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Short-time behaviour of the quantum survival probability

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Abstract. – The short-time behaviour of the quantum survival probability is examined. The origin of previous discrepancies on the short-time behaviour is explained by means of a discrete decomposition of the survival amplitude into a sum of decaying exponential terms and w-functions. Several possible non-exponential dependences are described and exemplified.

The quantum-mechanical decay of unstable states has been studied in many different ways [1]-[8]. An ideal description of the decay would handle arbitrarily complex initial states and potentials in simple terms, and allow an understanding of both the dominant exponential decay and the deviations from it. Much progress in this direction has been achieved by representing the *survival amplitude* $A(t,\psi) \equiv \langle\psi(0)|\psi(t)\rangle$ as a discrete sum over resonant terms [9], [10]. The discretization provides a means for clearly identifying the physically dominant contributions to the *survival probability* $S = |A|^2$, different terms being important in different time regimes.

We have recently used a discretization formalism to examine the deviation from exponential decay at large times [11]. The objective of the present letter is to discuss the short-time behaviour of the decay of the survival probability of quantum states. Several authors have described a short-time t^2-dependence of the *decay probability* $P_{\text{decay}} \equiv 1 - S$, provided the mean energy and second energy moment of these states exist, see, *e.g.*, [6], and papers related to the "quantum Zeno paradox" [12]-[15]. Less attention has been paid to the short-time behaviour if these conditions are not fulfilled. On the other hand, a formal treatment and examples by Moshinsky and coworkers suggest a $t^{1/2}$-dependence of the decay probability at short times [16], [17]. We shall clarify how these two seemingly different claims can be compatible. Other possible dependences will be justified and exemplified.

The discretization of the survival amplitude has been discussed by García Calderón and coworkers [9], [10]. We find it convenient to use here a variant of their approach [11], [18](1). The survival amplitude $A(t,\psi)$ requires the diagonal matrix elements of the unitary evolution

(1) We have preferred this route because the treatment in [10] is formally restricted to cut-off potentials, while our model potential is not cut off. This does not mean that *any* potential can be treated in the same fashion. It is necessary to examine the analytical properties of the corresponding $I(q)$ function, which depends on the behaviour of the potential at large distances. It is expected that the method is applicable, with some modifications depending on the case, whenever $I(q)$ is analytical except for poles and possibly branch points on the negative imaginary axis.

operator $\exp[-iHt/\hbar]$. When this operator is expressed in terms of the resolvent, $A(t,\psi)$ takes the form

$$A(t,\psi) = \langle\psi|\exp[-iHt/\hbar]|\psi\rangle = \frac{i}{2\pi m}\int_C \mathrm{d}q\, q \left\langle \psi \left| \frac{\exp[-izt/\hbar]}{z-H} \right| \psi \right\rangle = \frac{i}{2\pi}\int_C \mathrm{d}q \exp[-izt/\hbar] I(q)\,, \tag{1}$$

where $z = q^2/2m$ and the q contour, C, goes from $-\infty$ to $+\infty$ passing above all of the singularities of the resolvent due to the spectrum of H (discrete poles for bound states and the natural boundary of the real axis for the continuum).

The function

$$I(q) \equiv \frac{q}{m}\left\langle \psi \left| \frac{1}{z-H} \right| \psi \right\rangle \tag{2}$$

can be evaluated in the upper half q-plane and then analytically continued into the lower half plane. Provided that the continuation exists, $I(q)$ has in general a set of *core* singularities, depending only on the potential, plus possibly other *structural* singularities depending on the particular state ψ. It is then useful to deform the original integration contour to being along the diagonal D of the second and fourth quadrants of the q-plane. This provides both physical insight by identifying the most relevant time dependence (exponential decay) of the survival, and a calculational advantage for the remainder (for positive t the exponential $\exp[-izt/\hbar] = \exp[-iq^2t/(2m\hbar)]$ is a real Gaussian on this diagonal).

Let us assume that a pole expansion of the form

$$I(q) = \sum_k \frac{a_k}{(q-q_k)}, \qquad \Im\mathrm{m}\, q_k < 0 \tag{3}$$

is possible. (The presence of higher-order poles can be treated in a similar fashion.) Here $k = 1, 2, 3, \ldots$ indexes the poles. On deforming the q integration from contour C to D, the poles crossed on carrying out this deformation provide contributions to the survival amplitude that decay exponentially with time. For a pole at q_k this contribution to $A(t)$ takes the form

$$E_k(t) = a_k \exp[-iq_k^2 t/(2m\hbar)] = a_k \exp[-u_k^2]\,, \tag{4}$$

where

$$u_k \equiv q_k/f, \qquad f \equiv (1-i)\sqrt{(m\hbar/t)}\,. \tag{5}$$

Independently of being crossed or not crossed by the contour deformation, all poles contribute, because of the integral along the diagonal. Each pole contribution is of the form

$$D_k(t) = -\frac{a_k}{2}\mathrm{sign}(\Im u_k)\, w[\mathrm{sign}(\Im u_k) u_k]\,. \tag{6}$$

This is expressed in terms of the w-function, see [19]. Numerical values and asymptotic properties of this function for small or large times are easily computable. The exponential term (4) can be added to this contribution to give the compact result [19]

$$A(t) = \sum_k [E_k(t) + D_k(t)]\,, \tag{7}$$

$$= \sum_k \frac{1}{2} a_k w(-u_k)\,. \tag{8}$$

(It is understood that $E_k(t) = 0$ for poles that have not been crossed when deforming the contour.) In the first form, (7), the exponential decay contribution is clearly separated from the "correction" D_k in terms of a w-function. However, the second compact form in (8) is very useful in formal manipulations and in particular for studying the short-time behaviour.

The Taylor series of the w-function [19] gives a series in powers of $t^{1/2}$,

$$A(t) = \sum_k \frac{a_k}{2} \sum_{n=0}^{\infty} \frac{[2^{-1} q_k (1-i)(t/m\hbar)^{1/2}]^n}{\Gamma(\frac{n}{2}+1)} . \tag{9}$$

This suggests a short-time $t^{1/2}$-dependence of the decay probability, as claimed by Moshinsky and coworkers [16], [17]. On the other hand, the formal series based on expanding the evolution operator,

$$A(t,\psi) = \langle\psi|\exp[-iHt/\hbar]|\psi\rangle = 1 - \frac{it}{\hbar}\langle\psi|H|\psi\rangle - \frac{t^2}{2\hbar^2}\langle\psi|H^2|\psi\rangle + \cdots , \tag{10}$$

provides a t^2-dependence,

$$P_{\mathrm{decay}} = \frac{t^2}{\hbar^2}\left(\langle\psi|H^2|\psi\rangle - \langle\psi|H|\psi\rangle^2\right) + \cdots . \tag{11}$$

However, the expectation values of H and/or higher powers of H may not exist. Several behaviours are possible depending on the existence of these moments. The question of the physical realizability of states with infinite first or second energy moments is subject to debate [7]. In principle, if they are states in the Hilbert space of square integrable functions, they are physically valid states according to the standard interpretation of the quantum formalism. Lamb discussed idealized experiments to create arbitrary Hilbert space states by means of a previous creation of appropriate potential functions [20]. Nowadays molecular beam epitaxy allows the growth of structures with arbitrary potential profiles [21] and provides a means to approach Lamb's idealized experiments. In any case even if the moments of the quantum state are not strictly infinite, for a particular time scale they may be large enough so that the analysis below (which assumes the existence of states with diverging moments) is relevant.

Let us consider the first two derivatives of A at time $t = 0$ first from (10) and then by assuming a general short-time dependence of the form $A \sim 1 + b\,t^c$, where b and c are finite constants,

$$\left.\frac{\mathrm{d}A}{\mathrm{d}t}\right|_{t=0} = \frac{-i}{\hbar}\langle\psi|H|\psi\rangle = b\,c\,t^{c-1}\big|_{t=0} \tag{12}$$

$$\left.\frac{\mathrm{d}A^2}{\mathrm{d}t^2}\right|_{t=0} = -\frac{1}{\hbar^2}\langle\psi|H^2|\psi\rangle = b\,c\,(c-1)t^{c-2}\big|_{t=0} . \tag{13}$$

If the mean energy of the initial state does not exist, a $t^{1/2}$-dependence of the decay probability is possible. An explicit example in one dimension is provided in the appendix. Another example is provided in ref. [17] for a delta-shell model potential. The initial state considered in that paper takes (in three dimensions) the form $\sin(\pi r/R)/r$, $r \le R$. Its mean energy is infinite (a fact not commented upon in [17]), as can be seen by performing the integral in momentum representation.

If the mean energy is finite so that $\mathrm{d}S/\mathrm{d}t|_{t=0} = 2\Re\mathrm{e}(\mathrm{d}A/\mathrm{d}t|_{t=0}) = 0$, then $c \ge 1$. This rules out a $t^{1/2}$-dependence of A since a $t^{1/2}$-dependence implies an infinite time derivative of A at $t = 0$. The corresponding coefficient for $t^{1/2}$ in (9) must vanish, by compensation between the different pole contributions.

The second derivative is only finite at time zero if $c \geq 2$. This means that if the first energy moment exists but not the second, a dependence t^c where $1 \leq c < 2$ is possible for A (and for the decay probability), in particular $t^{3/2}$. (The coefficient for $t^{1/2}$ must also vanish in this case.) Otherwise, one can expect that the series (10) will be effective at short times for states with finite moments $\langle\psi|H^n|\psi\rangle$ leading to a t^2 behaviour. We shall provide next examples where $t^{3/2}$ and t^2 dominate the short-time behaviour of P_{decay}.

A simple separable (non–cut-off) potential [22]-[25] in one dimension is used to illustrate the previous general discussion,

$$V = |\chi\rangle V_0\langle\chi|, \tag{14}$$

$$\langle p|\chi\rangle = \left(\frac{2a^3}{\pi}\right)^{1/2}\frac{1}{a^2+p^2}. \tag{15}$$

For this potential,

$$\begin{aligned} I(q) &= \frac{1}{m}\left\langle\psi\left|\frac{q}{z-H_0}\right|\psi\right\rangle + \\ &+\left\langle\psi\left|\frac{1}{z-H_0}\right|\chi\right\rangle\frac{V_0\,q^2(q+ia)^2}{m\mathcal{C}(q)}\left\langle\chi\left|\frac{1}{z-H_0}\right|\psi\right\rangle, \end{aligned} \tag{16}$$

where H_0 is the free-particle Hamiltonian and $\mathcal{C}(q)$ is a cubic polynomial. The "motion" of its roots q_k in the complex q-plane as the potential strength V_0 changes has been previously analysed [24]. For $mV_0/a^2 > (-11+5\sqrt{5})/4$ the roots of the cubic $\mathcal{C}(q)$ (core singularities of $I(q)$) are a resonance pole in the fourth quadrant at $q_1 = \alpha - i\beta$, α, $\beta > 0$, the corresponding "antiresonance" at $q_2 = -q_1^*$, and a virtual state pole on the negative imaginary axis at $q_3 = -2ia + 2i\beta$.

The survival probability of the state χ is examined: In this case

$$I(q) = \frac{q}{m}\left\langle\chi\left|\frac{1}{z-H}\right|\chi\right\rangle = \frac{2q(q+2ia)}{\mathcal{C}(q)} \tag{17}$$

and the only singularities correspond to the roots of the cubic equation. This rational fraction can then be decomposed into partial fractions, $I(q) = \sum_k a_k/(q-q_k)$, where $a_k = \mathrm{res}[I(q)]_{q=q_k}$. For the state χ the first moment $\langle\chi|H|\chi\rangle$ is finite but the expectation values of H^2 and higher powers of H do not exist. The small t series for $A(t,\chi)$ takes the form

$$A(t,\chi) = \sum_{n=0}\frac{[(1-i)(t/m\hbar)^{1/2}/2]^n}{\Gamma(\frac{n}{2}+1)}A_n. \tag{18}$$

Using the standard relations between the roots of the cubic $\mathcal{C}(q)$, it is easy to prove that

$$A_0 = 1, \qquad A_1 = 0, \qquad A_2 = A_2^*. \tag{19}$$

The first result is a consistency check of the correct normalization. The second and third relations imply that there are no terms depending on $t^{1/2}$ or t in the corresponding expansion of P_{decay}. The first non-vanishing term is proportional to $t^{3/2}$.

Finally, a numerical check is made for an initial state having all finite moments $\langle\psi|H^n|\psi\rangle$, specifically a Gaussian packet $\mathcal{G}$. It is found that the decay probability of this *Gaussian state* behaves as t^2 for short times ([2]).

([2]) For the Gaussian wave function $I(q)$ is meromorphic but the pole expansion of $I(q)$ is not feasible in the form (3) because of the need to add an entire function. In such a case the exponential contribution can still be calculated in the same manner, but the integral along D needs to be evaluated numerically. Since it is weighted by a real Gaussian, $\exp[-u^2]$, this is a much simpler task than the original integral along the real axis with its oscillatory exponentials.

In summary, different possible short-time dependences of the decay probability have been justified with a discretization formalism. Examples have been provided that demonstrate that the decay probability may behave at short times as $t^{1/2}$ for states with divergent mean energy (χ_1 in the appendix), as $t^{3/2}$ for states with divergent second energy moment (χ), and as t^2 for states with finite first and second energy moments ($\mathcal{G}$).

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Appendix: Example of $t^{1/2}$ *behaviour of the decay probability at short times.* – We shall use here a separable potential model different from the one in the main text, namely

$$V_1 = |\chi_1\rangle V_0 \langle\chi_1| \,, \tag{A.1}$$

$$\langle p|\chi_1\rangle = \left(\frac{a}{\pi}\right)^{1/2} \frac{1}{(p^2+a^2)^{1/2}} \,. \tag{A.2}$$

Assuming $2mV_0 > a^2/4$, there are two core poles at $q_1 = -ia/2 + (2mV_0 - a^2/4)^{1/2}$ and $q_2 = -q_1^*$. Following the same procedure leading to (18), the survival of χ_1 can be written as

$$A(t,\chi_1) = \frac{1}{q_2 - q_1}[q_2 w(-u_2) - q_1 w(-u_1)] \,. \tag{A.3}$$

By substituting the series expansion of the w it is found that the first non-vanishing term of the decay probability is of order $t^{1/2}$ ([3]).

([3]) This behaviour is also described in ref. [9], sect. 17.6, by assuming a "one level" formula for the survival amplitude without specification of the potential function.

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