Decay processes in an open Hamiltonian system

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A complex spectral decomposition is developed for the survival probability and spectral density of a simple metastable state in an open quantum system. The time interval before exponential decay occurs is shown to be dominated by the short-lived quasibound states of the system. [S1050-2947(98)05710-2]

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The detailed mechanisms by which metastable states form and decay are of great interest for mesoscopic and atomic physics because they dominate the conductance and scattering properties of open quantum systems. In this paper we consider a model that can describe the process by which a localized particle can tunnel out of a potential well and into the continuum. The model we consider consists of a single particle in a δ potential well in the presence of a constant field. Ludviksson [1] showed that for this model the singularities of the energy Green's function can be found fairly easily. We will obtain numerical values for the dominant poles (quasibound states) of the energy Green's function for this system and show under what conditions these poles can be used to construct a spectral decomposition of the survival probability and spectral density of initial states. As Misra and Sudarshan [2] proved, the very short time decay of metastable states cannot be exponential. In this paper we find the spectral features that give rise to early nonexponential decay of our metastable particle.

The spectral decomposition of the survival probability and spectral density makes use of generalized eigenstates associated with complex eigenvalues that are found by analytic continuation of the energy Green's function. A theoretical framework for the complex spectral decomposition has been developed by Grossmann [3] (called nested Hilbert spaces) and also by Bohm *et al.* [4] (called rigged Hilbert spaces), based on mathematical concepts introduced by Gel'fand and Vilenkin [5]. The method has been used by a number of authors to discuss properties of open quantum systems [6,7,4] and it has been used in the study of chaotic maps [8].

In the present paper we use a complex spectral decomposition to study the dynamical properties of Ludviksson's model. We will first derive complex spectral decompositions of the survival probability and spectral density, respectively, for a certain class of initially localized states. We then compute the survival probability and spectral density for a specific example and show the mechanism by which exponential decay begins to emerge. We end with some concluding remarks.

We consider the motion of a particle of mass m in one space dimension moving in the presence of a constant force F and an attractive δ-function potential $V(r) = -\Omega\,\delta(r)$. The Hamiltonian operator is

$$\hat{H}'(r) = -\frac{\hbar^2}{2m}\left(\frac{\partial}{\partial r}\right)^2 - \Omega\,\delta(r) - Fr \tag{1}$$

and has a continuum of energy eigenvalues E'. If we introduce a dimensionless length $x = k_0 r$, with $k_0 = (2mF/\hbar^2)^{1/3}$, and a dimensionless potential strength $V = \Omega k_0^2/F$, the Hamiltonian becomes

$$\hat{H}(x) = -\left(\frac{\partial}{\partial x}\right)^2 - V\delta(x) - x, \tag{2}$$

with the eigenenergies changed to $E = E' k_0/F$.

Ludviksson [1] has computed the retarded and advanced energy Green's functions $G^R(x,x';E+i\delta) = \langle x|(E-\hat{H}+i\delta)^{-1}|x'\rangle$ and $G^A(x,x';E-i\delta) = \langle x|(E-\hat{H}-i\delta)^{-1}|x'\rangle$, respectively, for this system (E and δ are real and $\delta > 0$). He finds

$$G^{R/A}(x,x';z) = G_0^{R/A}(x,x';z) - \frac{G_0^{R/A}(x,0;z)G_0^{R/A}(0,x';z)}{\frac{1}{V} + G_0^{R/A}(0,0;z)}, \tag{3}$$

where $z = E \pm i\delta$ and $G_0^R(x,x';z)$ and $G_0^A(x,x';z)$ are the retarded and advanced energy Green's functions, respectively, when $V = 0$. They are given by

$$G_0^{R/A}(x,x';z) = -\pi \times \begin{cases} \mathrm{Ai}(-x-z)\mathrm{Ci}^{\pm}(-x'-z), & x \leqslant x' \\ \mathrm{Ci}^{\pm}(-x-z)\mathrm{Ai}(-x'-z), & x \geqslant x', \end{cases} \tag{4}$$

where $\mathrm{Ci}^{\pm} := \mathrm{Bi} \pm i\,\mathrm{Ai}$ and Ai and Bi are Airy functions [9]. The Green's functions $G^R(x,x';E+i\delta)$ and $G^A(x,x';E-i\delta)$ ($\delta > 0$) have no singularities other than a cut along the entire real axis. For $x,x' \to \pm\infty$ and $E \pm i\delta$ fixed, $G^R(x,x';E+i\delta)$ and $G^A(x,x';E-i\delta)$ are bounded, i.e., they satisfy the same boundary conditions as do the solutions of the stationary Schrödinger equation.

If we are given an initial state $\psi(x,0) = \psi_i(x)$ at $t = 0$, its time evolution *towards the future* ($t > 0$) is determined by the retarded Green's function [10]

$$\psi(x;t) = \frac{i}{2\pi}\lim_{\delta\to 0}\int_{-\infty}^{\infty} dx' \int_{-\infty+i\delta}^{\infty+i\delta} dz\; e^{-izt} G^R(x,x';z)\psi_i(x'). \tag{5}$$

The contour for the z integration must be closed by a semicircle in the lower half of the complex plane. Therefore, it is necessary to analytically continue $G^R(x,x';z)$ into the lower half plane because of the cut along the real axis. For complex

z in the lower half plane, $G^R(x,x';z)$ is not bounded for $x,x' \to \pm\infty$. Furthermore, it has simple poles at complex values $z=z_n$, determined by the condition

$$\frac{1}{V} + G_0^R(0,0;z_n) = 0. \tag{6}$$

The integral on the semicircle part of the contour vanishes once its radius goes to infinity [1,11]. By the theorem of residues one obtains

$$\psi(x;t) = \int_{-\infty}^{\infty} dx' \sum_n \operatorname*{Res}_{z=z_n} [e^{-izt} G^R(x,x';z)] \psi_i(x'). \tag{7}$$

The sum goes over the poles of $G^R(x,x';z)$, all of which lie in the lower half of the complex z plane ($-\pi \leqslant \arg z \leqslant 0$).

Ludviksson found that the poles are simple and that the residues at these poles take the form

$$\operatorname*{Res}_{z=z_n} [e^{-izt} G^R(x,x';z)] = e^{-iz_n t} \psi_n(x) \psi_n(x')$$

$$\equiv e^{-iz_n t} \psi_n(x) \tilde{\psi}_n^*(x'). \tag{8}$$

The explicit form of $\psi_n(x)$ is

$$\psi_n(x) = \pi \left(-\frac{\partial}{\partial z} G_0^R(0,0;z) \Big|_{z=z_n} \right)^{-1/2}$$

$$\times \begin{cases} \mathrm{Ci}^+(-z_n)\mathrm{Ai}(-x-z_n), & x \leqslant 0 \\ \mathrm{Ai}(-z_n)\mathrm{Ci}^+(-x-z_n), & x \geqslant 0. \end{cases} \tag{9}$$

In order to retain the usual form of the duality $\langle\,|\,\rangle$ [cf. Eqs. (16) and (17) below], we have defined

$$\tilde{\psi}_n(x) = \psi_n^*(x), \tag{10}$$

where $*$ denotes complex conjugation. Ludviksson [1] also found that the function ψ_n satisfies the condition

$$\hat{H}(x)\psi_n(x) = z_n \psi_n(x) \text{ [and hence } \hat{H}(x)\tilde{\psi}_n^*(x) = z_n \tilde{\psi}_n^*(x)], \tag{11}$$

so ψ_n is the right eigenstate and $\tilde{\psi}_n$ is the left eigenstate of $\hat{H}$ with respect to the eigenvalue z_n. The states ψ_n and $\tilde{\psi}_n$ are called generalized eigenstates because they do not belong to the Hilbert space of possible physical states. They are not square integrable ($\notin L^{(2)}$). They do, however, belong to a larger space Φ'_α. Using the asymptotic expressions for Airy functions [9], one can prove that

$$\psi_n, \tilde{\psi}_n \in \Phi'_\alpha := \left\{ \psi; \int_{-\infty}^{\infty} dx |\psi(x)|^2 e^{-|x|^\alpha} < \infty \right\} \tag{12}$$

for any $\alpha > 1/2$.

The fact that the functions ψ_n and $\tilde{\psi}_n$ are not square integrable implies that the integrals

$$I_n = \int_{-\infty}^{\infty} dx\ \psi_n(x)\psi_i(x) \tag{13}$$

do not necessarily exist for an arbitrary initial state ψ_i even though ψ_i is square integrable. Therefore, we may not always exchange the infinite sum and the integral in Eq. (7). We may only do this if Eq. (13) exists for all n. This imposes restrictions on the set of initial states $\psi_i(x)$ we can work with if we want to perform the integration in the specific way we are considering here.

Let us define another space

$$\Phi_\alpha := \left\{ \psi; \int_{-\infty}^{\infty} dx |\psi(x)|^2 e^{|x|^\alpha} < \infty \right\}. \tag{14}$$

From the definitions (12) and (14) it is obvious that $\Phi_\alpha \subset L^{(2)} \subset \Phi'_\alpha$. If $\varphi \in \Phi_\alpha$ and $\psi \in \Phi'_\alpha$, then

$$\int_{-\infty}^{\infty} dx\ \psi^*(x)\varphi(x) \tag{15}$$

exists and by such an integral one can denote the duality between Φ_α and its dual space Φ'_α. The three spaces Φ_α, $L^{(2)}$, and Φ'_α form a ''Gel'fand triplet.''

If the initial state ψ_i belongs to the space Φ_α, then the integrals (13) exist and Eq. (7) can be written

$$\psi(x;t) = \sum_n e^{-iz_n t} \psi_n(x) \left(\int_{-\infty}^{\infty} dx' \tilde{\psi}_n^*(x') \psi_i(x') \right) \tag{16}$$

or, more formally,

$$|\psi(t)\rangle = \sum_n e^{-iz_n t} |\psi_n\rangle \langle \tilde{\psi}_n | \psi_i \rangle. \tag{17}$$

Note that $\langle \tilde{\psi}_n | \psi_i \rangle$ is not the usual scalar product defined in Hilbert space since $\psi_n \notin L^{(2)}$, but it is the duality between the spaces Φ'_α and Φ_α.

Equation (17) can lead to exponential decay of some physical quantities including the survival probability. The survival amplitude $A_i(t)$ for an initial state ψ_i is defined $A_i(t) = \langle \psi_i | \psi(t) \rangle$. If $\psi_i \in \Phi_\alpha$, then the survival amplitude can be written

$$A_i(t) = \langle \psi_i | \psi(t) \rangle = \sum_n e^{-iz_n t} \langle \psi_i | \psi_n \rangle \langle \tilde{\psi}_n | \psi_i \rangle \tag{18}$$

and the survival probability can be written

$$P_i(t) = |A_i(t)|^2 = \sum_{n'} \sum_n e^{i(z_{n'}^* - z_n)t} \gamma_n \tilde{\gamma}_n^* \gamma_{n'}^* \tilde{\gamma}_{n'}, \tag{19}$$

where γ_n and $\tilde{\gamma}_n$ are the overlap integrals

$$\gamma_n = \langle \psi_i | \psi_n \rangle, \quad \tilde{\gamma}_n = \langle \psi_i | \tilde{\psi}_n \rangle. \tag{20}$$

If only a single term $n = n' = n_0$ contributes in Eq. (19), then the survival probability decays in a purely exponential manner with a lifetime $\tau_{n_0} = 1/2|\mathrm{Im}(z_{n_0})|$. However, if two or more terms contribute, the decay will be much more complex and generally will contain oscillations.

The complex spectral decomposition given in Eq. (17) allows for an *explicit* description of decay phenomena rather than just an average lifetime estimate as it is usually obtained

TABLE I. The most important poles and associated overlap integrals for the example from Sec. IV.

n	Position z_n	Overlap integral $\gamma_n(=\tilde{\gamma}_n^*)$	Product $\gamma_n\tilde{\gamma}_n^*$
−7	$-5.08948-i9.08886$	$0.0023812+i0.0058470$	$-0.0000285+i0.0000278$
−6	$-4.59265-i8.22096$	$-0.0019365-i0.0149192$	$-0.0002188+i0.0000578$
−5	$-4.06889-i7.30278$	$-0.0278465+i0.0106945$	$0.0006611-i0.0005956$
−4	$-3.51134-i6.31988$	$0.0308708+i0.0196142$	$0.0005683+i0.0012110$
−3	$-2.90949-i5.24829$	$-0.0156032-i0.0895955$	$-0.0077839+i0.0027959$
−2	$-2.24564-i4.04168$	$-0.1995118+i0.0554497$	$0.0367303-i0.0221257$
−1	$-1.48770-i2.57804$	$0.0917629+i0.3441265$	$-0.110003\ +i0.0631561$
0	$-1.14764-i0.18960$	$1.0325811-i0.0264531$	$1.0655240-i0.0546300$
1	$2.65495-i0.20418$	$-0.1259114-i0.0387222$	$0.0143543+i0.0097511$
2	$4.35897-i0.20322$	$-0.0073700-i0.0075198$	$-0.0000022+i0.0001108$
3	$5.76665-i0.20034$	$-0.0118315-i0.0060227$	$0.0001037+i0.0001425$
4	$7.01597-i0.19733$	$-0.0050012-i0.0034528$	$0.0000131+i0.0000345$
5	$8.16084-i0.19449$	$-0.0040785-i0.0025945$	$0.0000099+i0.0000212$
6	$9.22943-i0.19186$	$-0.0027452-i0.0019065$	$0.0000039+i0.0000104$
7	$10.23880-i0.18944$	$-0.0021746-i0.0015086$	$0.0000025+i0.0000066$

from discussions of the energy-time uncertainty relation. It is important to note that the lifetimes are determined by the poles of the retarded energy Green's function, which is independent of the initial state. In this sense, the lifetimes are intrinsic to the physical system. The choice of a particular initial state only ''picks'' those lifetimes that are most important for it via the overlap integrals γ_n and $\tilde{\gamma}_n$.

The initial state ψ_i is unstable. It will decay and therefore it has associated with it a spectral width that is determined by the poles of the energy Green's function.

In terms of the energy eigenstates $|E\rangle$ of the Hamiltonian ($\hat{H}|E\rangle = E|E\rangle$ with E real) the survival probability is

$$A_i(t) = \theta(t)\langle\psi_i|e^{-i\hat{H}t}|\psi_i\rangle = \theta(t)\int_{-\infty}^{\infty} dE\ e^{-iEt}\langle\psi_i|E\rangle\langle E|\psi_i\rangle. \tag{21}$$

The spectral density of the state ψ_i is proportional to the discontinuity of the energy Green's function across the cut [10] and is defined

$$\begin{aligned}\rho_i(E) &= \langle\psi_i|E\rangle\langle E|\psi_i\rangle \\ &= \frac{i}{2\pi}\lim_{\delta\to 0}[\langle\psi_i|G^R(E+i\delta)|\psi_i\rangle \\ &\quad -\langle\psi_i|G^A(E-i\delta)|\psi_i\rangle].\end{aligned} \tag{22}$$

However,

$$\begin{aligned}&\lim_{\delta\to 0}\langle\psi_i|G^R(E+i\delta)|\psi_i\rangle \\ &= \lim_{\delta\to 0}\int_{-\infty}^{\infty} dE'\ \frac{\rho_i(E')}{E-E'+i\delta} \\ &= \lim_{\delta\to 0}\lim_{\epsilon\to 0}\frac{i}{2\pi}\left[\int_{-\infty}^{\infty} dE'\ \frac{\langle\psi_i|G^R(E'+i\epsilon)|\psi_i\rangle}{E-E'+i\delta}\right. \\ &\quad \left. -\int_{-\infty}^{\infty} dE'\ \frac{\langle\psi_i|G^A(E'-i\epsilon)|\psi_i\rangle}{E-E'+i\delta}\right].\end{aligned} \tag{23}$$

The second integral involving the advanced Green's function in Eq. (23) is zero. The first integral picks up the poles of the retarded Green's function and gives (for $\psi_i\in\Phi_\alpha$)

$$\lim_{\delta\to 0}\langle\psi_i|G^R(E+i\delta)|\psi_i\rangle = \sum_n\ \frac{\gamma_n\tilde{\gamma}_n^*}{E-z_n}. \tag{24}$$

The second term in Eq. (22) is just the complex conjugate of the first, so we finally obtain

$$\rho_i(E) = \frac{i}{2\pi}\sum_n\left[\frac{\gamma_n\tilde{\gamma}_n^*}{E-z_n} - \frac{\gamma_n^*\tilde{\gamma}_n}{E-z_n^*}\right]. \tag{25}$$

After some algebra the spectral density of the initial state takes the form

$$\begin{aligned}\rho_i(E) = \sum_n &\left[\frac{\left(\frac{1}{2\tau_n}\right)^2}{(E-E_n)^2+\left(\frac{1}{2\tau_n}\right)^2}\right] \\ &\times\left[\frac{(2\tau_n)^2}{\pi}\left(\frac{1}{2\tau_n}\,\mathrm{Re}(\gamma_n\tilde{\gamma}_n^*) - (E-E_n)\,\mathrm{Im}(\gamma_n\tilde{\gamma}_n^*)\right)\right].\end{aligned} \tag{26}$$

The first term in square brackets is a ''Lorentzian'' centered at energy $E_n = \mathrm{Re}(z_n)$ and of width $1/\tau_n$. The second term in square brackets is not quite a constant, so that $\rho(E)$ is not simply a sum of Lorentzians. However, close to the peak of the Lorentzian $|E-E_n|$ becomes very small, so each term is well approximated by a Lorentzian for $E\approx E_n$.

The positions of the peaks as well as their widths are determined by the positions of the poles of the energy Green's function and the choice of an initial state only picks those poles that are most relevant for it. It is important to remember that the spectral decomposition derived here holds only for those initial states that are elements of Φ_α and not for all possible initial physical states $\psi_i\in L^{(2)}$.

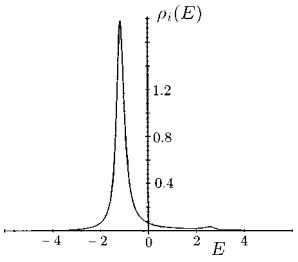

FIG. 1. Spectral density of $\psi_i=\sqrt{V/2}e^{-(V/2)|x|}$ for $V=2$ taking into account only the contributions from the poles at z_0 and z_1 (in dimensionless units).

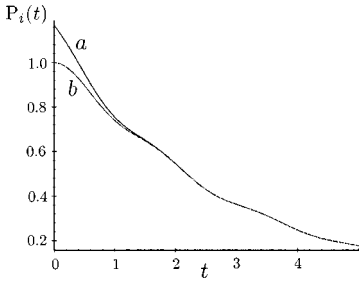

FIG. 2. Survival probability $P_i(t)$. Curve *a* shows $P_i(t)$ when only the poles z_0 and z_1 are taken into account (in dimensionless units). Curve *b* shows $P_i(t)$ when poles $z_{-5},\ldots,z_1$ are included. Already for $t>1.5$, the two graphs can hardly be distinguished from each other.

In order to illustrate the techniques described above, we consider the following example. For the Hamiltonian in Eq. (2) we have chosen $V=2$ and we have computed numerically the positions z_n of the poles in the energy range $-6\leqslant \mathrm{Re}(z_n)\leqslant 6$ (see Table I). We take $\psi_i(x)=\sqrt{V/2}e^{-(V/2)|x|}\in\Phi_\alpha$ as our initial state. This is the bound eigenstate of the δ potential alone, in the absence of the constant field. With the constant field ''turned on'' ψ_i is unstable. We have computed the ''overlap integrals'' γ_n for the poles in Table I and have listed them in Table I.

The Lorentzians that are peaked in the range $-6\leqslant E\leqslant 6$ are those corresponding to poles $z_{-7},\ldots,z_3$. The lifetimes $\tau_n=1/2|\mathrm{Im}(z_n)|$ and the values of the overlap integral products $\gamma_n\tilde{\gamma}_n^*$ can be found in Table I. These indicate that the poles z_0 and z_1 give the most important contributions to the spectral density $\rho_i(E)$. In Fig. 1 we plot the spectral density using only the contributions from the poles z_0 and z_1. These results agree qualitatively with the results of Cocke and Reichl [12], who computed the short-time behavior of this open system using a discrete set of energy eigenstates of a finite model (a wall was placed far down the hill from the δ potential).

We might expect that the survival probability $P_i(t)$ is also dominated by z_0 and z_1 at least for not too short times and $z_2,z_3,\ldots$ can again be left out. However, we have found that for short times, $z_{-1},\ldots,z_{-5}$ must be taken into account to obtain the correct short-time behavior of the survival probability. The overlap integral products corresponding to z_{-6} and z_{-7} make these negligible for *all* times. After an initial time interval, the survival probability has an exponential decay, superposed by oscillations due to interference of the terms from z_0 and z_1. The time interval before exponential decay sets in is determined by poles with a short lifetime (Fig. 2). (It is useful to note that the long-time decay of this system is dominated by exponential decay because there is no lower bound to the energy spectrum. For systems with a lower bound, the long-time decay is dominated by power-law behavior [13].)

We have used the Gel'fand triplet of spaces $\Phi_\alpha\subset L^{(2)}\subset\Phi'_\alpha$ to describe decay processes in this simple open quantum system. The idea of using extended spaces to describe quantum mechanical systems is not new. The mathematical justification [14] of the Dirac formalism uses exactly this pattern. Eigenstates of the position operator (i.e., δ functions in the position representation) or the momentum operator (plane waves in the position representation) are allowed, although they are not at all elements of $L^{(2)}$, but rather they belong to the Schwartz space S' of tempered distributions [15]. Such non-normalizable eigenstates are extremely useful for the description of physical processes.

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