Survival Probability for the Yamaguchi Potential

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Different decay behaviours of the survival probability are examined. Technically, the survival probability of an arbitrary state ψ is determined by the ψ matrix element of the resolvent of the full Hamiltonian. The analytical properties of this matrix element can be analyzed in terms of the properties of the kernel of the Lippmann–Schwinger equation. For the Yamaguchi potential and several initial states, all functions are explicitly calculated. This approach allows the decomposition of the survival amplitude into a sum of decaying exponential terms and w -functions associated with the pole positions of the resolvent matrix element in the complex momentum plane. Novel decay behaviours are found for the decay of states associated with the resolvent poles and the decay of a state which is dominated by the form of the wave function rather than by the resolvent poles. Certain anomalous short time decay behaviour is also exemplified. © 1996 Academic Press, Inc.

I. INTRODUCTION

The quantum mechanical decay of unstable states can be described in many different ways [1–8]. In spite of being an old and recurrent subject, surprises and new effects are frequently being found in the literature, see e.g. [9], even though in many theoretical works the emphasis has been on justifying the approximately valid exponential decay law. Traditional fields where decay has been of interest are high-energy, nuclear, atomic and molecular physics, but recent interest is also due to the development of artificial semiconductor structures where an understanding and the control of the time response of such a device are crucial [10]. In these structures the potential shapes can be basically built at will [11] so that they may serve as ideal tests for “anomalous” decay behaviours. Ultrafast, time resolved spectroscopy is also changing the conventional picture that associates the *preparation* of an initial unstable state and the *detection* procedures with asymptotic ingoing and outgoing packets in *collision* experiments. In fact, in optical excitation experiments the standard assumptions are not necessarily met. Packets can be excited from a lower to an upper potential surface by an initial laser pulse. Later pulses are then able to

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prove the wave packet motion accurately [12, 13]. Observation of deviations from a purely exponential decay law are thus entirely feasible.

A possible treatment for the survival amplitude $A(t, \psi) \equiv \langle \psi(0) | \psi(t) \rangle$ decomposes the state ψ by the usual resolution into proper and improper eigenstates of the Hamiltonian H , corresponding to bound, $|E_k\rangle$, and continuum states $|E, \alpha\rangle$,

$$A(t, \psi) = \sum_k e^{-iE_k t/\hbar} |\langle E_k | \psi(0) \rangle|^2 + \sum_\alpha \int dE e^{-iEt/\hbar} |\langle E, \alpha | \psi(0) \rangle|^2. \quad (1)$$

Even though it contains all the information, this is not convenient in general either for calculational purposes or for rationalizing the decay behaviour in a simple manner, except in favourable circumstances where the integral is easily approximated and parameterized, e.g. for isolated resonances and particular initial states. An ideal description 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 representating $A(t, \psi)$ as a discrete sum over resonant terms [9]. The discretization allows a clear identification and separation of the physically dominant contributions, different terms being important for different time regimes. The objective of this paper is to analyze and provide simple explanations for a series of novel decay behaviours (not purely exponential) in terms of a discrete decomposition of the survival amplitude. In particular, we examine the successive decay regimes and their association with those poles of the matrix element of the resolvent specifically due to the form of the wave function rather than due to the potential shape. A controversy on the short time behaviour of the decay of quantum states is discussed and clarified.

II. GENERAL THEORY

In this section the theoretical basis for the present study of the survival is summarized. The plausibility of the arguments is demonstrated with examples in the next section. One dimensional motion is assumed throughout.

The discretization of the survival amplitude has been discussed by García Calderón and coworkers [9]. Our method achieves essentially the same goal, but involves some technical differences that are detailed next. In a nutshell, we explicitly evaluate the relevant matrix element of the resolvent of the Hamiltonian and *then* study its analytical properties. This implies that there is no need to consider the analytical properties of any wavefunction, in particular in position representation. Only after calculating a matrix element of the resolvent and for the matrix element as a whole, are analytical properties explored. In particular, the analytical continuation of the resolvent element as a function of its energy (momentum) parameter is performed and the singularities of this function used for predicting the time dependence of the survival. Compared to the treatment in [9], this route has the

advantage that while the treatment in [9] is *formally* restricted to cut-off potentials our method is not. (The method used in [9] can surely be generalized by different routes. For example, the time dependent Green's function for at least one example of a non cut-off potential was obtained by Lozano and Moshinsky in [14].) Our method is restricted by a number of analyticity assumptions associated with the assumed nature of the singularities in the analytically continued matrix element of the resolvent. These must be checked in any application. The assumed analyticity properties are verified for the Yamaguchi potential. Again, for this simple potential, all functions are calculable so that the observed behaviours are easily traced to specific properties of the resolvent and its matrix elements.

The present approach is summarized by a sequence of steps: (a) The starting point is a contour integral expression of the survival amplitude in terms of the resolvent $G(z) \equiv (z - H)^{-1}$; (b) The full resolvent $G(z)$ is separated into a free part $G_0(z) \equiv (z - H_0)^{-1}$, which can be treated easily, and a scattering part $R(z) \equiv G(z) - G_0(z)$; (c) The operator $R(z)$ is expanded in a discrete biorthogonal basis of square integrable functions in the upper half q -plane [$q \equiv (2mz)^{1/2}$]; (d) All matrix elements are evaluated in this upper half q -plane as functions of q . This step requires only square integrable functions and convergent integrals; (e) These functions are analytically continued into the lower half plane; (f) The original integration contour is deformed to be along the diagonal of the second and fourth quadrants of the q -plane and the resulting integral evaluated.

II.a The Survival

The survival amplitude $A(t, \psi) = \langle \psi(0) | \psi(t) \rangle$ requires the diagonal matrix elements of the unitary evolution operator $e^{-iHt/\hbar}$. When this operator is expressed in terms of the resolvent, $A(t, \psi)$ takes the form

$$\begin{aligned} A(t, \psi) &= \langle \psi | e^{-iHt/\hbar} | \psi \rangle = \frac{i}{2\pi m} \int_C dq q \langle \psi | \frac{e^{-izt/\hbar}}{z - H} | \psi \rangle \\ &= \frac{i}{2\pi} \int_C dq e^{-izt/\hbar} I(q) \end{aligned} \quad (2)$$

where the q contour C (see Fig. 1) goes from $-\infty$ to $+\infty$ passing above all 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) and

$$I(q) \equiv \frac{q}{m} \langle \psi | \frac{1}{z - H} | \psi \rangle. \quad (3)$$

The survival probability is to be calculated as $S(t, \psi) = |A(t, \psi)|^2$. An analysis is presented in Section II.c for understanding the time dependence of the survival. This is based on the analytical continuation of $I(q)$ into the lower q -plane. For a number of model potentials, and in particular for the Yamaguchi potential studied in this paper, this can be explicitly carried out. However, for an arbitrary potential,

FIG. 1. Contour C (dashed line) in the complex q -plane, see Eq. (2). The two dots, one on the positive imaginary axis, and one in the fourth quadrant represent, respectively, are the locations of a bound state and a proper resonance. The contour is deformed into the straight line D and the circles around the singularities above D (solid lines).

a general theory for the structure of the resolvent and its analytical continuation is described next, in Section II.b. This section is also important to provide for the introduction of certain square integrable states that are associated with resonances and virtual states, and thus responsible for special decay behaviour.

II.b The Resolvent

It is useful to separate the resolvent into its free $(z - H_0)^{-1}$ and scattering parts

$$R(z) \equiv \frac{1}{z - H} - \frac{1}{z - H_0} = \frac{1}{z - H_0} \left[V + V \frac{1}{z - H} V \right] \frac{1}{z - H_0}. \quad (4)$$

The free part poses no technical problem and determines the contribution to decay from purely free motion. The scattering part is discretized by using the properties of the kernel of the Lippmann–Schwinger equation [15–20],

$$K(z) \equiv (z - H_0)^{-1} V. \quad (5)$$

For $\Im q > 0$ ($q \equiv \sqrt{2mz}$) and square integrable potentials, this is a compact operator. Thus it has a discrete set of eigenvalues associated with square integrable right and left eigenvectors,

$$K(z) |\zeta_n(z)\rangle = \eta_n(z) |\zeta_n(z)\rangle \quad (6)$$

$$\langle \zeta_n(z) | K(z) = \langle \zeta_n(z) | \eta_n(z) \quad (7)$$

$$\langle \zeta_n(z) | \zeta_{n'}(z) \rangle = \delta_{nn'}. \quad (8)$$

These are related by

$$|\zeta_n(z)\rangle = \frac{1}{z - H_0} N_n(z)^{-1} |\zeta_n(z^*)\rangle, \quad (9)$$

where

$$N_n(z) = \langle \xi_n(z) | \frac{1}{z - H_0} | \xi_n(z^*) \rangle \quad (10)$$

assures the proper normalization (8) of the biorthonormal set.

The eigenvalues $\eta_n(z)$ are real for $z < 0$ (positive imaginary q -axis) and equal to one for bound states. The Schwartz reflection principle then implies

$$\eta_n(z^*) = \eta_n(z)^*. \quad (11)$$

It is assumed here that the phase of the eigenvectors expressed in momentum representation is chosen so that, for $z < 0$, $\langle p | \zeta(z) \rangle$ is real. Thus the Schwartz reflection principle also applies to them, namely

$$\langle p | \zeta_n(z^*) \rangle = \langle p | \zeta_n(z) \rangle^*. \quad (12)$$

The difference in resolvents $R(z)$ is related to $K(z)$ and the free resolvent $G_0(z)$ by $R(z) = [1 - K(z)]^{-1} K(z) G_0(z)$ so in terms of the set of right and left square integrable eigenvectors of $K(z)$, the difference of resolvents can be written as the discrete sum:

$$\begin{aligned} R(z) &= \sum_n |\zeta_n(z)\rangle \frac{\eta_n(z)}{1 - \eta_n(z)} \langle \xi_n(z) | \frac{1}{z - H_0} \\ &= \sum_n |\zeta_n(z)\rangle \frac{\eta_n(z) N_n(z)}{1 - \eta_n(z)} \langle \xi_n(z^*) | \\ &= \sum_n \frac{1}{z - H_0} |\xi_n(z^*)\rangle \frac{\eta_n(z)}{[1 - \eta_n(z)] N_n(z)} \langle \xi_n(z) | \frac{1}{z - H_0}. \end{aligned} \quad (13)$$

Eq. (9) has been used to write the last two forms. When taking matrix elements of the resolvent $\langle \phi | G(z) | \psi \rangle$ a distinction can be made between a *core* factor $\eta_n/(1 - \eta_n)$ which does not depend on the states ϕ or ψ , overlaps between these states and the biorthonormal set of eigenfunctions of K , and the matrix element of the free resolvent which depends only on the states ϕ and ψ .

The resolvent has a natural boundary at the full real q axis. While all the above equations are valid for z not on the positive real axis (upper half q -plane, so z^* in the above equations corresponds to $-q^*$), matrix elements of $G(z)$ calculated in the upper half q -plane can be analytically continued into the lower half q -plane. This provides both physical insight (by separating the most relevant temporal dependence of the survival) and a calculational advantage. The analytical continuation of the matrix elements of the resolvent $\langle \phi | G(z) | \psi \rangle$ has in general a set of “core poles” at those z where $\eta_n(z) = 1$ for some n (depending *only* on the potential) plus possibly other *structural* singularities due to the matrix elements $\langle \phi | \zeta(z) \rangle$, $\langle \xi_n(z) | G_0(z) | \psi \rangle$ and $\langle \phi | G_0(z) | \psi \rangle$ which depend on the particular states ϕ and

ψ considered. In general, core and structural singularities are located at different points of the q -plane but there is also the possibility of finding a higher order pole due to the combined effect of the core and structure singularities as is demonstrated in the examples below. It is also possible that the singularities of some of the matrix elements are cancelled in the full integrand $I(q)$.

If the only singularities for finite q are poles, the resolvent matrix elements, and the quantities associated with them can be expanded in terms of their poles with the possible inclusion of an entire function. Of physical significance are the residues at those poles of $R(z)$ determined as the l th root $z_{n,l}$ of $\eta_n(z_{n,l}) = 1$. Assuming that they are first order poles, the residues, $\lim_{z \rightarrow z_{n,l}} \langle \phi | G(z) | \psi \rangle$ will have the factorized form

$$\langle \phi | \zeta_n(q_{n,l}) \rangle f_{n,l} \langle \zeta(-q_{n,l}^*) | \psi \rangle, \quad (14)$$

where all functions are well defined for $\Im q > 0$ and then analytically continued to the pole position in the lower half plane if $\Im q_{n,l} < 0$. For $\Im q_{n,l} > 0$, $q_{n,l}$ must be on the imaginary axis and the factors $\langle \phi | \zeta_n(q_{n,l}) \rangle$ and $\langle \zeta(-q_{n,l}^*) | \psi \rangle$ are proportional to the overlaps between the functions ϕ and ψ with a bound state. In fact $|\zeta_n(q_{n,l})\rangle$ is then, up to a constant, a bound state vector. However, for a pole in the lower half q -plane, different representations of the eigenvector $|\zeta_n(q_{n,l})\rangle$ have different analytical properties. In coordinate representation the analytical continuation of $\langle x | \zeta_n(q) \rangle$ to $q = q_{n,l}$ is (proportional to) a Gamow state with diverging behaviour for large x . On the contrary, if momentum representation is used, the analytical continuation of $\langle p | \zeta_n(a) \rangle$ to $q = q_{n,l}$ is a normalizable square integrable function. These latter functions have been described in the past [21, 18] but no attempt has been made to examine their use for time dependent problems. As used here, the $|\zeta_n(q_{n,l})\rangle$ appear only in the overlaps $\langle \psi | \zeta_n(q_{n,l}) \rangle$ and $\langle \zeta_n(-q_{n,l}^*) | \psi \rangle$, which are to be calculated for $\Im q > 0$ (where all representations of the states are well defined) and then analytically continued to $q_{n,l}$.

II.c Predicted Time Behaviour

Insertion of one of the expressions (13) for the resolvent difference, together with an expression for the free resolvent, into Eq. (3) provides a way to obtain $I(q)$ and localize its poles in the lower half q -plane by analytical continuation. It is assumed that a pole expansion is possible for $I(q)$ in the form

$$I(q) = \sum_k \sum_j \frac{a_k^{(j)}}{(q - q_k)^j} \quad (15)$$

where $k = 1, 2, 3, \dots$ indexes the poles (being a composite label for the pair n, l) and v_k is the order of the k th pole. Since for positive time t the exponential $e^{-iq^2 t/(2mh)}$ decays as a function of q in the second and fourth quadrants but grows in the first and third quadrants, it is not possible to close the contour at $|q| = \infty$ by a semicircle and evaluate the survival by a direct residue calculation. However by deforming the contour as indicated in Fig. 1, the poles crossed by the contour provide

exponential contributions, $E_k(t)$, to the survival amplitude. These will be purely oscillatory for poles in the upper half plane (bound states) but a combination of oscillation and decay for poles in the lower half plane (resonances): For a first order pole the contributions to $A(t)$ takes the form

$$E_k(t) = a_k^{(1)} e^{-iq_k^2 t/(2m\hbar)}, \quad (16)$$

while for a second order pole the contribution is

$$E_k(t) = e^{-iq_k^2 t/(2m\hbar)} [a_k^{(1)} - ia_k^{(2)} q_k t/(m\hbar)]. \quad (17)$$

Independently of being crossed or not crossed during the deformation of the contour, all poles contribute, because of the integral along the diagonal D , as w -functions (closely related to the Moshinsky functions [2, 22–24] see Appendix A for a list of their main properties). By changing the integration variable (when $t > 0$) to $u = q/f$, where

$$f = (1 - i) \sqrt{m\hbar/t}, \quad f^{-1} = \frac{1 + i}{2} \sqrt{t/m\hbar}, \quad (18)$$

the D integral of a given partial fraction of (15) becomes

$$\int_{-\infty}^{\infty} du f e^{-u^2} \frac{a_k^{(j)}}{(q - q_k)^j}. \quad (19)$$

On taking into account the integral definition of the w -function, first order poles contribute to A as

$$D_k(t) = -\frac{a_k^{(1)}}{2} \text{sign}(\Im u_k) w[\text{sign}(\Im u_k) u_k] \quad (20)$$

where $u_k \equiv q_k/f$. For the poles above the diagonal (proper resonances and bound states) the exponential term (16) can be added to this contribution to give the compact result, see Eq. (A.3),

$$D_k(t) + E_k(t) = \frac{1}{2} a_k^{(1)} w(-u_k). \quad (21)$$

The compactness gained by this combination may be useful for certain manipulations, for example in Appendices B and C, but buries the relevant exponential dependence into the new w -function.

Noting that the derivative of the w -function can be expressed in terms of w , Eq. (A.5) in Appendix A, second order poles contribute as

$$\begin{aligned} D_k(t) = & \frac{1}{f} a_k^{(2)} \left\{ \text{sign}(\Im u_k) u_k w[\text{sign}(\Im u_k) u_k] - \frac{i}{\pi^{1/2}} \right\} \\ & - \frac{1}{2} a_k^{(1)} \text{sign}(\Im u_k) w[\text{sign}(\Im u_k) u_k]. \end{aligned} \quad (22)$$

Contributions from higher order poles can be obtained in a similar fashion so that $A(t) = \sum_k [E_k(t) + D_k(t)]$. (It is understood that $E_k(t) = 0$ for poles below D since these have not been crossed when deforming the contour.)

In this manner the exponential decay contribution of a resonance pole is clearly separated. The "correction" to exponential decay is given in terms of the known entire function $w(y)$ parameterized by the pole position and time. Numerical values and asymptotic properties of this function for small or large times are easily computable.

If the function $I(q)$ is meromorphic but the pole expansion of $I(q)$ is not feasible in the form (15) because of the need to add an entire function, the exponential contribution can still be calculated in the same manner. But apart from w -functions, the integral along D has to be evaluated numerically. Since it is weighted by a real Gaussian, this is a much simpler task than the original integral along the real axis having oscillatory exponentials.

III. SEPARABLE POTENTIAL MODEL

A simple separable potential for one-dimensional motion [25–28] is used to illustrate the general formalism described in the last section,

$$V = |\chi\rangle V_0 \langle \chi| \quad (23)$$

with χ expressed in momentum and position representation,

$$\langle p|\chi\rangle = \left(\frac{2a^3}{\pi}\right)^{1/2} \frac{1}{a^2 + p^2}, \quad \langle x|\chi\rangle = \left(\frac{2\pi a}{h}\right)^{1/2} e^{-a|x|/\hbar}. \quad (24)$$

Note that $|\chi\rangle$ is normalized to one. For this potential the kernel operator is $K(z) = (z - H_0)^{-1} |\chi\rangle V_0 \langle \chi|$. The eigenvalues and right and left eigenstates of $K(q)$ for $\Im q > 0$ are given by

$$\eta(q) = V_0 Q_0(q),$$

$$\langle \xi(q)| = \langle \chi|,$$

and

$$|\zeta(q)\rangle = \frac{1}{Q_0(q)(z - H_0)} |\chi\rangle, \quad (25)$$

where

$$Q_0(q) = \langle \chi| \frac{1}{z - H_0} |\chi\rangle = \frac{2m(q + 2ia)}{q(q + ia)^2}, \quad \Im q > 0 \quad (26)$$

plays the role of the normalization factor $N(z)$. [The sum in Eq. (13) involves now only one term so the index n of the general theory can be dropped.] The equation $1 - \eta(z) = 1 - V_0 Q_0(z)$ can be zero on the positive imaginary axis only when $V_0 < 0$ at the imaginary momentum corresponding to the bound state negative energy [27]. However if $Q_0(q)$ is continued analytically into the lower q -plane by allowing q in (26) to have a negative imaginary part there are in general three roots q_1, q_2, q_3 corresponding to the cubic $\mathcal{C}(q)$ defined according to

$$1 - V_0 Q_0(q) - \frac{q(q + ia)^2 - 2mV_0(q + 2ia)}{q(q + ia)^2} = \frac{\mathcal{C}(q)}{q(q + ia)^2}. \quad (27)$$

The matrix element of the difference of resolvents takes the form

$$\begin{aligned} \langle \psi | R(z) | \psi \rangle &= \langle \psi | \frac{1}{z - H_0} | \chi \rangle \frac{V_0}{(1 - V_0 Q_0(q))} \langle \chi | \frac{1}{z - H_0} | \psi \rangle \\ &= \langle \psi | \frac{1}{z - H_0} | \chi \rangle \frac{V_0 q(q + ia)^2}{\mathcal{C}(q)} \langle \chi | \frac{1}{z - H_0} | \psi \rangle, \end{aligned} \quad (28)$$

so that

$$I(q) = \frac{1}{m} \langle \psi | \frac{q}{z - H_0} | \psi \rangle + \langle \psi | \frac{1}{z - H_0} | \chi \rangle \frac{V_0 q^2(q + ia)^2}{m\mathcal{C}(q)} \langle \chi | \frac{1}{z - H_0} | \psi \rangle. \quad (29)$$

The “motion” of the roots q_k in the complex q -plane obtained as the value of V_0 changes has been previously analyzed [27]. Provided $mV_0/a^2 > (-11 + 5\sqrt{5})/4$ then the core singularities are a resonance pole in the fourth quadrant at $q_1 = \alpha - i\beta$, $\alpha, \beta > 0$, 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 five different initial wave functions is examined: χ , $\zeta(q_1)$, $\zeta(q_3)$, a Gaussian and a Lorentzian function. In each case this requires calculating the matrix elements $\langle \psi | (z - H_0)^{-1} | \psi \rangle$, $\langle \psi | (z - H_0)^{-1} | \chi \rangle$ and $\langle \chi | (z - H_0)^{-1} | \psi \rangle$, together with the identification of the resulting poles of $I(q)$ and their orders.

III.a *Survival of χ*

The decay of this state is possibly the simplest illustration of the general formalism since in this case

$$I(q) = \frac{q}{m} \langle \chi | \frac{1}{z - H} | \chi \rangle = \frac{2q(q + 2ia)}{\mathcal{C}(q)} \quad (30)$$

and the only singularities correspond to the roots of the cubic equation. This rational fraction can then be decomposed into partial fractions

$$I(q) = \frac{2q(q + 2ia)}{\mathcal{C}(q)} = \sum_k \frac{a_k}{q - q_k} \quad (31)$$

where

$$a_k = \text{res}[I(q)]_{q=q_k} = \frac{2q_k(q_k + 2ia)}{3q_k^2 + 4iaq_k - a^2 - 2mV_0}. \quad (32)$$

Figure 2 shows $\ln S(\tau, \chi)$ versus the dimensionless time $\tau \equiv ta^2/m\hbar$. The same figure also shows the separate contributions from the exponential decay term associated with the resonance at q_1 , $|E_1(\tau)|^2$, and from the combination of the w -function terms, $|\sum_k D_k(\tau)|^2$. Clearly these two contributions alone account for the overall behaviour of the survival as a function of τ and the dominance of one or the other determines the different decay regimes. When these two main contributions are of comparable magnitude the interference between them can no longer be neglected and causes oscillations. The scale of the figure allows the transition from the resonance dominated time regime to the w -function dominated (large τ) regime to be clearly distinguished. The asymptotic (large time) survival decay as τ^{-3} . This power law can be understood in general from the symmetry properties of the integral at small values of q (which dominate in this case the integral along D [22]) and is also found for the other initial wave functions investigated in this paper. The short time behaviour requires a more careful analysis and is treated in the Discussion section.

III.b Survival of Correlated States

An eigenvector $\langle p|\zeta(z)\rangle$ in “momentum” representation, of $K(z)$ for $\Im q = \sqrt{2mz} > 0$ can be analytically continued as a function of the q parameter, into the

FIG. 2. $\ln S(\tau, \chi)$ versus τ for $mV_0/a^2 = 5$ (solid line); $|\sum_k D_k(\tau)|^2$ (long dash); $|E_1(\tau)|^2$ (short dash).

lower half q -plane. For q at the resonance ($q = q_1$), such a square integrable function of p will be referred to as a correlated state, see also [18]. This is given by

$$\langle p | \zeta_1 \rangle = \frac{2m\mathcal{N}_1}{q_1^2 - p^2} \langle p | \chi \rangle. \quad (33)$$

$\mathcal{N}_1$ is a normalization constant chosen so that $\langle \zeta_1 | \zeta_1 \rangle = 1$ (note that $\mathcal{N}_1 \neq N_1$),

$$|\mathcal{N}_k|^2 = (z_k - z_k^*) [Q_0(q_k^*) - Q_0(-q_k)]^{-1}. \quad (34)$$

The integrand for the survival amplitude is then

$$I(q) = \frac{q}{m} \langle \zeta_1 | \frac{1}{z - H} | \zeta_1 \rangle = [F(q, q_1) + f(q, -q_1^*)] |\mathcal{N}_1|^2 \quad (35)$$

where

$$F(q, q_1) = \frac{8m^2 q [1 - V_0 Q_0(q_1^*)] [(q_1 - q)(q_1 - 2ia)(q + 2ia) - 2ia^3]}{(q - q_1)^2 (q_1^2 - q_1^{*2}) q_1 (q_1 - ia)^2 (q + q_1^*)(q - q_3)}. \quad (36)$$

The important point is that, apart from a first order pole at q_3 , $I(q)$ has *double poles* at both q_1 and $q_2 = -q_1^*$. The decomposition into partial fractions then takes the form

$$I(q) = \frac{a_1^{(1)}}{q - q_1} + \frac{a_2^{(1)}}{q - q_2} + \frac{a_3^{(1)}}{q - q_3} + \frac{a_1^{(2)}}{(q - q_1)^2} + \frac{a_2^{(2)}}{(q - q_2)^2} \quad (37)$$

where explicit expressions for these coefficients can be easily obtained from Eqs. (35) and (36).

The double poles have a twofold origin: The resonant and antiresonant singularities of the resolvent core are first order poles, while the structural matrix elements $\langle \psi | (z - H_0)^{-1} | \chi \rangle$ and $\langle \chi | (z - H_0)^{-1} | \psi \rangle$, see Eq. (29), have poles respectively at q_1 and q_2 , leading to the double poles. The double pole at q_1 is crossed during the deformation of the contour and contributes according to (17). The w contributions from q_1 and q_2 are also influenced by their double pole character, see Eq. (22). In Fig. 3 the special nature of the decay at short times, due to the double pole, is clearly seen (compare with the straight line of Fig. 2).

III.c Survival of the Square Integrable Virtual State

The square integrable virtual state (defined analogously to the correlated state of the last section) is associated with the pole q_3 of the resolvent on the negative imaginary axis. When normalized, compare Eqs. (33) and (34), it is given by

$$\langle p | \zeta_3 \rangle = \frac{2m\mathcal{N}_3}{q_3^2 - p^2} \langle p | \chi \rangle. \quad (38)$$

FIG. 3. $\ln S(\tau, \zeta(q_1))$ versus τ for $mV_0/a^2 = 5$ (solid line); $|\sum_k D_k(\tau)|^2$ (long dash); $|E_1(\tau)|^2$ (short dash).

FIG. 4. $\ln S(\tau, \zeta(q_3))$ versus τ for $mV_0/a^2 = 5$ (solid line); $|\sum_k D_k(\tau)|^2$ (long dash); $|E_1(\tau)|^2$ (short dash).

Since both structural matrix elements in the scattering part of Eq. (29) have a pole at q_3 , these combine with the core pole to make this a triple pole. This fact however only affects the w -function contribution since this pole is not crossed during the contour deformation so the decay is dominated by the residue at the resonance pole q_1 . In this case

$$\begin{aligned}
 I(q) = & \frac{8m^2 q \mathcal{N}_3^2}{q_3^3 (q_3 - ia)^4 \mathcal{C}(q)(q - q_3)^2} \\
 & \times \{ q_3 (q_3 - 2ia)^2 (q - q_3) [(q - q_2)(q - q_1) + 2iaq - 2q_1 q_2] \\
 & - 4iaq_3 (q_3 - 2ia)(q - q_3)(q_3 + q_1)(q_3 + q_2) \\
 & + ia^3 (q - q_1)(q - q_2)(q - 3q_3) + 4iq_3^2 a^3 (q + 2ia) \}. \quad (39)
 \end{aligned}$$

Figure 4 illustrates the resonance dominated decay of the square integrable virtual state.

III.d *Survival of a Gaussian State*

In all previous cases $I(q)$ is a simple rational fraction with a finite discrete pole expansion. The Gaussian packet

$$\langle p | \mathcal{G}(p_0, \sigma) \rangle = (2\pi\sigma^2)^{-1/4} \exp \left[-\frac{(p - p_0)^2}{4\sigma^2} \right] \quad (40)$$

provides an example where this does not occur. The relevant matrix elements are

$$\begin{aligned}
 \langle \mathcal{G} | \frac{1}{z - H_0} | \chi \rangle = & \left(\frac{2\pi a^2}{\sigma^2} \right)^{1/4} \frac{m}{q^2 + a^2} \left[w \left(\frac{p_0 + ia}{2\sigma} \right) + w \left(\frac{-p_0 + ia}{2\sigma} \right) \right. \\
 & \left. - \frac{ia}{q} w \left(\frac{-p_0 + q}{2\sigma} \right) - \frac{ia}{q} w \left(\frac{p_0 + q}{2\sigma} \right) \right] \quad (41)
 \end{aligned}$$

and

$$\langle \mathcal{G} | \frac{1}{z - H_0} | \mathcal{G} \rangle = \frac{-im\pi^{1/2}}{2^{1/2}\sigma q} \left[w \left(\frac{q - p_0}{2^{1/2}\sigma} \right) + w \left(\frac{q + p_0}{2^{1/2}\sigma} \right) \right]. \quad (42)$$

The quantity in (41) has no pole at $q = ia$ since the w -functions cancel each other at this point. In Fig. 5 the decay of the Gaussian state is shown. There is a sharp initial decay dominated by $|\sum_k D_k(\tau)|^2$ followed by an exponential decay due to the resonance term $|E_1(\tau)|^2$ and finally by the asymptotic τ^{-3} behaviour dominated again by $|\sum_k D_k(\tau)|^2$.

III.e *Survival of a Lorentzian State*

In all previous cases the behaviour of the decay is determined primarily by the resonance pole, i.e., by the core part of Eq. (29). The structural contribution has

been either a minor correction or a reinforcement of these core poles by increasing their order. Another interesting possibility is that, by properly choosing the initial state, a structural pole at a different position from the core poles may arise. If this pole is in the fourth quadrant of the complex q -plane it plays a role similar to a regular resonance core pole, and can actually dominate the decay for a period of time. This case is illustrated by a state that is Lorentzian in momentum representation, centered about momentum p_b ,

$$\langle p | \mathcal{L}_b \rangle = \left(\frac{2b^3}{\pi} \right)^{1/2} \frac{1}{b^2 + (p - p_b)^2}. \quad (43)$$

The required matrix elements are then [28]

$$\langle \mathcal{L}_b | \frac{1}{z - H_0} | \chi \rangle = \frac{4m(ab)^{1/2} F(q)}{q(q + ia)[(q + ib)^2 - p_b^2][p_b^2 + (a + b)^2]}, \quad (44)$$

where $F(q)$ is a quadratic polynomial

$$F(q) = (a + b)(q + ia)(q + 2ib) + b(a^2 - b^2 - p_b^2) \quad (45)$$

and

$$\langle \mathcal{L}_b | \frac{1}{z - H_0} | \mathcal{L}_b \rangle = \frac{2mJ(q)}{q[(q + ib)^2 - p_b^2]^2}, \quad (46)$$

where

$$J(q) = q^3 + 4ibq^2 - q(p_b^2 + 5b^2) - 2ib^3. \quad (47)$$

Note the poles of the first matrix element at $q = 0$, $q = -ia$, $q = p_b - ib$ and $q = -p_b - ib$. The first two are cancelled by the core factor to give

$$I(q) = \frac{2}{[(q + ib)^2 - p_b^2]^2} \left\{ J(q) + \frac{8abmV_0 F(q)^2}{\mathcal{C}(q)[p_b^2 + (a + b)^2]^2} \right\}. \quad (48)$$

By selecting p_b and b appropriately, a variety of decay behaviours may be found. Figure 6 shows a case where three different time regimes are observed: first a decay associated with the structural double pole, then an exponential decay due to the resonance pole, and finally the asymptotic behaviour. As usual the transitions between the regimes are characterized by oscillations due to the interference between the dominant terms.

For comparison, the decay in the absence of the potential is also presented. This essentially agrees with the first decay regime. Our rationale of this is that the chosen wave packet is broader than the potential (in coordinate representation) and most of it decays, via free motion, without being affected by the presence of the potential. This is only true at sufficiently large momentum. If the packet has nearly zero

FIG. 5. $\ln S(\tau, \mathcal{G})$ versus τ for $mV_0/a^2=5$, $p_0/a=2$, $\sigma/a=2.5$ (solid line); $|\sum_k D_k(\tau)|^2$ (long dash); $|E_1(\tau)|^2$ (short dash).

FIG. 6. $\ln S(\tau, \mathcal{L}_b)$ versus τ for $mV_0/a^2=30$, $p_b/a=2$, $b/a=0.2$ (solid line); $|\sum_k D_k(\tau)|^2$ (squares); $|E_4(\tau)|^2$ (short dash, straight line); $|E_4(\tau)|^2$ (dash-dotted); $\ln S(\tau, \mathcal{L}_b)$ for same state parameters as before and free motion ($V_0=0$) (long dash).

FIG. 7. $\ln S(\tau, \mathcal{L}_b)$ versus τ for $mV_0/a^2=5$, $p_b/a=0.2$, $b/a=0.3$ (solid line); $|\sum_k D_k(\tau)|^2$ (squares); $|E_1(\tau)|^2$ (short dash); $\ln S(\tau, \mathcal{L}_b)$ for free motion and same parameters for the state (long dash).

average momentum with a narrow spread (b value), this is no longer true and the survival is predominantly determined by the resonance pole, see Fig. 7.

IV. DISCUSSION

The survival of several different states ψ has been examined using the Yamaguchi potential. The *method* of calculation exploits the analytical properties of the resolvent matrix elements $\langle \psi | G(z) | \psi \rangle$. The most important components of the decay have been associated with singularities (state and/or potential dependent) of $\langle \psi | G(z) | \psi \rangle$. Anomalous decay behaviour due to a double pole of mixed structural and core origin has been described. Decay dominated by structural (state dependent) poles has also been exemplified. The possibility of finding an arbitrary decay law by an appropriate choice of *asymptotic* initial state before collision has already been pointed out e.g. by Goldberger and Watson [29]. In the present approach, this possibility is associated with the choice of initial state at time $t=0$, which can in principle be selected by an appropriate laser excitation.

The long time behaviour fits into the known t^{-3} dependence. A detailed analysis of this long time limit for several model potentials as well as a comparison with the free motion case (in one dimension the survival probability of a freely moving packet decays as t^{-1} asymptotically and in three dimensions as t^{-3}) has been recently described in ref. [30]. The short time behaviour deserves careful examination, since different authors find contradictory results. Moshinsky and coworkers

claim that the first correction to unity should be proportional to $t^{1/2}$ [2, 22, 23]. This can be easily understood in terms of the w -functions contributing to the survival amplitude since their short time series is an expansion in powers of $t^{1/2}$. On the other hand, the formal series

$$A(t, \psi) = \langle \psi | e^{-iHt/\hbar} | \psi \rangle = 1 - \frac{it}{\hbar} \langle \psi | H | \psi \rangle - \frac{t^2}{\hbar} \langle \psi | H^2 | \psi \rangle + \dots \quad (49)$$

suggests a t^2 correction (the imaginary t^1 term combines with its complex conjugate when calculating the survival probability as $|A(t, \psi)|^2$ to yield only a t^2 contribution). The difficulty with this second argument is that the series can diverge. The present calculations provide clear illustrations of this fact: For the state χ the expectation values of H^2 and higher powers of H do not exist. But this does not immediately imply an initial $t^{1/2}$ dependence of the *decay probability* $1 - S(t)$, since the corresponding coefficients in the short time expansion of the w -functions (one for each pole) may cancel each other, and this is indeed the case, as shown explicitly in Appendix B for the decay of χ . The first non-vanishing term for $1 - S(t, \chi)$ is proportional to $t^{3/2}$. One can expect that the series (49) will be better behaved for states with finite moments $\langle \psi | H^n | \psi \rangle$. In particular, a numerical check for the decay probability of the Gaussian state of the previous section gives a t^2 behaviour at short times. This agrees with the general argument by Fonda *et al.* [6] that $dS(t)/dt = 0$ at $t = 0$, *provided* the first moment of the Hamiltonian (mean energy) exists. If this is the case, then one may rule out at t^n ($n < 1$) dependence quite generally because this dependence leads to an infinite derivative at $t = 0$. However, 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 Appendix C. In [23], the initial state considered takes (in three dimensions) the form $\sin(\pi r/R)/r$, $r \leq R$. Its mean energy is infinite, as can be seen in momentum representation, with is consistent with the $t^{1/2}$ short time dependence of the decay probability described using a delta-shell model potential [23]. In summary, 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 Appendix C), 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 ($\mathcal{G}$). The short time behaviour is relevant for the so called Zeno effect [31]. All discussions of this effect assume a t^2 behaviour for the decay probability. The effect considers the successive measurement at small time intervals Δt with its implied loss of phase coherence at each measurement. As a consequence, the probability that a decay has occurred after a finite time t involving $t/\Delta t$ steps, is of order Δt , thus vanishing if $\Delta t \rightarrow 0$. With an exceptional short time behaviour such as the $t^{1/2}$ or $t^{3/2}$ described here, the effects can be greatly changed. If the decay probability, equivalently the short time behaviour of the survival, goes as $(\Delta t)^g$, $g > 1$, then for a finite time t , the cumulative decay probability when “successively” measuring the system is proportional to $(\Delta t)^{g-1}$. Thus for a finite mean energy but divergent second energy

moment g can be $3/2$ and the Zeno effect is predicted. More interesting is the case in which the mean energy is infinite with a possible $g = 1/2$. In this case the decay probability for a successively observed system tends to one as the number of observations increases to infinity. These anomalous behaviours depend on the realizability of states with diverging (first or second) energy moments, which is subject to debate [32]. In any case, it is plausible that even if such states do not exist, for states with sufficiently large energy moments, the described short time behaviour should remain valid over a limited time interval. These are all interesting questions far beyond the objective of the present work, which is to illustrate different decay behaviours of the survival.

APPENDIX A. PROPERTIES OF W -FUNCTIONS

For completeness the properties of the w -functions used in this work are listed [33]. It is an entire function defined in terms of the complementary error function as,

$$w(y) = e^{-y^2} \operatorname{erfc}(-iy). \quad (\text{A.1})$$

An alternative integral expression which is used in the text is

$$\int_{-\infty}^{\infty} \frac{e^{-u^2}}{u - y} du = i\pi \operatorname{sign}(\Im y) w[\operatorname{sign}(\Im y) y] \quad (\text{A.2})$$

Basic symmetry properties of $w(y)$ are

$$w(-y) = 2e^{-y^2} - w(y) \quad (\text{A.3})$$

and

$$w(y^*) = [w(-y)]^*, \quad (\text{A.4})$$

while any derivative of the w -function can be expressed in terms of the w -function itself since

$$w'(y) = -2yw(y) + \frac{2i}{\sqrt{\pi}}. \quad (\text{A.5})$$

Using this equation the integral

$$\int_{-\infty}^{\infty} \frac{e^{-u^2}}{(u - y)^2} du = -2i\pi \{ \operatorname{sign}(\Im y) y w[\operatorname{sign}(\Im y) y] - i/\pi^{1/2} \} \quad (\text{A.6})$$

can be written in terms of w -functions with a similar result for integrals having higher inverse powers of $(u - y)$. $w(y)$ has the series expansion

$$w(y) = \sum_0^{\infty} \frac{(iy)^n}{\Gamma((n/2) + 1)}. \quad (\text{A.7})$$

The w -function is a particular case of the Moshinsky function [2], which can be regarded as “the basic propagator for a Schrödinger transient mode”.

APPENDIX B. SHORT TIME BEHAVIOUR OF $A(t, \chi)$

In this appendix the asymptotic behaviour of $A(t, \chi)$ is examined explicitly at short times.

According to Eqs. (31) and (21) the survival of χ can be written in the compact form

$$A(t, \chi) = \frac{1}{2} \sum_k a_k^{(1)} w(-u_k). \quad (\text{B.1})$$

Using (A.7) and (32) the small t series for $A(t, \chi)$ takes the form

$$A(t, \chi) = \sum_{n=0} \frac{[(1-i)(t/mh)^{1/2}/2]^n}{\Gamma((n/2) + 1)} A_n \quad (\text{B.2})$$

where

$$A_n = \sum_k \frac{q_k^{n+1}(q_k + 2ia)}{3q_k^2 + 4iaq_k - a^2 - 2mV_0} \quad (\text{B.3})$$

Using the relations between the roots of the cubic $\mathcal{C}(q)$

$$\begin{aligned} q_1 + q_2 + q_3 &= -2ia \\ 3q_j^2 + 4iaq_j - a^2 - 2mV_0 &= (q_j - q_l)(q_j - q_k) \quad j \neq k, l, \quad k \neq l \\ q_2 &= -q_1^* \end{aligned} \quad (\text{B.4})$$

it is easy to prove that

$$A_0 = 1, \quad A_1 = 0, \quad A_2 = A_2^* \quad (\text{B.5})$$

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 $|A(t, \chi)|^2 - 1$. The first nonvanishing term is therefore proportional to $t^{3/2}$.

APPENDIX C. EXAMPLE OF $t^{1/2}$ BEHAVIOUR OF DECAY PROBABILITY AT SHORT TIMES

In this appendix we shall use a separable potential model different from the one in the main text, namely

$$V_1 = |\chi_1\rangle V_0 \langle \chi_1| \quad (\text{C.1})$$

$$\langle p|\chi_1\rangle = \left(\frac{a}{\pi}\right)^{1/2} \frac{1}{(p^2 + a^2)^{1/2}}. \quad (\text{C.2})$$

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 Eq. (B.1) the survival of χ_1 can be written as

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

By substituting the series expansion of the w , Eq. (A.7), it is found that the first non-vanishing term of the decay probability is of order $t^{1/2}$. A similar result was obtained in [2] by making other assumptions about the interaction.

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