Double-Barrier Resonances and Time Decay of the Survival Probability: A Toy Model

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Abstract In this talk we consider the time evolution of a one-dimensional quantum system with a double barrier given by a couple of repulsive Dirac's deltas. In such a *pedagogical* model we give, by means of the theory of quantum resonances, the asymptotic behavior of $\langle \psi, e^{-itH}\phi \rangle$ for large times, where H is the double-barrier Hamiltonian operator and where ψ and ϕ are two test functions. In particular, when ψ is close to a resonant state then explicit expression of the dominant terms of the survival probability defined as $|\langle \psi, e^{-itH}\psi \rangle|^2$ is given.

Keywords Lambert special functions • Quantum resonances • Quantum survival probability • Singular barrier potential

1 Introduction

The phenomenon of exponential decay associated with quantum resonances is well known since the pioneering works on the Stark effect in an isolated hydrogen atom. Atomic hydrogen in an external electric field was first studied experimentally in 1913 by Stark [18] and Lo Surdo [11], and quantum mechanically in 1926 by Schrödinger [16]. The time independent Schrödinger equation for a hydrogen atom of nuclear charge Z, electron charge e, electron (reduced) mass m, in a uniform external electric field F directed along one axis (i.e. the z axis) has the form

$$H(F)\psi = \mathcal{E}\psi \, , \; H(F) := -\frac{\hbar^2}{2m}\Delta + \frac{eZ}{r} + Fez \, . \tag{1}$$

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When the external electric is absent, i.e. $F = 0$, then $H(0)$ has discrete negative eigenvalues given by (we set $\hbar = 1$, $2m = 1$ and $e = 1$)

$$\mathscr{E} = \mathscr{E}_{n,n_1,m} = -\frac{Z^2}{2n^2}$$

where $n = n_1 + n_2 + |m| + 1 = 1, 2, \ldots$ is the *principal quantum number*, $|m| = 0, 1, 2, \ldots, n-1$ and the quantum number n_1 is the number of nodes of the wave function.

In fact, when we switch on the electric field then the eigenvalues problem (1) has no eigenvalues at all as soon as $F \neq 0$. Thus, the quantum states experimentally observed in the Stark effect are not truly bound, but are instead *quantum resonances* associated with a *decay effect* of the *survival probability*. In fact, they are *s*hape resonances, which correspond to confinement of a particle by a barrier, through which tunneling occurs; although the strength of the electric field may be small, the perturbation interaction remains large somewhere far from the origin.

In order to explain the decay effect due to resonances let us consider, in a more general context, an Hamiltonian with a discrete eigenvalue $\mathscr{E}_0$ and an associated normalized eigenvector ψ_0. We suppose to weakly perturb such an Hamiltonian and that the new Hamiltonian H has purely absolutely continuous spectrum, that is the eigenvalue of the former Hamiltonian disappears into the continuous spectrum. Then we physically expect that, after a very short time, the *survival amplitude* has the following asymptotic behavior

$$\langle \psi_0, e^{-itH} \psi_0 \rangle \sim e^{-it\mathscr{E}} \tag{2}$$

where $\mathscr{E}$ is a quantum resonance close to the unperturbed eigenvalue $\mathscr{E}_0$, i.e. $\Re\mathscr{E} \sim \Re\mathscr{E}_0$ and $\Im\mathscr{E} < 0$ is such that $|\Im\mathscr{E}| \ll 1$. The *survival probability* is defined as the square of the absolute value of the survival amplitude (sometimes in the literature, with abuse of notation, both objects are named survival probability).

The validity of (2) has been proved when the perturbation term is given by a Stark potential. In such a case Herbst [10] proved that (2) holds true with an estimate of the error term. However, we should remark that Simon [17] pointed out that the exponentially decreasing behavior is dominant for large times only when the perturbed Hamiltonian H is not bounded from below. In fact, in the case of Hamiltonian H bounded from below we expect to observe a time decay for the survival amplitude of the form

$$\langle \psi_0, e^{-itH} \psi_0 \rangle = e^{-it\mathscr{E}} + b(t) \tag{3}$$

where the *remainder* term $b(t)$ is dominant for small and large times, and the exponential behavior is dominant for intermediate times. On the other hand, dispersive estimates for one-dimensional Schrödinger operators suggest that for large times the remainder term $b(t)$ is bounded by ct^{-r}, for some $c > 0$ and $r > 0$, as in the free model where $r = \frac{1}{2}$. However, this estimate is very raw because it does not take into account the resonances effects.

The analysis of the problem of the exponential decay rate *versus* the power decay rate in the time dependent survival amplitude defined by (3) is a research argument since the '50. In the seminal paper by Winter [20] it has been numerically conjectured that a transition effect between the two different kind of decays starts around some instant t. Recently a more rigorous analysis of the Winter's model, consisting of a one-dimensional model with one Dirac's delta potential at $x = R > 0$ and Dirichlet boundary condition at $x = 0$, has been done [7]. Such a transition effect has been also observed in ultra-cold sodium atoms trapped in an accelerating periodic optical potential [19]; more precisely, they show a transition from non-exponential decay for short times to exponential decay for intermediate time. Furthermore, Winter-like models, where a more general singular potential is considered, have been recently studied, see e.g. [4].

In this paper we consider a simple one-dimensional model with a symmetric double barrier potential with Hamiltonian

$$H_\alpha = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \alpha\delta(x+a) + \alpha\delta(x-a)$$

on the whole real axis [13, 14]. The two barriers are modeled by means of two symmetric repulsive Dirac's deltas at $x = \pm a$, for some $a > 0$, with strength $\alpha \in (0, +\infty]$. This model has been considered by [9], as a *pedagogical* model for the explicit study of quantum barrier resonances. However, H_α also has some physical interest as a model for ultra-thin double-barrier semiconductor heterostructures [12].

When $\alpha = +\infty$ the spectrum consists of a sequence of discrete eigenvalues $\mathscr{E}_{\infty,n}$, $n = 1, 2, 3, \ldots$, embedded in the continuum $[0, +\infty)$. When $\alpha < +\infty$ the spectrum of H_α is purely absolutely continuous and the eigenvalues obtained for H_∞ disappear into the continuum. More precisely, such eigenvalues becomes quantum resonances $\mathscr{E}_{\alpha,n}$ and the time decay of $\langle \psi, e^{-iHt}\phi \rangle$, where ψ and ϕ are two test functions, has the form (3) where

$$b(t) = c_\alpha t^{-3/2} + O(t^{-5/2}) \tag{4}$$

for large t and for some $c_\alpha > 0$ (see Theorem 1 below); in particular, in the case where the two test functions coincide with the unperturbed eigenvector then c_α may be explicitly computed (see Theorem 2 below) and it turns out that $c_\alpha \sim \alpha^{-2}$ in agreement with the fact that the asymptotic behavior (4) cannot uniformly hold true in a neighborhood of $\alpha = 0$.

In fact, we prove that a cancellation effect occurs and that the $t^{-1/2}$ factor coming from the free evolution propagator e^{-itH_0}, as usually occurs for the free one-dimensional Laplacian problem, is canceled by means of an opposite term coming from the two Dirac's deltas barrier. Hence, we can conclude that the effect of the double barrier is twice:

- the time-decay becomes faster, for t large for any $\alpha > 0$;
- for intermediate times the time-decay is slowed down because of the effect of the quantum resonant states.

Finally, we also find out the asymptotic value, for large α, of the instant t around which the transition between exponentially and power decay rate starts.

We should mention some papers where a weighted $t^{-3/2}$ dispersive estimate has been proved for the evolution operator under some assumptions on the potential. In particular, [8] (see also [15]) assumed that the potential is a L^1 function and that zero energy is not a resonance. We have to point out that the condition about the absence of zero energy resonance is crucial. In fact, in our model we see that the first resonance $\mathcal{E}_{\alpha,1}$ has limit zero when α goes to zero and the asymptotic behavior (4) does not hold true in such limit because c_α goes to infinity. We could overcome this problem by choosing the test vector ψ in a suitable subspace [3].

2 Description of the Model and Quantum Resonances

We consider the resonances problem for a one-dimensional Schrödinger equation with two symmetric potential barriers. In particular we model the two barriers by means of two Dirac's δ at $x = \pm a$, for some $a > 0$. The Schrödinger operator is formally defined on $L^2(\mathbb{R}, dx)$ as (let $\hbar = 1$ and $2m = 1$)

$$H_\alpha = -\frac{d^2}{dx^2} + \alpha\delta(x+a) + \alpha\delta(x-a)$$

where $\alpha \in (0, +\infty]$ denotes the strength of the Dirac's δ.

When $\alpha < +\infty$ it means that the wavefunction ψ should satisfies to the matching conditions

$$\psi(x+) = \psi(x-) \text{ and } \psi'(x+) = \psi'(x-) + \alpha\psi(x) \text{ at } x = \pm a\,, \tag{5}$$

and H_α has self-adjoint realization on the space of functions $H^2(\mathbb{R} \setminus \{\pm a\}) \cap H^1(\mathbb{R})$ satisfying the matching conditions (5). When $\alpha = +\infty$ it means that H_∞ has self-adjoint realization on a domain of functions satisfying the Dirichlet conditions $\psi(\pm a) = 0$. In this latter case then the eigenvalue problem $H_\infty\psi = \mathcal{E}_\infty\psi$ has simple eigenvalues $\mathcal{E}_{\infty,n} = k_n^2$ where $k_n = \frac{n\pi}{2a}$, $n = 1, 2, \ldots$, with associated (normalized) eigenvectors

$$\psi_n(x) = \begin{cases} 0 & \text{if } x < -a \\ \frac{1}{\sqrt{a}}\cos\left[k_n x - \frac{\pi}{4}(1+(-1)^n)\right] & \text{if } -a < x < +a \\ 0 & \text{if } +a < x \end{cases} . \tag{6}$$

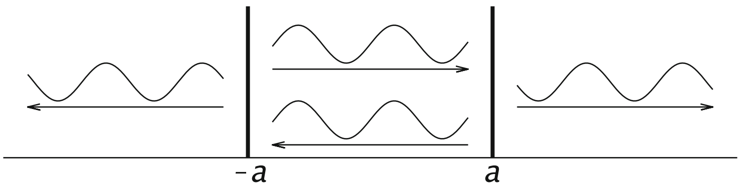

Fig. 1 Double-barrier model with two repulsive Dirac's δ at $x = \pm a$. Resonances are associated with the *outgoing* conditions $A = F = 0$ or, equivalently, to the poles of the kernel of the resolvent operator in the *unphysical complex half-plane* $\Im\mathscr{E} < 0$

The spectrum of H_∞ is then given by the continuum $[0, +\infty)$ with embedded eigenvalues $\mathscr{E}_{\infty,n}$.

In the case $\alpha \in (0, +\infty)$ then the eigenvalue problem

$$H_\alpha \psi = \mathscr{E}_\alpha \psi$$

has no real eigenvalues, but resonances; where resonances correspond to the complex values of $\mathscr{E}_\alpha$ such that the wavefunction

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & \text{if } x < -a \\ Ce^{ikx} + De^{-ikx} & \text{if } -a < x < +a \\ Ee^{ikx} + Fe^{-ikx} & \text{if } +a < x \end{cases}, \quad k = \sqrt{\mathscr{E}_\alpha}, \ \Im k \geq 0,$$

satisfying the matching condition (5), satisfies the *outgoing* conditions too (see Fig. 1)

$$A = 0 \text{ and } F = 0. \tag{7}$$

We should remark that the *outgoing condition* $A = F = 0$ implies that the wavefunction behaves like $e^{ik|x|}$ and thus it exponentially decays when the energy belongs to the *unphysical complex half-plane* $\Im\mathscr{E} < 0$.

The matching condition (5) and the resonance condition (7) imply that k satisfies to the following equation $M_{2,2} = 0$, where M is the transfer matrix $\begin{pmatrix} E \\ F \end{pmatrix} = M \begin{pmatrix} A \\ B \end{pmatrix}$. A straightforward calculation gives that equation $M_{2,2} = 0$ takes the form

$$\frac{1}{4k^2}\left[e^{4ika}\alpha^2 + 4k^2 + i4k\alpha - \alpha^2\right] = 0$$

that is

$$\left(e^{2ika}\alpha\right) \pm i\,(2k + i\alpha) = 0 \tag{8}$$

which has two families of complex-valued solutions

$$k_{1,m} = \frac{i}{2a}\left[W_m(-a\alpha e^{a\alpha}) - a\alpha\right] \text{ and } k_{2,m} = \frac{i}{2a}\left[W_m(a\alpha e^{a\alpha}) - a\alpha\right] \tag{9}$$

where $W_m(x)$ is the m-th branch, $m \in \mathbb{Z}$, of the Lambert special function. The Lambert function [2], denoted by $W(z)$ and introduced by Johann Heinrich Lambert (1728–1777), is defined to be the multivalued analytic function satisfying the equation $W(z)e^{W(z)} = z$, $z \in \mathbb{C}$.

It turns out that $\Im k_{j,m} < 0$ for any j and m, but $k_{2,0} = 0$, and thus equation $H_\alpha \psi = \mathscr{E}_\alpha \psi$ has no eigenvalues for any $\alpha > 0$. However, we have to remark that for $m < 0$ then $\Re k_{j,m} > 0$ and $\Im k_{j,m} < 0$ and then $\mathscr{E}_\alpha = \left(k_{j,m}\right)^2$ belongs to the *unphysical sheet* with $\Im \mathscr{E}_\alpha < 0$ for $m = -1, -2, -3, \ldots$. Therefore, we conclude that the spectral problem $H_\alpha \psi = \mathscr{E}_\alpha \psi$ has a family of resonances given by

$$\mathscr{E}_{\alpha,n} = \begin{cases} k^2_{1,-(n+1)/2} = \left[\frac{i}{2a}\left(W_{-\frac{n+1}{2}}(-a\alpha e^{a\alpha}) - a\alpha\right)\right]^2 & \text{if } n = 1,3,5,\ldots \\ k^2_{2,-n/2} = \left[\frac{i}{2a}\left(W_{-\frac{n}{2}}(a\alpha e^{a\alpha}) - a\alpha\right)\right]^2 & \text{if } n = 2,4,6,\ldots \end{cases} .$$

Let $a > 0$ be fixed, then it follows that for n fixed and α large enough the asymptotic behavior of the resonances follows from the asymptotic expansion of the Lambert function (see Eq. (4.18) by [2]) and it is given by (see [14] where the correct asymptotic expansion of the imaginary part of the resonance is reported)

$$\begin{aligned}\mathscr{E}_{\alpha,n} &= \left(\frac{n\pi}{2a}\right)^2 \left[1 - \frac{1}{a\alpha} + \frac{1}{a^2\alpha^2} - \frac{i}{a^2\alpha^2}\frac{n\pi}{2} + \mathscr{O}\left(\frac{1}{\alpha^3}\right)\right]^2 \\ &\sim \left(\frac{n\pi}{2a}\right)^2 - i\frac{n^3\pi^3}{4a^4\alpha^2}\end{aligned}$$

The explicit form of the resolvent of H_α, $\alpha \in (0, +\infty)$ is given by [1]

$$\left(\left[H_\alpha - k^2\right]^{-1} \phi\right)(x) = \int_{\mathbb{R}} K_\alpha(x,y;k)\phi(y)dy, \quad \phi \in L^2(\mathbb{R}),\ \Im k \geq 0,$$

where the integral kernel K_α is given by

$$K_\alpha(x,y;k) = K_0(x,y;k) + \sum_{j=1}^{4} K_j(x,y;k)$$

with $K_0(x,y;k) = \frac{i}{2k} e^{ik|x-y|}$ and $K_j(x,y;k) = L_j(x,y;k)/g(k)$ where $g(k) = 0$ is the resonance's equation,

$$g(k) := -2k\left((2k + i\alpha)^2 + \alpha^2 e^{i4ka}\right),$$

and

$$L_1(x,y;k) = -\alpha(2k+i\alpha)\, e^{ik|x+a|}e^{ik|y+a|},\; L_4(x,y;k) = L_1(-x,-y;k)$$
$$L_2(x,y;k) = i\alpha^2\, e^{2ika}\;\, e^{ik|x+a|}e^{ik|y-a|},\; L_3(x,y;k) = L_2(-x,-y;k).$$

Resonances can be defined as the complex poles in the *unphysical sheet* $\Im\mathscr{E}_\alpha < 0$ of the kernel of the resolvent, too; that is the pole of the function $g(k)$ in agreement with (8).

3 Time Decay: Main Results

Let ϕ and ψ two well localized wave-functions, we are going to estimate the time decay of the term

$$\langle\psi, e^{-itH_\alpha}\phi\rangle \tag{10}$$

Theorem 1 *Let us assume that ϕ and ψ have compact support. Then we have that*

$$\langle\psi, e^{-itH_\alpha}\phi\rangle = c_\alpha t^{-3/2} + \sum_{n=1}^{\infty}\beta_n c_n e^{-i\mathscr{E}_{\alpha,n}t} + O(t^{-5/2}) \tag{11}$$

for some constants c_α and c_n and where

$$\beta_n = \begin{cases} 1 & \text{if } \left|\Im\sqrt{\mathscr{E}_{\alpha,n}}\right| < \left|\Re\sqrt{\mathscr{E}_{n,\alpha}}\right| \\ \frac{1}{2} & \text{if } \left|\Im\sqrt{\mathscr{E}_{\alpha,n}}\right| = \left|\Re\sqrt{\mathscr{E}_{\alpha,n}}\right| \\ 0 & \text{if } \left|\Im\sqrt{\mathscr{E}_{\alpha,n}}\right| > \left|\Re\sqrt{\mathscr{E}_{\alpha,n}}\right| \end{cases}. \tag{12}$$

We may remark that in the case $\alpha = 0$, that is when there are no barriers, then $\langle\psi, e^{-itH_0}\phi\rangle \sim t^{-1/2}$ and an apparent contradiction appears. The point is that the asymptotic expansion (11) is not uniform as α goes to zero. In fact, in an explicit model, see Theorem 2, it results that $c_\alpha \to \infty$ as $\alpha \to 0$. We can explain this apparent contradicion by remarking that the first resonance $\mathscr{E}_{\alpha,1} \to 0$ when $\alpha \to 0$ and that H_0 has a zero energy resonance.

Remark 1 Some authors [5, 6] discuss if and how the smoothness of the wave-functions ψ and ϕ plays a special role in the asymptotic behavior of the survival probability. Although this is a quite interesting question we don't treat it in such a paper.

We consider now, in particular, the asymptotic behavior of (10) when the test vectors ϕ and ψ coincide with one of the *localized* states, e.g. with $\psi_1(x) = \chi_{[-a,+a]}(x)\cos(k_1 x)$ defined by (6) for $n = 1$.

Theorem 2 *Let $\psi = \phi$ coinciding with the eigenvector ψ_1 of H_∞ associated with $\mathcal{E}_{\infty,1} = \left(\frac{\pi}{2a}\right)^2$, let $\ell(k)$ be the function defined as*

$$\ell(k) = 2\pi\sqrt{a}\frac{e^{2kai}+1}{\pi^2 - 4k^2a^2}, \tag{13}$$

and let $\mathcal{E}^2_{\alpha,1} = k_{1,-m}$ be the resonances defined by (9). Then

$$\langle \psi_1, e^{-itH_\alpha}\psi_1\rangle = c_\alpha t^{-3/2} + \sum_{m=1}^{\infty} \beta_m c_m e^{-i\mathcal{E}_{\alpha,1}t} + O(t^{-5/2}) \tag{14}$$

where β_m is defined by (12) and

$$c_\alpha = -\frac{2^{3/2}(1+i)a}{\pi^{5/2}\alpha^2}, \quad c_m = -\frac{\alpha\ell(k_{1,-m})^2}{1+\alpha a\left(1+\frac{2k_{1,-m}}{i\alpha}\right)}$$

This result agrees with the limit case when $\alpha = +\infty$. Indeed, we check that

$$\ell(k_{1,-m}) = \frac{4i\pi\sqrt{a}k_{1,-m}}{\alpha(\pi^2 - 4k^2_{1,-m}a^2)}$$

Hence

$$\ell(k_{1,-m}) \sim O(\alpha^{-1}) \text{ if } m \neq 1$$

as $\alpha \to +\infty$. For $m = 1$, from the asymptotic behavior of $k_{1,-1}$ it follows that

$$\pi^2 - 4k^2_{1,-1}a^2 \sim \pi^2 - 4a^2\left[\frac{\pi^2}{4a^2}\left(1 - \frac{2}{a\alpha}\right)\right] = \frac{2\pi^2}{a\alpha}$$

and then

$$\ell(k_{1,-1}) \sim i\sqrt{a}, \text{ as } \alpha \to +\infty.$$

Hence, as α goes to infinity it follows that the dominant term of $\langle \psi_1, e^{-itH_\alpha}\psi_1\rangle$ is given by

$$\langle \psi_1, e^{-itH_\alpha}\psi_1\rangle = e^{-i\left(\frac{\pi}{2a}\right)^2 t} + O(\alpha^{-1})$$

in agreement with the fact that $\langle \psi_1, e^{-iH_\infty t}\psi_1\rangle = e^{-i\mathcal{E}_{\alpha,1}t}$.

The proof of the Theorems is given by [13] and it is based on the explicit calculation of the evolution operator, obtained by the expression of the kernel of the resolvent operator, on the stationary phase theorem and the residue theorm.

4 Decay Transition

Let us compare, in the limit of large α and a fixed such that $a\alpha \gg 1$, the absolute values of the two dominant terms of $\langle \psi_1, e^{-itH_\alpha}\psi_1 \rangle$ given by (14); that is the power term $\frac{d_1}{\alpha^2 t^{3/2}}$, where $d_1 = \left| \frac{2^{3/2}(1+i)a}{\pi^{5/2}} \right| = \frac{4a}{\pi^{5/2}}$, and the exponential term

$$\left| c_1 e^{-i\mathscr{E}_{\alpha,1} t} \right| = d_3 e^{\Im \mathscr{E}_{\alpha,1} t} \sim d_3 e^{-d_2 t/\alpha^2} ,$$

where

$$d_2 = \frac{\pi^3}{4a^4} \text{ and } d_3 = |c_1| = \left| \frac{\alpha \ell (k_{1,-1})^2}{1 + \alpha a \left(1 + \frac{2k_{1,-1}}{i\alpha} \right)} \right| \sim 1 .$$

In order to understand when the power behavior dominates and when the exponential behavior dominates we have to solve the inequality

$$\frac{d_1}{\alpha^2 t^{3/2}} < d_3 e^{-d_2 t/\alpha^2} .$$

A straightforward calculation gives that this inequality is satisfied for any $t \in [t_1, t_2]$, where $0 < t_1 < t_2$ are given by

$$t_1 = -\frac{3\alpha^2}{2d_2} W_0(z) \text{ and } t_2 = -\frac{3\alpha^2}{2d_2} W_{-1}(z) \tag{15}$$

where

$$z = -\frac{2}{3} \frac{d_2 d_1^{2/3}}{\alpha^{10/3} d_3^{2/3}} .$$

This interval is not empty provided that the argument z of the Lambert function is between $(-1/e, 0)$; which holds true for α large enough. Furthermore, we should remark that

$$t_1(\alpha) \sim \frac{d_1^{2/3}}{\alpha^{4/3} d_3^{2/3}} \ll 1 \text{ and } t_2(\alpha) \gg 1$$

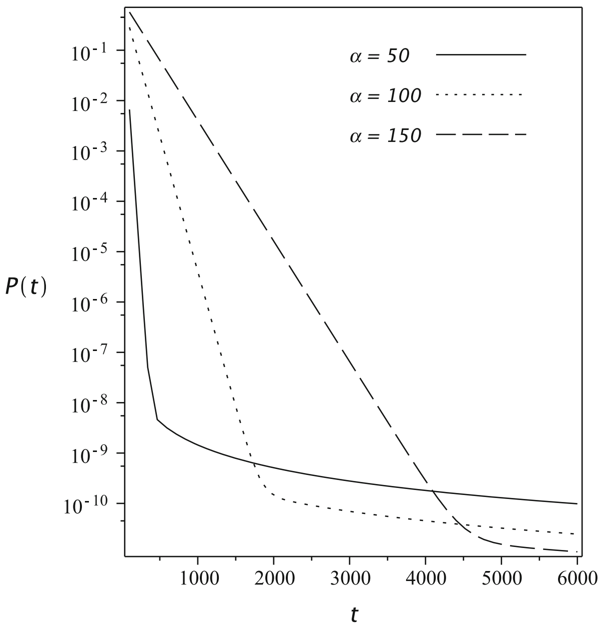

Fig. 2 Plot of the absolute value of the survival amplitude $P(t) = \left|\langle \psi_1, e^{-itH_\alpha}\psi_1\rangle\right|$ given by the dominant terms of (14) for large times $t \in [100, 6000]$ and for different values of α, here we fix $a = \frac{1}{2}$. Around $t = t_2(\alpha)$ a transition of the decay law starts; for $t < t_2(\alpha)$ the exponential decay dominates, while for $t > t_2(\alpha)$ the power law decay dominates

because $W_0(\zeta) \sim \zeta$ if $|\zeta| \ll 1$ and

$$W_{-1}(-\xi) \sim \ln(\xi) - \ln\left(-\ln(\xi)\right)$$

if $0 < \xi \ll 1$.

Finally, we can resume these results in the following statement.

Proposition (decay transition) *Let $\alpha > 0$ be large enough, and let $t_2(\alpha)$ given by (15). Let $\langle \psi_1, e^{-itH_\alpha}\psi_1\rangle$ be the survival amplitude of the state ψ_1 given by (14) and consisting by a superposition of the exponential and power law decay terms. Then a transition from the exponential to the power law decay term starts around $t_2(\alpha)$. More precisely, for $t < t_2(\alpha)$ the exponential decay term dominates, while for $t > t_2(\alpha)$ the power law decay term dominates (see Fig. 2).*

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