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The decay law can have an irregular character

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Abstract

Within a well-known decay model describing a particle confined initially within a spherical δ potential shell, we consider the situation when the initial state has an unusual energy distribution decaying slowly as $k \to \infty$; the simplest example corresponds to a wavefunction constant within the shell. We show that the non-decay probability as a function of time then behaves in a highly irregular, most likely fractal way.

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The decay of an unstable quantum system is one of the effects frequently discussed and various aspects of such processes were considered. To name just a few, recall the long-time deviation from the exponential decay law [1, 2], the short-time behaviour related to the Zeno and anti-Zeno effects [3–6], revival effects such as the classical one in the kaon–antikaon system, etc. In all the existing literature³, however, the decay law is treated as a smooth function, either explicitly or implicitly, e.g., by dealing with its derivatives. The aim of this paper is to show there are situations when it is not the case.

A hint why it could be so comes from the behaviour of Schrödinger wavefunctions during the time evolution. While in most cases the evolution causes smoothing [8], it may not be true for a particle confined in a potential well and the initial state does not belong to the domain of the Hamiltonian. A simple and striking example was found by Berry [9] for a rectangular hard-wall box and independently by Thaller [10] for a one-dimensional infinite potential well. It appears that if the initial wavefunction is constant, it evolves into a steplike-shaped $\psi(x, t)$ for times which are rational multiples of the period, t = qT with q = N/M, and the number of steps increases with growing M, while for an irrational q the function $\psi(x, t)$ is fractal with respect to (w.r.t.) the variable x.

One can naturally ask what will happen if the hard wall is replaced by a semitransparent barrier through which the particle can tunnel into the outside space. In a broad sense, this is one of the most classical decay model which can be traced back to [11]. We will deal with its particular case when the barrier is given by a spherical δ potential which is sometimes

³ The bibliography concerning unstable systems is vast; most part can be derived from sources such as [2, 5, 7].

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called *Winter model* being introduced for the first time, to our knowledge, in [12]. A thorough analysis of the model can be found in [13]; it has also various generalizations, we refer to [14] for a bibliography. The described behaviour of the wavefunction in the absence of tunnelling suggests that in the decaying system the irregular⁴ time dependence could also be visible, both in the wavefunction and in various quantities derived from it, at least in the weak coupling case⁵. The aim of the present paper is to demonstrate that this conjecture is indeed valid.

To be concrete, we will study a spinless nonrelativistic quantum particle described by the Hamiltonian

$$H_{\alpha} = -\Delta + \alpha \delta(|\vec{r}| - R), \qquad \alpha > 0, \tag{1}$$

with a fixed R > 0; we use rational units, $\hbar = 2m = 1$. For simplicity, we restrict our attention to the s-wave part of the problem, writing thus the wavefunctions as $\psi(\vec{r}, t) = \frac{1}{\sqrt{4\pi}}r^{-1}\phi(r, t)$ with the associated Hamiltonian

$$h_{\alpha} = -\frac{d^2}{dr^2} + \alpha \delta(r - R) \tag{2}$$

in the lowest partial wave. We are interested in the time evolution determined by the Hamiltonian (1), $\psi(\vec{r}, t) = e^{-iH_{a}t}\psi(\vec{r}, 0)$ for a fixed initial condition $\psi(\vec{r}, 0)$ with the support inside the ball of radius *R*; the advantage of the used model is that the propagator can be computed explicitly. The time evolution is naturally defined for *all* vectors in the Hilbert space, not only for those of the domain of the Hamiltonian, and it is in fact states *outside* the domain we will be primarily concerned with. Of a particular interest is the decay law,

$$P(t) = \int_0^R |\phi(r, t)|^2 \,\mathrm{d}r,$$
(3)

i.e. the probability that the system localized initially within the shell will be still found there at the measurement performed at an instant t. We are going to derive an exact formula for the decay law which will then allow us to evaluate the function (3) numerically for a given initial state.

It is straightforward to check [13] that the Hamiltonian (1) has no bound states. On the other hand, it has infinitely many resonances with the widths increasing logarithmically w.r.t. the resonance index. A natural and well-known idea [17, 18] is to employ them as a tool to expand the quantities of interest.

First of all, we have to find Green's function g(k, r, r'), i.e. the integral kernel of $(h_{\alpha} - k^2)^{-1}$ which determines the time evolution in the standard way [19],

$$e^{-ih_{\alpha}t} = \frac{1}{\pi} \lim_{\varepsilon \downarrow 0} \int_0^\infty e^{-i\lambda t} \operatorname{Im} \frac{1}{h_{\alpha} - \lambda - i\varepsilon} \, d\lambda, \tag{4}$$

recall that $\sigma(h_{\alpha}) = [0, \infty)$ for $\alpha > 0$; we are going to perform a resonance expansion of the integral (4). The Green function for a system with singular potential is obtained from Krein's formula

$$\frac{1}{\mathsf{h}_{\alpha}-k^{2}}=\frac{1}{\mathsf{h}_{0}-k^{2}}+\lambda(k)(\Phi_{k},\cdot)\Phi_{k}(r),$$

where $\Phi_k(r) := G_0(r, R)$ is the free Green function with one argument fixed; in particular, $\Phi_k(r) = \frac{1}{k} \sin(kr) e^{ikR}$ holds for r < R, and $\lambda(k)$ is determined by δ -interaction matching conditions at the singular point *R*; by a direct calculation [13] one finds

$$\lambda(k) = -\frac{\alpha}{1 + \frac{i\alpha}{2k}(1 - e^{2ikR})}.$$
(5)

⁴ We use this term in the sense common in mathematics, namely as characterization of a depart from smoothness.

⁵ This conjecture is also supported by the study of revivals in an infinite square well with a δ -barrier, see [15]; another example of highly complex evolution is a similar situation that can be found in [16].

By (4) we then get $\phi(r, t) = \int_0^\infty u(t, r, r')\phi(r', 0) dr'$ with the kernel expressed through Fourier transformation of Im $g(k + i\varepsilon, r, r')$; since h_α has no eigenvalues we may pass to the limit $\varepsilon \to 0$ obtaining

$$u(t, r, r') = \int_0^\infty p(k, r, r') \exp(-ik^2 t) \, 2k \, dk, \tag{6}$$

where $p(k, r, r') = \frac{1}{\pi} \text{Im } g(k, r, r')$. Using equation (5) this can be written explicitly as

$$p(k, r, r') = \frac{2k\sin(kr)\sin(kr')}{\pi(2k^2 + 2\alpha^2\sin^2 kR + 2k\alpha\sin 2kR)}.$$
(7)

The resonances of the problem are identified with the poles of $g(\cdot, r, r')$ continued analytically to the lower momentum half plane. They exist in pairs, those in the fourth quadrant, denoted as k_n in the increasing order of their real parts and $-\bar{k}_n$. The set of singularities of the kernel (7) then also includes the mirrored points, being

$$S = \{k_n, -k_n, \bar{k}_n, -\bar{k}_n : n \in \mathbb{N}\}.$$
(8)

In the vicinity of the singular point k_n the function $p(\cdot, r, r')$ can be written as

$$p(k, r, r') = \frac{1}{2\pi} \frac{v_n(r)v_n(r')}{k^2 - k_n^2} + \chi(k, r, r'),$$
(9)

where $v_n(r)$ solves the differential equation $h_\alpha v_n(r) = k_n^2 v_n(r)$ and the function χ is locally analytic.

The factor $\frac{i}{2\pi}$ is chosen to get the conventional normalization of the resonant state $v_n(r)$ [17]. For fixed r, r' < R and $\alpha > 0$, the function $p(\cdot, r, r')$ decays exponentially in the sector $\Omega_{\alpha} = \{k \in \mathbb{C} : \pi - \alpha > | \arg k | > \alpha\}$. Moreover, putting $l_n(\varphi) = \frac{1}{2R}(2n\pi + \pi/2)(1 + i \tan \varphi)$ we find that $p(l_n(\varphi), r, r')$ is bounded independently of φ and n. Thus considering the integration curves $\Gamma_n(\varphi) = \{l_n(\varphi) \text{ if } \varphi \notin \Omega_{\varphi_n} \text{ and } |l_n(\varphi_n)| e^{i\varphi} \text{ if } \varphi \in \Omega_{\varphi_n}\}$ with properly chosen $\varphi_n \to 0$, one can express p(k, r, r') as the sum over the pole singularities

$$p(k, r, r') = \sum_{\tilde{k} \in S} \frac{1}{k - \tilde{k}} \operatorname{Res}_{\tilde{k}} p(k, r, r')$$
(10)

and derive the following useful formula from the residue theorem:

$$\sum_{\tilde{k}\in S} \operatorname{Res}_{\tilde{k}} p(k, r, r') = 0.$$
⁽¹¹⁾

The last two equations can be rewritten in view of equation (9) and the symmetry of the set *S* in the form

$$p(k, r, r') = \sum_{n \in \mathbb{Z}} \frac{i}{2\pi} \frac{1}{k^2 - k_n^2} \frac{k}{k_n} v_n(r) v_n(r'), \qquad (12)$$

$$\sum_{n\in\mathbb{Z}}\frac{1}{k_n}v_n(r)v_n(r') = 0,$$
(13)

where we denote $k_{-n} := -\bar{k}_n$ and v_{-n} is the associated solution of the equation $H_{\alpha}v_{-n}(r) = k_{-n}^2 v_{-n}(r)$.

Next, we substitute equation (12) into (6) and using the identity (13) we arrive at the formula

$$u(t, r, r') = \frac{i}{2\pi} \int_0^\infty \sum_{n \in \mathbb{Z}} \frac{\exp(-ik^2 t)}{k^2 - k_n^2} \frac{2k^2}{k_n} v_n(r) v_n(r') dk$$

= $\sum_{n \in \mathbb{Z}} M(k_n, t) v_n(r) v_n(r')$ (14)

with $M(k_n, t) = \frac{1}{2} e^{u_n^2} \operatorname{erfc}(u_n)$ and $u_n := -e^{-i\pi/4}k_n\sqrt{t}$. Indeed, using $2k^2 = 2(k^2 - k_n^2) + 2k_n^2$ we write u(t, r, r') as a sum of two terms, the first of which vanishes in view of (13). The second one decomposes again into a sum of two integrals containing $k_n \pm k$ in their denominators, which gives the right-hand side of (14) with

$$M(k_n, t) = \frac{\mathrm{i}}{2\pi} \int_{-\infty}^{\infty} \frac{\mathrm{e}^{-\mathrm{i}k^2 t}}{k - k_n} \,\mathrm{d}k,\tag{15}$$

in other words, the above expression.

Now a straightforward calculation using (3) and (14) allows us to express the decay law in the form

$$P(t) = \sum_{n,l} C_n \overline{C}_l I_{nl} M(k_n, t) \overline{M(k_l, t)}, \qquad (16)$$

with the coefficients

$$C_n := \int_0^R \phi(r, 0) v_n(r) \, \mathrm{d}r, \qquad I_{nl} := \int_0^R v_n(r) \bar{v}_l(r) \, \mathrm{d}r.$$
(17)

This expression is valid for more general potentials, e.g., finite-range ones [18]; in our particular case of the Hamiltonian (2) we can specify $v_n(r) = \sqrt{2}Q_n \sin(k_n r)$ with the coefficient Q_n as follows:

$$Q_n = \left(\frac{-2ik_n^2}{2k_n + \alpha^2 R \sin 2k_n R + \alpha \sin 2k_n R + 2k_n \alpha R \cos 2k_n R}\right)^{1/2}$$

Now we are ready to compute the decay law for a given initial state. Without loss of generality we may put R = 1, we choose the value $\alpha = 500$ for numerical evaluation⁶ and replace the infinite series by a cut-off one with $|n| \leq 1000$; this guarantees numerical stability of the result. As the first example we consider initial wavefunction constant within the well, i.e.,

$$\phi(r,0) = R^{-3/2} \sqrt{3}r, \qquad r < R.$$
(18)

The corresponding decay law is plotted in figure 1. It is irregular having numerous steps⁷, the most pronounced at the period $T = 2R^2/\pi$ of motion in the inner part of the corresponding decoupled system (in other words, the infinite potential well) and its simple rational multiples. To make them more visible, we plot the logarithmic derivative of the function P(t) in the inset; it is locally smeared, otherwise the picture would be a fuzzy band. The irregular structure is expected to be fractal; it persists at higher time but its amplitude decreases relatively w.r.t. the smooth background.

In the next example, we choose the initial state having constant reduced wavefunction, $\phi(r, 0) = R^{-1/2}$ for r < R, so $\psi(r, 0)$ has a (square integrable) singularity at the origin; the advantage is that the reduced problem offers a straightforward comparison to the onedimensional example treated in [10] including the shapes of the wavefunctions. The decay law for this case is plotted in figure 2; it again exhibits derivative jumps around simple rational multiples of the period. The corresponding function $|\phi(r, t)|^2$ for three such values is plotted in figure 3. To compare with [10] one has to take the symmetry into account to conclude that the revival period of the infinite-well states is T/8. In the absence of decay the function for t = T/8 is just constant, the other two are simple step functions. We see that the tunnelling

⁶ The effect is expected to be present for any $\alpha > 0$; however, for a numerical demonstration we seek here it is reasonable to choose a large value at which the particle leaks out only slowly.

⁷ Another striking deviation from the exponential decay law is that the decay rate explodes as $t \to 0$, which is due to the fact that the energy distribution of the state ψ decays too slowly at high energies, cf [6].



Figure 1. Decay law for the initial state $\phi(r, 0) = R^{-3/2}\sqrt{3}r$. In the inset we plot the logarithmic derivative averaged over intervals of the length approximately T/200.



Figure 2. Decay law for initial state $\phi(r, 0) = R^{-1/2}$ and its logarithmic derivative, locally smeared, in the inset.

through δ -barrier modifies the shape of the function mostly in the vicinity of the origin, the barrier and the jump points.



Figure 3. The probability density inside the sphere with R = 1 multiplied by r^2 at the instants t = T/8, T/16 and T/27.

To support the conjecture about the fractal character of P(t) let us look how its derivative behaves in the limit $\alpha \to \infty$ when $\phi(r, t)$ expands asymptotically as

$$\phi(r,t) \approx \sum_{n} C_n \exp\left(-\mathrm{i}k_n^2 t\right) v_n(r).$$
(19)

It is easy to see that for a fixed *n* and $\alpha \to \infty$ the resonance position expands around $k_{n,0} := n\pi/R$ as

$$k_n \approx k_{n,0} - \frac{k_{n,0}}{\alpha R} + \frac{k_{n,0}}{(\alpha R)^2} - i\frac{k_{n,0}^2}{\alpha^2 R} + \cdots$$
 (20)

which shows that in the leading order we have $v_n(r) \approx \sqrt{\frac{2}{R}} \sin(k_n r)$ and, furthermore, that the substantial contribution to the sum in (19) comes from terms with $n \leq \left[\alpha^{1-\varepsilon} \frac{R}{\pi}\right]$ for some $0 < \varepsilon < 1/3$.

The derivative $\dot{P}(t)$ can be computed from the probability current conservation $J'(r) = -\frac{d}{dt}|\phi(r,t)|^2$; integrating it over the interval (0, *R*) and using J(0) = 0 we get

$$\dot{P}(t) = -2 \operatorname{Im}(\phi'(R, t)\bar{\phi}(R, t)).$$
(21)

We plug the above expansion into (19) obtaining

$$\phi(R,t) \approx \sqrt{\frac{2}{R}} \sum_{n=1}^{\infty} (-1)^n C_n \exp\left[-ik_{n,0}^2 t \left(1 - \frac{2}{\alpha R}\right)\right] \exp\left(-\frac{2k_{n,0}^3}{\alpha^2 R}t\right) \left(-\frac{k_{n,0}}{\alpha} - i\frac{k_{n,0}^2}{\alpha^2}\right)$$
(22)

and a similar expansion for $\phi'(R, t)$ with the last bracket replaced by $k_{n,0}$. We observe that for j > -1 we have

$$\sum_{n=1}^{\infty} \exp\left(-2\frac{k_{n,0}^3}{\alpha^2 R}t\right) k_{n,0}^j \approx \frac{R}{\pi} \left(\frac{R}{2t}\right)^{(j+1)/3} \alpha^{2(j+1)/3} I_j,$$

where we have denoted $I_j := \int_0^\infty e^{-x^3} x^j dx = \frac{1}{3} \Gamma(\frac{j+1}{3}).$

Let us now we assume that the coefficients in (19) satisfy $C_n \sim k_{n,0}^{-p}$ as $n \to \infty$. First suppose that the decay is fast enough, p > 1; note that this is certainly true in the finite-energy case with p > 3/2. The term $-k_{n,0}/\alpha$ in (22) obviously does not contribute to the imaginary part, hence we find that $|\dot{P}(t)| \leq \text{const } \alpha^{4/3-4/3p} \to 0$ holds as $\alpha \to \infty$ uniformly in the time variable.

The situation is different if the decay is slow⁸, $p \leq 1$. As an illustration take $C_n = (-1)^{n+1} \frac{\sqrt{6}}{Rk_n}$, which corresponds to the first one of the above numerical examples. Since the real part of the resonances changes with α , cf (20), it is natural to study the limit of $\dot{P}(t_{\alpha})$ as $\alpha \to \infty$ at the moving time value $t_{\alpha} := t(1 + 2/\alpha R)$. Up to higher order terms the appropriate value $\phi(R, t_{\alpha})$ is obtained by removing the bracket $(1 - 2/\alpha R)$ on the right-hand side of (22) and $\phi'(R, t_{\alpha})$ is obtained similarly.

First consider irrational multiples of *T*. We use the observation made in [21] that the modulus of $\sum_{n=1}^{L} e^{i\pi n^2 t}$ is for an irrational *t* bound by $CL^{1-\varepsilon}$ where *C*, ε depend on *t* only. In combination with a Cauchy-like estimate, $\sum_{n=1}^{\infty} a_n b_n \leq \sum_{n=1}^{\infty} \left| \sum_{j=1}^{n} a_j \right| |b_n - b_{n+1}|$, which yields

$$\sum_{n=1}^{\infty} \exp\left(-ik_{n,0}^{2}t\right) \exp\left(-\frac{2k_{n,0}^{2}}{\alpha^{2}R}t\right) k_{n,0}^{j} \lesssim \operatorname{const} \alpha^{2/3(j+1-\varepsilon)}$$

and, consequently, $\dot{P}(t_{\alpha}) \rightarrow 0$ as $\alpha \rightarrow \infty$ similarly as in the case of fast decaying coefficients.

Let us next assume rational times, $t = \frac{p}{q}T$. If pq is odd then $S_L(t) := \sum_{n=1}^{L} e^{i\pi n^2 t}$ repeatedly retraces by [21] the same pattern, hence $\dot{P}(t_{\alpha}) \rightarrow 0$, cf figure 1 at the half period. On the other hand, for pq even $|S_L(t)|$ grows linearly with L and, consequently, $\lim_{\alpha\to\infty} \dot{P}(t_{\alpha}) > 0$. As an example let us compute this limit for the period T, i.e. p = q = 1. Using (21) we find

$$\lim_{t \to \infty} \dot{P}(T_{\alpha}) = -\frac{24}{R^2} \lim_{\alpha \to \infty} \operatorname{Im} \left(\sum_{n=1}^{\infty} \exp\left(-\frac{2k_{n,0}^3}{\alpha^2 R}T\right) \right)$$
$$\times \sum_{n=1}^{\infty} \exp\left(-\frac{2k_{n,0}^3}{\alpha^2 R}T\right) \left(-\frac{1}{\alpha} + i\frac{k_{n,0}}{\alpha^2}\right)$$
$$= -\frac{24}{R^2} \left(\frac{R}{\pi}\right)^2 \frac{1}{2T/R} I_1 I_0 = -\frac{4}{3\sqrt{3}} \approx -0.77;$$

this is approximately the value obtained by numerical calculations⁹.

С

Summarizing this paper, we have reexamined time decay in the Winter model and found indications that the decay law is a highly irregular function if the energy distribution decays slowly as $k \to \infty$.

⁸ Resonance regime change due to momentum–space delocalization was also observed in a different context, see [20].

⁹ This is not obvious from the inset of figure 1. The difference is due to the smearing. The true width of the peak is about T/α with $\alpha = 500$; a comparison to the chosen scale of local averaging explains the factor of order 2 by which the value differs from the height of the peak there.

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