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Description of resonance decay by Lindblad operators

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Abstract

Using an analytical model potential which contains resonant and bound states, we show that the decay of the resonances can be simulated by Lindblad operators. For that purpose, the unitary time evolution of an initial Gaussian wave packet in the model potential is compared with the non-unitary time evolution, obtained by solving the Lindblad equation, of the same wave packet in a potential which coincides with the model potential in the region of interest but does not contain resonances. In the latter case, dissipative effects are accounted for by Lindblad operators which lead to phenomenological friction and diffusion constants in the equations of motion. We suggest how those constants can be determined in a non-heuristic way, being directly connected to the width of the resonance in the model potential which we calculate using the complex rotation method.

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1. Introduction

Open quantum systems have been studied quite intensively in recent decades, covering a wide spectrum of applications in surface [1, 2], atomic [3–6], nuclear [7–11] and particle [12, 13] physics and in decay [14, 15], decoherence [16–20] and tunnelling [21–23] processes, to mention just a few examples. They also present an important framework in quantum information theory which allows us to study fundamental aspects like e.g., dephasing and entanglement dynamics of qubits [24–26]. Open quantum systems are characterized by dissipative interaction with the environment which leads, in general, to a non-unitary time evolution, and a common approach to describe such a time evolution are master equations for the density matrix ρ. Among those, the Markovian master equation derived by Lindblad [27] presents the most general form:

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -\frac{\mathrm{i}}{\hbar}[H, \rho] + \frac{1}{2\hbar}\sum_j \left(\left[V_j\rho, V_j^\dagger\right] + \left[V_j, \rho V_j^\dagger\right]\right). \tag{1}$$

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Here, H denotes the Hamiltonian of the open quantum system, and V_j are operators defined on the Hilbert space of H, representing the dissipative interaction of the open system with the environment. There are no further general restrictions on these operators, and their choice in physical applications is often heuristic, as are also the numerical values of the phenomenological constant(s), which may appear in the resulting equations of motion as a consequence. Such a phenomenological approach allows the treatment of problems where the nature of the dissipative effects is far too complex to be described in detail, such as, for example, in deep inelastic heavy-ion collisions, where dissipation arises from the excitation of the internal degrees of freedom, i.e. the nucleons. On the other hand, it is not obvious to what extent the true dynamics of the system is reflected in such calculations, since in many cases no experimental data or theoretical results from independent models are available for comparison. The aim of the present work is to investigate whether the phenomenological constant(s) can be obtained from external parameters of the considered open system. Hence, we require an appropriate open system, so that its true time evolution can be obtained independently, and a subsequent comparison can be made in order to either confirm or disprove the choice of the phenomenological constant(s).

Resonances present a special case of open systems, where the dissipative character occurs due to the coupling to the continuum. There exists a number of reliable methods to determine their positions, widths and time evolution (see, e.g., a recent work by Jentschura *et al* [28] where their dissipative terms are also explicitly mentioned). As is well known, the decay of a resonance is driven by the width, so if we try to describe the effect of resonances on a physical system in the framework of the Lindblad theory instead of an *ab initio* treatment, one can expect the appearing phenomenological constant(s) to be connected to the width in some way. To investigate this connection, we proceed as follows. In section 2, we propose a model potential for our analysis and calculate the energy positions of the bound and resonant states, and the widths of the latter ones using the complex rotation method. In section 3, we repeat the derivation of the equations of motion including the phenomenological constants from the Lindblad equation (1) for the given case, and present their solutions. The time evolution of an initial Gaussian wave packet in the model potential is calculated in section 4, and a comparison to the Lindblad dynamics is made. From that, the main conclusion of the present work is formulated. This conclusion is further discussed in section 5. Restrictions and limitations of the used approach are also discussed at the end. Atomic units are used throughout unless stated otherwise.

2. The model potential

The Lindblad equation is known to be analytically solvable for a harmonic oscillator potential. Such a potential, of course, has only bound states but no resonances. On the other hand, multiplying this potential with a smooth analytical cutoff yields a potential barrier, and hence resonances do occur. If we consider a one-dimensional harmonic oscillator potential, $U_h(q)$, (q being the coordinate) with a minimum U_0 at $q = q_0$, that is

$$U_h(q) = \tfrac{1}{2}m\omega^2(q - q_0)^2 - U_0, \tag{2}$$

where ω is the oscillator frequency, and m is the mass of the particle; the cutoff in the model potential U_m can be implemented in the following form:

$$U_m(q) = U_h(q)\left(1 - \frac{1}{1 + \exp(-(q - q_B)/\tau)}\right). \tag{3}$$

The parameter τ gives the smoothness of the cutoff (in the limit $\tau \to 0$, one obtains the Heaviside step function), and q_B is the point at which the cutoff is switched on, thus it

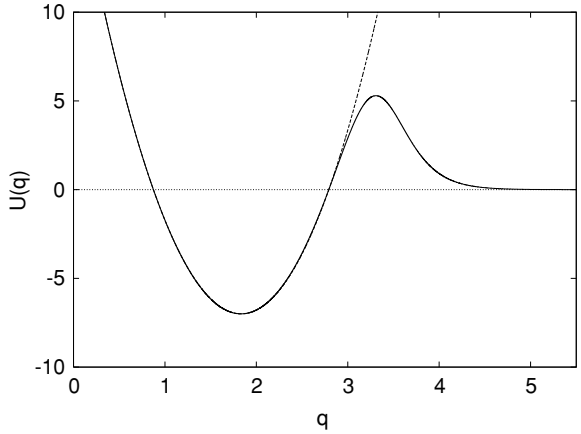

Figure 1. The model potential U_m (3) (solid line) shown together with a harmonic oscillator potential U_h (2) (dashed line) for $m = 1.0$, $\omega = 3.9$, $q_0 = 1.833$, $q_B = 3.35$, $U_0 = 7.0$ and $\tau = 0.19$.

corresponds approximately to the position of the barrier. For a better visualization, the model potential is shown together with a harmonic oscillator potential in figure 1. This model potential has the advantage that it coincides with a harmonic oscillator potential in the region $q < q_B$, and hence we can adopt the following approach: while the true time evolution of the Gaussian wave packet which is initially situated in the region of interest is obtained from the Schrödinger equation with the full model Hamiltonian

$$H_m = \frac{p^2}{2m} + U_m(q), \tag{4}$$

the time evolution given by the Lindblad master equation (1) is calculated for *the same* initial wave packet, but with the harmonic oscillator Hamiltonian

$$H_h = \frac{p^2}{2m} + U_h(q), \tag{5}$$

since the effect of the resonances is already accounted for by Lindblad operators, i.e., by the fact that we use the Lindblad equation. Such an approach seems justified as long as we are interested only in the local dynamics in the region of interest ($q < q_B$). However, we would like to emphasize here that the time propagation itself has, of course, to be calculated for the whole space including the asymptotic region in the first case.

We now proceed with the calculation of the energy positions of the bound states and resonances, and the widths of the latter ones in the model potential U_m. Complex rotation [29–31] is a widely used tool to treat resonances. If a Hermitian Hamiltonian of the form,

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial q^2} + U(q), \tag{6}$$

is transformed as $q \to q\exp(\mathrm{i}\theta)$ (where θ is a real rotation angle), the resonances are obtained as its complex eigenvalues:

$$E = E_r - \mathrm{i}\Gamma/2, \tag{7}$$

that is, the real part gives the energy position of the resonance, and the negative imaginary part gives the half width. Bound states are unaffected by the transformation. They appear as

Table 1. Bound and resonant states in the model potential U_m. The same parameters as listed in the caption of figure 1 were used.

State	$\mathrm{Re}(E)$	$-\mathrm{Im}(E) = \Gamma/2$
Bound	-5.045	–
Bound	-1.155	–
Resonance	2.62	3.3×10^{-2}
Resonance	6.21	0.44

eigenvalues of the complex Hamiltonian matrix, but their imaginary parts vanish. Continuum energies are rotated by the angle 2θ, and can be easily separated from the resonances, whose positions are independent of the rotation angle. To carry out this procedure, in practice, for the Hamiltonian (4) we use a B-splines expansion. B-splines are piecewise polynomial functions, defined on a so-called knot sequence and have several desirable properties (a detailed overview can be found in [32]). The combination of B-splines with complex rotation is a common method, mainly in atomic and molecular physics (e.g., [33–36]). The standard numerical procedure is to embed a knot sequence in a box of sufficient size, and subsequently project the Schrödinger equation $H\psi_j = E_j\psi_j$ onto the chosen B-splines set B_i (thus, the eigenfunctions are expanded as $\psi_j = \sum_i c_i^j B_i$). By solving the resulting generalized eigenvalue equation

$$H\mathbf{c} = EB\mathbf{c}, \tag{8}$$

(where $H_{ij} = \langle B_i|H|B_j\rangle$ and $B_{ij} = \langle B_i|B_j\rangle$) we can directly obtain the energies. The four lowest physical states are given in table 1. The two bound states lie close to the analytically known positions of an ideal harmonic oscillator ($E_1 = \hbar\omega/2 - U_0 = -5.05$ and $E_2 = 3\hbar\omega/2 - U_0 = -1.15$), and their distance approximately equals $\hbar\omega$ ($\Delta E = 3.89, \hbar\omega = 3.9$). This shows that the cutoff influences the bound states only weakly. Moreover, even the energy gap between the highest bound state and the lowest resonance is of about the same order ($\Delta E = 3.775$), due to the fact that this resonance is situated below the barrier. The second resonance lies above the barrier and is, as will be seen later, not relevant for our study. For this reason, further resonances, which were found at even higher energies are not listed in the table.

3. Equations of motion in the Lindblad theory

In this section, we will give a brief derivation of the equations of motion for a harmonic oscillator from the Lindblad equation and their solutions. This problem has been intensively studied in the last two decades, and a very detailed treatment can be found, e.g., in [37, 38] which we are closely following here.

It is convenient to transform the master equation (1) to the Heisenberg picture with time-dependent operators. For an operator A, it reads

$$\frac{\mathrm{d}A}{\mathrm{d}t} = \frac{\mathrm{i}}{\hbar}[H, A] + \frac{1}{2\hbar}\sum_j \left(V_j^\dagger[A, V_j] + \left[V_j^\dagger, A\right]V_j\right), \tag{9}$$

where H is the Hamiltonian (5). For simplicity, we will omit the shift q_0 in this part which is only a trivial coordinate transformation that does not change the equations of motion. The Lindblad operators for a harmonic oscillator are chosen as first-order polynomials in p and q (this choice is sometimes referred to as the quantum-mechanical analogue of Hook's law and

is, to the best of our knowledge, the only one ever used for a harmonic oscillator). This restricts the number of the Lindblad operators to two due to the fact that $\{p, q\}$ gives a basis of such non-commuting first-order polynomials, and hence only two independent linear combinations can be constructed. Thus, we have

$$V_j = a_j p + b_j q, \qquad V_j^\dagger = a_j^* p + b_j^* q, \qquad j = 1, 2, \tag{10}$$

where a_j, b_j are complex numbers.

First, we consider the expectation values of the coordinate q and momentum p, which are denoted by

$$\sigma_q = \mathrm{Tr}(\rho q), \qquad \sigma_p = \mathrm{Tr}(\rho p). \tag{11}$$

Setting $A = q$ ($A = p$ respectively) in (9) and evaluating the commutators, we arrive at two coupled first-order differential equations which, by introducing a phenomenological friction constant

$$\lambda = -\mathrm{Im} \sum_{j=1}^{2} a_j^* b_j, \tag{12}$$

can be written in the following form:

$$\frac{\mathrm{d}}{\mathrm{d}t}\sigma_q(t) = -\lambda\sigma_q(t) + \frac{1}{m}\sigma_p(t), \tag{13a}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\sigma_p(t) = -m\omega^2\sigma_q(t) - \lambda\sigma_p(t). \tag{13b}$$

With given initial conditions $\sigma_q(t = 0) = \sigma_q^0, \sigma_p(t = 0) = \sigma_p^0$, the analytical solutions of (13*a*), (13*b*) are (here and in the following, we assume $0 < \lambda < \omega$ which will be justified in section 4)

$$\sigma_q(t) = \mathrm{e}^{-\lambda t}\left(\cos(\omega t)\sigma_q^0 + \frac{1}{m\omega}\sin(\omega t)\sigma_p^0\right), \tag{14a}$$

$$\sigma_p(t) = \mathrm{e}^{-\lambda t}\left(-m\omega\sin(\omega t)\sigma_q^0 + \cos(\omega t)\sigma_p^0\right). \tag{14b}$$

Next, we consider the second moments which, for two operators A and B, are defined as

$$\sigma_{AB} = \sigma_{BA} = \tfrac{1}{2}\mathrm{Tr}(\rho(AB + BA)) - \mathrm{Tr}(\rho A)\mathrm{Tr}(\rho B). \tag{15}$$

For the three cases $A = q, B = q$; $A = p, B = p$ and $A = q, B = p$ one obtains (again by inserting the operator products in (9) and evaluating the commutators) a set of differential equations that describes the time behaviour of the variances of p and q (denoted by σ_{pp} and σ_{qq}, respectively), and their covariance σ_{pq}. To write these equations in a compact form, it is convenient to define the symmetrical covariance matrix:

$$\sigma(t) = \begin{pmatrix} \sigma_{qq}(t) & \sigma_{pq}(t) \\ \sigma_{pq}(t) & \sigma_{pp}(t) \end{pmatrix}. \tag{16}$$

It is worth mentioning that its determinant appears in the generalized uncertainty relation,

$$\sigma_{qq}(t)\sigma_{pp}(t) - \sigma_{pq}^2(t) \geqslant \hbar^2/4. \tag{17}$$

Then, the equations can be written in the matrix form as

$$\frac{\mathrm{d}}{\mathrm{d}t}\sigma(t) = Y\sigma(t) + \sigma(t)Y^T + 2D, \tag{18}$$

where we used the abbreviations

$$Y = \begin{pmatrix} -\lambda & 1/m \\ -m\omega^2 & -\lambda \end{pmatrix}, \qquad D = \begin{pmatrix} D_{qq} & D_{pq} \\ D_{pq} & D_{pp} \end{pmatrix}. \tag{19}$$

The elements of D are usually called 'diffusion coefficients' and are defined as

$$D_{qq} = \frac{\hbar}{2}\sum_{j=1}^{2}|a_j|^2, \qquad D_{pp} = \frac{\hbar}{2}\sum_{j=1}^{2}|b_j|^2, \qquad D_{pq} = -\frac{\hbar}{2}\,\mathrm{Re}\sum_{j=1}^{2}a_j^* b_j. \tag{20}$$

Their determination and properties have been thoroughly discussed, especially for the case of a harmonic oscillator, and different sets of diffusion coefficients were proposed [8, 39–42]. We just mention that, from definitions (12) and (20) and the Cauchy–Schwartz inequality, one obtains the fundamental constraint

$$D_{qq} > 0, \qquad D_{pp} > 0, \qquad D_{qq}D_{pp} - D_{pq}^2 \geqslant \lambda^2\hbar^2/4, \tag{21}$$

which ensures the non-negativity of the density matrix for all times. Such diffusion coefficients are often referred to as 'quantum mechanical' while those which do not obey (21) are called 'classical' due to the violation of the non-negativity condition. However, the diffusion coefficients can be determined by postulating a certain asymptotic state (e.g., a Gibbs state), and they may depend on the thermodynamical temperature of the system. In this case, the asymptotic state presents an input parameter (this rather general problem of the Lindblad equation was recently pointed out by Dietz [43]). If one considers the low-temperature limit, the following set of diffusion coefficients can be derived [8]:

$$D_{qq} = \frac{\hbar\lambda}{2m\omega}, \qquad D_{pp} = \frac{1}{2}\hbar\lambda m\omega, \qquad D_{pq} = 0. \tag{22}$$

This set satisfies (21) and does not depend on the temperature. Moreover, it has the advantage that the diffusion coefficients are fully determined by the phenomenological friction constant, and thus λ becomes *the only* phenomenological parameter to be found. We can conclude that the given set (22) is very suitable for our study, and thus it will be used in all further calculations. For a more comprehensive discussion, we refer to the articles mentioned above.

Now we return to the differential equations (18). Their solutions can also be given in an analytical form,

$$\sigma(t) = \mathrm{e}^{tY}(\sigma^0 - \sigma^\infty)(\mathrm{e}^{tY})^T + \sigma^\infty, \tag{23}$$

where $\sigma^0 = \sigma(t=0)$ is the initial covariance matrix, and $\sigma^\infty = \sigma(t\to\infty)$ is its asymptote. The latter one can be determined from the diffusion coefficients by inserting (23) in (18) which leads to

$$Y\sigma^\infty + \sigma^\infty Y^T = -2D. \tag{24}$$

The above matrix equation can also be written as a system of three linear equations (since both sides of (24) are symmetrical matrices), which then can be solved for the elements of σ^∞. The result is

$$\begin{aligned}
\sigma_{qq}(\infty) &= \frac{(m\omega)^2(2\lambda^2+\omega^2)D_{qq} + \omega^2 D_{pp} + 2m\omega^2\lambda D_{pq}}{2(m\omega)^2\lambda(\lambda^2+\omega^2)},\\
\sigma_{pp}(\infty) &= \frac{(m\omega)^2\omega^2 D_{qq} + (2\lambda^2+\omega^2)D_{pp} - 2m\omega^2\lambda D_{pq}}{2\lambda(\lambda^2+\omega^2)},\\
\sigma_{pq}(\infty) &= \frac{-\lambda(m\omega)^2 D_{qq} + \lambda D_{pp} + 2m\lambda^2 D_{pq}}{2m\lambda(\lambda^2+\omega^2)}.
\end{aligned} \tag{25}$$

Inserting the diffusion coefficients (22) in the above expressions, the asymptotic values can be shown to simplify to

$$\sigma_{qq}(\infty) = \frac{\hbar}{2m\omega}, \qquad \sigma_{pp}(\infty) = \hbar m\omega/2, \qquad \sigma_{pq}(\infty) = 0. \tag{26}$$

The exponential of the matrix that appears in (23) is found by diagonalizing Y:

$$\mathrm{e}^{tY} = \mathrm{e}^{-\lambda t}\begin{pmatrix} \cos(\omega t) & \frac{1}{m\omega}\sin(\omega t) \\ -m\omega\sin(\omega t) & \cos(\omega t) \end{pmatrix}. \tag{27}$$

Hence, the time evolution of the first and second moments of the open quantum system is fully determined by (14*a*), (14*b*) and (23) (provided given initial conditions σ_q^0, σ_p^0 and σ^0 which, however, do not influence the asymptotic values), and contains λ as the only free parameter. Its connection to the resonance widths in the model Hamiltonian will be suggested from a comparison in the following section.

4. Time evolution, comparison and main conclusion

We consider an initial Gaussian wavefunction of the form

$$\psi(q, t=0) = \frac{1}{\left(2\pi\sigma_{qq}^0\right)^{1/4}} \exp\left(-\frac{1}{4\sigma_{qq}^0}\left(q-\sigma_q^0\right)^2 + \frac{\mathrm{i}}{\hbar}q\sigma_p^0\right), \tag{28}$$

which is centered around σ_q^0 in q-space with the initial spread σ_{qq}^0, and σ_p^0 is the momentum expectation value. By means of a Fourier transformation it can also be shown that the initial spread in p-space, σ_{pp}^0, is given by the initial spread in q-space as $\sigma_{pp}^0 = \hbar^2/\left(4\sigma_{qq}^0\right)$. The corresponding probability density $|\psi(q)|^2$ ($|\psi(p)|^2$ respectively) preserves the initial Gaussian form for all times in a potential that is quadratic in q [11, 21, 23], which means that, for a harmonic oscillator within the Lindblad theory, the time propagation can be obtained by inserting the first and second moments as they are given by (14*a*), (14*b*) and (23) at any time t. In order to propagate the initial wavefunction (28) in the model potential, we use the same numerical tools as in section 2 but without complex rotation (i.e., $\theta = 0$). In particular, the Schrödinger equation for the Hamiltonian (4) is solved numerically in a box of sufficient size, yielding the box energies ϵ_j and the box eigenfunctions φ_j in terms of B-splines:

$$\varphi_j(q) = \sum_i c_i^j B_i(q). \tag{29}$$

In the following step, the initial wavefunction (28) is expanded in the box eigenstates as

$$\psi(q, t=0) = \sum_k d_k\varphi_k(q), \qquad d_k = \langle\varphi_k|\psi(t=0)\rangle, \tag{30}$$

and thus the wavefunction for any time t is obtained as a solution of the time-dependent Schrödinger equation:

$$\psi(q, t) = \sum_k d_k\varphi_k(q)\exp(-\mathrm{i}\epsilon_k t/\hbar). \tag{31}$$

For a suitable comparison between the two approaches we will, as already indicated at the beginning, restrict ourselves to the region where the model potential overlaps with the harmonic oscillator, i.e. $q \leqslant q_B$. We consider the wave packet to be located at rest around the minimum of the model potential (which is also the minimum of the harmonic oscillator potential), in other words, $\sigma_p^0 = 0$, $\sigma_q^0 = q_0$. We define the norm P contained in the region of interest as

$$P(t) = \int_{-\infty}^{q_B} |\psi(q, t)|^2\,\mathrm{d}q, \tag{32}$$

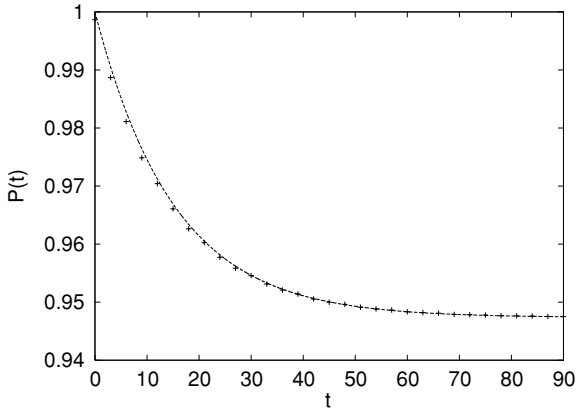

Figure 2. Calculated time evolution of P (crosses), shown with a function as given in (34) (dashed line) with $\alpha = \Gamma = 6.6 \times 10^{-2}$. The calculated population of the bound states P_B (33) is found to be $P_B = 0.947$, which agrees with the calculated asymptotic value of P. The slight deviation at the beginning occurs probably due to the fact that the initial wave packet has small components above the barrier which are classically allowed outside the region $q < q_B$, and hence they can leave this region directly without tunnelling. In addition, the presence of a second resonance with a larger width may also play a role for those components.

and with a moderate choice of σ^0_{qq}, the initial norm is very close to unity (e.g., $P(t = 0) = 0.9987$ for $\sigma^0_{qq} = 0.25$ in our following illustrative calculations, and the deviation is most likely caused by the numerics). Due to the presence of a resonance, we expect this quantity to decay exponentially and to converge towards the initial population of the bound states P_B, defined as

$$P_B = |d_1|^2 + |d_2|^2, \tag{33}$$

with the coefficients d_1, d_2 from the expansion (30) that correspond to the two bound states (cf table 1). Indeed, if the calculated time evolution of P is compared with a function of the form

$$P(t) = (1 - P_B)\,\mathrm{e}^{-\alpha t} + P_B, \tag{34}$$

a very good agreement is achieved for $\alpha = \Gamma$, where Γ is the width of the lowest resonance (table 1), as shown in figure 2. Hence, we can conclude that only the lowest resonance plays a role in our case. However, it is not clear how the described norm loss in the region of interest can be related to Lindblad dynamics, since the latter one is norm conserving. On the other hand, the energy expectation value is time dependent, and hence it seems more appropriate to look for a suitable definition of the amount of energy contained in the region of interest in order to make a reasonable comparison. We propose thus the following definition:

$$\langle E\rangle(t) = \frac{1}{P(t)}\mathrm{Re}\left(\int_{-\infty}^{q_B} \psi^*(q,t) H_m \psi(q,t)\,\mathrm{d}q\right), \tag{35}$$

which will be discussed below.

The box states in which the wavefunction ψ is expanded (30) are orthogonal with respect to the scalar product:

$$\int_{-\infty}^{+\infty} \varphi_j^*(q)\varphi_k(q)\,\mathrm{d}q = \delta_{jk}. \tag{36}$$

They are, however, not orthogonal if the integration is taken only from $-\infty$ to q_B. Hence, the expression $\int_{-\infty}^{q_B} \psi^*(q,t) H_m \psi(q,t)\,\mathrm{d}q$ is, in general, complex since the last term in the equation below does not vanish:

$$\int_{-\infty}^{q_B} \psi^*(q,t) H_m \psi(q,t) = \sum_k |d_k|^2 \epsilon_k \int_{-\infty}^{q_B} |\varphi_k(q)|^2\,\mathrm{d}q + \sum_{k\neq j} d_j^* d_k \epsilon_k \,\mathrm{e}^{\mathrm{i}(\epsilon_j-\epsilon_k)t/\hbar} \int_{-\infty}^{q_B} \varphi_j^*(q)\varphi_k(q)\,\mathrm{d}q. \tag{37}$$

However, the disregard of the complex part in definition (35) can be motivated as follows. Consider two equivalent expressions for the energy expectation value E_H for a usual Hermitian quantum system with a Hamiltonian, H, and a wavefunction, ψ,

$$\frac{1}{N}\int \psi^* H \psi = E_H = \frac{1}{N}\int (H\psi)^* \psi, \qquad N = \int |\psi|^2, \tag{38}$$

so that it can also be written as

$$E_H = \frac{1}{2N}\left(\int \psi^* H \psi + \int (H\psi)^* \psi\right). \tag{39}$$

Going back to our case, the analogue of the above expression is

$$\begin{aligned}\langle E\rangle(t) &= \frac{1}{2P(t)}\int_{-\infty}^{q_B} (\psi^*(q,t) H_m \psi(q,t) + (H_m\psi(q,t))^* \psi(q,t))\,\mathrm{d}q \\ &= \frac{1}{2P(t)}\int_{-\infty}^{q_B} (\psi^*(q,t) H_m \psi(q,t) + \text{h.c.})\,\mathrm{d}q \\ &= \frac{1}{P(t)}\mathrm{Re}\left(\int_{-\infty}^{q_B} \psi^*(q,t) H_m \psi(q,t)\,\mathrm{d}q\right),\end{aligned} \tag{40}$$

which is exactly definition (35).

Now, we return to the time propagation of $\langle E\rangle$. In an ideal harmonic oscillator, the energy associated with the initial wave packet (28) is given by

$$E_0 = \frac{1}{2m}\left(\sigma_{pp}^0 + \left(\sigma_p^0\right)^2\right) + \frac{1}{2}m\omega^2\left(\sigma_{qq}^0 + \left(\sigma_q^0\right)^2\right), \tag{41}$$

where $\sigma_{pp}^0 = \hbar^2/\left(4\sigma_{qq}^0\right)$. Again, since initially the wave packet is almost completely located in the region $q < q_B$ in the model potential, we expect $\langle E\rangle(t=0)$ to be very close to this value (shifted by U_0). Calculating $\langle E\rangle$ confirms this expectation ($E_0 - U_0 = -4.60$ versus $\langle E\rangle(t=0) = -4.61$). Asymptotically, we expect $\langle E\rangle$ to converge towards the energy initially contained in the two bound states, that is

$$E_\infty = \frac{|d_1|^2\epsilon_1 + |d_2|^2\epsilon_2}{|d_1|^2 + |d_2|^2}, \tag{42}$$

which is also rather well confirmed by the calculation ($E_\infty = -5.03$ versus $\langle E\rangle(t\to\infty) = -5.04$). The calculated overall time evolution of $\langle E\rangle$ suggests a fit with a function of the same form as in (34), i.e.

$$\langle E\rangle(t) = (E_0 - U_0 - E_\infty)\,\mathrm{e}^{-\beta t} + E_\infty, \tag{43}$$

and again good agreement is achieved for $\beta = \Gamma$ (see figure 3). On the other hand, the time evolution of the energy expectation value for a harmonic oscillator within the Lindblad theory

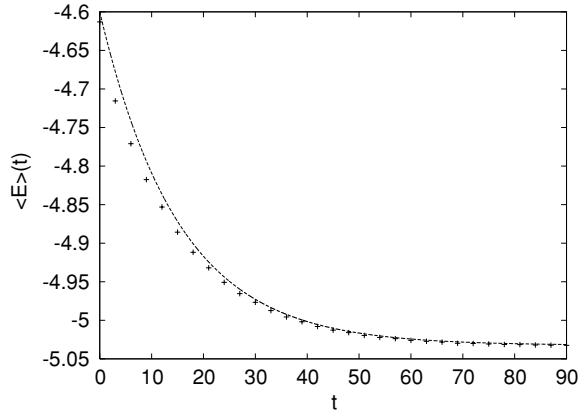

Figure 3. Calculated time evolution of $\langle E\rangle$ (crosses) shown together with the fit (43) (dashed line) with $\beta = \Gamma$. As in figure 2, the deviation at the beginning can be explained by the high-energetic components of the wave packet that leave the region $q < q_B$ very fast.

(including the shift U_0) reads

$$E_L(t) = \frac{1}{2m}(\sigma_{pp}(t) + \sigma_p(t)^2) + \frac{1}{2}m\omega^2(\sigma_{qq}(t) + \sigma_q(t)^2) - U_0, \tag{44}$$

where $\sigma_p(t), \sigma_q(t), \sigma_{pp}(t)$ and $\sigma_{qq}(t)$ are given by (14*a*), (14*b*) and (23). For the initial conditions, which were used to calculate $\langle E\rangle$, that is, a wave packet at rest centered in the potential minimum with no initial covariance $\left(\sigma^0_{pq} = 0\right)$, expression (44) can be analytically shown to simplify to

$$E_L(t) = \left(E_0 - \frac{\hbar\omega}{2}\right)\mathrm{e}^{-2\lambda t} + \frac{\hbar\omega}{2} - U_0. \tag{45}$$

Comparing this with (43) (where $\beta = \Gamma$), we see that for the case

$$E_\infty \approx \frac{\hbar\omega}{2} - U_0, \tag{46}$$

(which is fulfilled in our calculations, $E_\infty = -5.03$ versus $\hbar\omega/2 - U_0 = -5.05$) the time dependence is *the same*, which leads us to the main conclusion:

$$\lambda = \frac{\Gamma}{2}, \tag{47}$$

in other words, to describe the dissipative effect of a resonance by Lindblad operators of the form (10), a suitable choice for the phenomenological friction constant (12) is the half width of the resonance.

5. Discussion and restrictions

The derived conclusion provides certain information about how the phenomenological friction constant can be determined. This allows a less heuristic approach if the Lindblad equation is used for the description of resonances, opening new possibilities of applications in nuclear, atomic and molecular physics. To ensure that the agreement displayed in figure 3 is not random (i.e., that $\langle E\rangle$ generally behaves as suggested in (43)), other numerical values of the parameters in the potential (3) were imposed, which gives different positions and widths of

the resonances, and yet the same qualitative behaviour was obtained. However, the result (47) should be seen more as a tendency rather than an absolutely universal recipe, since some restrictions apply in our calculations. The considered wave packet (28) has a very high overlap with the bound states, which provides the condition (46) that is necessary for the agreement between (43) and (45) from which (47) was derived. Furthermore, at high energies (e.g., if σ_p^0 is large in (28)) the exponential behaviour is disturbed, since a large part of the wave packet is classically allowed to cross the barrier, and the decay of the norm and the energy contained in the region of interest occurs faster. Also the role of highly lying resonances can become more significant, and the dynamics is no longer dominated by one single width. In that case, extensions of the model to more than one phenomenological constant can be necessary. Furthermore, it is not clear to what extent definition (35) can really be interpreted as the amount of energy in the space $q < q_B$. We hope that it was sufficiently motivated, but a deeper investigation for arbitrary potentials would definitely shed more light on this question (although the obtained agreement with the Lindblad equation seems encouraging).

Also the potentials that one is confronted with in physical applications are often more complex than that treated here. Thus, if the Lindblad theory is applied, the local approximation of the true potential by a harmonic oscillator may not be the best choice, and hence other forms of Lindblad operators than (10) may be more appropriate, eventually leading to a different set of phenomenological constants in the equations of motion. Altogether, we can conclude that in an open system approach to resonances the obtained result may reflect the true dynamics quite well in some cases. However, in complex resonant systems where a heuristic approach is inevitable and phenomenological constants similar to (12) appear, relation (47) can still be adopted at least as a first guess, especially if no other more elaborated alternatives are available.

Finally, there exist also more fundamental limitations of the approach adopted in the present work. A rigorous study of master equations for the damped harmonic oscillator [44] shows that an exact general Liouville operator $\mathcal{L}$, which satisfies $\dot{\rho} = \mathcal{L}\rho$, does not exist for arbitrary environment conditions. The Lindblad form is only valid in the weak coupling limit on a coarse grained time scale. This is, to a rather good extent, fulfilled in the case studied here ($\lambda/\omega \approx 10^{-2} \approx \omega^{-1}/\Delta t$), but these restrictions should be kept in mind when master equations of the form (1) are used to describe the reduced dynamics of open quantum systems.

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