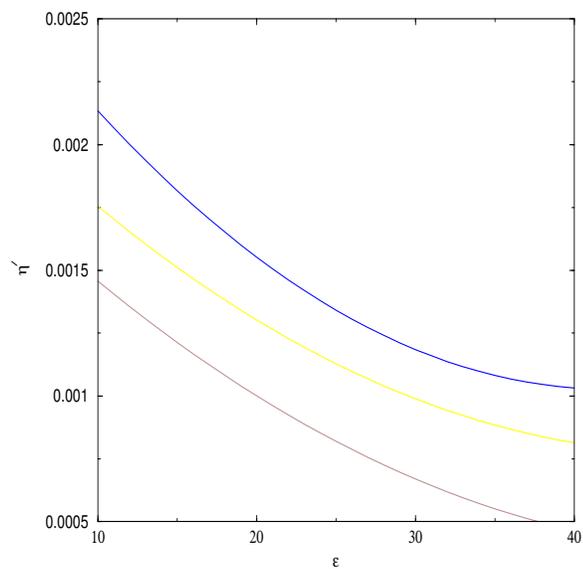


Figure 5.6: Superarrivals in the transmitted wave packet are shown to decrease with increase in  $\epsilon$ , the time taken for barrier raising. The three different curves correspond to three different values of the detector position  $x'$ .

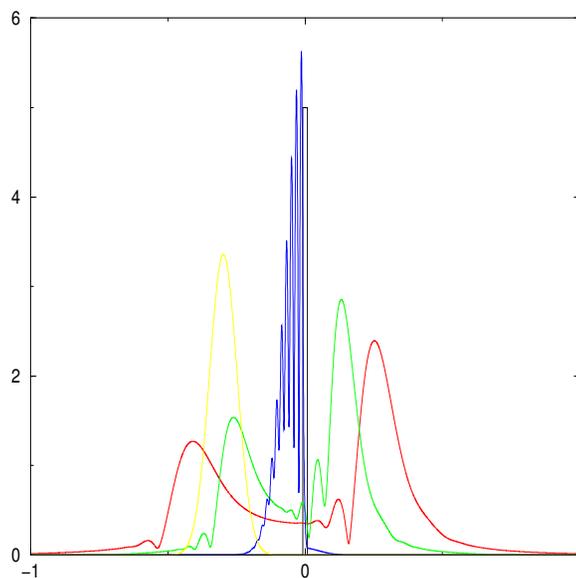


Figure 5.7: Snapshots of the wave packet are plotted at four different instants of time. The initial narrow Gaussian is heavily distorted upon striking the barrier. It splits up into two, with the reflected part possessing a secondary peak shifted towards the detector.

splits into two pieces, one of which moves towards the right (transmitted particles). The reflected packet has a secondary peak shifted towards the left. It is thus not possible to uniquely define a group velocity  $v_g$  for the reflected packet in this case.

The action due to a local perturbation (reduction of barrier height) propagates across the wave packet with a signal velocity  $v_e$  which affects the time evolving reflection probability that can be measured at different points. Thus a distant observer who records the growth of reflection probability becomes aware of the perturbation of the barrier (occurring from an instant  $t_p$ ) at the instant  $t_d$  when the time varying reflection probability starts deviating from that in the unperturbed case. Then  $v_e$  is given by

$$v_e = \frac{D}{t_d - (t_p - \epsilon/2)} \quad (5.30)$$

We compute  $v_e$  and  $v_g \equiv \langle p \rangle / m$  for a range of parameters and plot  $v_e/v_g$  versus  $\epsilon$  in Figure 5.8. Both  $\Delta t$  (the duration of superarrivals) and  $v_e$  (the signal velocity) *decrease* with *increasing*  $\epsilon$  (or, decreasing rate of perturbation). The magnitude of superarrivals ( $\eta$ ) also *decreases* with *increasing*  $\epsilon$  (Figure 5.4). From such behaviours of  $\eta$ ,  $\Delta t$  and  $v_e$  we infer the following *explanation* for the origin of superarrivals. The barrier pertur-

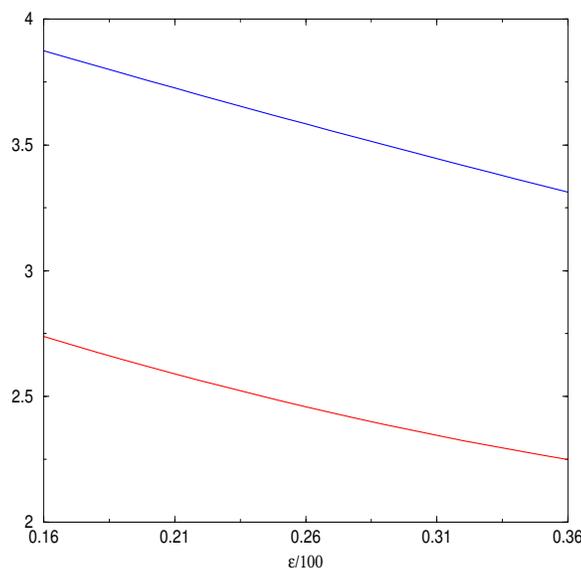


Figure 5.8: The upper curve represents a plot of  $\Delta t$  (duration of superarrivals) versus  $\epsilon$ . The lower curve is a plot of  $v_e/v_g$  versus  $\epsilon$ . Here the detector position  $x' = -0.4$ .

bation imparts a “kick” on the impinging wave packet which splits, and a part of it is reflected with a distortion. A finite disturbance proportional to this “kick” or the rate of perturbation propagates from the reducing barrier to the reflected packet, which results in a proportional magnitude of superarrivals  $\eta$ . Note that information about the barrier perturbation reaches the detector at the instant  $t_d$  with a velocity  $v_e$  which decreases with the decreasing magnitude of impulse imparted to a wave packet. These results therefore suggest that information about the barrier perturbation propagates with a *definite speed* across the wave function which plays the role of a “field”.

We have seen that a counter intuitive enhancement of probabilities takes place in both the cases as a result of barrier perturbation. In the next section we shall discuss a possible scheme of secure transfer of continuous information by exploiting the above feature of superarrivals caused by the dynamical effect of perturbation of the boundary conditions on the wave function.

### 5.3 Information transfer using the wave function through a time-varying boundary

Superarrivals become more pronounced for larger rate of perturbation. It appears as if the effect of reducing or rising the barrier imparts a dynamical “kick” to the wave packet, which is then propagated to the detector. A local change in potential affects a wave packet globally, the global effect being manifested through the time evolution of the packet. The action due to a local perturbation (barrier height reduction or raising) propagates across the wave packet at a finite speed,  $v_e$ , affecting the time evolving reflection (or transmission) probability. Thus a distant observer who records the growth of reflection probability becomes aware of perturbation of the barrier (starting at an instant  $t_p$ ) from the instant  $t_d$  when the time-varying reflection (or transmission) probability starts deviating from that measured in the unperturbed case.

It can be seen from Figures 5.4 and 5.8 that the magnitude of superarrivals  $\eta$ , the signal velocity  $v_e$  and the *duration* of superarrivals  $\Delta t$  all decreases monotonically with increasing  $\epsilon$  (or decreasing the rate of barrier reduction or raising). The reducing (or rising) barrier imparts a kick (the magnitude of which is proportional to the rate of reduction) on the wave packet. This disturbance is propagated across the wave packet to reach the detector. We see that information about barrier perturbation taking place at location  $x_c$  and starting at time  $t_p$  propagates through the wave packet and reaches the detector located at  $x'$  at time  $t_d$  with a finite velocity  $v_e$ .

A lot of interest is currently being devoted to study and develop new schemes of quantum information transfer (see, for instance, Alber *et al* [111] ), and much work is going on to optimize the capacity of classical and quantum channels. Let us see how the present scheme of superarrivals could, in principle, be used for information transfer through the wave function. In order to do so, it is important to focus on the variation of  $\Delta t = t_c - t_d$  (the duration of superarrivals) as a function of  $\epsilon$  (the time taken for barrier perturbation). This is plotted in Figure 5.9 for three different values of the detector position  $x'$ . Note that  $\Delta t$  decreases monotonically with increasing  $\epsilon$  for a wide range of values of  $\epsilon$ . Now suppose a particular curve in Figure 5.9 (functional relation between  $\Delta t$  and  $\epsilon$  for a fixed value of detector position  $x'$ ) is chosen as a key which is shared by

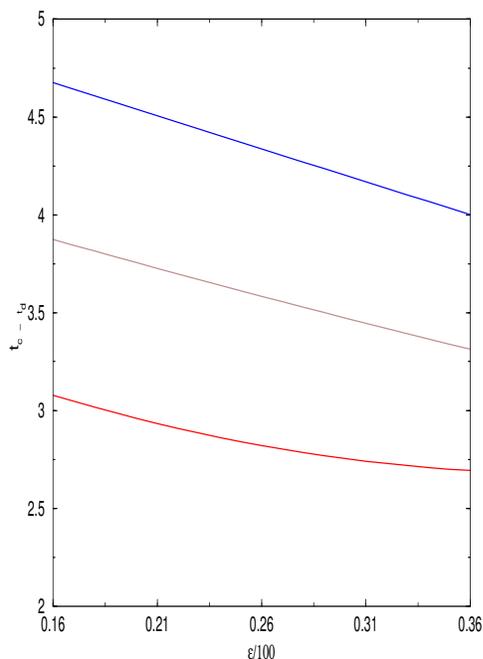


Figure 5.9: The duration of superarrivals  $\Delta t = (t_c - t_d)$  is plotted versus  $\epsilon$ . The three different curves denote three different values of the detector position  $x'$ .

two persons Alice and Bob who want to exchange information. Alice is at the barrier and receives a continuous inflow of particles whose wave function is given by the initial Gaussian. Alice has the choice of reducing (or raising) the barrier height at completely random different rates. She chooses one particular value of  $\epsilon$  for a single run of the experiment, and she wants Bob who is at the detector to be able to decipher this value of  $\epsilon$ . Bob monitors the time evolution of  $|R_p(t)|^2$  (or  $|T_p(t)|^2$ ) through the detector counts and is able to decipher  $t_c$ ,  $t_d$ , and hence  $\Delta t$  by comparison with the curve  $|R_s(t)|^2$  (or  $|T_s(t)|^2$ ) for the static case. He then uses his key to infer the exact value of  $\epsilon$  corresponding to the particular value of  $\Delta t$  he has measured. The whole procedure can be repeated with different rates of barrier reduction (or raising) as many times as required by Alice and Bob. This exchange is secure because it would not be possible for any eavesdropper to decipher Alice's chosen value of  $\epsilon$  without having access to the key. It is important to note that information transfer [112] takes place in this scheme without any shared entanglement between the two players Alice and Bob. Also, the variable  $\epsilon$  can vary continuously in the allowed parameter range.

Before concluding the present chapter let us focus on the manifestation of wave-particle duality in the context of the phenomenon of superarrivals. We argue that both classical wave-like and classical particle-like properties can be exhibited in the same gedanken experimental set-up for obtaining superarrivals through Schrödinger dynamics.

## 5.4 Quantum superarrivals: Bohr's wave-particle duality revisited

The phenomenon of quantum superarrivals is manifested in the probabilities for Schrödinger wave packets scattered from perturbed potential barriers. The purpose of this section is to focus on the manifestation of wave-particle duality in the context of the phenomenon of superarrivals. Here we argue that both classical wave-like and classical particle-like properties can be exhibited in the same gedanken experimental set-up for obtaining superarrivals through Schrödinger dynamics [113]. An interesting question regarding the tenet of mutual exclusiveness, *a la* Bohr, of these two properties is raised in the context of this phenomenon.

Over the years, the double-slit experiment has remained the archetypical example for displaying the key features of the superposition of quanta, as well as of the discreteness of quanta. Interference experiments like the double-slit experiment, are however, not the only ones featuring aspects of wave-particle duality. By the present example we would like to emphasize that the curious aspects of wave-particle duality could also be exhibited in other quantum phenomenon. A number of recent experiments in optical and condensed matter systems have exhibited novel and interesting characteristics of Schrödinger dynamics [98]. Here we propose one such example in the particular arena of time-dependent wave packet dynamics which leads to quantum superarrivals. Let us here restrict ourselves to one particular manifestation of superarrivals, namely, the superarrivals observed in the reflection probability when the barrier height is reduced to zero. As was discussed in the previous sections, other kinds of barrier perturbations may also lead to superarrivals. Since our purpose here is to bring forth an example highlighting certain curious features of wave-particle duality, we will consider without the loss of generality the following experimental scenario.

We consider a Gaussian wave packet initially centered at  $x_0$ , which moves to the right and strikes a potential barrier of height  $V_0$  and width  $w$  centred at a point  $x_c$ . A detector placed at a point  $x'$  far to the left of  $x_0$  measures the time-dependent reflection probability by counting the reflected particles arriving there *up to* various instants. Another detector placed to the right of the barrier at a point  $x''$  such that both the detectors are equidistant from the barrier, i.e.,  $x_c - x' = x'' - x_c$ , measures the time-dependent transmission probability by counting the transmitted particles arriving there *up to* various instants. Both the detectors record the cumulative number of particles arriving at them for the following two separate cases: (i) for a static barrier, and (ii) when the barrier is perturbed by reducing its height to zero linearly in time during the time interval  $\epsilon$  which may be varied for different runs of the experiment. At any instant *before* the asymptotic value of the reflection probability is attained, the time evolving reflection probability in the region  $-\infty < x \leq x'$  is given by

$$|R(t)|^2 = \int_{-\infty}^{x'} |\psi(x, t)|^2 dx \quad (5.31)$$

We denote the reflection probability for the static and the perturbed cases as  $|R_s(t)|^2$  and  $|R_p(t)|^2$  respectively. Similarly, at any instant *before* the asymptotic value of the transmission probability is attained, the time evolving transmission probability in the region  $x'' \leq x \leq \infty$  is given by

$$|T(t)|^2 = \int_{x''}^{\infty} |\psi(x, t)|^2 dx \quad (5.32)$$

The transmission probability for the static and the perturbed cases are denoted as  $|T_s(t)|^2$  and  $|T_p(t)|^2$  respectively. It is important to stress again that these four functions  $|R_s(t)|^2$ ,  $|R_p(t)|^2$ ,  $|T_s(t)|^2$  and  $|T_p(t)|^2$ , all measure the cumulative number of particles that arrive at the detectors *up to* various instants of time  $t$ .

Let us now concentrate on certain specific features of superarrivals, that are relevant to the argument of the present section. In Figure 5.10 we provide plots of the four probabilities  $|R_s(t)|^2$ ,  $|R_p(t)|^2$ ,  $|T_s(t)|^2$  and  $|T_p(t)|^2$  versus time for a particular choice of the parameter  $\epsilon$  (barrier reduction time). The initial height of the barrier  $V_0$  is chosen such that there is no transmission for the static barrier, as represented by the horizontal line for  $|T_s(t)|^2$  in the figure. The intersection of the curves  $|R_s(t)|^2$  and  $|R_p(t)|^2$  clearly reveals, as

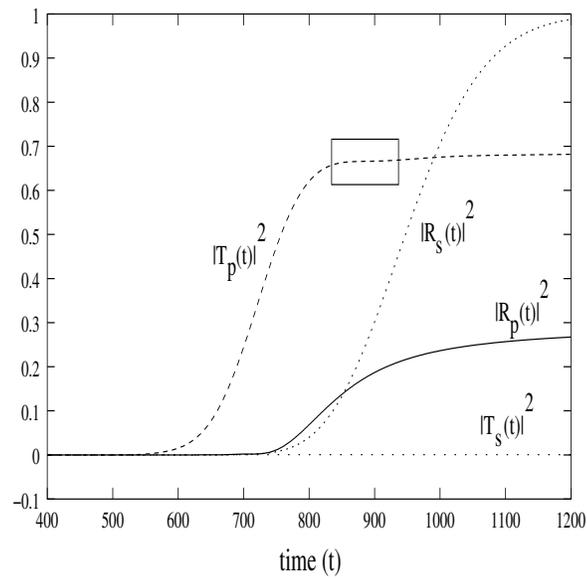


Figure 5.10: The reflection and transmission probabilities are plotted with time for the static as well as perturbed cases. The barrier reduction time  $\epsilon = 10$ . The region within the small box exhibits a kink in the transmitted probability.

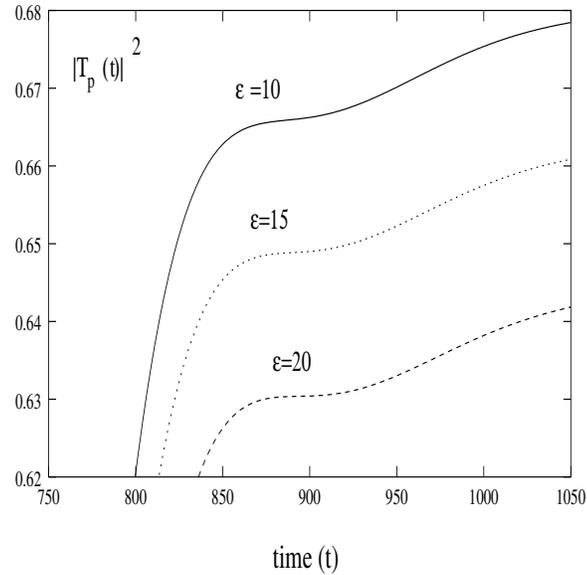


Figure 5.11: The transmission probability for the perturbed barrier is plotted versus time for three different values of the barrier reduction time. The flat regions of the curves indicate no transmission during these time intervals

discussed above, the occurrence of superarrivals in the time-dependent reflection probability. The time-dependent transmission probability for the perturbed barrier,  $|T_p(t)|^2$  starts to rise monotonically, and then stays *constant* for a small duration of time. The latter behaviour is seen as a kink in the curve  $|T_p(t)|^2$  highlighted by the box inside Figure 5.10. Finally,  $|T_p(t)|^2$ , rises again to reach its asymptotic value symbolising the passage of the entire transmitted portion of the wave packet. Note that that the asymptotic values of the transmitted and reflected probabilities add up to 1, i.e.,  $|R_p(t_\infty)|^2 + |T_p(t_\infty)|^2 = 1$ , since there is no loss of probability (no particle disappears undetected). The highlighted region of Figure 5.10 representing the kink or the stoppage of growth in  $|T_p(t)|^2$ , is magnified and shown in Figure 5.11 where we also plot portions of  $|T_p(t)|^2$  with time for two other values of  $\epsilon$ . It is clear from these curves that there exists a finite interval of time during which the detector at  $x''$  registers no counts symbolised by the flat regions of the plots.

It is interesting to look for interpretations of the results of this experiment. Let us first focus on the reflection probability. The very origin of superarrivals in the reflection probability can be ascribed to a “kick” or disturbance affected on the wave packet due to the perturbing barrier. The magnitude of this impact on the wave packet is proportional to the rate of barrier perturbation, and as was observed, results in a proportionate magnitude of superarrivals. This quantitative feature can only be understood in terms of the *classical* wave-like nature of the impinging wave packet, since the information about barrier perturbation reaches the detector  $x'$  with a definite velocity  $v_e$ . This velocity of information transfer again *varies* with the rate of barrier reduction [107, 109]. This latter feature is only possible if the wave function acts as a classical field transmitting the information about barrier perturbation.

Next, consider the transmission probability. If we now think in terms of the wave-like nature of the impinging wave packet, a part of it will be transmitted due to barrier reduction. Thus  $|T_p(t)|^2$  is expected to grow monotonically at *all* times till it reaches its asymptotic value at  $t_\infty$  signalling the passage of the whole transmitted packet. At *no* interval of time does one expect  $|T_p(t)|^2$  to remain constant signifying no arrival of particles at  $x''$  during this interval. A constant value for  $|T_p(t)|^2$  over a finite interval of time that one gets is the very antithesis of wave-like behaviour representing the *continuous* flow of probability. The very fact that one obtains flat regions in the curves for  $|T_p(t)|^2$

for several different values of the rate of barrier perturbation, can only be explained with the interpretation of a *discrete* classical particle-like behaviour for the impinging wave packet. This is how one can understand the lack of clicks in the detector located at  $x''$  during a specific interval of time.

We see that wave-particle duality is exhibited in the same phenomenon of superarrivals if one observes both the reflected and the transmitted probabilities, respectively on the two sides of the barrier. One may proceed even further in trying to find an interpretation of the phenomenon of superarrivals in the context of Bohr's complementarity principle (BCP) [114] between the wave and particle pictures of fundamental quantum entities. According to the BCP the classical concepts like wave or particle description are indispensable for describing quantum mechanical formula, but nonetheless, these very classical concepts are subject to certain rudimentary limitations elucidated by the principle of *mutual exclusiveness* (ME), a precise statement for which was provided by Bohr in Ref. [114]: "... any given application of classical concepts precludes the simultaneous use of other classical concepts which in a different connection are equally necessary for the elucidation of the phenomena". Bohr regarded this ME as a necessary ingredient in BCP to ensure its inner consistency. In the present gedanken experiment we see that the reflected and the transmitted probabilities arise from the same wave packet, or in other words, a part of the incident wave packet is reflected, and another part transmitted from the barrier *at the same time*. The above picture seems to imply that the sense in which ME is usually talked about, is not satisfied in the present experiment. One is forced to invoke both classical wave-like, *and* classical particle-like properties for the Schrödinger wave packet at the same time to describe the complete results of this experiment.

## 5.5 Summary

In this chapter we have discussed a new quantum mechanical effect which occurs in the time dependent reflection/transmission probabilities for a propagating Gaussian wave packet which encounters a localised time-dependent rectangular potential barriers. We have shown that a counter intuitive enhancement of probabilities takes place in both the cases as a result of barrier perturbation. By reducing the height of the barrier to zero in

a short span of time during which there is a significant overlap of it with the wave packet, we observed that the reflection probability is larger compared to the case of reflection from a static barrier for a small but finite interval of time. The particular example of superarrivals in the reflection probability when the barrier height is brought down is not the only example of superarrivals with time dependent barriers. Indeed, other cases of time dependent barriers with oscillating height and width can be considered to lead to superarrivals in the reflected as well as transmitted probabilities. We have seen that superarrivals occur both in the reflection and transmission probabilities when the barrier height is reduced/increased (theses two cases are complementary to each other). In both the cases (superarrivals in reflection/transmission probabilities) the wave function plays the role of a field or carrier through which information is transmitted.

This phenomenon of quantum superarrivals can be explained in terms of the dynamical kick imparted on the wave packet by the time-evolving barrier. Note that the information content of a *wave packet* does not always propagate with its group velocity  $v_g$  which is usually identified with the velocity of the peak of the wave packet. What we see is that a local change in potential affects the wave packet globally, the global effect being manifested through the time evolution of the packet. Information about barrier perturbation, or change in the boundary conditions, propagates across the wave function and then reaches the detector with a finite speed (signal velocity,  $v_e$ ) which is also proportional to the rate at which the barrier height is reduced. We also found the magnitude of superarrivals to be proportional to the rate of reduction of the potential barrier. We argued that superarrivals occur because of the “objective reality” of a wave function acting as a “field” which mediates across it the propagation of a physical disturbance, *viz.* perturbation of the potential barrier. We have discussed a possible scheme of secure transfer of continuous information by exploiting the above feature of superarrivals caused by the dynamical effect of perturbation of the boundary condition on the wave function.

Next, we have presented a new manifestation of wave-particle duality in the context of the phenomenon of superarrivals where we have argued that both classical wave-like and classical particle-like properties can be exhibited in the same gadenken experimental set-up for obtaining superarrivals through Schrödinger dynamics. Further work involving detailed analyses of the various aspects of superarrivals is needed to understand the tenet

of “*mutual exclusiveness*” (ME) in the context of the present experiment. The observational status of Bohr’s complementarity principle (BCP) [114], as regards ME between the wave and particle descriptions, has been debated upon in recent years. It has been argued [115] that as far as interference type experiments are concerned, the quantum mechanical formalism guarantees the validity of ME because it contains a built-in mechanism that ensures the disappearance of the interference pattern whenever one has which-path information. Note however, that a claim for a counterexample using a variant of the Mach-Zehnder interferometer exists in literature [116]. An entirely different category of experiments are those involving the tunneling of single quanta. It has been shown using the quantum-optical formalism that a double-prism experiment involving the reflection and tunneling of single photons predicts anti-coincidences at two separate detectors, thus countering ME [117]. Such an experiment has actually been performed to observe these anti-coincidences [118], and thereafter, a further proposal has been made to improve the statistical viability of the coincidence counts [119]. The desired outcome of the present analysis is to motivate investigation of more such experiments and inspire further debate [120] which should bring forth all issues concerning wave-particle duality into a sharper focus. We conclude by noting that the phenomenon of superarrivals has a distinct quantum mechanical significance. Its ramifications call for further studies. In particular, different types of perturbations may be studied to probe the viability of single particle experiments [121, 122] for demonstrating this effect.

## Chapter 6

### A Bohmian perspective

In the previous chapters we have discussed several new and interesting quantum effects. Two such effects that could be highlighted are the spin dependent contribution to the arrival time distribution, and the phenomenon of quantum superarrivals manifested in the reflection and transmission probabilities of wave packets scattered from time dependent potential barriers. The purpose of the present chapter is to obtain a clearer physical insight into these results by invoking the Bohmian interpretation of quantum theory [123]. It should be emphasized that though all our previous results are obtained within the standard framework of quantum mechanics, here we will strive towards a sounder pedagogical footing in the context of Bohmian mechanics. This is especially true regarding the use of the probability current density in calculating the arrival time distribution, as we argue in section 6.2. Further, we will see in section 6.3 that a clear understanding as to how superarrivals originate is obtained with the help of the quantum potential of the Bohm model. We will compute the “particle trajectories” and will derive a quantitative estimate of the magnitude of superarrivals using the Bohmian interpretation of quantum mechanics to have a deeper insight into the nature of superarrivals. In the next section we begin with a brief review of some essential aspects of the Bohm model.

#### 6.1 A brief review of the Bohm model

The Bohm model (BM) provides an ontological and a self-consistent interpretation of the formalism of quantum mechanics [123]. Predictions of BM are in agreement with that of standard quantum mechanics. Born’s interpretation of the squared modulus of a wave

function ( $|\psi|^2$ ) as the probability density of *finding* a particle within a specified region of space is a key ingredient of the standard framework of quantum mechanics. Thus the standard interpretation of quantum mechanics is inherently *epistemological*. On the other hand, the possibility of an *alternative interpretation* of quantum mechanics by interpreting ( $|\psi|^2$ ) as the probability density of a particle *being* actually present within a specified region was first suggested by de Broglie [124]. Later, Bohm [123] developed the details of such an *ontological* model of quantum mechanics by using the notion of an *observer-independent spacetime trajectory* of an *individual particle* which is determined by its wave function through an equation of motion which is formulated in a way consistent with the Schrödinger time evolution. Bohm's model thus explicitly refuted the counterarguments (such as the ones put forward by Pauli [125] and von Neumann [126]) prohibiting the formulation of such a model. Subsequently, much work has been done on various aspects of the Bohmian model [44, 127, 128]. That such a model is *not* unique has also been pointed out [48] and different versions of the ontological model of quantum mechanics have been proposed [34, 46, 47, 129]. Although any such ontological model hinges on the notion of a definite *spacetime track* used to provide a description of the objective motion of a single particle, such trajectories are not directly measurable. Hence these trajectories have been essentially viewed as conceptual aids for understanding the various features of quantum mechanics. Recently a study has been reported which shows an application of such trajectories as computational aids for solving the time-dependent Schrödinger equation [49].

In BM a wave function  $\psi$  is taken to be an incomplete specification of the state of an individual particle. An objectively real “position” coordinate (“position” existing irrespective of any external observation) is ascribed to a particle apart from the wave function. Its “position” evolves with time obeying an equation that can be justified in the following way from the Schrödinger equation

$$i\hbar \frac{\partial \psi(\mathbf{x}, t)}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{x}, t) + V(\mathbf{x}, t) \psi(\mathbf{x}, t) \quad (6.1)$$

by writing

$$\psi = R(\mathbf{x}, t) e^{iS(\mathbf{x}, t)/\hbar} \quad (6.2)$$

and using the continuity equation

$$\nabla \cdot (\rho v) + \frac{\partial \rho}{\partial t} = 0 \quad (6.3)$$

with the probability distribution  $\rho(\mathbf{x}, t)$  being given by

$$\rho(\mathbf{x}, t) = |\psi(\mathbf{x}, t)|^2. \quad (6.4)$$

It is important to note that  $\rho$  in BM is ascribed an *ontological* significance by regarding it as representing the probability density of “particles” occupying *actual* positions and the velocity  $v$  is interpreted as an ontological (premeasurement) velocity. On the other hand, in the standard interpretation,  $\rho$  is interpreted as the probability density of *finding* (*not being*) particles around specific positions and there is no concept of an ontological velocity. Integrating Eq.(6.3) by using Eqs.(6.1), (6.2) and (6.4) and requiring that  $v$  should vanish when  $\rho$  vanishes leads to the Bohmian equation of motion where the particle velocity  $v(\mathbf{x}, t)$  is given by

$$v(\mathbf{x}, t) = \dot{\mathbf{x}} = \frac{\nabla S}{m} \quad (6.5)$$

The particle trajectory is thus deterministic and is obtained by integrating the velocity equation for a given initial position. Another perspective on the notion of particle trajectories in BM is obtained by decomposing the Schrodinger equation in terms of two real equations for the modulus  $R$  and the phase  $S$  of the wave function  $\psi$  [44]

$$\frac{\partial S}{\partial t} + \frac{(\nabla S)^2}{2m} - \frac{\hbar^2}{2m} \frac{\nabla^2 R}{R} + V = 0 \quad (6.6)$$

$$\frac{\partial R^2}{\partial t} + \nabla \cdot \left( \frac{R^2 \nabla S}{m} \right) = 0 \quad (6.7)$$

and by indentifying

$$Q(\mathbf{x}, t) = -\frac{\hbar^2}{2m} \frac{\nabla^2 R}{R} \quad (6.8)$$

as the “quantum potential” [44, 123], the equation of motion of a particle along its trajectory can now be written in a form analogous to Newton’s second law

$$\frac{d}{dt}(m\dot{\mathbf{X}}) = -\nabla(V + Q)|_X \quad (6.9)$$

(with  $d/dt = \partial/\partial t + \dot{\mathbf{X}} \cdot \nabla$ ) where the particle is subjected to a quantum force  $-\nabla Q$  in addition to the classical force  $-\nabla V$ . The effective potential on the particle is  $(Q + V)$ . We can now summarise the essential part of Bohm's trajectory interpretation of non-relativistic quantum mechanics as follows: The motion of a quantum *particle* is causally determined by an objectively real complex-valued field  $\psi$  and *it* has a well-defined position and velocity at each instant of time. Although this is diametrically opposed to the fundamental tenets of conventional quantum mechanics, precisely the same results are obtained for all experimentally observable quantities when the above postulate is augmented by the following three secondary ones:

- (1) The guiding field  $\psi(\mathbf{x}, t)$  satisfies the time-dependent Schrödinger equation.
- (2) The velocity of the particle located at the position  $\mathbf{x}$  at time  $t$  is given by

$$v(\mathbf{x}, t) = \frac{\hbar}{m} \text{Im} \frac{\nabla \psi}{\psi} \quad (6.10)$$

- (3) The quantity  $|\psi(\mathbf{x}, t)|^2 d\mathbf{x}$  is the probability of the particle *being* between  $\mathbf{x}$  and  $\mathbf{x} + d\mathbf{x}$  at time  $t$  even in the absence of a position measurement.

With this interpretation, we are now going to find out the arrival time probability distribution for a free particle moving in one dimension.

## 6.2 Probability current as the arrival time distribution from the Bohmian interpretation

Let the initial wave function for the free particle moving in one dimension be a Gaussian wave packet,

$$\psi(x, t = 0) = \frac{1}{(2\pi\sigma_0^2)^{1/4}} e^{ikx - \frac{x^2}{4\sigma_0^2}} \quad (6.11)$$

and after time  $t$ , the free Schrödinger time evolved wave function is given by

$$\psi(x, t) = \frac{1}{(2\pi\sigma_t^2)^{1/4}} e^{ik(x - \frac{1}{2}ut) - \frac{(x-ut)^2}{4\sigma_t\sigma_0}} \quad (6.12)$$

where  $\sigma_t = \sigma_0(1 + i\hbar t/2m\sigma_0^2)$  and the group velocity is  $u = \hbar k/m$ . Then solving the Bohmian trajectory equation given by

$$\dot{x} = \frac{\hbar}{m} \operatorname{Im} \frac{\nabla \psi(x, t)}{\psi(x, t)} = u + \frac{(x - ut) \hbar^2 t}{4m^2 \sigma_0^4 \left(1 + \frac{\hbar^2 t^2}{4m^2 \sigma_0^4}\right)} \quad (6.13)$$

we get

$$x(t) = ut + x_0 \left(1 + \frac{\hbar^2 t^2}{4m^2 \sigma_0^4}\right)^{1/2} \quad (6.14)$$

where  $x_0$  is the initial position of the particle. Now, let us put a detector at  $x=X$  so that a particle starting from the initial position  $x_0$  arrives at the detector located at  $x=X$  at time  $t=T$ ; then

$$X = uT + x_0 \left(1 + \frac{\hbar^2 T^2}{4m^2 \sigma_0^4}\right)^{1/2} \quad (6.15)$$

Consequently,

$$x_0 = \frac{(X - uT)}{\left(1 + \frac{\hbar^2 T^2}{4m^2 \sigma_0^4}\right)^{1/2}} \quad (6.16)$$

So the particle arrives at the detector located at  $X$  at time  $T$  if it starts from this initial position  $x_0$ . Now we will equate the following two probabilities:

(1) The probability of the particle to start from the initial position between  $x_0$  and  $x_0 + dx_0$ , which is equal to  $|\psi(x_0, t = 0)|^2 dx_0$ .

(2) The probability of the particle to arrive at the detector between the time  $T$  and  $T + dT$ , which is equal to  $\Pi(T) dT$

$$\Pi(T) dT = |\psi(x_0, t = 0)|^2 dx_0 \quad (6.17)$$

$$\Rightarrow \Pi(T) = |\psi(x_0, t = 0)|^2 \frac{dx_0}{dT} \quad (6.18)$$

Here if we put the value of  $x_0$  from Eq.(6.16), then we get

$$\Pi(T) = \frac{1}{(2\pi\sigma_0^2)} \frac{1}{\left(1 + \frac{\hbar^2 T^2}{4m^2 \sigma_0^4}\right)} \exp\left(-\frac{(X - uT)^2}{2\sigma_0^2 \left(1 + \frac{\hbar^2 T^2}{4m^2 \sigma_0^4}\right)}\right) \left[ u + \frac{(X - uT) T}{4m^2 \sigma_0^4 \left(1 + \frac{\hbar^2 T^2}{4m^2 \sigma_0^4}\right)} \right] \quad (6.19)$$

This is exactly equal to the probability current density  $\mathbf{J}(X, T)$  of the particle at the detector computed by substituting the expression of  $\psi(x, t)$  from Eq.(6.12) in the definition of  $\mathbf{J}$  given in Eq.(2.2). Here we have ignored an overall negative sign which merely implies that  $x_0$  decreases as  $T$  is increased. Hence finally we have

$$\Pi(T) = \mathbf{J}(X, T) \tag{6.20}$$

We thus see that the Bohmian model of quantum mechanics in terms of the causal trajectories of individual particles implies the interpretation of probability current as the arrival time distribution on a firmer footing. Here it is relevant to reemphasize certain points on the uniqueness of the probability current in the context of Bohmian mechanics. Note that the current  $\mathbf{J}(X, T)$  is not uniquely determined by the continuity equation. It is determined only up to a divergenceless vector. For example, one can construct a new current  $\bar{\mathbf{J}}$  by adding the divergenceless current  $\mathbf{J}_a$  to the current  $\mathbf{J}$ . The newly defined current  $\bar{\mathbf{J}} = \mathbf{J} + \mathbf{J}_a$  then also satisfies the continuity equation with the same probability density. Hence we are left with an apparent ambiguity in the definition of the probability current. Now, the Bohmian guidance equation is derived from the quantum mechanical probability current and the possibility of an additional contribution to the particle current leads to an ambiguity at the level of the Bohmian interpretation. Deotto and Ghirardi [46] considered different currents compatible with the continuity equation from which different guidance laws (apart from Bohmian law) for the particle could be derived. Holland [48] showed in the context of analyzing the uniqueness of the Bohmian model of quantum mechanics that the Dirac equation implies a *unique* expression for the probability current density for spin-1/2 particles. With the demand that the non-relativistic spin-1/2 particle current should be obtained by taking the non-relativistic limit of the Dirac current, this non-relativistic particle current which contains a generally nonvanishing, spin-dependent term, is also unique. This implies a guidance law for the particle which differs by an additional spin-dependent term from that originally proposed by de Broglie and Bohm and it is argued [48] that this guidance equation for spin-1/2 particle is unique. Unique expressions for the conserved currents have been explicitly derived for Dirac equation, the Klein-Gordon equation, coupled Maxwell-Dirac equation [48, 49] and the relativistic Kemmer equation [50, 51].

### 6.3 Understanding quantum superarrivals using Bohmian mechanics

In the previous chapter we have discussed a new quantum mechanical effect which occurs in the time dependent reflection/transmission probabilities for a propagating Gaussian wave packet which encounters a localised time-dependent rectangular potential barriers. By reducing the height of the barrier to zero in a short span of time during which there is a significant overlap of it with the wave packet, we observed that the reflection probability is larger compared to the case of reflection from a static barrier for a small but finite interval of time. We have seen that superarrivals occur both in the reflection and transmission probabilities when the barrier height is reduced/increased (theses two cases are complementary to each other). The aim of this section is to have a deeper insight into the phenomenon of superarrivals and also to understand *how* superarrivals occur. In order to understand how superarrivals originate in the particle picture, we compute particle trajectories using the Bohmian interpretation of quantum mechanics. Using such computed trajectories of individual particles we show that the Bohm model provides a clear understanding of the phenomenon of superarrivals. We derive a *quantitative estimate* of the magnitude of superarrivals using the Bohmian trajectories. We illustrate this by considering the case of a wave packet which is reflected from the perturbed barrier. Similar analysis can be done for the transmitted wave packet also.

We compute the Bohmian trajectories for a given set of initial positions with a Gaussian distribution corresponding to the initial wave packet. This procedure is carried out for both the cases of lowering and raising the barrier. Since our purpose is to obtain conceptual clarity of the phenomenon of superarrivals, it suffices to illustrate our scheme through the example of superarrivals in the reflection probability when the barrier is reduced. All the qualitative as well as quantitative features of superarrivals are similar in the case where one observes the transmitted probability from a rising barrier. Thus, henceforth we consider only the former case in the following discussion.

We first plot the profile of  $Q$  versus  $x$  at various instants of time near the potential barrier (when its height is reduced) in Figure 6.1. It is then transparent how the perturbation of the classical potential  $V$  affects  $Q$  away from the vicinity of the boundary of  $V$ .

This in turn accounts for the sharp turn experienced by those particles which contribute towards *superarrivals* (as we shall see explicitly later).

The following approach is used to study *superarrivals* in terms of the Bohmian trajectories. First, a particular value of the barrier reduction rate, or  $\epsilon$  is chosen. We then choose a range of initial positions for which the trajectory arrival times at the detector lie between  $t_d$  and  $t_c$  (i.e., we select only those trajectories which *contribute* to superarrivals). We consider  $N$  such trajectories whose initial positions form a Gaussian distribution. Let us denote *one* such trajectory by  $S_{ip}$  having the initial position  $x_i$  and the arrival time  $t_{ip}$ . Taking the static case, the trajectory  $S_i$  for that initial position  $x_i$  is computed. Let the corresponding arrival time be  $t_i$ . A superarrival parameter  $\beta_i$  for the  $i$ -th Bohmian trajectory is then defined as

$$\beta_i = \frac{t_i - t_{ip}}{t_i} \quad (6.21)$$

which provides a measure of superarrivals for a *particular value* of initial position. Next we define an *average value*

$$\tilde{\beta} = \frac{\sum_i \beta_i}{N} \quad (6.22)$$

which provides a *quantitative estimate* of superarrivals obtained through Bohmian trajectories.

Our results show that the arrival time  $t_{ip}$  for the perturbed case is sensitive to the value of initial position  $x_i$ . We have checked that for a particular initial position,  $t_i$  *exceeds*  $t_{ip}$  for *only* those trajectories which *contribute* to superarrivals. This is a distinct feature associated with the superarrivals that can be identified in terms of the Bohmian trajectories. We plot a set of Bohmian trajectories in Figure 6.3. Note that the trajectories of the particles corresponding to the perturbed case take a sharp turn and arrive at the detector *earlier* than they would have for a static barrier. Any abrupt perturbation of the potential barrier has thus a *global effect* on the wave function and affects the values of the quantum potential  $Q(x, t)$  at various points. Then, through the Bohmian equation of motion the velocities of the incident particles get correspondingly affected *much before* reaching the vicinity of the potential barrier. Superarrivals originate from *those* particles in the perturbed case which reach the detector *earlier* than those corresponding to the *same* initial positions in the static case. This accounts for why a detector records more counts in the perturbed case during a particular time interval as compared to that in a

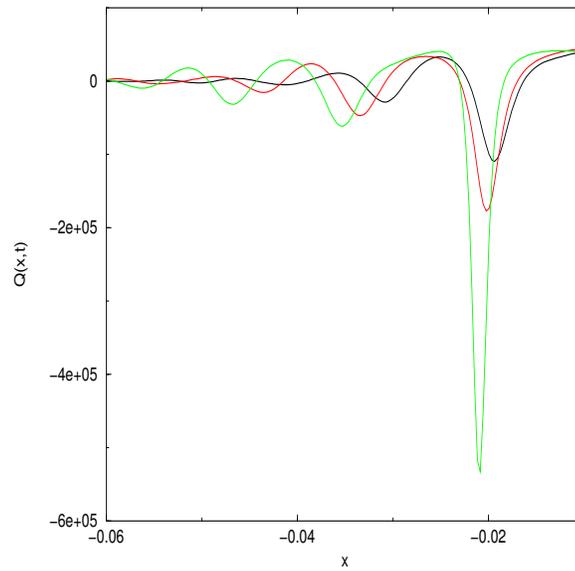


Figure 6.1: Snapshots of the quantum potential  $Q(x, t)$  are plotted versus  $x$  at various instants of time. The potential barrier is located in the region  $-0.008 < x < 0.008$ . Barrier perturbation is from  $t = 400$  to  $t = 410$ . The full, dashed and dotted curves represent  $Q$  at times  $t = 420$ ,  $425$  and  $430$  respectively. The wells in the quantum potential move towards the left with time and reflect incoming particles away from the vicinity of the classical barrier. This explains why certain particles arrive at the detector earlier than they would have done if reflected from a static barrier.

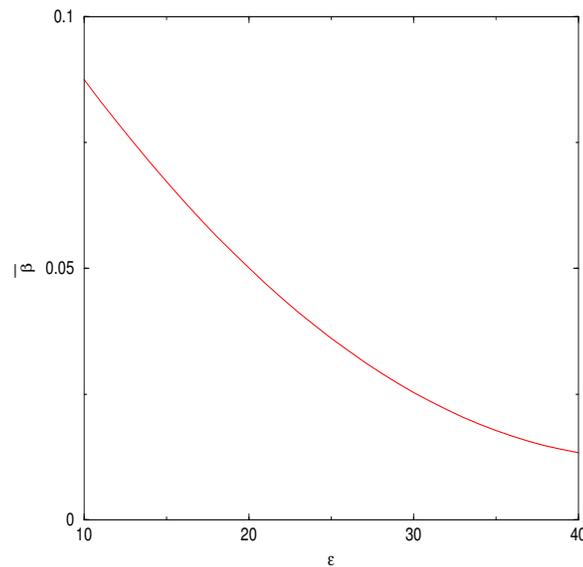


Figure 6.2: The Bohmian superarrival parameter  $\bar{\beta}$  is plotted versus  $\epsilon$ .

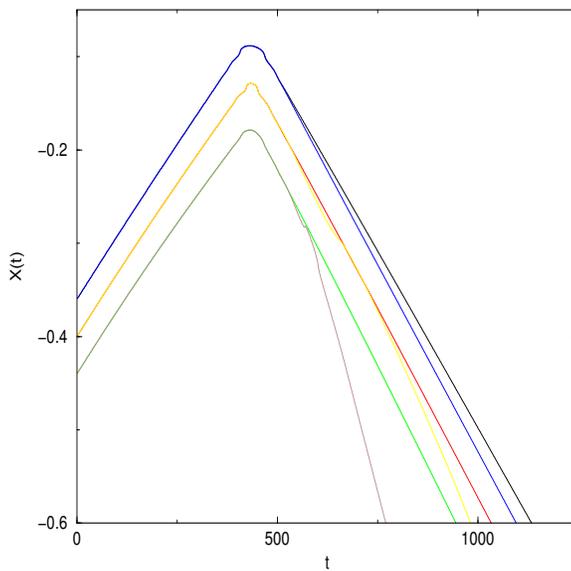


Figure 6.3: Bohmian trajectories for particles originating from the same initial positions get reflected differently from the static and the perturbed barriers. The trajectories undergo sharper turns when the barrier is perturbed and arrive the detector earlier than they would have done for the static barrier case. The barrier is placed at  $x = -0.008$  to  $x = 0.008$ . Perturbation takes place from  $t = 400$  to  $t = 410$ .

static situation. The origin of superarrivals can thus be understood in this way by using the Bohmian trajectories.

The effect of altering the barrier perturbation time  $\epsilon$  on the magnitude of superarrivals  $\bar{\beta}$  can be studied by computing  $\bar{\beta}$  for various values of  $\epsilon$ . We display the results of this study in Figure 6.2. Note that the the magnitude of superarrivals decreases monotonically with increasing  $\epsilon$ , or decreasing rate of perturbation. This effect was also discussed in the previous chapter where we obtained a similar behaviour for the superarrival parameter  $\eta$ . The similarity of these two results obtained through entirely different techniques reinforces our contention about the dynamical nature of superarrivals originating from a “disturbance” provided by the lowering of potential barrier, which propagates across the wave function with a definite speed.

## 6.4 Summary

The purpose of the present chapter has been to secure clearer physical insights into some results obtained in the earlier chapters by invoking the Bohmian interpretation of quantum theory [123]. We have shown that the concept of the probability current density in obtaining the arrival time distribution is uniquely derived in the Bohm model. Further, we have seen that a clear understanding as to how superarrivals originate is obtained with the help of the quantum potential. We have computed the “particle trajectories” and derived a quantitative estimate of the magnitude of superarrivals using the Bohmian interpretation of quantum mechanics. This analysis substantiates our earlier contention that superarrivals arise from a dynamical disturbance provided by the perturbed barrier which propagates across the wave packet with a definite speed.

Such time dependent quantum phenomena could be useful in furnishing examples of the *conceptual utility* of the Bohm model from a perspective different from other examples studied recently [130] for this purpose. Superarrivals is a special case of barrier crossing problem of a quantum wave packet. A very important problem related to barrier crossing which remains controversial at present is that concerned with the formal definition of traversal and tunneling times, *viz.*, “how much time a quantum particle spends inside the barrier before tunneling”. A variety of proposals have been made for the definition of the time (actual and mean) spent by a tunneling particle inside the barrier [131]. The Bohmian approach gives a clear definition of the time taken for an individual particle to cross a barrier, and hence the mean time over an ensemble, as well.

## Chapter 7

### Conclusions

In this thesis we have studied the arrival time distribution and the time-dependent probability of arrival for quantum wave packets evolving under different kinds of potentials. The important implications obtained from the dynamical evolution of the wave packets under these potentials have been discussed. Some of the key results obtained in this thesis are (i) spin-dependence of arrival time of free particles (ii) smooth quantum to classical transition of the arrival time distribution, (iii) demonstration of the quantum violation of the weak equivalence principle, and (iv) understanding quantum superarrivals. The main framework used for this study is the probability current density approach to the problem of arrival time distribution for quantum particles.

In order to motivate the necessity of formalising arrival time distributions, we began with a brief review of the status of time in quantum theory and the difficulties in constructing a time operator with desired properties. This sets up our description of the probability current density approach in calculating the arrival time distribution for free particles. Here we first discussed that in the non-relativistic quantum mechanics the form of the probability current is not *unique* and leads to an ambiguity in the arrival time distribution. As shown by Holland [48] the probability current can be uniquely fixed if one starts from a relativistic quantum wave equation and this *uniqueness* is also preserved in the non-relativistic limit of the relevant relativistic equation [43]. A novel spin dependent effect on the arrival time distribution for free particles was shown by demonstrating the uniqueness of the conserved probability current in the non-relativistic limit of Dirac equation. The mean arrival time was computed using the modulus of the unique

(spin-dependent) probability current density for spin-1/2 free particles associated with a propagating Gaussian wave packet.

This spin-dependent effect highlights the feature that the spin of a particle is an *intrinsic* property and is *not* contingent on the presence of an external field. The scheme we have discussed shows that the magnitude of total spin can be measured *without* subjecting the particle to an external field. The measurability of the property of spin of a free particle arises from the relativistic nature of the dynamical evolution of the wave function where the relevant wave function is fundamentally 4-component (or, 2-component), even in the *non relativistic limit*. Since the spin-dependent term which may contribute significantly to the arrival time distribution has been computed in the nonrelativistic regime by starting from the relativistic Dirac equation, this provides a rather rare example of an empirically detectable manifestation of a relativistic dynamical equation in the *non relativistic regime*. A future line of investigation as an offshoot of this analysis could be to explore the possibilities of using the relativistic quantum mechanical wave equations of particles with spins other than spin 1/2 (such as using the relativistic Kemmer equation for spin 0 and spin 1 bosons) in order to compute the spin-dependent terms in the probability current densities and their effects on the arrival time distribution. We have also outlined the sketch of an experimentally realizable scheme which needs to be developed further to test any postulated quantum mechanical approach for calculating the arrival time distribution.

We then proceed to investigate the classical limit [71] of arrival time defined through the probability current in the context of *macroscopic limit problem* of quantum mechanics. Here we have considered the evolution of a quantum *free* particle represented by a Gaussian wave packet. We have formulated the classical analogue of the arrival time distribution for an ensemble of *free* particles represented by a phase space distribution function evolving under the classical Liouville's equation. We show that the quantum results for the probability current and through it the arrival time distribution, approach smoothly to the classical result in the large mass limit. It needs to be emphasized that it is worthwhile to investigate the classical limit of arrival time distribution calculated from different theoretical approaches that have been suggested in the literature [5, 15, 31, 39, 42]. Such studies, if undertaken extensively, are not only expected to throw light on the com-

paritive merits of different arrival time formulations, but could also be of relevance to the behaviour of mesoscopic systems where a great deal of experimental activity is presently underway [75]. Our outlook is concerned about an approach to test the quantitative equivalence between the classical statistical prediction and the prediction obtained in the macroscopic limit of quantum mechanics. What we have seen is that the *mean time* of arrival of a freely moving quantum particle computed through the probability current depends on the mass of the particle even if its group velocity is fixed. The predicted mass dependence of mean arrival time is, in principle, amenable for experimental verification, and is a clear signature of the probability current approach to time in quantum mechanics [33, 36, 42, 43].

The free fall of quantum wave packets is an interesting arena of study vis-a-vis the issue of compatibility of quantum mechanics with the equivalence principle of gravitation [82]-[91]. We have studied the evolution of quantum *wave packets* under the gravitational potential in the context of a gedanken quantum analogue of Galileo's leaning tower experiment. We have shown that the position probability density and the arrival time distribution for the particle calculated through probability current density exhibits mass dependence. The observable position probability and the *mean time* (computed through the quantum probability current) taken by the freely falling particle to arrive at a particular location are also shown to be mass dependent. Our results of mass-dependence of these observable quantities indicate the manifest violation of a particular form of the quantum analogue of the weak equivalence principle [79]. The variation of the detection probability with mass disappears in the limit of large mass of the freely falling particles, as is expected for classical objects. This saturation of the detection probability is also reflected in the mean arrival time distribution defined through the quantum probability current, which approaches the classical result in a continuous manner with the increase of mass. We have seen that the compatibility of the weak equivalence principle with quantum mechanics can be achieved in the classical limit within this framework for particles falling freely under gravity. The predicted mass dependence of the arrival time of freely falling molecular mass particles offers a distinct possibility of checking the empirical status of the equivalence principle at the quantum level.

The manifestation of nonlocality is ubiquitous in quantum mechanics. The dynamics

of wave packets is certainly not left untouched by implications of quantum nonlocality as was shown by Greenberger in the context of a particle in a box with varying boundaries [93]. The phenomenon of quantum superarrivals [107] is an offshoot of this effect. We have discussed how this recently uncovered phenomena occurs in the time dependent reflection/transmission probabilities for a propagating Gaussian wave packet which encounters localised time-dependent rectangular potential barriers. We have argued that quantum superarrivals can be explained in terms of the dynamical kick imparted on the wave packet by the time-evolving barrier. Information about barrier perturbation, or change in the boundary conditions, propagates across the wave function and then reaches the detector with a finite speed (signal velocity,  $v_e$ ) which is also proportional to the rate at which the barrier height is reduced. It can be interpreted that superarrivals occur because of the “objective reality” of a wave function acting as a “field” which mediates across it the propagation of a physical disturbance, *viz.* perturbation of the potential barrier. We have discussed a possible scheme of secure transfer of continuous information by exploiting the above feature of superarrivals caused by the dynamical effect of perturbation of the boundary condition on the wave function. Next, we have presented a new manifestation of wave-particle duality in the context of the phenomenon of superarrivals where we have argued that both classical wave-like and classical particle-like properties can be exhibited in the same gedanken experimental set-up for obtaining superarrivals through Schrödinger dynamics. According to the Bohr’s complementarity principle the classical concepts like wave or particle description are indispensable for describing quantum mechanical formula, but nonetheless, these very classical concepts are subject to certain rudimentary limitations elucidated by the principle of *mutual exclusiveness* [114]. Further work involving detailed analyses of the various aspects of superarrivals as could be elaborated in different types of dynamical potentials, is needed to understand the tenet of *mutual exclusiveness* in the context of the present example that we have furnished. This issue is of relevance because of certain recent claims in the literature related to the status of *mutual exclusiveness* in tunneling and other experiments [116]-[120].

Finally, we make use of the Bohmian interpretation of quantum theory [123] to obtain a clearer physical insight into some of our key results. The probability current density in calculating the arrival time distribution can be placed on a sounder pedagogical footing

within the context of Bohmian mechanics. Further, we have shown that a clear understanding as to how superarrivals originate is obtained with the help of quantum potential of the Bohm model. We have computed the “particle trajectories” and derived a quantitative estimate of the magnitude of superarrivals using the Bohmian interpretation of quantum mechanics to have a deeper insight into the nature of superarrivals. This analysis substantiates our earlier contention that superarrivals arise from a dynamical disturbance provided by the perturbed barrier which propagates across the wave packet with a definite speed and affects the “particles”. Such time dependent quantum phenomena could be useful in furnishing examples of the *conceptual utility* of the Bohm model.

We conclude by noting that other aspects of the foundations of quantum mechanics are intertwined to make the study of the arrival time problem even more attractive: the “measurement problem”, the quantum Zeno effect, the interpretation of wave- particle duality, and the difficulty in explaining quantum mechanically the occurrence of actual classical-like events are important ingredients of this research. A very important question is raised by Rovelli [132] that “can we compute the exact time at which a quantum measurement happens ?” Without addressing the measurement problem (i.e. *what* causes the wave function to collapse) he discussed the problem of the *timing* of the quantum measurement. Another problem related to barrier crossing which remains controversial at present is that concerned with the formal definition of traversal and tunneling times [133, 134]. This subtle question has received considerable attention in recent years, motivated in part by the possible applications of tunneling in semiconductor devices. A variety of proposals have been made for the definition of the time (actual and mean) spent by a tunneling particle inside the barrier[131]. The Bohmian interpretation can provide a deeper insight into the problem as to how much time a physical corpuscle can take to traverse a region. Research in foundational problems of quantum theory of which the arrival or traversal time is an integral part, is exciting due to the scope of empirical probes made possible by the advance of modern technology, particularly in the fabrication of nano materials.

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