Quantum time of arrival distribution in a simple lattice model

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Abstract
Imagine an experiment where a quantum particle inside a box is released at some time in some initial state. A detector is placed at a fixed location inside the box and its clicking signifies arrival of the particle at the detector. What is the time of arrival (TOA) of the particle at the detector? Within the paradigm of the measurement postulate of quantum mechanics, one can use the idea of projective measurements to define the TOA. We consider a setup where a detector keeps making instantaneous measurements at regular finite time intervals until it detects the particle at time $t$, which is defined as the TOA. This is a stochastic variable and, for a simple lattice model of a free particle in a one-dimensional box, we find interesting features such as power-law tails in its distribution and in the probability of survival (non-detection). We propose a perturbative calculational approach which yields results that compare very well with exact numerics.

Keywords: quantum time of arrival, first passage problem, quantum measurement

(Some figures may appear in colour only in the online journal)
There are several aspects that are involved in discussions of the TOA:

(i) First there is the question of the effect of measurements made to detect the particle’s arrival. The question of repeated ideal measurements in a quantum system was discussed in the seminal paper of Misra and Sudarshan [16] who studied this question in a general setting and showed the surprising result, the so-called quantum Zeno effect, that the probability of detecting a particle (or decay from the initial state) vanishes in the limit that the time interval between measurements $\tau \to 0$ [17, 18]. This means that continued measurements to find the TOA leads to the particle never being detected. The Zeno effect has been experimentally verified [19] though questions of interpretation remain [21]. Hence the question of making measurements at regular finite intervals arises and it becomes necessary to study the effect that null measurements have on the time evolution of a quantum system and on the TOA distribution [6]. A related issue is that of defining positive-operator valued measures corresponding to TOA measurements [14];

(ii) There is then the question of defining a self-adjoint time operator and some progress has been made here [9]. Determining arrival time distributions from these definitions has its own issues [10];

(iii) Finally there is the important question of trying to connect to real experiments. One then needs to incorporate into the picture the entire measurement process by also modeling the measuring device and its interaction with the particle. This has been discussed in, for example, [7, 8, 13].

In this paper, our focus is on aspect (i); we discuss the distribution of TOA resulting from repeated ideal measurements made at regular finite time intervals. In particular, with the aim of being able to explicitly compute the TOA distribution, we study a lattice version of a free particle in one-dimension (1D). We consider a quantum particle that is prepared in a given initial state at some time instant (say $t = 0$) and a detector is placed at some fixed location (schematically shown in figure 1). The detector makes instantaneous quantum measurements at regular intervals of time $\tau$, and keeps doing so until it detects the particle, say on the $n$th observation, at time $\tau_n$. This is taken to be the TOA, which is a stochastic variable. The time evolution of the system undergoing repeated measurements constitutes a non-unitary dynamic. Here we examine the survival probability $P(t)$ that the particle is undetected until time $t$. The limit of continuous measurements $\tau \to 0$ gives $P(t) \to 1$ but we will see that any finite $\tau$ leads to a non-trivial survival probability with interesting power-law tails.

We note that a closely related work is that by Anastopoulos and Savvidou [6] who consider a free particle on the infinite real line. The particle is initially prepared in the negative half line and then subjected to regular measurements that correspond to projections onto the positive half space. The approach followed in this paper is similar to their paper, however, while their main emphasis was in trying to understand the $\tau \to 0$ limit and the related problems, here we focus on the finite $\tau$ problem. Our study is also different from earlier studies on the effect of finite-time-interval measurements on the Zeno effect which have typically looked at few-level unstable systems and examined their decay and survival
probabilities [17, 18, 20]. In contrast, our set-up is that of an extended system where measurements are made in part of the space and the system’s time evolution is altered by the measurements. Another related study is that of Yi et al [22] who consider the effect of multiple measurements involving observation at a single site on the density matrix of a particle in a 1D box. However, there the focus was not on first arrival and the effective evolution equation of the density matrix is completely different from that considered by us.

Our model consists of a particle moving on a discrete lattice of \( N \) sites and its dynamic is described by a tight-binding type Hamiltonian of the form

\[
H = \sum_{\ell,m=1}^{N} H_{\ell,m} |\ell\rangle \langle m|,
\]

where \( H \) is a symmetric matrix. The free time evolution of \(|\psi\rangle\) is given by \(|\psi(t)\rangle = U^{t}|\psi(0)\rangle\), where \( U^{t} = e^{-itH/\hbar}\). Let us define the projection operator \( A = \sum_{i\in D}|i\rangle \langle i| \) corresponding to a measurement to detect the particle in the domain \( D \) containing a fixed set of sites and the complementary operator \( B = 1 - A \). According to the measurement postulate of quantum mechanics, the probability of detecting the particle on performing a measurement on the state \(|\psi\rangle\) is \( p = \sum_{i\in D}|\langle i|\psi\rangle|^{2} = \langle \psi|A|\psi\rangle \). The probability of non-detection or the survival probability is then \( P = \langle \psi|B|\psi\rangle = 1 - p \). The measurement postulate also tells us that measurements alter the Hamiltonian time evolution of the system. Thus if a measurement does not detect the particle then the wavefunction immediately after a measurement projects to \(|\psi_{n}\rangle = |\psi(0)\rangle \). We now consider a sequence of measurements \( n = 1, 2, \ldots \) at intervals of time \( \tau \) which continue until a particle is detected. Thus the time evolution is given by a sequence of unitary evolutions followed by projections into the subspace corresponding to \( B \) until the particle is detected. Let \(|\psi_{n}^{-}\rangle\) and \(|\psi_{n}^{+}\rangle\) be the wavefunctions (un-normalized) of the system immediately before and after the \( n \)th measurement respectively. We note that \(|\psi_{0}^{-}\rangle = U^{1}|\psi_{-1}^{-}\rangle\) and \(|\psi_{0}^{+}\rangle = B|\psi_{-1}^{+}\rangle\). Hence, defining \( \widetilde{B} = BU^{t} \), it follows that

\[
|\psi_{n}^{-}\rangle = U^{t}\widetilde{B}^{n-1}|\psi(0)\rangle, \quad |\psi_{n}^{+}\rangle = \widetilde{B}^{n}|\psi(0)\rangle.
\]

Let \( P_{n} \) be the probability of survival after \( n \) measurements. Then clearly

\[
R_{1} = \langle \psi_{1}^{-} | B | \psi_{1}^{-} \rangle = \langle \psi(0) | \widetilde{B} \widetilde{B} \psi(0) \rangle = \langle \psi_{1}^{+} | \psi_{1}^{+} \rangle.
\]

Note that \( P_{1} \) is thus the normalizing factor for \(|\psi_{1}^{+}\rangle\) and also for \(|\psi_{1}^{-}\rangle\). The survival probability after the second measurement is obtained as the product of non-detection at \( n = 1 \) times the probability of non-detection at \( n = 2 \) and this is

\[
P_{2} = P_{1} \times \frac{\langle \psi_{2}^{-} | B | \psi_{2}^{-} \rangle}{\sqrt{R_{1}}} = \langle \psi(0) | \widetilde{B} \widetilde{B} \widetilde{B} | \psi(0) \rangle = \langle \psi_{2}^{+} | \psi_{2}^{+} \rangle.
\]

Proceeding iteratively in this way, we get

\[
P_{n} = \langle \psi(0) | \widetilde{B} \widetilde{B} \cdots \widetilde{B} | \psi(0) \rangle = \langle \psi_{n}^{+} | \psi_{n}^{+} \rangle.
\]
In the rest of the paper, we shall consider the special case of a 1D lattice where the measurement is made at a single site $N$. In the position basis, the complementary operator $B$ corresponds to an $N \times N$ matrix with elements $B_{ij} = \delta_{i,j-1} \delta_{j,N}$. Our main interest will be in the survival probability, $P_n$ (or equivalently, $P(t)$, where $t = n\tau$) given by equation (3). An explicit solution of this problem requires one to diagonalize the non-Hermitian evolution operator $\tilde{B}$ which in general is difficult.

We study a Hamiltonian that incorporates nearest neighbor hopping of a particle and first consider the case of an open chain corresponding to a free particle inside a 1D box. Thus, the Hamiltonian is given by

$$H = -\sum_{k=1}^{N-1} \gamma (|k+1\rangle \langle k| + |k\rangle \langle k+1|).$$

Without loss of generality we can set $\gamma = 1$, $\hbar = 1$. The eigenvalues and eigenvectors of this Hamiltonian are given by $\epsilon_n = -2\cos \left(s\pi/(N+1)\right)$ and $\psi_n(\ell) = [2/(N+1)]^{1/2} \times$ sin $[s\pi/(N+1)]$ with $s = 1, 2, \ldots, N$. The orthogonal matrix $V$ with matrix elements $V_{\ell,m} = \psi_m(\ell)$ diagonalizes $H$ and the time evolution of the state, from $|\psi_n^-\rangle$ to $|\psi_n^+\rangle = U^\dagger |\psi_n^-\rangle$ with $U_{\ell,m} = \sum_n V_{\ell,n} e^{-i\epsilon_n \tau}/V_{m,n}$, is easy to implement numerically. The projection to $|\psi_n^-\rangle = |\psi_n^-\rangle$ is then simply obtained, in the position basis, as

$$\psi_n^+(\ell) = \begin{cases} \psi_n^- (\ell) & \text{for } \ell \neq N, \\ 0 & \text{for } \ell = N. \end{cases}$$

Thus, numerically it is easy to start with any initial wavefunction $\psi_0^+(\ell)$ and evolve it using the above iteration scheme.

We now present a perturbative calculation of the time evolution of the wavefunction and of the survival probability. The small parameter here is the time $\tau$ between successive measurements (compared to the time for the wavefunction to spread which is $\hbar/\gamma$). Let us use the notation $H_N$ to denote the Hamiltonian matrix on an $N$-site lattice and let $h_N = (0, 0, \ldots, 1)^T$ be an $N$-dimensional column vector with only the last element non-zero. We note that the vector $\tau h_N$ is an exact eigenstate of $\tilde{B}$ with eigenvalue 0 and find the other eigenvalues and eigenstates perturbatively. Expanding $\tilde{B}$ to second order in $\tau$ we have

$$\tilde{B} = B (1 - i\tau H - H^2\tau^2/2 + \ldots)$$

$$= \begin{pmatrix} I_{N-1} & 0 \\ 0 & 0 \end{pmatrix} \left[ \begin{pmatrix} I_{N-1} & 0 \\ 0 & 1 \end{pmatrix} - i\tau \begin{pmatrix} H_{N-1} & -h_{N-1} \\ -h_{N-1}^T & 0 \end{pmatrix} \right]$$

$$- \frac{\tau^2}{2} \begin{pmatrix} H_{N-1}^2 + h_{N-1}h_{N-1}^T & -H_{N-1}h_{N-1} \\ -h_{N-1}^T H_{N-1} & 1 \end{pmatrix}$$

$$= \begin{pmatrix} I_{N-1} - i\tau H_{N-1} - \tau^2 H_{N-1}^2/2 + Z_{N-1} & C_{N-1} \\ 0 & 0 \end{pmatrix},$$

where $I_N$ denotes an $N$-dimensional unit matrix, $Z_{N-1} = -(\tau^2/2)h_{N-1}h_{N-1}^T = -(\tau^2/2)[N-1](N-1)$ is a $(N-1) \times (N-1)$ matrix with one non-vanishing element and $C_{N-1} = i\tau h_{N-1} - (\tau^2/2)H_{N-1}h_{N-1}$. Let the $N-1$ eigenstates and eigenvalues of the matrix $Q_{N-1} = I_{N-1} - i\tau H_{N-1} - \tau^2 H_{N-1}^2/2 + Z_{N-1}$ be denoted by $|\chi_i\rangle$ and $\mu_i$ respectively, satisfying
\( Q_{N-1} | \chi_\ell \rangle = \mu | \chi_\ell \rangle. \) (6)

Denoting the components \( \chi_\ell (\ell) = \langle \ell | \chi_s \rangle \), it is easily seen that the vectors \( (\chi_1 (1), \chi_2 (2), \ldots, \chi_{N-1} (N-1), 0) \) form the remaining \((N-1)\) eigenstates of \( \hat{B} \). We now find \( \chi_\ell (\ell) \) and \( \mu \) using perturbation theory.

The eigenfunctions and eigenvalues of \( H_{N-1} \) are respectively given by

\[
\phi^s = \frac{1}{2} \sin \left( \frac{s \pi}{N} \right) \quad \text{and} \quad e_s = -2 \cos \left( \frac{s \pi}{N} \right), \quad \text{with} \quad s = 1, 2, \ldots, N-1 \quad \text{and} \quad \ell = 1, 2, \ldots, N-1.
\]

Treating the part \( Z_{N-1} \) of \( Q_{N-1} \) as a perturbation, we get from first order perturbation theory

\[
\langle \chi_\ell | H_{N-1} | \chi_\ell \rangle = \frac{e_s^2}{2} + O\left( \ell^3 \right)
\]

\[
\mu = 1 - ire_s - \frac{e_s^2}{2} + \langle \phi | Z_{N-1} | \phi \rangle + O\left( \ell^3 \right)
\]

where \( \alpha_s = -(2/\tau) \langle \phi | Z_{N-1} | \phi \rangle = \tau \phi_s^2 (N-1) = \tau \phi_s^2 (1) \). Now we can use equation (2) to find the state of the system at time \( t = n\tau \) after \( n \) measurements. If the initial state is an eigenstate of \( H_{N-1} \), i.e. \( \langle \psi_0^s \rangle = \langle \phi \rangle \), then we have approximately

\[
| \psi_t^+ \rangle = \mu^s | \phi \rangle = e^{-i\alpha_s \tau} e^{-\frac{e_s^2}{2} \tau} | \phi \rangle = P_s^{1/2}(t) e^{-i\alpha_s \tau} | \phi \rangle.
\]

where \( P_s(t) \), the survival probability (of the \( s \)th energy eigenstate) given by

\[
P_s(t) = \langle \psi_t^+ | \psi_t^+ \rangle = e^{-\alpha_s \tau}.
\]

Thus, \( \alpha_s \) represents the decay rate of the state \( | \phi \rangle \). We see that when the initial state is an eigenstate of the Hamiltonian, the survival probability decays exponentially with time with the rate of decay depending on the measurement interval \( \tau \) and the probability density of the wavefunction near the detection point. In the limit \( \tau \to 0 \), the decay rate vanishes implying the Zeno effect.

For the case where the particle is initially at site \( \ell \), the initial position eigenstate can be expanded as \( | \ell \rangle = \sum_i c_i | \phi_i \rangle \), with \( c_\ell = \phi_\ell (\ell) \), so that at time \( t \) we now get

\[
| \psi_t^+ \rangle = \sum_s \phi_s (\ell) P_s^{1/2}(t) e^{-i\alpha_s \tau} | \phi \rangle.
\] (8)

The survival probability is then obtained as

\[
P_s(t) = \langle \psi_t^+ | \psi_t^+ \rangle = \sum_s \phi_s^2 (\ell) P_s(t)
\]

\[
= \sum_{s=1}^{N} 2 \sin^2 \left( \frac{s\pi}{N} \right) e^{-\frac{e_s^2}{2N} \sin^2 \left( \frac{s\pi}{N} \right)}.
\] (9)

The difference between the \((s + 1)\)th and \(s\)th term of this summation will be small for large \( N \) and small \( \tau \pi/N^3 \). We can then convert the sum to an integral and get

\[
P_s(t) = \frac{2}{\pi} \int_0^\pi dq \sin^2 (q\ell) e^{-\frac{2q^2}{N^2} \sin^2 q}.
\] (10)
Thus we find that $P_t(\ell)$ has the scaling form $P_t(\ell) = f(\tau t/N)$. Defining,

$$x \equiv \frac{\tau t}{N},$$

we also see that when $x$ is large, only small values of $q$ in this integral will matter and hence

$$P_t(\ell) = \frac{1}{\pi} \int_{-\infty}^{\infty} dq \sin^2(q\ell) e^{-2\pi^2} = \frac{1}{\sqrt{8\pi x}} \left[ 1 - e^{-\ell^2/2x} \right].$$

For points close to the boundary, $\ell \sim O(1)$, we get $P_t(\ell) \sim 1/\ell^{1/2}$ at times $1 \ll \tau t/N \ll \ell^2$, and then a cross-over to $P_t(\ell) \sim 1/\ell^{3/2}$ at large times $\tau t/N \gg \ell^2$. For points in the bulk of the sample, $\ell \sim O(N)$, $\ell^2/\ell(xN^2/\tau t)$ is large in the time domain where $\tau t/N^3 \ll 1$, hence one observes only the behaviour $P_t(\ell) \sim 1/\ell^{3/2}$. The power-law decay with time changes to an exponential decay at time $t \sim N^3$ when the sum in equation (9) is dominated by one term, namely the one corresponding to the smallest eigenvalue. The first arrival probability is obtained as $p(t) = -dP/dt$. In figure 2 we show the comparison between the analytic predictions for the survival probability with the exact numerical results. The agreement is very good.

We shall now discuss the case of periodic boundary condition. The Hamiltonian is now given by

$$H_p = -\sum_{k=1}^{N-1} \{\varepsilon_k + 1\} \langle k | + | k \rangle \langle k + 1 | - | 1 \rangle \langle N | - | N \rangle \langle 1 |. \quad (12)$$

For even values of $N$, there are $(N-2)/2$ eigenvalues $\varepsilon_j = -2 \cos (2\pi j/N)$, each with two degenerate eigenvectors

$$\psi_{\ell}(\ell) = (2/N)^{1/2} \sin (2 s\ell\pi/N)$$

$$\psi_{\ell+N/2-1}(\ell) = (2/N)^{1/2} \cos (2 s\ell\pi/N)$$
for \( s = 1, 2, \ldots, N/2 - 1 \). The remaining two eigenvectors (non-degenerate) are \( \psi_{N-1}(t) = (-1)^{t}/N^{1/2} \) and \( \psi_{N}(t) = 1/N^{1/2} \) with eigenvalues \(-2\) and \(2\) respectively. However, in this case we notice that the eigenstates \( \phi_{s}(t) \) of \( H_{N-1} \) (with open boundary condition) for \( s = 1, 2, \ldots, N/2 - 1 \) are also exact eigenstates of \( H_{P} \) and they all vanish at the site \( N \). Hence these are also exact eigenstates of \( \tilde{H}( = B e^{-i\tau H_{P}}) \) with eigenvalue \( e^{-i\tau \ell} \) and do not decay. Also, one observes that the vector \( e^{i\tau H_{P}}(0,0, \ldots,1)^T \) is an exact eigenvector of \( \tilde{B} \) with eigenvalue zero. However, this eigenvector does not contribute to the dynamics as the eigenvalue is only zero. Thus, we now have \( N/2 \) exact eigenvectors of \( \tau \). The remaining eigenvectors can be found perturbatively as before. We note that writing Hamiltonian \( H_{P} \) in block form now gives us the same form as \( -H_{N-1} \) before while the vector \( \tilde{h}_{N-1} \) now has the form \( \alpha_{0} \) and \( Z_{N-1} \) is therefore given by

\[
Z_{N-1} = -(t^{2}/2) h_{N-1} h_{N-1} = -\left(t^{2}/2\right)\left(1\right)\left(1\right) + \langle 1 \rangle \langle N - 1\rangle + \left|\psi_{s}\right|^{2} \langle N - 1\rangle + \left|\psi_{s}\right|^{2} \langle N - 1\rangle.
\]

Let the initial state of the system be any one of \( \left|\psi_{2s+1}\right\rangle, s = 0, 1, \ldots, N/2 - 1 \). The decay rate is then given by

\[
\alpha_{2s+1} = -(2/\tau)\left\{ \phi_{2s+1}\right\} \left\{ Z_{N-1}\right\} \left|\phi_{2s+1}\right\rangle = 4\tau\phi_{2s+1}^{2}(1).
\]

Thus, initial eigenstates which are symmetric about the centre \( (N/2) \) of the ring decay with this rate while the odd states remain undetected and do not decay.

If the initial state is a position eigenstate \( \neq \ell N \) then we expand in the basis of \( H_{N-1} \) and obtain

\[
\psi_{s} = \sum_{s=1}^{N/2-1} \phi_{2s}(t)e^{-i\varphi_{2s}t}\phi_{2s} + \sum_{s=0}^{N/2-1} \phi_{2s+1}(t)P^{2s+1}_{2s+1}(t)e^{-i\varphi_{2s+1}t}\phi_{2s+1}.
\]

Taking the inner product we get

\[
P(t) - P(\infty) = \frac{1}{\pi} \int_{0}^{\pi} dq \sin^{2}(q\ell)e^{-8\pi^2 q^{2}/N}\sin^{2} q,
\]

For large \( \tau t/N = x \), this integral becomes

\[
P(t) - P(\infty) = \frac{1}{8\sqrt{\pi x}} \left[ 1 - e^{-t^{2}/8x} \right].
\]

Thus, as before we find that, for initial starting points close to detector \( \ell \sim O(1) \) or \( N - \ell \sim O(1) \), \( P(t) \) decays to its asymptotic limiting value as \( \sim 1/t^{3/2} \) while for initial starting points in the bulk of the sample we get a decay as \( \sim 1/t^{1/2} \). It can also be shown that for \( \ell = N \) we get \( P(\infty) = 0 \) and a \( 1/t^{1/2} \) decay. We note here that a recent paper [23] considered the motion of a quantum particle on a ring in the presence of trapping sites (modeled by non-Hermitian potentials) and found similar results.

**Conclusion**

In this paper we considered the example of a particle inside a box that is released at time \( t = 0 \) with an initial wavefunction \( |\psi(0)\rangle \), which could either be an extended energy...
eigenstate or a spatially localized state. A detector placed at a fixed location is turned on at regular small intervals of time $\tau$ and makes instantaneous measurements. The first click of the detector, say on the $n$th measurement, gives the TOA (or time of first detection) $t = n \tau$. One can imagine an ensemble of such experiments being performed such that, once a particle is detected in any of the realizations, it is no longer studied and we carry on with the remaining realizations. Thus each different realization of the experiment ends at a different time and we get a distribution of times. For this process, the probability distribution of the TOA and the corresponding survival probability can be defined unambiguously according to the measurement postulates of quantum mechanics. The effective time evolution constitutes an interesting example of non-unitary time evolution for which we show that an accurate solution is given from standard perturbation theory. Using this, we obtained non-trivial results for the survival probability for a simple lattice Hamiltonian model of a free particle. Interesting features, including non-trivial power-law tails of the survival probability, are observed and these features are different from the first passage behaviour in a classical system [24].

Our formalism and results are easily extendable to more realistic systems, e.g. those in higher dimensions with extended detectors. Cold atoms on optical lattices would be ideal experimental systems where some of our predictions can be tested. These tests are interesting since they offer a direct test of the measurement postulate of quantum mechanics.

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