Long time deviation from exponential decay: non-integral power laws.

J. Martorell
Department d’Estructura i Constituents de la Materia, Facultat Física, University of Barcelona, Barcelona 08028, Spain

J. G. Muga
Departamento de Química-Física, UPV-EHU, Apdo 644, 48080 Bilbao, Spain

D. W. L. Sprung
Department of Physics and Astronomy, McMaster University
Hamilton, Ontario L8S 4M1 Canada

Quantal systems are predicted to show a change-over from exponential decay to power law decay at very long times. Although most theoretical studies predict integer power-law exponents, recent measurements by Rothe et al. of decay luminescence of organic molecules in solution [Phys. Rev. Lett. 96 (2006) 163601] found non-integer exponents in most cases. We propose a physical mechanism, within the realm of scattering from potentials with long tails, which produces a continuous range of power law exponents. In the tractable case of the repulsive inverse square potential, we demonstrate a simple relation between the strength of the long range tail and the power law exponent. This system is amenable to experimental scrutiny.

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Repeating to this apparent contradiction, we explore physical mechanisms which could lead to long-time deviations from exponential decay with arbitrary, non-integer power law exponents. On the mathematical side, an “explanation” of an arbitrary power-law exponent follows from the expression for the survival amplitude in terms of an energy density \( \omega(E) \). As defined in Section II,

\[
A(t) = \int_0^\infty dE \omega(E) e^{-iEt/\hbar},
\]

where we have assumed no bound states and an energy threshold at \( E_m = 0 \). The large-time asymptotics depend on the behaviour of \( \omega(E) \) near the origin \( E \to 0 \). In fact, under mild conditions on \( \omega(E) \) as a function of the complex variable \( E \), \( A(t) \sim t^{-(\nu+1)} \) as \( t \to \infty \) if \( \omega(E) \sim E^\nu \) as \( E \to 0 \). This implies \( P(t) \equiv |A(t)|^2 \sim t^{-2(\nu+1)} \).

One puzzling aspect of the experimental results of Rothe et al. [1] is that their inferred algebraic exponents \( \mu \) are patently non-integral, except in one case (PtOE, frozen solution), for which \( \mu = 4 \). Other values range from \( \mu = 2.08 \) to 4.07. These non-integer exponents are in sharp contrast to theoretical studies of long-time deviation from exponential decay which predict or postulate integral exponents for the algebraic decay

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1 In fact the perturbing effect of measurement depends on the particular process. It has been shown to be negligible for distant detectors in solvable models [2].

*Electronic address: martorell@ecm.ub.es
†Electronic address: jg.muga@ehu.es

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I. INTRODUCTION

Rothe et al. [1] have recently presented experimental evidence for “Violation of the Exponential Decay-Law at Long Times”. Deviations from exponential decay of an unstable quantum system had been predicted long ago as a result of the semiboundedness of the energy spectrum [2]. However, the transition into the non-exponential regime at long times occurs in most decaying systems after many lifetimes, where the minute survival probability had previously frustrated verification. In addition, it had been argued that interaction with the environment and/or the measurement process would suppress the long time deviation [2]. Rothe et al. measured the decay of luminescence of various dissolved organic molecules after pulsed laser excitation. The results clearly show a range of times over which the decay of the survival probability \( P(t) \) is exponential, followed by another where it is algebraic, \( P(t) \sim t^{-\mu} \).

One puzzling aspect of the experimental results of Rothe et al. [1] is that their inferred algebraic exponents \( \mu \) are patently non-integral, except in one case (PtOE, frozen solution), for which \( \mu = 4 \). Other values range from \( \mu = 2.08 \) to 4.07. These non-integer exponents are in sharp contrast to theoretical studies of long-time deviation from exponential decay which predict or postulate integral exponents for the algebraic decay
decay of a wavepacket in a spherically symmetric potential well, in a given partial wave. This is done with the hope that the lessons learned here may be useful elsewhere, although there is no guarantee that our results can be extended to such diverse fields as auto-ionizing states, photo-ionization, particle physics or spontaneous photon emission, because of the particular constructions of their distributions $\omega(E)$.

One of the advantages of the decay of unstable states in 1D and spherically symmetric 3D potential models is that it is a well-studied subject, reviewed by Fonda, Ghirardi and Rimini some time ago \cite{3}. The conditions leading to integer exponents are well understood. If the initial unstable state has angular momentum $\ell$ and the potential is “well behaved” at short and large distances, then the algebraic exponent is generally $\mu = 2\ell + 3$. In particular, for the most studied case of s-waves, $\mu = 3$; the $\ell = 0$ contribution would be in any case the dominant one at very large times since it is the slowest decaying term. This algebraic decay law also applies in 1D decaying systems \cite{14}. The derivation of these integral power laws will facilitate identification of the complementary cases in which the exponents may be non-integers, so we shall devote Section II to a review of the basic elements of potential scattering theory relevant for our purposes. (This presentation differs from \cite{3} in some respects, but we shall conclude that potentials with long tails are natural candidates for providing non-integral decay exponents. The case of inverse square potentials, \(V(r) = 2m\beta(\beta + 1)/(h^2 r^2)\) for \(r > r_d\), and $\beta > 0$ (repulsive tail), is particularly suitable for theoretical treatment and provides as a first approximation a very simple relation between the strength of the interaction and the exponent, $\mu = 2\beta + 3$ (The attractive tail case ($-1/2 < \beta < 0$) will also be studied but the decay law is more involved.) The predicted algebraic exponent varies continuously with $\beta$, with $\mu = 3$ when $\beta = 0$ corresponding to a short range potential. This is shown in detail in Section III, for a potential model with inverse square tail in which $\omega(E)$ is obtained analytically, and the conditions for the validity of the simple prediction for the algebraic exponent can be easily studied. In the final discussion we comment on the experimental feasibility of inverse square interactions.

II. POWER LAWS FOR LONG TIME DECAY IN POTENTIAL SCATTERING

We consider a system that is initially in a normalized non-stationary state $|\Psi_0\rangle$. The survival amplitude of that state is defined as the overlap of the initial state with the state at time $t$, and is the expectation value of the time evolution operator

\[
A(t) = \langle \Psi_0 | \exp(-iHt/\hbar) | \Psi_0 \rangle, \tag{2}
\]

$H$ being the Hamiltonian. The survival probability, sometimes called “non-decay probability” \cite{3}, is

\[
P(t) = |A(t)|^2. \tag{3}
\]

This is the function whose asymptotic time behaviour we will study. The stationary states of the Hamiltonian, $H|\Phi_{E,\lambda}\rangle = E|\Phi_{E,\lambda}\rangle$, where by $\lambda$ we indicate any other quantum numbers characterizing states of energy $E$, determine a basis. In our models we have only a continuous spectrum, so the range of energies will be $E_m < E < \infty$, and the origin of energies is taken at threshold $E_m = 0$. The completeness relation is then

\[
\sum_{\lambda} \int_0^\infty dE \langle \Phi_{E,\lambda} | \Phi_{E,\lambda} \rangle = 1, \tag{4}
\]

which gives

\[
A(t) = \int_0^\infty dE \omega(E) e^{-iEt/\hbar} \tag{5}
\]

We will call $\omega(E)$ the “energy density” or “energy distribution” of the initial state. To construct $\omega(E)$, we therefore need the continuum solutions denoted $|\Phi_{E,\lambda}\rangle$. For a spherically symmetric potential, the Schrödinger equation has separable solutions $\Phi(\vec{r}) = u_\ell(r)Y^m_\ell(\Omega)/r$. For each partial wave

\[
\frac{d^2u_\ell}{dr^2} - \frac{\ell(\ell + 1)}{r^2}u_\ell + [k^2 - v(r)]u_\ell = 0, \tag{6}
\]

where $v(r) = (2m/\hbar^2)V(r)$ and $k^2 = (2m/\hbar^2)E$. For convenience, in the following we work with solutions $w_\ell(k, r)$ normalized as

\[
\int_0^\infty dr w_\ell(k', r)^* w_\ell(k, r) = \delta(k' - k) \tag{7}
\]

and obeying the boundary condition

\[
\lim_{r \to \infty} w_\ell(k, r) = (2/\pi)^{1/2} \sin(kr - \pi\ell/2 + \delta_\ell), \tag{8}
\]

where $\delta_\ell$ is the phase shift for the partial wave $\ell$. These solutions are related to the regular solutions $\hat{\phi}_\ell$ defined by their behaviour as Riccati-Bessel functions $\hat{j}_\ell, \hat{\phi}_\ell(r) \sim \hat{j}_\ell(kr)$ when $r \to 0$) by

\[
w_\ell = (2/\pi)^{1/2} \frac{\hat{\phi}_\ell}{f_\ell(k)} \tag{9}
\]

where $f_\ell(k)$ is the Jost function. Among the different definitions we use the one by Taylor \cite{24} so that

\[
f_\ell(k) = 1 + \frac{1}{k} \int_0^\infty dr \hat{h}^+_\ell(kr)v(r)\hat{\phi}_\ell(k, r), \tag{10}
\]

see the Appendix A for a minimal account of Riccati-Bessel functions.
We now sketch the arguments that justify integral power laws for the long time deviation from exponential decay in scattering from “well-behaved” potentials, defined as those falling off faster than \( r^{-3} \) at infinity and by being less singular than \( r^{-3/2} \) at the origin [24]. We shall assume for simplicity that the initial non-stationary state is in a particular partial wave \( \ell \) without bound states, and localized,

\[ u_i(r) = 0 \quad \text{for} \quad r > r_a. \]

Then the survival amplitude takes the form

\[ A(t) = \frac{2m}{\pi \hbar^2} \int_0^\infty \frac{dE}{k} \left| \left\langle u_i|\hat{\phi}_\ell \right\rangle \right|^2 e^{-iEt/\hbar}. \]

The function \( \langle \hat{\phi}\rangle \) for \( \ell > 0 \) vanishes at \( k = 0 \) if and only if there is a zero energy bound state whereas for \( \ell = 0 \) such an occurrence represents a zero-energy resonance [24]. We disregard these exceptional possibilities and concentrate on the generic case \( f_1(0) \neq 0 \).

The main properties of concern for the long-time behaviour of the survival probability are analyticity of \( \hat{\phi} \) in the complex \( k \)-plane, its asymptotic behaviour near the origin (the same as the Ricatti-Bessel function) and at infinity [24],

\[ |\hat{\phi}_\ell(k, r)| \leq \gamma_\ell \left( \frac{|kr|}{1 + |kr|} \right)^{\ell + 1} e^{\text{Im}(kr)}, \]

where \( \gamma_\ell \) is some constant, and the behaviour of the Jost function at \( k = 0 \) and at infinity. Eq. [10] can be continued analytically in the upper \( k \)-plane (zeroses on the positive imaginary axis would represent bound states), and tends to one uniformly as \( |k| \to \infty \) in \( \text{Im}(k) \geq 0 \).

Now we deform the energy contour from the positive axis in Eq. [12] to one directed upwards along the lower imaginary axis on the first energy sheet. A long closing arc at infinity does not contribute because the exponential growth of \( \hat{\phi}_\ell \) implied in Eq. [13] is limited by the localization [11] and thus compensated by the decaying time exponent. The behaviour of the integrand near threshold is thus, from Eq. [13] and the zero energy asymptotics of the Jost function, of order \( E^{\ell+1/2} \), so the long-time asymptotic of the survival amplitude is, according to Watson’s lemma, \( A \sim t^{-(\ell+3/2)} \), and therefore

\[ P(t) \sim t^{-(2\ell+3)}. \]

This is easily generalized to cases with a zero energy resonance or bound states, since the zero energy behaviour of the Jost function is known in these cases [24], and again provides integer exponents. Another type of exception arises from the possible cancellation of the threshold dependence in Eq. [13] by integration over the coordinate in \( \langle \hat{\phi}|u_i \rangle \), by a suitable choice of \( u_i(r) \). In the context of 1D potential models, Miyamoto [19] has studied the long time behaviour of wavepackets scattered by a finite range potential. He showed that by careful adjustment of the low momentum components of the initial wave packet, initially located outside the interaction region, an exponent 5 for the decay power law may occur, instead of the generic value 3. As presented, such state manipulation produces only odd integer values.

Comparing the result [14] with the dependence on \( \ell \) of the centrifugal barrier, it is tempting to speculate that a \( v(r) = \beta(\beta + 1)/r^2 \) potential tail, where \( \beta > 0 \), may produce long-time decay power laws of the form \( t^{-(2\beta+3)} \) for \( \ell = 0 \), based on the fact that the long tail plays for large \( r \) the role of a centrifugal term with a non-integer, effective \( \ell \). That this is indeed the case, will be demonstrated in a solvable model below. A proof of generality of this result is however far from trivial, since the properties of the functions used to arrive at Eq. [14] depend on fast fall-off conditions which are not satisfied for an inverse square tail. Instead of using \( \ell = 0 \), we could alternatively assume from the start a non-integer, effective \( \ell = \beta \) and its corresponding “partial wave” stationary equation to extend the usual results, but this requires a redefinition of the potential \( V(r) \) in the internal region to compensate exactly for the unphysical inverse square term. The consequence is an inverse square divergence in \( V(r) \) at \( r = 0 \) which, again, makes the formal treatment non-standard. We shall therefore be content with a demonstration, via exactly solvable models, that the proposed long-time decay behaviour with non-integer exponents does indeed occur, and leave a more general and abstract theory for a further publication.

III. DECAY OF AN UNSTABLE STATE IN POTENTIAL MODELS

A. General results

Consider a point particle of mass \( m \) in 3D subject to a central force. First we will derive some general results assuming only that beyond a certain radius, \( r = r_d \), the potential is inversely proportional to the square of the distance. We call this a “boundary condition model”. For convenience, we write

\[ V(r) = \frac{2m}{\hbar^2} \frac{\beta(\beta + 1)}{r^2}, \quad r > r_d. \]

The inner part is also assumed to be free of singularities, even at the origin, so that the existence of regular solutions of the Schrödinger equation is guaranteed. To have a vanishing survival probability when \( t \to \infty \), we choose a potential with no bound states. Later, in order to have explicit analytic expressions for the properties of \( \omega(E) \) and the asymptotic survival probability, we will use the more detailed “WB” (well-barrier) model. In that case, the inner part of \( V(r) \) will be a square well, depth \( -V_0 < 0 \) and extending from 0 to \( r_a \), followed by a square
barrier of height $V_b > 0$ located between $r_a$ and $r_d$. An example is shown in figure. With suitable parameters for the well and barrier this model has well defined quasibound states, which lead to the exponentially decaying part of $P(t)$.

As announced in the Introduction, we will show that for simplicity we take the initial state to have $\ell = 0$, and drop the subindex $\ell$ in the following. It is also convenient to define a different regular solution $\phi(k;r) = \phi(k, r)/k$ that satisfies the boundary conditions

$$\phi(k; 0) = 0, \quad \phi'(k; 0) = 1$$

and, as shown in [23], provided that the potential goes to zero faster than $1/r$ when $r \to \infty$, its asymptotic form is, see Eqs. (20),

$$\phi(k, r) \approx \frac{|f(k)|}{k} \sin(kr + \delta).$$

where $f(k) \equiv |f(k)|e^{-i\delta} = f^*(-k)$ on the real $k$-axis. In addition, to be consistent with Eq. (21), we define solutions normalized with respect to energy, $w_E(r)$,

$$w_E(r) = \sqrt{\frac{m}{\hbar^2}} w(k; r) = \sqrt{\frac{2mk}{\pi\hbar^2 |f(k)|}} \phi(k; r),$$

such that

$$\langle w_E|w_E' \rangle = \delta(E - E') = \frac{m}{\hbar^2} \delta(k - k').$$

Finally, we assume that the chosen potential allows a regular solution at zero energy, denoted $\phi_0(r) = \phi(0; r)$.

For the potential in Eq. (15), the regular solution for $r > r_d$ can be written as a linear combination of Riccati-Bessel functions,

$$\phi(k, r) = a_{III} \hat{y}_\beta(kr_d) + b_{III} \hat{y}_\beta(kr_d).$$

(The reason for the subindex III is the consideration of two spatial regions for the inner part of the potential in the following subsection.) For repulsive potentials $\beta > 0$. We will also consider weakly attractive potentials with $\beta > -1/2$ so that the order of the related cylinder functions $\nu = \beta + 1/2$ remains positive; see Appendix A. For a detailed and updated discussion of the problems arising when the $1/r^2$ potential becomes too strongly attractive, $\beta < -1/2$, see reference [28]. The constants $a_{III}, b_{III}$, can be written in terms of the regular solution and its derivative at $r_d$ by matching the inner and outer solutions at this boundary,

$$\phi(k, r_d) = a_{III} \hat{y}_\beta(kr_d) + b_{III} \hat{y}_\beta(kr_d)$$

$$\frac{\partial \phi(k, r)}{\partial r} \bigg|_{r=r_d} = k \left[ a_{III} \hat{y}_\beta(kr_d) + b_{III} \hat{y}_\beta(kr_d) \right].$$

where the prime means derivative with respect to the argument of the Bessel function, $x = kr$.

Using their asymptotic forms and comparing to Eq. (17),

$$|f(k)| = k \sqrt{a_{III}^2 + b_{III}^2},$$

with

$$C^2 \equiv a_{III}^2 + b_{III}^2$$

$$= (|\hat{y}_\beta'|^2 + |\hat{y}_\beta|^2)\phi(k, r_d)^2 + \frac{1}{k^2} \phi'(k, r_d)^2 (\hat{n}_\beta^2 + \hat{j}_\beta^2)$$

$$- \frac{2}{k} \phi(k, r_d) \phi'(k, r_d) (\hat{n}_\beta \hat{n}_\beta' + \hat{j}_\beta \hat{j}_\beta').$$

where, to simplify notation, $\phi'(k, r_d) = (\partial \phi(k, r)/\partial r)|_{r=r_d}$, and the argument of the Bessel functions is $x_d = kr_d$. In subsection C we will need the asymptotic forms when $k \to 0$. In this limit, $\phi(k, r_d) \to \phi_0(r_d)$, which will always be finite and non vanishing unless we have made a rather unfortunate choice for the point $r_d$. The value of the derivative will also be finite. Eqs. (22) and (23) then show that in this limit the explicit $k$ dependence of the Jost function is determined by that of the Ricatti-Bessel functions: Eq. (24) gives an example of this.

Since our initial state has $\ell = 0$, the sum over $\lambda$ in Eq. (5) may be dropped, and writing the radial part of the initial state as $|u_i\rangle$, the energy density is

$$\omega(E) = |\langle w_E|u_i \rangle|^2.$$
with \( k_a = n_a \pi / r_a \) and \( n_a \) integer. In this paper we take \( n_a = 1 \). Then \( |u_i \rangle \) coincides with the ground state of the inner well in the limit of infinite barrier height. This initial state is widely used in simulations of unstable systems. Its advantage is its simple analytic form. At intermediate times only the lowest quasibound state contributes significantly, which leads to exponential decay of \( P(t) \). For this choice of \( |u_i \rangle \)

\[
\langle w_E | u_i \rangle = \frac{2}{h} \sqrt{\frac{mk}{\pi r_a |f(k)|}} \int_0^r \phi(k;r) \sin k_ar \ dr,
\]

which, combined with Eq. (24), expresses \( \omega(E) \) in terms of the regular solutions.

**B. The well-barrier (WB) model**

We now choose a specific model for the inner potential, consisting of an inner square well enclosed by a square barrier. In this case,

\[
\phi(k;r) = \begin{cases} \frac{1}{k_I} \sin k_Ir, & r < r_a \\ a_I e^{\kappa_r r} + b_I e^{-\kappa_r r}, & r \in (r_a, r_d), \end{cases}
\]

where \( k_I^2 = k^2 + v_0 \), \( v_0 = 2mV_0/\hbar^2 \), \( \kappa^2 = v_0 - k^2 \) and \( v_b = 2mV_i/\hbar^2 \). The constants \( a_I \) and \( b_I \) are determined by matching at \( r = r_a \) and from them we get the expressions for \( \phi(k;r_d) \) and its derivative,

\[
\phi(k;r_d) = \frac{1}{k_I} \left( \cosh \kappa r_b \sin k_I r_a + \frac{k_I}{\kappa} \sinh \kappa r_b \cos k_I r_a \right),
\]

\[
\phi'(k;r_d) = \frac{\kappa}{k_I} \left( \sinh \kappa r_b \sin k_I r_a + \frac{k_I}{\kappa} \cosh \kappa r_b \cos k_I r_a \right),
\]

with \( r_d = r_d - r_a \).

Inserting these into Eqs. (22) and (23) determines the Jost function. The overlap is now given by

\[
\langle w_E | u_i \rangle = \frac{2}{h} \sqrt{\frac{mk}{\pi r_a |f(k)|}} \int_0^r \phi(k;r) \sin k_ar \ dr = \frac{2}{h} \sqrt{\frac{mk}{\pi r_a |f(k)|}} \left( \frac{(-)^n a}{k_I} \right) k_a \sin k_I r_a \]

and therefore when \( k_a = \pi / r_a \) (\( n_a = 1 \)),

\[
\omega(E) = \frac{4\pi mk \sin^2 k_I r_a}{h^2 r_a^3 k_I^2 |f(k)|^2 (\pi / r_a)^2 - k_I^2}.
\]

Since \( k_I^2 = k^2 + v_0 \), even in this simple model the \( k \)-dependence is non-trivial. To illustrate our results, we fix on specific parameter values for our inner potential. We use units such that \( \hbar = 2m = 1 \) and set \( r_a = 3.0, r_d = 3.4, v_0 = 0.5 \) and \( v_b = 1.8 \). Fig. 2 shows the computed energy spectra when the outer part of the potential has \( \beta \) ranging from -0.4 to 0.7. Fig. 3 shows the corresponding survival probabilities. It can be seen that for this choice of inner parameters a strong resonance peak dominates the energy density in all cases, and that there is exponential decay of \( P(t) \) at intermediate times. Other smaller peaks present in \( \omega(E) \) at higher energies, not shown in the figure, affect the corresponding \( P(t) \) only at very small times. We are not interested in that regime here. At long times the survival probability shows algebraic decay in all cases. To determine the form of \( P(t) \) when \( t \to \infty \), we need the asymptotic properties of \( \omega(E) \) near threshold. We find them now in the context of the boundary condition model.

**C. The threshold energy density**

From Eq. (18),

\[
w_E(r) \sim \sqrt{\frac{2mk}{\pi \hbar^2}} \frac{1}{|f(k)|} \phi_0(r).
\]
and therefore
\[ \langle w_E | u_i \rangle \simeq \frac{2}{\hbar} \sqrt{\frac{mk}{\pi \tau_a}} \frac{1}{|f(k)|} \int_0^\infty \phi_0(r) \sin k_a r \, dr. \tag{32} \]

Clearly in this limit all the \( k \)-dependence is in the factor multiplying the integral, while the latter is to this order a constant. For the specific case of the WB model, the analytic expression for the integral can be obtained from Eq. (29), replacing \( k_I \) by \( k_{I,0} = \sqrt{\omega_0} \).

We look first at the behaviour of the Jost function, Eqs. (22) and (23), also to lowest order in \( k \). Using standard expansions, (see Appendix A,) the behaviour when \( \beta > 0 \) as \( x = kr_d \to 0 \) is
\[ \tilde{j}_\beta(x) \simeq \frac{\pi^{1/2} x^{\beta+1}}{2^{\beta+1}(\beta + 1/2)!}, \]
\[ \tilde{n}_\beta(x) \simeq \frac{(\beta - 1/2)! 2^\beta}{\pi^{1/2} x^{\beta}}, \tag{33} \]
and the contribution from the Neumann function will dominate in Eq. (23). One easily finds that
\[ |f(k)| \simeq D \; k^{-\beta} \quad \text{with} \]
\[ D \equiv \frac{2\pi}{\pi^{1/2} \beta!} \left| \frac{\phi_0}{r_d} + \phi'_0 \right|, \tag{34} \]
where \( \phi_0 \equiv \phi_0(r_d) \) and \( \phi'_0 \equiv \phi'_0(r_d) \). For the WB model, these are given explicitly in Eqs. (28).

Inserting Eq. (34) into Eq. (23) we arrive finally at the desired result,
\[ \omega(E) \simeq \frac{4m \pi \sin^2 (k_{I,0} r_a)}{h^2 r_a^3 (k_a^2 - k_{I,0}^2)^2} k_{I,0}^2 D^2 \; k^{2\beta+1} \equiv \zeta \; k^{2\beta+1}. \tag{35} \]

D. Decay at long times

Usually, when an explicit expression for the energy density is available, to find analytic approximations for the asymptotic contribution to \( P(t) \) one replaces the integration path in Eq. (5) by an equivalent one in the complex plane. Examples of these methods can be found in [12, 3] and [13]. In our case, we choose a closed path consisting of the positive real energy axis, a quarter circle of infinite radius joining the positive real axis to the negative imaginary axis, and the latter. As shown in the Appendix B, integration along the circular arc gives a vanishing contribution. Therefore
\[ A(t) = \int_0^\infty dE \; \omega(E) \; e^{-iEt/\hbar} \]
\[ = \int_0^\infty dE \; \omega(E) \; e^{-iEt/\hbar} + \int_{-\infty}^0 dE \; \omega(E) \; e^{-iEt/\hbar} \]
\[ \equiv A_p(t) + A_v(t). \tag{36} \]

We have analytically continued \( \omega(E) \) into the lower half plane, and placed the cut running from the origin in the upper half plane. The term \( A_v(t) \) has contributions from the poles enclosed in the contour. These are related to the resonances and lead to exponentially decaying terms, so we will not discuss \( A_v(t) \) further.

The second term, \( A_p(t) \), gives the dominant contribution to the decay at long time. To evaluate it, we make the change of variable \( E = -ix \).

\[ A_v(t) = i \int_0^\infty dx \; e^{-xt} \; \omega(-ix). \tag{37} \]

In our examples the exponential decay becomes negligible beyond \( t \simeq 200 \), so (assuming \( \omega(-ix) \) is smooth), the range of values of \( x \) giving significant contributions to the integral is \( 0 < x < x_c \simeq 1/200 \). Therefore, in a first approximation we use the small \( k \) expansion of \( \omega(E) \), Eq. (35), to extend this function to the relevant part of the negative imaginary axis, and write
\[ \omega(-ix) \simeq (-i)^{\beta+1/2} \zeta \; x^{\beta+1/2}. \tag{38} \]

Inserting this into Eq. (37) one immediately finds
\[ A_v(t) \simeq (-i)^{\beta+3/2} \zeta \; \Gamma(\beta + 3/2) \; t^{-(\beta+3/2)}. \tag{39} \]

and therefore asymptotically
\[ \mathcal{P}(t) \simeq |A_v(t)|^2 = \zeta^2 \; \Gamma^2(\beta + 3/2) \; t^{-(2\beta+3)}. \tag{40} \]

![FIG. 4: Effective \( \mu_I \) v.s. \( \beta \). Continuous line with filled circles: standard choice of parameters for the inner part of the potential. Dotted line with filled diamonds: standard set except \( v_0 = 1.6 \), dashed line with crosses: standard set except \( r_d = 3.5 \). The straight dashed line is \( \mu = 2\beta + 3 \).](image)
Eq. (33) is negligible. Within the WB model we have checked that other choices of parameters for the inner part of the potential lead to the same conclusions. This will be further confirmed in figure 4.

However, the above approximation fails for values of $\beta$ that make the outer potential attractive, especially when approaching the lowest value we considered, $\beta = -1/2$. This is shown in Fig. 5 for $\beta = -0.4$. Empirically we have found that for the range of times shown in the figure the asymptotic decay can still be well fitted by an algebraic form, but the exponent determined from such a fit deviates from the simple law that holds for positive $\beta$. Intuitively, the simple algebraic behaviour of the repulsive case $\beta > 0$ may be understood as a consequence of the dominance of the long centrifugal-like tail of the potential in near threshold scattering. However if the tail is attractive the particle is drawn to explore the inner part of the potential. This makes the decay more complex and also more sensitive to this inner part. We will now discuss that in further detail.

![Pic: Fig. 5: Survival probability, $P(t)$, for $\beta = -0.4$, $\nu = 0.1$.](image)

Looking again at the expansions of the Ricatti-Bessel functions in Eq. (A2) one sees that when $\beta \rightarrow -1/2$ the series for $j_\beta$ and $\tilde{a}_\beta$ both begin with $x^{1/2}$ and therefore the contribution from the $j_\beta$ cannot be discarded. At this stage it is convenient to use the auxiliary index, $\nu = \beta + 1/2$, that corresponds to the index of the cylindrical Neumann and Bessel functions in Eq. (A1). We will be interested in small values of $\nu$. Our representative example will be that of Fig. 5 $\nu = 0.1$. Including only the lowest order terms, $p = 0$ in Eq. (A2), but for both functions, one finds

$$|f(k)|^2 \simeq k (\lambda_- k^{-2 \nu} + \lambda_0 + \lambda_+ k^{2 \nu}) \quad (41)$$

with

$$\lambda_- \equiv \frac{[\Gamma(\nu)]^2}{\pi r_d^{2 \nu-1}} \left[\left(\nu - \frac{1}{2}\right) \frac{\phi_0}{r_d} + \phi_0'\right]^2$$

$$\lambda_0 \equiv \frac{\cot(\nu \pi)}{\nu} r_d \left[\left(\nu - \frac{1}{2}\right) \frac{\phi_0}{r_d} + \phi_0'\right] \times \left[\left(\nu + \frac{1}{2}\right) \frac{\phi_0}{r_d} - \phi_0'\right]$$

$$\lambda_+ \equiv \frac{\nu^{2 \nu+1} \Gamma(1-\nu)^2}{\pi^2 2^{2n+1} \nu^2} \left[\left(\nu + \frac{1}{2}\right) \frac{\phi_0}{r_d} - \phi_0'\right]^2 \quad (42)$$

Therefore

$$\omega(E) \simeq \frac{\zeta k^{2 \nu}}{1 + (\lambda_0/\lambda_-)k^{2 \nu} + (\lambda_+/\lambda_-)k^{4 \nu}} \quad (43)$$

replaces Eq. (39). To have a result for $A_\nu(t)$ similar in form to the earlier one, we expand the denominator and write

$$\omega(E) \simeq \sum_{m=1}^\infty \zeta_{2m} k^{2m \nu} \quad (44)$$

with $\zeta_2 = \zeta$ already defined, and the other $\zeta_{2m}$ obtained from Eqs. (42) and (43). Repeating the derivation in Eqs. (38) to (40), we obtain

$$A_\nu(t) \simeq -\sum_{m=1}^\infty \zeta_{2m} \Gamma(1+m \nu) (it)^{-(1+m \nu)} \quad (45)$$

The first term in this expansion reproduces Eq. (39), but when $\nu \simeq 0.1$ the algebraic exponents of the first few terms in the series will be comparable, and keeping only the first would be insufficient. Confirming this, figure 5 shows that with a single term in the series the prediction is wrong by an order of magnitude, and that one has to include at least four terms in the series to reproduce the exact $P(t)$ for $t > 200$. When we use the approximation for $\omega(E)$ of Eq. (33) in Eq. (37), the agreement is even better.

These results show that for positive $\beta$ one can neglect the $k$-dependence in $\phi(k, r_d)$ and its derivative, and also the higher order terms in the series for the Ricatti-Bessel functions, and still have a satisfactory approximation for the asymptotic decay of the survival probability over the range of time included in the figures. But when $\beta$ becomes negative (outer potential attractive) the truncation leading to the asymptotic law in Eq. (40) ceases to be valid. Even then, we have empirically found that the exact $P(t)$ can be well fitted with a formally similar algebraic expression in a range of times that we will specify as the interval $400 < t < 800$. To be more precise, and to try to simulate the way in which the algebraic exponents could be extracted in experiments like that of Rothe et al, we have made linear least square fits to the exact values of $\ln P(t)$ v.s. $t$ in $t$ for equally spaced values of $t$ in the
above range. The fits are always excellent, so that in that range of times one can hardly distinguish in the figures the exact $P(t)$ from the fitted form $P_f(t) = \mathcal{M} t^{-\mu_f}$. The effective algebraic exponents, $\mu_f$, thus found are shown in figure 4. One sees that when $\beta < 0$ the effective exponents depend on the parameters of the potential, and deviate from the simple law $\mu = 2\beta + 3$. Making the barrier wider or higher, increases the values of $\mu_f$ for a given $\beta$, but in all cases as $\beta \to -1/2$ one finds that the values of $\mu_f$ become constant.

We tried to derive explicit analytic expressions for $P(t)$ in the limit $\nu = 0$. Using only the first order term in the expansion of the Neumann function, $N_0(z)$, the first term in the asymptotic series for $A_n(t)$ goes like $1/[t \ln(t/r_0^2)]$ with the next order terms involving higher powers of the logarithm. However, using only the first order term of the series for $N_0$ is not enough; one needs at least one more term in both $J_0$ and $N_0$. With these added terms, we were unable to find a useful analytic expression for $A_n(t)$. Still, the fact that the lowest order results include $\ln t$ and powers thereof indicates that the algebraic form of decay for the asymptotic part of $P(t)$ is not as universal as previously thought. It is only for potentials with a vanishing or repulsive outer part that such a simple algebraic decay law can be established.

IV. DISCUSSION

Our study of the long-time deviations from exponential decay, was motivated by the apparent contradiction between the recent (and so far only) experimental results which unambiguously show such deviations, and theoretical models: the power laws in the experiments have non-integer exponents whereas the models predict integral exponents? The complexity of the system studied experimentally (large, excited organic molecules in solution), made us consider, instead of an ab initio or realistic approach, the more modest goal of understanding and answering the question in a tractable system.

Limiting ourselves to a single-particle model of wave-packet decay from a scattering potential region, we have established a link between non-integer exponents and long potential tails, which is expressed by a simple formula for repulsive inverse square potentials. Before arriving at these results we explored several other possible sources of “anomalous” long-time decay: in particular, we tried to simulate the effects of the solvent molecules and of temperature by introducing randomly fluctuating perturbations in the potential and averaging over many realizations. This lead to localization effects and a non-vanishing constant value of $P(t)$ at long times but non-integer exponents were not found. Another attempt was consideration of complex potentials that could simulate the effect of coupled channels due to measurement or other effects. However the result of an imaginary term is similar to that described in [4], Eq. (11): the long-time deviation is altered but not in the sought for algebraic form.

Despite our retreat from the arena of the organic molecule experiments, the long-time decay described here is not simply academic. Attractive inverse square potentials occur physically as effective radial potentials between a charged wire and a polarizable neutral atom [30], the strength factor being proportional to the square of the linear charge density of the wire and thus controllable [31, 32]. Combined with a repulsive centrifugal term, an arbitrary $\alpha/r^2$ potential may be implemented. In addition, it is possible to modify the inner region and implement a potential minimum by a time varying sinusoidal voltage in the high frequency limit [32], or by replacing the wire by a charged optical fiber with blue detuned light propagating along the fiber and the cladding removed [31]. Decay experiments with cold atoms showing exponential laws have been performed [31], and the ability to modify the potential parameters makes the observation and study of the long-time power-law in these systems a realistic prospect.

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APPENDIX A

The Riccati-Bessel functions $\hat{j}_\beta(x)$, $\hat{n}_\beta$, and $\hat{j}_\beta^2(x) = \hat{n}_\beta \pm i \hat{j}_\beta$ are defined as $x$ times the corresponding spherical functions, or, in terms of cylindrical Bessel and Neumann functions,

\begin{align*}
\hat{j}_\beta(x) &= \sqrt{\frac{\pi}{2}} J_{\beta+1/2}(x), \\
\hat{n}_\beta(x) &= \sqrt{\frac{\pi}{2}} N_{\beta+1/2}(x).
\end{align*}

(A1)

In this paper $\beta$ may be non-integer.

Their series representations are [29],

\begin{align*}
\hat{j}_\beta(x) &= \sqrt{\pi} \left(\frac{x}{2}\right)^{\beta+1} \sum_{p=0}^{\infty} \frac{(-)^p}{p! \Gamma(\beta + p + 3/2)} \left(\frac{x}{2}\right)^{2p}, \\
\hat{n}_\beta(x) &= \cot \left(\beta + \frac{1}{2}\right) \pi \hat{j}_\beta(x) - \frac{\sqrt{\pi}}{\sin(\beta + 1/2)\pi} \\
&\times \left(\frac{x}{2}\right)^{-\beta-1} \sum_{p=0}^{\infty} \frac{(-)^p}{p! \Gamma(p - \beta + 1/2)} \left(\frac{x}{2}\right)^{2p}.
\end{align*}

(A2)
APPENDIX B

We will prove here that the energy density extended to the quarter circle at infinity, in the fourth quadrant of the energy plane, is vanishingly small and therefore does not contribute to $A(t)$ in Eq. (30). To do so, we first rewrite the energy density as

$$\omega(E) = \frac{4m\pi}{h^2\pi^3r_\alpha^2k_\alpha^2(\pi/r_\alpha)^2 - k_\alpha^2} G(E)$$

$$G(E) = \frac{\sin^2k_\alpha r_\alpha}{C^2}. \quad (B1)$$

We will now extend these functions to the fourth quadrant in the energy plane and look at their asymptotic behaviour when $|E| \to \infty$. It is convenient to write

$$E = |E|e^{2i\phi},$$

$$k = |k|e^{i\phi},$$

and $\phi \in (-\pi/4, 0)$. Similarly we will write $k_\alpha = |k_\alpha|e^{i\phi_\alpha}$ and will now find an approximate expression for the latter valid in the limit when $|k| \to \infty$. From $k_\alpha^2 = k^2 + v_0$, we can write

$$|k_\alpha|^2 e^{2i\phi_\alpha} = |k|^2 e^{2i\phi} + v_0 \approx \left( |k|e^{i\phi} + \frac{v_0}{2|k|e^{i\phi}} \right)^2,$$

$$|k_\alpha|^2 e^{i\phi_\alpha} \approx |k|^2 e^{i\phi} + \frac{v_0}{2|k|} e^{-i\phi} + O(|k|^{-2}),$$

$$k_\alpha \approx k + \frac{v_0}{2|k|} e^{-i\phi} + O(|k|^{-2}). \quad (B3)$$

Similarly, since $k_\alpha^2 = k^2 - v_0$,

$$k_\alpha \approx k - \frac{v_0}{2|k|} e^{-i\phi} + O(|k|^{-2}). \quad (B4)$$

In the same limit, the sine in the numerator of $G(E)$ will give

$$\sin k_\alpha r_\alpha \approx \frac{1}{2i} e^{ik_\alpha r_\alpha} \to \infty \quad (B5)$$

since $\text{Im}(k_\alpha) < 0$. Let us now consider the denominator: from Eq. (29) one sees that both the Ricatti-Bessel functions and the regular solutions at $r = r_\alpha$ must be extended to complex energies in the fourth quadrant and in the large $|E|$ limit. Using the asymptotic expansions given e.g. in [33], we find

$$\frac{n_\beta^2 + \frac{j_\beta^2}{2}}{\beta(\beta + 1)} + O(z^{-4})$$

$$\frac{n_\beta n_\beta + \frac{j_\beta j_\beta}{2}}{\beta(\beta + 1)} + O(z^{-5})$$

$$\frac{(n_\beta^2)^2 + (j_\beta^2)^2}{1 - \frac{\beta(\beta + 1)}{2z^2} + O(z^{-4})}, \quad (B6)$$

with $z = kr_\alpha$. Inserting these into Eq. (23) we find to order $z^{-4}$

$$C^2 \approx \phi^2 + \frac{1}{k^2} \left( \phi' \right)^2 + \frac{\beta(\beta + 1)}{2z^2} \left( -\phi^2 + \frac{1}{k^2} \left( \phi' \right)^2 \right)$$

$$+ 2\phi \phi' \frac{1}{k} \left( \beta(\beta + 1) \right) \left( -\phi' \right)^2. \quad (B7)$$

Now one has to deal with $\phi$ and $\phi'$, whose explicit expressions are given in Eqs. (28) Using the approximations in Eqs. (B3, B4) and (B5), one finds

$$\phi^2 + \left( \frac{\phi'}{k} \right)^2 \approx -\frac{v_0 + v_0}{4k^4} e^{2i(k_\alpha r_\alpha + k_\alpha r_\alpha)}$$

$$\frac{1}{k^2} \left( -\phi^2 + \frac{1}{k^2} \left( \phi' \right)^2 \right) \approx \frac{8}{k^4} e^{2i(k_\alpha r_\alpha + k_\alpha r_\alpha)}$$

$$\frac{1}{k^4} \phi \phi' \approx -\frac{1}{4k^5} e^{2i(k_\alpha r_\alpha + k_\alpha r_\alpha)}, \quad (B8)$$

so that all terms in the denominator of $G(E)$ diverge like $\exp(2i(k_\alpha r_\alpha + k_\alpha r_\alpha))$. Since the $\sin^2$ in the numerator diverges only like $\exp(2i(k_\alpha r_\alpha))$, see Eq. (B5), the result is that $|G(E)| \to 0$ and therefore the contribution to $A(t)$ due to the integral on the quarter circle at infinity is nil.

Note that this result can be easily extended to any value of $n_\alpha$, introduced in Eq. (29). Therefore any initial state, $|u_\alpha\rangle$, that can be expanded as a finite superposition of eigenstates of the infinite square well will have an energy density with similar properties.
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