Feasibility study of resonant antiproton capture by ions and an open system approach to resonance decay

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Abstract

The present thesis is based on two different projects. The first part deals with resonant capture of antiprotons by electron excitation in highly charged hydrogen-like ions. The search for this process was mentioned by an experimental group at the Max Planck Institute in Heidelberg (Germany) as a possible future project at the Facility for Low Antiproton and Ion Research (FLAIR) at the "Gesellschaft für Schwerionenforschung" (GSI) in Darmstadt (Germany), which motivated the theoretical feasibility study presented in this thesis. Illustrative calculations on the collision of antiprotons in the energy region \( E \approx 0.13 - 0.14 \text{ keV} \) with hydrogen-like calcium \( \text{Ca}^{19+} \) have been carried out using an approach which is common in dielectronic recombination (DR) calculations, justified by the fact that the process of interest can formally be seen as the exotic analogon of DR where the incoming electron is replaced by an antiproton. In particular, we investigated the doubly excited resonant electron-antiproton states that can eventually be formed in such a collision and estimated their positions as well as the rates of the possible decay channels. Based on this, first approximate predictions for the cross section of resonant antiproton capture are made.

The second part of the thesis is devoted to resonances as well, but in quite a different context. Due to the coupling to the continuum, a quantum system that contains resonances can be treated as an open quantum system. Such an approach, however, is often heuristic to a certain extent, because the theoretical description of the dissipative interaction of an open system with its environment in many cases requires phenomenological constants that cannot be determined from the first principles. To investigate whether such constants are connected to known parameters of a resonance (its width, in particular), the unitary time evolution of a model quantum system within the Schrödinger equation is compared to the non-unitary time evolution within the Lindblad master equation. For the chosen model potential, good agreement was achieved and a relation between the resonance width and the phenomenological constants that appear in the Lindblad-type equations of motion is suggested.
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Outline of the thesis

This thesis is divided in two independent parts dealing with resonance effects in quantum systems. The first part is devoted to a theoretical feasibility study of resonant antiprotonic capture by highly charged hydrogenlike ions. It was motivated by a proposal of a possible experimental setup [1] by a group at the Max Planck Institute in Heidelberg. The described setup could become relevant in connection with the FLAIR project at GSI [2]. This process is quite similar to dielectronic recombination (DR), with the only, but quite significant, difference that the incoming electron is replaced by an antiproton. Thus, the computational methods which were developed for a theoretical treatment of DR can also be used for the description of the exotic process after some modifications. The calculations and main results are presented in Paper I and will be described and discussed in more detail in chapter 1.

The second part deals with a formal treatment of resonances as open quantum systems. The term open implies that there exists some interaction of the considered system with its environment. There are, however, no restrictions if such an environment is real or if it is just postulated to simulate dissipative effects which often can be far too complex to be included in calculations explicitly. Thus, the presence of a resonance (which implies a coupling to the continuum) can also be treated in this framework. At the same time, for a sufficiently simple system the dynamics can also be obtained from the first principles, including the effect of the present resonances. Hence, the approaches can be compared in order to investigate in how far an open system treatment is appropriate. The purpose of such a study is the following. In many cases, the open system approach is heuristic, i.e. the equations of motion for the quantum system may contain one or several phenomenological operators or constant(s) that account for dissipative effects. There is, however, not always a reasonable way to determine the form of the operators or the numerical values of the constants so that heuristic values have to be adopted. Hence, a comparative study with \textit{ab initio} calculations can shed light on this question and eventually provide further constraints on the phenomenological quantities. We performed such a study for a rather simple model potential in the framework of the Lindblad theory of open quantum systems, and the obtained results can,
to some extent, also be generalized for more complex resonant systems. The pro-
cedure and main results are given in Paper II. A more detailed description of the
Lindblad theory, the adopted approach and achieved conclusion will be presented
in chapter 2.
Chapter 1

Resonant capture of antiprotons by ions

1.1 Introduction

Experiments with antimatter present a fascinating laboratory to test fundamental symmetries of nature. Among other examples, one can mention numerous efforts on high precision spectroscopy of antihydrogen at CERN (Geneva, Switzerland) within the ATHENA / ALPHA and ATRAP projects [3, 4] and subsequent comparison to the hydrogenic spectrum. Such measurements could not be performed yet, although formation of antihydrogen was experimentally observed a few years ago [5,6]. Another field of interest are antiprotonic atoms, where matter and antimatter coexist in one quantum system. Typically, they emerge if an antiproton $\bar{p}$ is captured into an atom or an ion, and information can be extracted from precision spectroscopy of the exotic system. For example, antiprotonic helium, an exotic three-particle system, consisting of an $\alpha$-particle, an electron and an antiproton, has been subject to intensive experimental [7–10] and theoretical [11–20] studies since it was discovered about fifteen years ago [21, 22] (see also [23] for a detailed review). These studies, among other achievements, led to a new improved value for the electron-antiproton mass ratio [10]. This value can be translated to a determination of the proton-antiproton mass ratio and hence it presents a test of CPT symmetry. Also more complex antiprotonic systems have been studied during the last years [24–26]. However, in the vast majority of the cases, collisions of antiprotons with neutral atoms are considered to form the exotic systems, and there exist only a few investigations on collisions of antiprotons with ions [27–29]. In both cases, the following formation process is considered:

$$A^q + \bar{p} \rightarrow [A^{(q+1)} + \bar{p}] + e$$

(1.1)

where $A$ can be either an ion with charge $q$ or a neutral atom ($q = 0$), in other words, an electron is replaced by an antiproton in the final state. Such a process
is non-resonant, i.e. the continuum energies of the incoming antiproton $\epsilon_p$ and the emitted electron $\epsilon_e$ only have to fulfill the condition

$$\epsilon_p + E_i = \epsilon_e + E_f$$

(1.2)

where $E_i$ is the energy of the initial atom or ion and $E_f$ the energy of the formed exotic system with the antiproton in a bound state.

Let us now try to establish an analogy between antiproton-ion collisions and the possible reactions in electron-ion collisions. In the latter ones, the mechanism (1.1) is not of much interest, since the number of bound and continuum electrons is the same in the initial and final states. There exist, however, two well-known recombination mechanisms, namely radiative recombination (RR) and dielectronic recombination (DR). If the incoming electron is captured into a bound state and the released energy is transferred to an emitted photon, one speaks of RR. This is a non-resonant direct one-step process, which dominantly occurs into low-lying states and scales as the inverse of the relative energy $\epsilon$ between the colliding ion and the electron. For collisions with bare ions, an empirical formula for the cross section was derived by Kramers [30] in a semi-classical approach almost 100 years ago:

$$\sigma(\epsilon) = 2.11 \cdot 10^{-22} \text{ cm}^2 \frac{E_{1s}^2}{n\epsilon(E_{1s} + n^2\epsilon)}$$

(1.3)

where $E_{1s}$ is the ground state energy of the given ion and $n$ the principle quantum number. This formula is also valid in a quantum mechanical treatment, as shown by Bethe and Salpeter [31]. The interfering process of DR is, in contrast, a resonant two-step process. It mainly contributes to recombination if, in the collision with a non-bare ion, the energy of the incoming electron is tuned such that an intermediate doubly excited state can be formed. The free electron is captured from the continuum, and the released energy is transferred to an inner electron which then is excited. The necessary resonance condition thus reads

$$\epsilon_e = E_d - E_i$$

(1.4)

where $E_i$ is the energy of the initial ion and $E_d$ that of the formed doubly excited state. Such a doubly excited state lies above the threshold of the initial ion and is, therefore, autoionizing. Hence, to complete the recombination process the ion has to stabilize by photon emission. The strength $S$ of the whole process (i.e. the integrated cross section) is then proportional to the product of the probabilities (rates) of the capture and subsequent radiative stabilization ($A_r$). The former one is, in fact, the time reverse process of autoionization so that the capture and autoionization rate are the same according to the principle of detailed balance. With all factors, the strength reads (cf. e.g [32])

$$S = \int \sigma(\epsilon) d\epsilon = \frac{\hbar^3 \pi^2}{2m_e(E_d - E_i)} g_d A_n A_r \frac{A_n^{\text{tot}} + A_r}{g_i}.$$
Here, \( m_e \) is the electron mass, \( g_d, g_i \) denote the multiplicity factors of the doubly excited state and the initial ion, respectively, and \( A_n^{\text{tot}} \) is the total autoionization rate of the doubly excited state. This expression may be simplified if one of the rates is significantly slower than the others. In that case, the rate fraction in (1.5) approximately equals the slowest rate and hence it is this rate that determines the strength of the process. For example, such a situation often occurs in light ions where \( A_r \ll A_a \) and hence \( S \sim A_r \). In heavy systems, the opposite can be the case because the radiative rate strongly increases with the nuclear charge \( (A_r \gg A_a, S \sim A_a) \).

The question is now whether analog processes also can occur in antiproton-ion collisions and in how far they are relevant for a subsequent high precision spectroscopy of the emerging exotic system. Let us first consider direct radiative capture. Qualitatively, the Kramers formula (1.3) will still be valid (at least approximately) which means that mainly low lying states are populated. Since the orbit radius \( r \) of a negative particle with mass \( m \) scales as \( r \sim n^2/m \) (where \( n \) is the principle quantum number), such a heavy particle as an antiproton \( (m_p \approx 1836 m_e) \) would, for low \( n \), be situated very close to the nucleus and annihilate very fast. Typical lifetimes of antiprotons in matter are about \( 10^{-12} \) s, which means that only exotic systems where the antiproton is situated far enough from the nucleus for a sufficient amount of time can be subject to a spectroscopic study. Thus, the previously mentioned successful experimental investigations of antiprotonic helium were only possible due to presence of metastable circular \( (l \approx n - 1 \) where \( l \) is the angular quantum number) orbits which prolong the lifetime of the antiproton in matter by six orders of magnitude. From this considerations, it is apparent that the direct radiative capture process is not suited for subsequent spectroscopic studies.

The situation can be quite different for the DR-like resonant process. The fact that the capture occurs into a well-defined state which can be controlled by tuning the antiproton energy certainly presents a spectroscopic advantage. Furthermore, an estimation from the Bohr formula yields a rather large antiprotonic principle quantum number. For example, if the electron is initially in the ground state, an excitation to \( n_e = 2 \) states would lead to antiproton capture into \( n_p \approx 45 - 50 \) states which are far enough from the nucleus to prevent immediate annihilation. Hence, from a theoretical point of view the resonant process looks like a promising candidate. A natural question that one can ask is, of course, if an experimental observation is possible. While a high intensity electron beam in DR experiments is nowadays easily achieved, a cooled intense antiproton beam presents an experimental challenge. In addition, a setup has to be provided where cooled antiprotons can collide with ions with a sufficient rate. Considering this, a rather recent proposal was made by an experimental group at the Max Planck institute for nuclear
physics in Heidelberg [1], which also motivated the present theoretical investigation. As described therein, the Heidelberg Electron Beam Ion Trap (HD-EBIT) would, in a nested trap configuration, allow the slow antiprotons to collide with the ions repeatedly. As for the intensity, with the anticipated beam at the future Facility for Low Antiproton and Ion Research (FLAIR [2]) the EBIT could be loaded with up to $10^7 \bar{p}$ per shot [1]. In view of this encouraging experimental outlook, a theoretical study is carried out here to obtain estimations for the feasibility of the process.

This part of the thesis is structured as follows. First, a schematical description of the considered process will be given. In particular, the decay channels of the exotic doubly excited states are qualitatively discussed and necessary modifications of the theoretical approach used in DR calculations are suggested. Subsequently, the computational methods to calculate the decay rates are presented, like complex rotation and Fermi Golden Rule. Thereafter, illustrative calculations are performed for a medium heavy hydrogenlike ion, Ca$^{19+}$, and the cross section for resonant capture of antiprotons is estimated. The obtained results are discussed in the last part of this chapter, followed by some concluding remarks.
1.2 Theory

1.2.1 Decay channels

The doubly excited electron-antiproton state that can emerge in the collision

\[ A^q^+ + \bar{p} \rightarrow [A^q^+ \bar{p} e]^{**} \]  

(1.6)

will now be considered in more detail. For simplicity, the treatment will be restricted to collisions with hydrogenlike ions, since even for this rather simple system the numerical treatment turns out to be rather challenging. The resonant condition to be fulfilled is the same as in the DR process (1.4), where \( \epsilon_e \) is replaced by \( \epsilon_{\bar{p}} \). However, contrary to DR, the involved particles are not identical, which changes the situation quite significantly. On the one hand, it makes life simpler because no care needs to be taken of antisymmetrization. On the other hand, it also leads to additional decay channels that are not present in the DR process.

As previously mentioned, a dielectronic doubly excited state can either autoionize or stabilize by photon emission. In the present case, these processes split up: The radiative transitions have to be considered both for the electron and antiproton. Also the autoionization can occur in two ways: The electron can relaxate to the ground state and eject the antiproton, or, vice versa, the antiproton can undergo a transition which leads to the emission of an Auger electron. The former process is the time reverse of antiproton capture (1.6) and, in analogy to DR, the rates are the same according to the principle of detailed balance. The latter process, in spite of its autoionizing nature, can be seen as stabilizing because the antiproton is bound in the final state. It should be noted that in this case both the initial and final state are the same as in the non-resonant process (1.1) and hence possible interference effects need to be discussed. The four processes can be schematically represented in terms of approximate one-particle quantum numbers \( n_e, l_e, n_p, l_p \) as

\[
\begin{align*}
|n_e l_e n_p l_p|^{**} & \rightarrow |n_e' l_e' n_p l_p| + \gamma, \quad (1.7) \\
|n_e l_e n_p l_p'|^{**} & \rightarrow |n_e l_e n_p' l_p| + \gamma, \quad (1.8) \\
|n_e l_e n_p l_p'|^{**} & \rightarrow |n_e' l_e' n_p| + \bar{p}, \quad (1.9) \\
|n_e l_e n_p l_p'|^{**} & \rightarrow |n_e' l_e' n_p'| + e. \quad (1.10)
\end{align*}
\]

where (1.7) is electronic and (1.8) antiprotonic radiative stabilization, and the lower two mechanisms describe antiproton (1.9) and electron (1.10) emission. In view of all these processes, one can think of a suitable modification of the relation (1.5) to express the recombination strength of the exotic process by means of the occurring rates. The similarity to DR can be exploited to a large extent, but the additional channels need to be incorporated in a reasonable way.
1.2.2 Recombination strength and cross section

Basically, the same argumentation as in the derivation of expression (1.5) applies, namely, that the resonant formation of antiprotonic atoms is a two-step process and hence the strength should be proportional to the product of the capture rate (which, as already mentioned, equals the one of the inverse process (1.9)) and the stabilization rate. However, in the given case, the stabilization rate should include not only radiative transitions (1.7,1.8) but also electron emission (1.10), and the denominator should contain all rates. Thus, we arrive at the following expression for the recombination strength of resonant antiproton capture:

\[
S_P = \frac{k^3 \pi^2}{2 \mu_P (E_d - E_i)} \frac{g_d}{g_i} \frac{A_P A_{\text{stab}}}{A_P + A_{\text{stab}}}.
\] (1.11)

Here, \(E_i, E_d, g_i, g_d\) are, as before, the energies and multiplicity factors of the initial and the doubly excited state, \(A_P\) denotes the antiproton ejection rate, and \(A_{\text{stab}}\) is the stabilization rate

\[
A_{\text{stab}} = A_e + A_{\text{rad}} + A_{\bar{p}}
\] (1.12)

where \(A_e\) is the Auger electron emission rate and \(A_{\text{rad}}, A_{\bar{p}}\) denote the total radiative rate for electronic and antiprotonic transitions, respectively. Note also that it is the reduced mass of the antiproton

\[
\mu_{\bar{p}} = \frac{m_p m_N}{m_{\bar{p}} + m_N} \quad (m_p, m_N : \text{mass of antiproton / nucleus})
\] (1.13)

that appears in (1.11), since for such a heavy particle the motion of the nucleus should not be neglected. From the obtained expression, it becomes evident that for a feasibility prediction all the decay rates have to be calculated, and the central aspect of the first part of this thesis is to develop, to validate and to test computational methods suitable for this purpose. As for the cross section, the latter can be directly obtained from the recombination strength if assumed as a resonant Lorentz profile with the total width \(\Gamma\):

\[
\sigma(\epsilon_{\bar{p}}) = \frac{1}{\pi} S \left( \frac{\Gamma/2}{(E_d - E_i - \epsilon_{\bar{p}})^2 + \Gamma^2/4} \right).
\] (1.14)

Such a parametrization is often used in DR calculations (e.g. [32, 33]) and presents a good approximation for isolated resonances, i.e. resonances with a width much smaller than the distance from the nearest threshold. As will be demonstrated in the illustrative calculations, this condition is fulfilled for some of the antiproton-electron resonances and hence cross sections for antiprotonic capture via these resonances can be estimated. Another aspect is the symmetric form of (1.14). In atomic systems, resonances occasionally show asymmetric behavior and appear as
so called Fano profiles [34] due to interference effects. As an example, one can mention the interference between DR and RR which, in principle, should lead to asymmetric profiles. Similarly, possible interference between the processes (1.1) and (1.6) followed by (1.10) could also disturb the symmetry in our case. However, for such effects to be visible, the interfering processes need to be of about the same importance, which, in general, is not the case for DR and RR. Also for the processes considered here, the illustrative calculations on the particularly chosen ion show that this effect should not be of high importance. This will be discussed in more detail at a later point.

1.3 Computational methods

1.3.1 Complex rotation

The method of complex rotation (also known as complex scaling, dilatation analyticity or Augilar-Balslev-Combes Theorem) was formally developed in the beginning of the 1970s [35–37]. It presents a powerful tool to calculate positions and widths of resonances and there is a wide spectrum of its applications in atomic and molecular physics. As an example related to the present study the description of metastable states in antiprotonic helium [20] should be mentioned. The formal mathematical aspects of complex rotation will not be discussed here, and we proceed straight to its practical use.

Let us consider a one-dimensional Hermitian Hamiltonian of the form

\[ H = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \]  

(1.15)

and assume that the time-independent Schrödinger equation

\[ H\psi = E\psi \]  

(1.16)

is to be solved in a box of sufficient size. Let us furthermore assume that the potential can be written as

\[ V(x) = \sum_{n=-N_1}^{N_2} \alpha_n x^n \]  

(1.17)

where \( N_1, N_2 \) are natural numbers and \( \alpha_n \) some coefficients. This is not a necessary condition, but makes the following argumentation simpler. However, it should be emphasized that complex rotation also works well for potentials which can not be written in this form. This is demonstrated in the second part of the thesis, where complex rotation is succesfully applied to a model potential with an exponential
cutoff (cf. chapter 2). The common procedure is now to calculate the matrix elements of $H$ within some suitable basis so that a Hamiltonian matrix is obtained. This is where complex rotation comes into play: The coordinate $x$ in (1.16) is replaced by $x \exp(i\theta)$ where $\theta$ is a real number $0 < \theta < \pi/4$ usually called rotation angle. In the matrix representation, it simply means that the kinetic term is to be multiplied with $\exp(-2i\theta)$ and the potential terms which are proportional to $x^n$ with $\exp(in\theta)$. So far, the whole procedure is a trivial coordinate transformation, but the decisive point is that the boundary condition (i.e. that the wave function should vanish outside the box) remains unchanged. In other words, we still demand that the solution of the rotated Schrödinger equation

$$H(xe^{i\theta})\psi(xe^{i\theta}) = E\psi(xe^{i\theta})$$

(1.18)

vanishes at $x = R$ rather than at $x = R\exp(i\theta)$ (where $R$ is the box size). The eigenvalues of the complex scaled Hamiltonian are now found by diagonalizing the Hamiltonian matrix. There are, in general, three major kinds of states: bound states, resonances and pseudo-continuum states. The latter ones are unphysical and depend on the rotation angle. To illustrate their behaviour, the following qualitative argumentation can be adopted. For large $x$, positive energy solutions behave like $\sim \sin(kx)$ (where $k = \sqrt{2mE}/\hbar$ is the wave number) and hence they fulfill $\sin(kR) = 0$. After complex rotation is imposed the unchanged boundary condition becomes $\sin(kR\exp(i\theta)) = 0$, which implies $k \rightarrow k \exp(-i\theta)$. From that it follows directly (because $E \sim k^2$) that the continuum energies transform as $E \rightarrow E \exp(-2i\theta)$. In other words, they are rotated into the complex plane by the angle $2\theta$. Next, we consider bound states. The corresponding wave functions fall off fast, and for a sufficiently large box the boundary condition is fulfilled automatically. Hence, bound states are unaffected by complex rotation and the corresponding energies remain real. Finally, and this is the crucial aspect, resonances are directly obtained as the eigenvalues of the complex Hamiltonian matrix in the form

$$E = E_r - i\Gamma/2,$$

(1.19)

that is, the real part of the energy gives the position of the resonance $E_r$ and the width $\Gamma$ is given by twice the negative imaginary part. The resonances can be distinguished from the pseudo-continuum because their positions in the complex plane are $\theta$-independent. In practice, the calculation is usually performed with different values for $\theta$, and the eigenvalues with non-vanishing complex part which are unaffected by changing $\theta$ are identified as resonances. The problems that naturally arise in a numerical treatment are mainly a reliable representation of the wave function and the diagonalization of the Hamiltonian matrix (which, in many applications, can have a quite enormous size). The latter aspect is rather a question of time, since there exists a number of elaborated algorithms and libraries
1.3. Computational methods

(in the illustrative calculations presented in this thesis the LAPACK library was used). A numerically efficient way to represent the wave functions is discussed in the following subsection.

1.3.2 B-Splines

B-Splines are a class of piecewise polynomial functions that have several numerical advantages and are widely used in physical applications. Here, only a few necessary definitions, the most important properties and a very brief introduction will be given. For a detailed description, deBoors book [38] can be recommended, and applications to problems in atomic and molecular physics were reviewed in [39].

**Definition:** A finite subset \( \{t_0, \ldots, t_{n+m+1}\} \subset \mathbb{R} \) is called knot sequence of order \( m \) if

\[
0 \leq t_1 \leq \cdots \leq t_{n+m+1}
\]

and

\[
t_j < t_{j+m+1}, \quad j = 0 \ldots n.
\]

**Definition:** For each knot \( t_j \), its multiplicity \( \mu \) is defined as the number for which

\[
t_{j-1} < t_j = \cdots = t_{j+\mu-1} < t_{j+\mu}.
\]

**Definition:** Given a knot sequence \( \{t_i\} \), the B-Splines of order \( k \) are recursively defined as

\[
B_{i,1} = 1 \text{ if } t_i \leq x < t_{i+1}, \quad B_{i,1} = 0 \text{ else}
\]

and

\[
B_{i,k}(x) = \frac{x - t_i}{t_{i+k-1} - t_i} B_{i,k-1}(x) + \frac{t_{i+k} - x}{t_{i+k} - t_{i+1}} B_{i+1,k-1}(x).
\]

Throughout this thesis, B-Splines of order \( k = 7 \) are used and hence the second index will be omitted in the following. Among others, some important advantages of using B-Splines are that

- If the calculations are confined to a box, the knots can be distributed freely inside, so that the knot density can be increased in the regions where the relevant wave functions are expected to oscillate and less knots can be placed in regions where the wave functions are very smooth.

- If a scheme is used where \( k \) knots are placed at the box boundaries and all other knots appear only once (i.e. the multiplicity of the first and last \( k \) knots is \( \mu = k \) and \( \mu = 1 \) else), the first and the last B-Spline are the only ones which are non-zero on the boundary (in general, \( B_{i,k} \) is non-zero only between \( t_i \) and \( t_{i+k+1} \)). Hence, the boundary condition is automatically fulfilled if those two B-Splines are removed.
• The derivative of a B-Spline of order $k$ can be recursively expressed in terms of B-Splines of order $k-1$

$$\frac{d}{dx} B_{i,k}(x) = \frac{1 - k}{t_{i+k} - t_{i+1}} B_{i+1,k-1}(x) + \frac{k - 1}{t_{i+k-1} - t_i} B_{i,k-1}.$$ (1.25)

This is helpful when the calculation of the matrix elements of the momentum operator $p = -i\hbar \partial / \partial x$ is required.

• Numerical integration of B-Splines can be carried out to machine accuracy if necessary (i.e. no numerical error is produced) if Gaussian quadrature is used. This is due to the fact that B-Splines of order $k$ are piecewise polynomials of degree $k - 1$ and Gaussian quadrature with $n$ knots is exact for polynomials of degree up to $2n - 1$.

• Finally, although not pairwise orthogonal, B-Splines present a finite basis of the linear Spline space $S_m$, that is, of the linear space of piecewise polynomials that are $(m - \mu)$ times differentiable in a knot of multiplicity $\mu$.

It should be mentioned that there are, of course, also other methods for numerical representation of the wave functions which are more suitable in some cases, like e.g. directly on a grid. However, for our purpose B-Splines seem to be an appropriate choice, and no alternative methods were used in the numerical representation.

Now the application of B-Splines to an atomic three-particle system with subsequent complex scaling will be introduced. The goal is to diagonalize the complex scaled non-relativistic three particle Hamiltonian, which, in the center of mass system, reads

$$H = \frac{\hat{p}_e^2}{2\mu_e} + \frac{\hat{p}_{\overline{p}}^2}{2\mu_{\overline{p}}} + \frac{\mathbf{p}_e \cdot \mathbf{p}_{\overline{p}}}{m_N} - \frac{e^2}{4\pi\epsilon_0} \left( \frac{Z}{r_e} + \frac{Z}{r_{\overline{p}}} - \frac{1}{r_{12}} \right).$$ (1.26)

Here, $Z$ is the nuclear charge, $\mu_e$ and $\mu_{\overline{p}}$ denote the reduced masses of the electron and antiproton (and $m_N$ the mass of the nucleus), $r_e$ and $r_{\overline{p}}$ their distance to the nucleus and $r_{12} = |r_e - r_{\overline{p}}|$ the distance between them. The kinetic energy of the nucleus is accounted for through the use of reduced masses in the first two terms and the inclusion of the term $\mathbf{p}_e \cdot \mathbf{p}_{\overline{p}}/m_N$, usually called mass polarization. As an adequate basis set for a matrix representation, products of the eigenfunctions to the one-particle Hamiltonian

$$\hbar(r) = -\frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial r^2} + \frac{l(l+1)\hbar^2}{2\mu r^2} - \frac{Ze^2}{4\pi\epsilon_0 r},$$ (1.27)

can be used (with $r = r_e, r_{\overline{p}}, \mu = \mu_e, \mu_{\overline{p}}$). We adopt the notation

$$|\phi_{ab}^{SL\pi}\rangle = |\{n_a, l_a, n_b, l_b\} SL\pi\rangle$$ (1.28)
where \( S \) is the total spin, \( \pi \) the parity and \( L \) the total angular momentum to which \( l_a \) and \( l_b \) are coupled. However, only the Coulomb interaction will be considered in our calculations, and the dynamics is treated non-relativistically. Hence, parity and spin do not affect the matrix elements and will be omitted in further notation. Now, the procedure is as follows. First, the reduced one-particle eigenfunctions \( P_{nl}(r) \), i.e. solutions to
\[
h(r)P_{nl}(r) = \epsilon P_{nl}(r)
\]
are obtained in terms of B-Splines as
\[
P_{nl}(r) = \sum c_i B_i(r).
\]
For this, the one-particle Schrödinger equation (1.29) (after inserting the expansion above) is multiplied with \( B_j(r) \) and integrated over \( r \). Introducing the matrices
\[
h_{ji} = \langle B_j | h | B_i \rangle = \int \text{d}r B_j(r) h(r) B_i(r), \quad B_{ji} = \langle B_j | B_i \rangle = \int \text{d}r B_j(r) B_i(r)
\]
we arrive at a generalized eigenvalue equation
\[
h\mathbf{c} = \epsilon \mathbf{B}\mathbf{c}
\]
where \( \mathbf{c} = (c_1..c_N)^T \) is the coefficient vector and \( N \) the number of B-Splines used. Although such generalized equations can be solved directly, for numerical reasons equation (1.32) is transformed into a common linear equation by multiplying both sides from the left with \( B^{-1} \). Thus, the problem reduces to diagonalization of the matrix \( B^{-1}h \) after which both the one-particle energies \( \epsilon \) and the expansion coefficients \( c_i \) in (1.30) (i.e. one-particle wave functions) are obtained.

In the next step, the full Hamiltonian (1.26) is set up in the basis (1.28) where the basis functions are expressed in B-Splines, as just described. This is straightforward, because their radial parts are products of the radial parts of one-particle orbitals \( P_{nl} \). Furthermore, the full Hamiltonian \( H \) can be written as
\[
H = h_e + h_\bar{\mu} + h_{12}
\]
where \( h_e \) and \( h_\bar{\mu} \) have the form as in (1.27) with \( r = r_e, r_\bar{\mu}, \mu = \mu_e, \mu_\bar{\mu} \) and
\[
h_{12} = \frac{P_e \cdot \mathbf{P}_{\bar{\mu}}}{m_N} + \frac{e^2}{4\pi\epsilon_0 r_{12}}.
\]
The calculation of the matrix elements of \( H \) in the basis (1.28) is performed in the following way. The matrix elements of \( h_e \) and \( h_\bar{\mu} \) simply give the corresponding hydrogenlike one-particle energies, since the electronic one-particle Hamiltonian
does not act on antiprotonic one-particle wave functions (and vice versa). The calculation of the matrix elements of the interaction Hamiltonian $h_{12}$ requires a little bit more work. It is convenient to separate the appearing integrals into a radial and an angular part. The former ones are evaluated numerically with Gaussian quadrature. In this context, the previously mentioned properties of the B-Splines are exploited. The angular part can be treated analytically by means of angular momentum graph theory [40] (also known as Racah algebra). More details will be given when necessary in section 1.4.

Finally, as discussed in the previous subsection, complex rotation is introduced in the full Hamiltonian matrix by multiplying the kinetic terms with $\exp(-2i\theta)$ and the potential terms with $\exp(-i\theta)$. The resulting matrix is then diagonalized and the positions and widths of the resonances are obtained in the form (1.19). The whole procedure follows closely that of Refs. [41, 42].

1.3.3 Fermi Golden Rule

The described method that combines complex rotation with B-Splines is quite challenging from a computational point of view. However, sometimes a rather simple method to approximate transition rates can be useful, be it due to lack of alternative methods, for a quick estimation of the order of magnitude or for a comparison with more elaborated calculations as a validation. For this purpose, the Fermi Golden Rule is known to be a quite universal approach. It states that the rate $A$ (or the corresponding width $\Gamma = hA$) for a transition from an initial state $|\psi_i\rangle$ to a final state $|\psi_f\rangle$, caused by an interaction $U$, is given by

$$\Gamma = 2\pi \rho |\langle \psi_f | U | \psi_i \rangle|^2,$$

where $\rho$ denotes the density of states. This formula is rather fundamental and can be used as a starting point to derive some well known laws (in a quantum mechanical derivation of Rutherford's scattering formula, for example). In the following illustrative calculations, this approach will be used for two purposes. One of them is to independently estimate the antiproton ejection rates in the exotic doubly excited states in order to check the previously described full method for numerical accuracy. Such an approach was applied to autoionization processes in usual [43] but also exotic [14] atomic three-body systems. The second purpose is the calculation of the radiative transition rates. At this point, it should be emphasized that the widths obtained with complex rotation by diagonalizing the full Hamiltonian do not include any transitions of that kind. The reason is that they do not occur due to electron-antiproton interaction but because of external fluctuations of the electromagnetic field. Such fluctuations can result either from the environment or, if one considers the atom to be in vacuum, from vacuum fluctuations, which is a QED effect.
The interaction operator $U$ in (1.35) can be approximated by the Coulomb interaction between the electron and the antiproton when calculating the antiproton ejection rate, or, for calculating the radiative rates, by the dipole operator. The latter approximation (often called dipole approximation) is valid as long as the wavelength of the electromagnetic field is much larger than the dimension of the atom. The space dependence of the vector potential can then be neglected ($\mathbf{A}(r, t) = \mathbf{A}(t)$) and hence no magnetic field but only an electric field arises from the vector potential:

\[
\begin{align*}
B &= \nabla \times \mathbf{A} = 0, \\
E &= -\frac{d\mathbf{A}}{dt} \neq 0.
\end{align*}
\]

For the case considered in the illustrative calculations, this condition is fulfilled. This approach has already been used to calculate radiative transitions in antiprotonic helium in [11], and further comments on its validity can be found in [13].

1.4 Illustrative calculations

Now the described methods will be applied in the following illustrative calculations. First, a suitable test system is to be chosen. In very light antiprotonic systems the correlation between the electron and antiproton can become very important. The usual "atomic" picture adopted in the previously described approach may not be the best choice in this case. Thus, antiprotonic helium can be successfully treated in a molecular framework (e.g. by means of Born-Oppenheimer approximation, as demonstrated in [12]). In very heavy systems, on the other hand, relativistic effects cannot be neglected. From this considerations, ions in the intermediate region ($Z \sim 20$) seem to present a reasonable test case: The electron-antiproton interaction is much weaker that the interaction of the particles with the nucleus, but at the same time a non-relativistic treatment is still meaningful. Hence, as an example, collisions of antiprotons with hydrogenlike calcium $\text{Ca}^{19+}$ will be investigated. As will be shown later, the decisive quantity for the feasibility of the process is the antiprotonic capture rate into the doubly excited state which is, to a first approximation, independent of $Z$ and so the results obtained can be at least qualitatively generalized to neighboring ions.

In particular, the calculations proceed as follows. First, the Fermi Golden Rule approach is used to estimate how the recombination strength depends on the total angular momentum at which the collision takes place. All further calculations are carried out at fixed angular momentum $L_{\text{max}}$ around which the recombination strength reaches its maximum. In the next subsection, the occuring numerical
difficulties are discussed in more detail and the combination of a B-Splines expansion with complex rotation is tested for convergence in second order perturbation theory calculations for single product states. Then, first estimations for the antiproton emission rates are made by imposing a simplified approach where only a few most important basis configurations are included in the representation of the doubly excited electron-antiproton states, both with Fermi Golden Rule and complex rotation. The results from the full complex rotation calculation (i.e. which includes a large number of configurations) are presented and discussed in subsection 1.4.4, followed by the calculation of the radiative rates. In the last subsection, the obtained results for the rates are used to estimate the recombination strengths and the cross sections for resonant antiproton capture via a few chosen resonances.

1.4.1 Role of angular momentum

To investigate how the total angular momentum influences the recombination strength (1.11), it should be noted that the latter is proportional to $g_dA_m$, i.e. to the antiproton emission rate scaled with the multiplicity of the state which itself is proportional to $2L + 1$. Within the Fermi Golden Rule approach, the transition rate is proportional to the absolute square of the corresponding matrix element. Hence, the following estimation procedure will be adopted: A few matrix elements which are most relevant for the transition of interest will be calculated with the Fermi Golden Rule for different angular momenta $L$ and subsequently scaled with the multiplicity factor $2L + 1$. The angular momentum region at which the resulting quantity has its maximum is then also the region where the highest recombination strength can be expected.

Let us now consider the mentioned matrix elements in more detail. First, the initial and final state in (1.35) have to be specified. In the final state, the electron is in the ground state ($1s$ state) while the antiproton is in a continuum state with some positive energy $\epsilon$. Such a situation can be rather well described by a single product wave function

$$|\psi_f\rangle = |\{1s \epsilon L\}L\rangle. \quad (1.38)$$

In this case, the angular momentum coupling of the two particles is trivial, since the electron is in an $s$-state and hence the angular momentum of the antiproton equals the total angular momentum. The radial parts are all known analytically. The bound states can be expressed in terms of associated Laguerre polynomials (this can be found in almost any book on quantum mechanics or atomic physics, e.g. [44]) and continuum states by means of regular Coulomb wave functions (a very detailed description considering their properties and normalization is given in [45]). The initial doubly excited state, however, cannot be represented that
easily. It can be expanded in the basis (1.28) as
\[ |\psi_i\rangle = \sum_{a,b} c_{ab} |\{n_a l_a n_b l_b\} L\rangle, \quad (1.39) \]
and for a proper representation a large amount of configurations has to be included. However, in the present study the approach can be simplified if one focuses on a particular group of resonances. Thus, for electron excitations from the ground state to \( n = 2 \) states, the minimum quantum number into which the antiproton is captured can be estimated from the Bohr formula to be about \( n_b \approx 49 \). The dominant contribution to the resulting doubly excited states will therefore arise from the following three basis states:
\[ |\phi_1\rangle = |\{2s 49 L\} L\rangle, \quad |\phi_2\rangle = |\{2p 49 L - 1\} L\rangle, \quad |\phi_3\rangle = |\{2p 49 L + 1\} L\rangle. \quad (1.40) \]
Note that the one-particle angular momenta have to be coupled to the total angular momentum, which is indicated by the brackets. The basis state \(|\{2p 49 L\} L\rangle\) has opposite parity and should not be included. Within this approximation, the antiproton emission rate is given by a coherent sum of the products of the following matrix elements (this will be discussed in more detail in subsection 1.4.3):
\[ \langle \psi_f | (r_{12})^{-1} | \phi_i \rangle, \quad i = 1, 2, 3 \quad (1.41) \]
where \((r_{12})^{-1}\) is the Coulomb interaction in atomic units. For their explicit calculation, one can apply the general expression for Coulomb matrix elements between coupled two-particle states [40]
\[ \langle \{n_a l_a n_b l_b\} L|(r_{12})^{-1}|\{n_c l_c n_d l_d\} L\rangle = \sum_{k=0}^{\infty} R_k(-1)^k l_a + l_c + L \left\{ \begin{array}{ccc} l_a & l_b & L \\ l_c & l_d & k \end{array} \right\} \langle l_a| C_k \| l_c \rangle \langle l_b| C_k \| l_d \rangle \quad (1.42) \]
where the standard notation for Wigner 6j-symbols and reduced matrix elements between spherical tensor operators \( C^k \) [40] is used. In our case, the state \( b \) is a continuum state which means that instead of the reduced bound wave function \( P_{n_b} \) a Coulomb function with energy \( \epsilon \) and angular momentum \( l_b \) (denoted by \( F^b_{\epsilon l_b} \)) should be inserted into the two-dimensional radial integral \( R^k \):
\[ R_k = \int \int \overline{d}r_1 \overline{d}r_2 P_{n_b l_b}(r_1) F^b_{\epsilon l_b}(r_2) \frac{r_1^k}{r_1^{k+1}} P_{n_c l_c}(r_1) P_{n_d l_d}(r_2). \quad (1.43) \]
Here, \( r_1 \) and \( r_2 \) denote the larger and smaller of \( r_1 \) and \( r_2 \), respectively (arising from the multipole expansion of the Coulomb interaction, see e.g. [46]). The angular part in (1.42) can, as already mentioned, be evaluated analytically by means
of angular momentum graph theory. The radial integration above is carried out numerically, where the regular Coulomb functions were implemented using Barnett's algorithm [47]. The matrix elements (1.41) were calculated at fixed energy $\epsilon = 4.95 \text{ a.u.} \approx 0.135 \text{ keV}$ for all possible $L$-values and their multiplicity scaled absolute squares were plotted versus $L$. The choice of energy approximately corresponds to the difference between the ground state energy of hydrogenlike calcium ($E_{1s} = -200 \text{ a.u.}$) and the energy position of the considered doubly excited states (around -195 a.u.). However, it should be mentioned that the matrix elements depend on the energy very weakly, so that no high precision is required at this point. The result is shown for the matrix element with $i = 1$ (Eq. (1.41)) in paper 1 (Fig. 2), and very similar behavior was also found for the matrix elements with $i = 2, 3$. The multiplicity scaled absolute squares show a maximum around $L = 12$, which determines the choice of the total angular momentum for the further calculations.

1.4.2 Fermi Golden Rule for single product states - a numerical validation

The previously calculated matrix elements allow us, apart from the study of angular momentum dependence, also to crosscheck the numerical method which is to be used for the full calculation for stability and accuracy. Although the procedure is well tested for purely electronic systems, a numerical validation seems necessary because of the high mass of the antiproton and, therefore, different spatial extensions of the involved one-particle orbitals. The behavior is illustrated in figure 1.1. The fast oscillations of the antiprotonic wave functions also explain the previously discussed high sensitivity of the matrix elements to the angular momentum (cf. Fig. 2 in paper 1). The numerical problem caused by the described behavior is that the difference in scaling is so strong that the antiprotonic and electronic wave functions cannot be represented properly (at least with a reasonable effort) on the same knot sequence. For this reason, a new scheme was applied in the present calculations, where two different knot sequences and two boxes of different size are used. As a test bench of this scheme, the antiproton emission rate for a single product state in second order perturbation theory with complex scaling presents a suitable candidate, because it can be directly compared to the matrix elements (1.41) which are calculated as given in (1.42). Let us consider the matrix element $\langle \psi_j | (r_{12})^{-1} | \phi_i \rangle$ as an example. If the numerical representation is proper, the second order expression must converge towards the analytical Fermi Golden
Figure 1.1: Some relevant reduced radial one-particle wave functions

The upper picture shows the antiprotonic bound state with \( n = 49, l = 12 \) and the antiprotonic continuum state with the energy \( \epsilon = 5 \) a.u. and \( l = 12 \). For comparison, the electronic 1s, 2s and 2p orbitals are also shown (lower picture). The fast oscillations are clearly visible in the upper plot compared to the lower one (note also the different scales on the x-axes). The normalization of the reduced bound states is given by \( \int |P_n(r)|^2 dr = 1 \) and the continuum state is represented by the regular energy normalized Coulomb function (that is, normalized to a delta function in energy space) generated with Barnett’s algorithm [47].
Rule result, i.e. the following equality should hold:

\[
2\pi|\langle \{1s 12\} 12 | \{1s 49 12\} 12 \rangle |^2 = \\
-2 \text{Im} \sum_{i=1}^{N} \frac{\langle \{1s i 12\} 12 | \{2s 49 12\} 12 \rangle^2}{E_{2s}^i + E_{49,12}^i - E_{1s}^i}.
\]

(1.44)

The factor $2\pi$ on the left hand side arises from the energy normalization of the Coulomb functions (this normalization can be formally seen as the density of states $\rho$ in (1.35)) and the energy $\epsilon$ is determined by the on-shell condition

\[
\epsilon = E_{2p}^e + E_{49,12}^\rho - E_{1s}^e = 0.812 \text{ a.u.}
\]

(1.45)

The expression in the brackets on the right hand side gives the energy in second order perturbation theory (this is discussed in several textbooks, e.g. [40]), and hence the width is given by twice the imaginary part of the latter. Note also that complex scaling is imposed and the energies $E_i$ are complex, so that the energy denominator is always different from zero. The sum on the right hand side runs over all antiprotonic states. In particular, a good representation of the continuum is necessary in order to describe the exotic autoionization-like process. This leads us to the main numerical question: How many knot points should be used in the B-Splines expansion and how many configurations need to be included? A convergence study of the expression in (1.44) gives an answer to that. The agreement between the analytical value and the asymptotic value of the sum in (1.44) can be seen as an indicator of how well the wave functions are represented by the B-Splines (i.e. if the used number of knot points $N_k$ is sufficient), while how fast the second order expression converges towards the asymptotic value is a measure of how many states need to be included. This is illustrated in Fig. 3 in paper I, where $N_k = 45$ knot points were used for the electronic wave functions (with a box size of 2.0 a.u.) and $N_k = 325$ knot points for the antiprotonic ones (with a box size of 0.2 a.u.). The electronic knot sequence is linear in the beginning and exponential further out. This is a scheme that is well tested. The knot sequence for the antiproton has to be dense enough to allow a precise description of the oscillating wave function (see Fig. 1.1). The strongest oscillations are found close to the nucleus, while further out the distance between the minima is slowly increasing. The knot sequence is adopted to this situation; the distance between the knots increases slowly with the distance to the nucleus. The maximum number of configurations $N_{\text{max}}$ is limited by $N_k$ and the order $k$ of the B-Splines as $N_{\text{max}} = N_k - k - 2$ (recall that the first and last B-Spline are removed from the set to ensure the boundary condition as discussed in subsection 1.3.2). The figure shows the convergence of the second order expression as a function of the number of included antiprotonic configurations $N$, and, as one can see, sufficient agreement is achieved already at
1.4. Illustrative calculations

\( N \approx 80 - 90 \) (while \( N_{\text{max}} = 316 \) for \( k = 7 \)). Another benchmarking quantity are the numerically calculated one-particle energies which can be compared to the analytical ones. For example, the analytical value of the antiprotonic \( n = 49 \) orbital is \( E = -149.1940989 \) a.u., and the corresponding numerically obtained value is \( E = -149.1940985 \) a.u.. The same convergence study was also performed for the matrix elements \( \langle \psi_f | (r_{12})^{-1} | \phi_2 \rangle \) and \( \langle \psi_f | (r_{12})^{-1} | \phi_3 \rangle \), and the convergence behavior was found to be practically the same as in the example discussed here. In conclusion, one can say that the implemented computational method is rather stable and seems to provide sufficient accuracy.

1.4.3 Extension to a few basis states

Before going over to the full calculation, it is interesting to see whether (and if yes, to what extent) the rather simple approach that was used so far can provide estimates of the true rates. It should be emphasized that the squared matrix elements by themselves, as considered in the previous subsections, do not provide true physical rates because only single product states are calculated rather than a coherent sum, and Eq. (1.44) should rather be seen as a numerical test model. For a more realistic picture, at least a few most contributing basis states should be included. Let us therefore impose a model space that is spanned by the three states (1.40) and approximate the doubly excited states \( |\psi_i\rangle \) by the expansion

\[
|\psi_i\rangle = \sum_{j=1}^{3} c_j |\phi_j\rangle. \tag{1.46}
\]

Within this model, the positions of the resonances and the coefficients in the expansion above are obtained by diagonalizing the full Hamiltonian (1.26) in the basis \( |\phi_i\rangle \). For further simplification, the mass polarization term will be neglected at this point. The diagonal matrix elements of \( H \) are then given by the sum of the one-particle energies and a correction from the Coulomb interaction, given by the relation (1.42), and the off-diagonal elements arise from this correction only (see table 1.1). Hence, the diagonalization will yield three eigenstates (which will be denoted by \( |\psi_I\rangle, |\psi_{II}\rangle, |\psi_{III}\rangle \)) with expansion coefficients \( c_I, c_{II}, c_{III} \). The widths of these resonances are then given by

\[
\Gamma_I = \hbar \left| \sum_{j=1}^{3} c_j^I \langle \psi_f | (r_{12})^{-1} | \phi_j \rangle \right|^2 \quad \text{(and for } \Gamma_{II}, \Gamma_{III} \text{ respectively)}, \tag{1.47}
\]

which is now a coherent sum. However, if we want to compare these rates with those obtained from complex rotation, it is important to account for antiproton
Table 1.1: Matrix elements of the Hamiltonian (1.26) in the model basis. The mass polarization term is neglected here.

\[
\begin{array}{|c|c|c|c|}
\hline
H & |\phi_1\rangle & |\phi_2\rangle & |\phi_3\rangle \\
\hline
(\phi_1) & -195.2041 & 0.5270 & -0.5453 \\
(\phi_2) & 0.5270 & -194.2764 & -0.4573 \\
(\phi_3) & -0.5453 & -0.4573 & -194.2357 \\
\hline
\end{array}
\]

emission only in the latter, because the final state in (1.47) involves the antiprotonic continuum state. Note that the continuum energy is now given by the energy difference between the electronic ground state (at -200 a.u.) and the energy position of the treated resonance. Therefore, at this point only the following configurations are included: To represent the antiprotonic continuum (while the electron is in the ground state) all the configurations of the form \(|1s i 12\rangle\) are taken into account. The index \(i\) runs over the whole antiprotonic spectrum. In addition, also the three basis states \(|\phi_i\rangle\) are included in order to represent the initial state. The widths obtained by such a truncation of the basis in the complex rotation approach should approximately correspond to the Fermi Golden Rule result (1.47). The comparison of the positions and widths calculated with the two methods is given in table 1.2 together with the coefficients from the diagonalization of the Hamiltonian matrix in the model space. As one can see, the positions agree to a

Table 1.2: Expansion coefficients of the resonances in the basis \(|\phi_i\rangle\) and their energy positions and antiproton emission half widths calculated with Fermi Golden Rule (FGR), Eq. (1.47) and complex rotation (CR) within a truncated basis (see text), given in atomic units \((a|b| = a \cdot 10^b)\).

\[
\begin{array}{|c|c|c|c|c|c|c|}
\hline
\text{Set} & c_1 & c_2 & c_3 & E & E_{CR} & \Gamma/2_{\text{FGR}} & \Gamma/2_{\text{CR}} \\
\hline
\text{I} & -0.9164565 & 0.2797662 & -0.2861758 & -195.5352 & -195.5138 & 3.48\times10^{-7} & 1.85\times10^{-7} \\
\text{II} & 0.00343 & 0.72067 & 0.69327 & -194.7138 & -194.7133 & 6.32\times10^{-6} & 8.55\times10^{-6} \\
\text{III} & -0.4000 & -0.63437 & 0.661423 & -193.4671 & -193.4607 & 1.52\times10^{-5} & 2.75\times10^{-5} \\
\hline
\end{array}
\]

rather high accuracy. The situation with the widths, however, is less satisfactory. The first resonance is very narrow, and the two approaches disagree by a factor of about five. Hence, this resonance cannot be resolved properly within the presented simplified framework. The description is apparently better for the second and third resonance. The FGR and CR results are at least of the same order of
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magnitude, but still with a relative deviation of about 30 percent (Res. II) and 60 percent (Res. III). In conclusion, one can say that the rather simple approach presented so far is able to qualitatively describe the main features of the resonances but cannot provide more or less precise quantitative results for the widths. Thus, there is a need for a more elaborated treatment like complex rotation calculations within a large basis. This method is the subject of the next subsection.

1.4.4 Full calculation

The number of the configurations that can be included is, of course, limited by the computational resources. The term "full" simply implies that as many basis states as possible will be used and the obtained results are converged. Strictly speaking, no configuration interaction calculation can be full in its true meaning since all basis sets used in practice are finite. An appropriate truncation of the basis presents therefore a crucial aspect, because one has to keep the balance between sufficient convergence and reasonable computation times. However, in the present computation, an additional challenge arises from the exotic nature of the considered system. If, after introducing complex rotation, the Hamiltonian matrix is diagonalized within the full basis, the obtained widths will be total, i.e. account for antiproton and electron emission. At the same time, to compute the recombination strength as given in Eq. (1.11), the partial widths for antiproton and electron emission are required distinctly. This can be handled by further truncation. If, for example, low lying antiprotonic states are excluded from the basis set, the resonances become virtually stable against Auger electron emission since in this case there are virtually no states into which the antiproton could relaxate by transferring energy to the electron. Similarly, to isolate the channel of electron emission, all configurations that include the electronic 1s state are removed from the basis set. The widths that are obtained within these "artificial" basis sets should approximately give the desired partial widths. To check if this picture is consistent, one can compare the sum of these partial widths with the full one (i.e. the one obtained within the full basis). In case the agreement between those is satisfactory, the approach can be seen as justified.

Basically, the same numerical setup as in the previously tested validative calculations (cf. subsection 1.4.2) was used, with a box size of 0.2 a.u. for the antiprotonic knot sequence with $N_k = 325$ knot points. To represent the electronic orbitals, $N_k = 45$ knot points were distributed in a box of size 2.0 a.u.. The angular symmetries were restricted to \{s, L\} and \{p, L \pm 1\}, under consideration of parity conservation. As before, the maximal number of antiprotonic orbitals is given by $N_{\text{max}} = 316$. Including all of them with all electronic orbitals, however, would yield a matrix size far beyond reasonable dimensions. Therefore, the maximum number of antiprotonic orbitals was included only in combination with the
Figure 1.2: Resonances in Ca\(^{19+}\)\(\bar{p}\)-collisions at fixed angular momentum \(L = 12\)

The figure shows the energy positions of doubly excited electron-antiproton states in the vicinity of the 1s threshold of Ca\(^{19+}\). The numbers to the right indicate the electronic and antiprotonic one-particle orbitals with dominant contribution. Dashed lines denote resonances with \(n_e = 2\) and solid lines those arising from higher electronic orbitals \((n_e = 3, 4)\). The latter ones (arising from the 3-45 and 4-44 configurations) lie very densely and could not be resolved. All energies are given in atomic units.

electronic 1s, 2s and 2p orbitals, while for all other electronic orbitals only 114 antiprotonic ones were included. As evident from subsection 1.4.2 (and a few other convergence tests which are not shown here), this number is sufficient. For this setup, the matrix size is about \(10^4 \times 10^4\) and the full calculation, including the calculation of the matrix elements and subsequent diagonalization, usually can be completed within a real-time of 48 hours per run. The channel isolation, as discussed above, is implemented by removing all antiprotonic orbitals with \(n < 44\) (to "eliminate" electron emission) or, respectively, by excluding all configurations with the electronic 1s state to "eliminate" antiproton emission.

The structure of the resonances near the 1s threshold of Ca\(^{19+}\) is shown in figure 1.2. Two of the resonances that arise from the \(n_e = 2, n_\bar{p} = 48\) configurations lie below the threshold and are, therefore, not of interest for the process considered here. The third resonance in this group is very close to the threshold. Such resonances are known to be very hard to describe numerically, and also in our
Table 1.3: Positions and half widths corresponding to antiproton \( \bar{p} \) and electron emission \( e \) and total half widths of the 2-49-resonances for \( L = 12 \) with and without mass polarization, given in atomic units \( (a[b] = a \cdot 10^b) \). See text for further details.

<table>
<thead>
<tr>
<th></th>
<th>Res. I</th>
<th>Res. II</th>
<th>Res. III</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Position</strong></td>
<td>-195.586</td>
<td>-194.786</td>
<td>-193.628</td>
</tr>
<tr>
<td><strong>Without</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( \Gamma/2(\bar{p}) )</td>
<td>7.3[-7]</td>
<td>8.8[-6]</td>
<td>2.0[-5]</td>
</tr>
<tr>
<td>( \Gamma/2(e) )</td>
<td>4.4[-5]</td>
<td>3.6[-7]</td>
<td>7.7[-6]</td>
</tr>
<tr>
<td>( \sum (\Gamma/2(\bar{p}, e)) )</td>
<td>4.5[-5]</td>
<td>9.2[-6]</td>
<td>2.8[-5]</td>
</tr>
<tr>
<td>( \Gamma/2(\text{total}) )</td>
<td>5.8[-5]</td>
<td>9.5[-6]</td>
<td>3.0[-5]</td>
</tr>
<tr>
<td><strong>With</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( \Gamma/2(\bar{p}) )</td>
<td>-</td>
<td>1.8[-5]</td>
<td>3.7[-5]</td>
</tr>
<tr>
<td>( \Gamma/2(e) )</td>
<td>6.2[-5]</td>
<td>8.5[-7]</td>
<td>1.3[-5]</td>
</tr>
<tr>
<td>( \sum (\Gamma/2(\bar{p}, e)) )</td>
<td>-</td>
<td>1.9[-5]</td>
<td>5.0[-5]</td>
</tr>
<tr>
<td>( \Gamma/2(\text{total}) )</td>
<td>7.8[-5]</td>
<td>1.9[-5]</td>
<td>5.3[-5]</td>
</tr>
</tbody>
</table>

In the case the obtained width cannot be considered reliable. Further resonances are found with dominant contributions from the \( n_e = 3, n_\bar{p} = 45 \) and \( n_e = 4, n_\bar{p} = 44 \) configurations. These lie very densely and are hence not very suitable for our study due to the fact that the adopted isolated resonance approximation for the cross section (cf. Eq. 1.14) is rather questionable in this case. Moreover, if an experimental search for the resonant antiproton capture process is intended, a very important aspect is to control via which resonance the exotic recombination takes place by tuning the antiproton energy (in view of subsequent high precision spectroscopy of the exotic system). Because of that, a very dense region seems not to be the best choice also from an experimental point of view. From these considerations, the resonance group arising from the \( n_e = 2, n_\bar{p} = 49 \) configurations looks like a reasonable candidate: They are not very close to the threshold and their positions are clearly resolved. The characteristics of these resonances are shown in more detail in table 1.3. Unfortunately, in spite of a rather large distance to the threshold \( (\sim 4.5 \text{ a.u.}) \) the partial antiproton emission width of the lowest one still could not be resolved, which indicates that this resonance is probably very narrow.

The two other resonances are broader, and converged results could be obtained for the partial half widths for antiproton \( (\Gamma/2(\bar{p})) \) and electron \( (\Gamma/2(e)) \) emission as well as for the total half widths. Also a comparison between the sum of the partial widths and the total width is shown in the table. As one can see, the agreement is quite good, with a relative deviation of less than seven percent. Hence, we
can conclude that the artificial truncation of the basis set is able to describe the channel isolation to a satisfactory extent. Another aspect visible from the results is the importance of the mass polarization term. The strong deviation of the results with and without the latter clearly indicates its significance. The reason is the large mass of the antiproton, which, even compared to the mass of a rather heavy nucleus, is not negligible.

To conclude, two suitable resonances (at \( E = -194.786 \) a.u., Res. II, and \( E = -193.628 \) a.u., Res. III) were found for which the recombination strengths and cross sections for resonant antiproton capture can be estimated as a test case. The only thing left to do is to calculate the radiative stabilization rates of these resonances, which is carried out in the following subsection.

1.4.5 Radiative transitions

As already briefly mentioned, complex rotation cannot provide radiative transition rates, because the field fluctuations that are responsible for these transitions are not included in the full non-relativistic three-body Hamiltonian (1.26). It should be emphasized that the half widths referred to as "total" in the previous part are only total in the sense that they account for all decay processes that arise from the electron-antiproton interaction. Thus, the Fermi Golden Rule method will be used. For the particular case of dipole transitions between some initial (\( |\psi_i\rangle \)) and final (\( |\psi_f\rangle \)) state, Eq. (1.35) then takes the following form:

\[
A_r = \frac{1}{4\pi \epsilon_0} \frac{4}{3h^4} \left( \frac{\Delta E}{c} \right)^3 |\langle \psi_f|E1|\psi_i\rangle|^2.
\]

(1.48)

Here, \( A_r \) is the radiative rate, \( \Delta E \) the energy difference between the initial and the final state (i.e. it corresponds to the frequency \( \omega \) of the emitted photon as \( \Delta E = \hbar \omega \)), \( c \) the speed of light in vacuum and \( E1 \) the dipole transition operator. If the transition occurs between coupled product states of the form \( |nl n' l' \rangle \rightarrow |nl n' l' \rangle \) (where \( L_i \) and \( L_f \) are the total angular momenta of the initial and final state, respectively), the matrix element in the above equation can be written out explicitly as

\[
A_r = \frac{e^2}{4\pi \epsilon_0} \frac{4}{3h^4} \left( \frac{\Delta E}{c} \right)^3 \left( 2L_f + 1 \right)
\times \left( \int P_{n'l'}(r) P_{n'l}(r) dr \right)^2 \left\{ \frac{L_f}{l'} \frac{1}{l} \frac{L_i}{l'} \right\}^2 \langle l'| \mathcal{C}^1 |l'\rangle^2.
\]

(1.49)

Note that the dipole selection rules are incorporated in the angular part of this expression. In order to apply this formula to the resonances of interest, a similar
1.4. Illustrative calculations

approach as in subsection 1.4.3 will be adopted, i.e. we will exploit the fact that the dominant contribution to the doubly excited states arises from only a few basis states. When the full Hamiltonian is diagonalized within the large basis (as done in the previous part), not only the positions and widths of the resonances but also their expansion coefficients are obtained. Recalling the expansion as given in (1.46), one can check in how far the coefficients that appear in front of the basis states \( \ket{\phi_j} \) as the result of the full calculation are complete by defining a parameter

\[
\delta = 1 - \sum_{j=1}^{3} |c_j|^2. \tag{1.50}
\]

If \( \delta \) is close to zero, the restricted expansion can indeed be seen as a good approximation of the resonances. For the three resonances given in table 1.3, we find \( \delta^I \approx 0.010, \delta^{II} \approx 0.004 \) and \( \delta^{III} \approx 0.010 \) which shows that such an approach is reasonable. The final state will depend on which particle it is that undergoes the transition (cf. Eqs. (1.7,1.8). For example, if we insert the basis state \( \ket{\phi_2} = \{|2p\, 49\, 11\}\, 12 \) as the initial state in (1.49), the possible final states will be \( \ket{\psi_f} = \{|1s\, 49\, 11\}\, 11 \) if the electron undergoes the transition or, for antiprotonic transitions, \( \ket{\psi_f} = \{|2p\, 49 - \Delta n\, 11\, 1\, 1\}\, 12 \pm 1 \) where \( \Delta n \) is the change in the principle quantum number of the antiproton. However, it turns out that the antiprotonic transitions are several orders of magnitude slower than the electronic ones. This can be understood by looking at the expression (1.49). The latter is proportional to \( (\Delta E)^3 \) and to the squared radial integral. On the one hand, transitions with small \( \Delta n \) are suppressed since, in the treated resonances, the antiprotonic principle quantum number is large and the energy difference \( \Delta E \) between the initial and the final state is small compared to the electronic \( 2p - 1s \) transition. On the other hand, if \( \Delta n \) is large, it is the radial integral that is responsible for the suppression of the transition because the initial and final wave function have almost no overlap. This means that the antiprotonic radiative transitions can safely be neglected and it is enough to treat the electronic ones only. As a direct consequence, it follows that no contribution will arise from the basis state \( \ket{\phi_1} \) where the electron is in the \( 2s \) state (due to dipole selection rules). The only possible final states are \( \{|1s\, 49\, 11\}\, 11 \), where the contribution comes from \( \ket{\phi_2} \) only, and \( \{|1s\, 49\, 13\}\, 13 \) with the contribution arising only from the basis state \( \ket{\phi_3} \). Thus, we arrive at the following picture: For each final state there is only one basis state that gives a contribution to the transition. Hence, to determine the distinct rates it is enough to evaluate the expression in (1.49) for the two basis states \( \ket{\phi_{2,3}} \) and the corresponding final state and multiply with the absolute squared expansion coefficient, i.e. no coherent summation, in contrast to Eq. (1.47), is necessary. The total radiative rate can then be approximated by the sum of the partial ones. The rates are shown in table 1.4 together with the absolute squared expansion coeffi-
Table 1.4: Partial half widths for electronic radiative transitions into the final states \(|\{1s\, 49\, 11\}\rangle \) \((\Delta L = -1)\) and \(|\{1s\, 49\, 13\}\rangle \) \((\Delta L = +1)\) and total radiative half widths of the 2-49 resonances from table 1.3, given in atomic units \((a[\text{b}] = a\cdot 10^b)\). The coefficients from the expansion of the doubly excited states correspond to the basis states \(|\phi_1\rangle = |\{2s\, 49\, 12\}\rangle \) \((c1)\), \(|\phi_2\rangle = |\{2p\, 49\, 11\}\rangle \) \((c2)\) and \(|\phi_3\rangle = |\{2p\, 49\, 13\}\rangle \) \((c3)\).

|          | \(|c_1|^2\) | \(|c_2|^2\) | \(|c_3|^2\) | \(\Delta L = -1\) \(\Delta L = +1\) | \(\Gamma_{\text{rad}}^{\text{tot}}/2\) |
|----------|-------------|-------------|-------------|----------------|-----------------|
| Res. I   | 0.83        | 0.08        | 0.08        | 8.5[-5]        | 8.5[-5]         | 1.7[-4]         |
| Res. II  | -           | 0.526       | 0.47        | 5.7[-4]        | 5.1[-4]         | 1.08[-3]        |
| Res. III | 0.16        | 0.39        | 0.44        | 4.3[-4]        | 4.9[-4]         | 9.2[-4]         |

coefficients. As one can see from comparison with table 1.3, the radiative transitions are much faster than the ones arising from the Coulomb interaction. This means that once the antiproton is captured into a doubly excited state, its loss via the inverse autoionization-like process is unlikely, and a stabilization through photoemission (arising from the relaxation of the electron back to the ground state) dominates. Now, with all rates calculated, the recombination strength and cross section can be estimated.

1.4.6 Recombination strength and cross section

An important consequence of the results of the preceding calculations is that, due to the dominance of stabilizing photoemission, the expression for the recombination strength (1.11) can be simplified. To illustrate it more clearly, let us define two dimensionless quantities:

\[
\xi = \frac{\pi^2}{2(\mu/\mu_e) E_{d} - E_{i}} \frac{g_{d}}{g_{i}},
\]

\[
F_s = \frac{A_{\text{stab}}}{A_{\bar{p}} + A_{\text{stab}}},
\]

The first quantity \(\xi\) contains the typical \(\sigma \sim \epsilon^{-1}\) behavior of the recombination cross section as function of collision energy, the multiplicity ratio \(g_{d}/g_{i}\), the formation rate of the doubly excited states (which equals the antiproton emission rate \(A_{\bar{p}}\)) and the electron-antiproton mass ratio. The second quantity \(F_s\) will be called stabilization fraction, since it is given by the ratio of the rates of stabilizing processes to the total decay rate. Comparing with (1.11), we see that the
Figure 1.3: Cross section profile as function of energy

The shown example for Res. II (at $-194.786$ a.u.) is given by a Lorentz profile (1.14) in the isolated resonance approximation and is therefore symmetrically centered around the antiproton energy $\epsilon_\rho = (200 - 194.786)$ a.u. = 5.214 a.u. $\approx 0.14$ keV.

The recombination strength can be written as

$$S_\rho = \frac{\hbar^2}{m_e} \xi F_s$$  \hspace{1cm} (1.53)

with $\hbar^2/m_e = 7.62 \cdot 10^{-16}$ eV cm$^2$. Now, the dominance of the radiative rate simply gives $F_s \approx 1$. This also means that, as long as the radiative rate is much larger than the rate for antiproton emission, the former one does not need to be calculated with very high accuracy (since it cancels in the ratio $F_s$) and it is the slowest rate ($A_\rho$) that is decisive. Hence, the approximate approach that was adopted for the calculation of the radiative rates is justified retrospectively. Also the electron emission rate turns out not to be important because it can be neglected in comparison to the radiative one in $A_{\mathrm{stab}} = A_e + A_{\mathrm{rad}}$. The multiplicity of the initial ion with the electron being in the 1s state is $g_i = 2$ due to spin, while the multiplicity of the doubly excited state $d$ is given by its total angular momentum $L_d = 12$ and four possible spin couplings to $g_d = 4 \cdot (2L_d + 1) = 100$. After inserting the previously calculated rates of the two resonances on which we focus (Res. II and Res. III from table 1.3) in (1.51,1.52), the following recombination strengths
are obtained:
\[ S_{II} = 7.1 \times 10^{-22} \text{ eV cm}^2, \quad S_{III} = 11.7 \times 10^{-22} \text{ eV cm}^2. \] (1.54)

These values are of the same order as found in some DR calculations and experiments (see e.g. [48] \((\text{He}^+)\) or [49] (lithiumlike beryllium)), so that an experimental observation does not look hopeless. The resulting cross section profiles are then given as Lorentz curves by Eq. (1.14). As an example, the one for Res. II is shown in figure 1.3. The maximum value is about a few barn for both resonances \((7.56 \text{ barn} \text{ for Res. II and } 14.06 \text{ barn} \text{ for Res. III})\), showing peaks at 0.14 keV (Res. II) and 0.17 keV (Res. III). Also from this point of view, the present feasibility estimation of a possible experiment is not discouraging. However, the absolute values of the recombination strengths and cross sections alone do not guarantee that the described exotic resonant capture process can be observed. There are further issues, such as interference effects with competing processes, that need to be discussed in this context. Also some comments about the generalization of the illustrative calculations presented here to hydrogenlike ions in different \(Z\)-regions will be given below.

### 1.5 Discussion and summary of the first chapter

To estimate the feasibility of resonant antiproton capture by electron excitation in highly charged hydrogenlike ions, a theoretical approach which is based on the one often used in calculations on dielectronic recombination was adopted. The choice is motivated by the similarity of the processes. The numerical method was tested for stability and convergence with a satisfactory result. Illustrative calculations for a few resonances in hydrogenlike \(\text{Ca}^{19+}\) lead to cross sections of about a few kilobarn in the 0.1-0.2 keV region. The decay rates of the resulting doubly excited electron-antiproton states could be calculated distinctly for the processes of antiproton, electron and photon emission. It was found that the stabilization is dominated by electronic radiative transitions, and consequently, the antiproton emission rate appears to be the decisive quantity for the feasibility of the process. To discuss the obtained results, mainly two questions will be addressed:

1. To what extent can these results be generalized to ions in other charge states?
2. How much do they really tell about the possibility of an experimental observation?

To answer the first question, it should be emphasized that the different decay rates depend on \(Z\) in different ways. The radiative rate scales as \(Z^4\), while the antiproton emission rate is, to a first approximation, independent of the nuclear
charge. Hence, as long as the former one is much larger than the latter, the qualitative picture as found in the example treated here remains valid, that is, a similar behavior can be expected for neighboring ions. However, for significantly lighter systems this may no longer be the case. If the antiproton emission rate and the radiative rate are about the same size, the stabilization fraction $F_s$ (1.52) cannot be approximated by unity, and the pure linear dependence of the recombination strength on the antiproton emission rate is disturbed. Also the correlation between the electron and antiproton and molecular features become more important as $Z$ decreases, so that an application of the approach used in the present work to significantly lighter systems is rather questionable. Much heavier systems, however, cannot be treated non-relativistically even approximately. Moreover, QED effects have to be considered. For the element we chose to study here, they play a role but should not be crucial ($Z\alpha \approx 0.146$ for calcium). Also $LS$-coupling of angular momenta can be adopted. This approach breaks down for high $Z$. To conclude, the presented approach is meaningful in the intermediate $Z$ region.

The second question is a little bit more speculative. As already mentioned, the estimated absolute values for the recombination strengths and cross sections are sufficient from an experimental point of view. Nevertheless, an experimental observation is not guaranteed: If competing processes of larger probability are present, the resonant process will vanish in the background. Such a competing process can arise from non-resonant capture of antiprotons by ions where the initially bound electron is scattered into the continuum, as schematically given in (1.1). Theoretical calculations of the cross sections for this process were carried out in Refs. [28, 29] for collisions of antiprotons with $\text{He}^+$ and in [27] for several singly charged ions. The cross sections in the center of mass energy region of about 1 a.u. are of the order of $a_0^2$ (where $a_0$ is the Bohr radius), that is, a few Mbarn, which is much larger than the cross sections presented here. However, the cross sections from Refs. [27–29] are total (i.e. summed over all angular momenta and antiprotonic final states) while in the present calculations the cross sections are partial, in other words, only one specific final quantum state at fixed angular momentum is considered. Therefore, it is not clear which process (resonant or not) will dominate the formation of the exotic system. Ref. [28] also estimates that the resonant process should give a significant contribution, but the latter can possibly arise from an overlap of many resonances in an energy region where they lie very densely. Such a region is not suitable if the aim is to control the state into which the antiproton is captured, which is another reason to focus on highly charged ions since the energy difference between different $n$-manifolds is larger. Another aspect that should be mentioned in this context is the possible interference between the resonant and non-resonant processes. Strictly speaking, this interference can arise if the initial and final state for both processes are the same. This is the case if, in
the resonant process, the doubly excited state decays by electron emission (1.10). For all other decay channels, the system ends up in a different charge state than in the non-resonant case. However, recalling that the decay of the resonances treated here is dominated by radiative transitions such interference effects do not seem very likely. The situation can, of course, be different for resonances where autoionizing processes are equally important as photoemission.

Summing up, we may say that from the theoretical estimations presented here the exotic DR-like process with antiprotons does not seem to be completely out of reach, but possible interference effects with non-resonant processes need to be studied more thoroughly for a definite conclusion.
Chapter 2

Open system approach to resonances

2.1 Introduction

The time evolution of a non-relativistic quantum system is completely governed by the fundamental Schrödinger equation. In the Schrödinger picture, its solution provides the wave function of the system for all times, from which expectation values of the observables can be determined. Alternatively, the dynamics can also be formulated in the Heisenberg picture with time-dependent operators and time-independent wave functions. As is well known, these pictures are equivalent in the sense that for any physical observable they yield the same results. If the Hamiltonian $H$ of the system is time-independent and Hermitian, the time evolution of a quantum state $|\psi\rangle$ from some initial time $t_0$ to a time $t$ is given by the operator

$$U_{t,t_0} = \exp(-iH(t - t_0)/\hbar)$$

(2.1)

as

$$|\psi\rangle(t) = U_{t,t_0}|\psi\rangle(t_0)$$

(2.2)

in the Schrödinger picture, and, equivalently, for an operator $A$ in the Heisenberg picture:

$$A(t) = U_{t,t_0}^\dagger A(t_0) U_{t,t_0}.$$  

(2.3)

The operator $U$ is unitary (i.e. $UU^\dagger = U^\dagger U = 1$) and hence it preserves the fundamental properties of a quantum system, like commutators or expectation values. Speaking more formally, the operators $U_t$ as defined in (2.1) ($t_0$ is set to 0 for simplicity here and in the following) build a group in the algebraic sense where $t$ is the group parameter and $H$ the generator. In particular, $t$ can take any real value from $-\infty$ to $+\infty$ and hence the considered quantum system can be propagated in time not only forwards but also backwards, in other words, for any time $t$ the future and the past can be obtained equivalently. Such systems,
where the Hamiltonian is a constant of motion (and hence the expectation value of the total energy is conserved) are referred to as closed. This picture is, although theoretically crucial, not fully realistic, because any kind of dissipative interaction of the quantum system with its environment is excluded per definition. Let us consider a macroscopic example as an illustration: If a body loses kinetic energy due to friction and heats up the environment, the process is irreversible in time, because there is no way that the environment cools down and accelerates the body. On a quantum scale, it means that a unitary group cannot describe irreversible quantum dissipation due to the incorporated reversibility condition (i.e. that the group parameter can take any real value). Therefore, a modification of the time evolution for the description of open quantum systems is necessary.

A widely used approach to open quantum systems are master equations, that is, equations governing the time evolution of the density matrix $\rho$ of the system. They are of the general form

$$\frac{d\rho}{dt} = \mathcal{L}(\rho)$$

(2.4)

where $\mathcal{L}$ is called the Liouville operator (or sometimes superoperator because it acts on density matrices). For example, the most simple Liouville operator is the particular case of a closed system

$$\mathcal{L}(\rho) = -\frac{i}{\hbar}[H, \rho].$$

(2.5)

This is exactly the von Neumann equation which is the equivalent of the Schrödinger equation if the description of the quantum system is formulated with a density matrix instead of a wave function. However, for an open quantum system it may be very non-trivial (or even impossible!) to determine the exact form of the Liouville operator. An illustrative and rather fundamental problem which was thoroughly studied in this context is the quantum damped harmonic oscillator interacting with the environment. In a rigorous treatment, it can be shown that for arbitrary environments no exact Liouville operator exists [50], but, under certain assumptions, approximate forms can be found. In the weak coupling limit, the most general form of a master equation was found and proven by Lindblad [51] in the 1970s. It will be discussed in detail in the next section. To mention the main idea only briefly, the von Neumann equation is modified by an additional term which contains operators that simulate the dissipative interaction with the environment (usually called Lindblad operators). A problem which often arises if master equations of this type are used is that the explicit form of these operators can be chosen freely, and the approach becomes heuristic. Even if appropriate Lindblad operators can be found, there are still phenomenological constants in the equations of motion for which numerical values are needed. It is, however, not clear in general how the latter ones can be obtained.
These problems motivated the present study. In many physical applications, the dissipative effects are far too complex to be treated in detail, and the phenomenological constants have to be fitted either to experimental data or independent theoretical calculations. As an example where the Lindblad equation is often used one can mention heavy ion collisions and non-equilibrium nuclear processes, where dissipation arises from the excitation of the internal degrees of freedom (i.e. the nucleons) [52–57]. However, if the open system is simple enough to be treated \textit{ab initio}, one can compare the phenomenological approach with the true dynamics to obtain information about the phenomenological constants. For this purpose, systems containing resonances seem to be a suitable candidate: The dissipative nature arises due to the coupling to the continuum, and there exists a number of reliable methods to determine the time evolution as well as the positions and widths of the resonances [58, 59]. Furthermore, since the decay of a resonance is driven by its width and, in the Lindblad case, by the magnitude of the phenomenological constants, one can expect these quantities to be related to each other. The outline of this part of the thesis is the following: First, the Lindblad equation will be discussed in detail (section 2.2). The fundamental problem of the damped quantum oscillator in its framework will be treated (section 2.3), covering the choice of Lindblad operators, the derivation of the equations of motions for the first and second moments and their solution as well as a brief discussion of the emerging phenomenological constants. Then, a suitable model potential for our study is suggested. The potential is required to coincide with a harmonic oscillator potential in the region where the comparison of the Lindblad dynamics to the true dynamics is made, but it should also contain resonances at the same time. The positions and widths of the latter ones are then calculated with the method of complex rotation, which was already introduced in the first part. Finally, the time evolution in the model potential is compared to the one given by the Lindblad equation, from which a relation between the phenomenological constants and the widths of the present resonances can be suggested. The applicability of the adopted approach, restrictions and limitations are discussed at the end.
2.2 The Lindblad master equation

2.2.1 Physical motivation

The previously introduced concept of open quantum systems has become more and more important in the last two decades. Nowadays, relevant examples in almost all areas of physics can be found, in the low energy range (e.g. in surface [60,61] and atomic [62–64] physics) as well as at higher energies, like in the previously mentioned applications in heavy ion physics and even in particle physics [65,66]. Also general physical effects like tunneling [67,68] or decoherence [69–75] are often studied in this framework. Especially in quantum information theory, master equations for open quantum systems present a very important tool, because they allow to treat crucial effects like dephasing and entanglement of qubits [76, 77]. But which properties do we expect from a master equation from a physical point of view, or, more formally, what are the physical restrictions if we are looking for a modified Liouville operator in (2.4) which is different from the von Neumann form (2.5)? First of all, the new time evolution \( \Phi_{t_1,t_0} \) (which replaces the unitary time evolution \( U_{t,t_0} \) (2.1) in closed systems) should obey the property

\[
\Phi_{t_1,t_0} \Phi_{t_2,t_1} = \Phi_{t_2,t_0},
\]

(2.6)

that is, if the system evolves in time from \( t_0 \) to \( t_1 \) and then from \( t_1 \) to \( t_2 \) it should end up in the same state as if it were directly propagated from \( t_0 \) to \( t_2 \). At the same time, \( \Phi \) should be irreversible in order to account for dissipation, in other words, the system is not allowed to propagate backwards in time. Furthermore, the Liouville operator should preserve all physically necessary conditions of a density matrix, such as hermicity, non-negativity and \( \text{Tr}(\rho) = 1 \). As one can imagine, to unify all these properties mathematically is a very non-trivial task. An explicit form of such a Liouville operator was found and proven by Lindblad [51], mathematically based on the theory of completely positive mappings and dynamical semigroups. This very formal treatment cannot be discussed here, and only a few most important aspects will be given below without any proof together with the main result, i.e. the explicit form of the Lindblad master equation.

2.2.2 Explicit form and validity

The reversibility of the time evolution in closed systems arises formally from the group condition \( t \in (-\infty, +\infty) \) for \( U_{t,t_0} \). Thus, this condition needs necessarily to be abandoned if one wants to introduce time irreversibility, but simultaneously the physically important properties of the density matrix (as previously mentioned) should be preserved. There exists, in fact, an algebraic structure that fulfills these conditions, namely so called dynamical semigroups. Without discussing the
mathematics behind, the decisive aspect is that if the time evolution is chosen to be a semigroup $\Phi_{t,t_0}$ with a real parameter $t$, the latter one is allowed to take positive values only (if we set $t_0 = 0$). This is often referred to as the semigroup condition. Physically speaking, a preferred direction in time is introduced and hence the system can evolve only forwards in time - exactly the property required in dissipative systems. Also the hermicity, the non-negativity and the trace of the density matrix are conserved under semigroup transformations. The next question is how the generator of such semigroups (i.e. the Liouville operator) looks like. The explicit most general form proven by Lindblad is the following:

$$L(\rho) = -i \frac{\hbar}{\hbar} [H, \rho] + \frac{1}{2\hbar} \sum_j \left( [V_j \rho, V_j^\dagger] + [V_j^\dagger, \rho V_j^\dagger] \right). \quad (2.7)$$

The first term is the same as in the von Neumann equation for closed systems. The second term accounts for dissipative interaction with an environment and contains a set of Lindblad operators $V_j$. These operators can be chosen freely and act on the Hilbert space of the Hamiltonian. Such an approach is often called reduced dynamics, because the system described by the Hamiltonian is virtually coupled to a reservoir via the Lindblad operators, but the resulting equations of motion describe only the dynamics of this reduced system and not the one of the reservoir. An important assumption which is incorporated in the master equation is weak coupling of the reduced system to the reservoir. The relaxation times of the latter have to be much shorter than the typical timescale of the reduced system (i.e. the reservoir is assumed to be very large compared to the subsystem). This also means that no memory effects occur, and hence Eq. (2.7) presents a Markovian master equation. Its general character is also confirmed by the fact that several master equations that are found in literature are particular cases of the Lindblad form, as shown in [78]. It can be equivalently formulated in the Heisenberg picture for a time-dependent operator $A$, which is often a more convenient approach in practical applications:

$$\frac{dA}{dt} = i \frac{\hbar}{\hbar} [H, A] + \frac{1}{2\hbar} \sum_j \left( V_j^\dagger [A, V_j] + [V_j^\dagger, A] V_j \right). \quad (2.8)$$

In the next section, this equation will be explicitly solved for a harmonic oscillator Hamiltonian. This special case is of particular interest, not only for the present study but also from a fundamental point of view, since it allows to investigate several properties of open quantum systems in a more general context.
2.3 Lindblad-type equations of motion for a harmonic oscillator

2.3.1 Derivation

The first thing that has to be specified in applications of the Lindblad equation to any physical problem is the explicit form (and number) of the Lindblad operators $V_j$. Qualitatively, a similar choice has to be made also in classical mechanics, where different types of dissipative effects can occur, e.g. the friction can depend linearly (Stokes-friction) or quadratically (Newton-friction) on the velocity. Here, the Lindblad operators will be chosen as a linear combination of the coordinate and momentum operators

$$V_j = a_j p + b_j q$$

(2.9)

where $a_j$ and $b_j$ are complex numbers (hence $V_j^\dagger = a_j^\ast p + b_j^\ast q$ since $p$ and $q$ are Hermitian operators). This choice is sometimes referred to as the quantum mechanical analogue of Hook's law and has the big advantage that the equations of motion for a harmonic oscillator are solvable exactly (similarly to classical mechanics where a friction term proportional to the velocity is the easiest and most convenient choice). To the best knowledge of the author, the form (2.9) is the only one ever used for a harmonic oscillator. The number of the Lindblad operators follows in this case directly from their form, because the operators $\{p, q\}$ give a basis of the linear space of first-order non-commuting polynomials and, therefore, only two linearly independent combinations of $p$ and $q$ can be constructed, i.e. $j = 1, 2$ in (2.9).

Let us now consider the time dependence of the expectation values of the canonical operators $p$ and $q$ (denoted by $\sigma_p$, $\sigma_q$) for a harmonic oscillator Hamiltonian

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2$$

(2.10)

with mass $m$ and frequency $\omega$. They are given by the trace of the product of the density matrix with the corresponding operator

$$\sigma_q = \text{Tr}(\rho q), \quad \sigma_p = \text{Tr}(\rho p).$$

(2.11)

Therefore, the time dependence in the Heisenberg picture is

$$\frac{d}{dt} \sigma_A(t) = \frac{d}{dt} \text{Tr}(\rho A) = \text{Tr} \left( \rho \frac{dA}{dt} \right), \quad (A = p, q)$$

(2.12)

where $dA/dt$ in the last term is now given by Eq. (2.8). This means that, to obtain the equations of motion, one has to insert $A = p$ and $A = q$ together with the
Lindblad operators from (2.9) into (2.8) and calculate all appearing commutators. Using the fundamental relation

\[ [q, p] = i\hbar, \]

(2.13)

they are evaluated as

\[
\begin{align*}
[H, q] &= -\frac{i\hbar}{m}p, \\
[H, p] &= i\hbar m\omega^2 q, \\
[V_j^\dagger, q]V_j &= i\hbar (|a_j|^2 p + a_j^* b_j q), \\
[V_j^\dagger, q]V_j &= -i\hbar (|a_j|^2 p + a_j^* b_j q), \\
[V_j^\dagger, p]V_j &= -i\hbar (a_j^* b_j p + |b_j|^2 q), \\
[V_j^\dagger, p]V_j &= i\hbar (a_j^* b_j^* p + |b_j|^2 q).
\end{align*}
\]

(2.14)

To write the expressions which involve the Lindblad operators in a more compact form, one can define a phenomenological friction constant

\[ \lambda = -\text{Im} \sum_{j=1}^{2} a_j^* b_j \]

(2.15)

so that the second term in (2.8) for \( A = q, p \) reads

\[
\sum_{j=1}^{2} \left( V_j^\dagger [q, V_j] + [V_j^\dagger, q]V_j \right) = -2\hbar \lambda q, \]

(2.16)

\[
\sum_{j=1}^{2} \left( V_j^\dagger [p, V_j] + [V_j^\dagger, p]V_j \right) = -2\hbar \lambda p. \]

(2.17)

Combining this with the commutators \([H, q]\) and \([H, p]\) from (2.14) and inserting the result into (2.12) yields the following coupled first-order differential equations for the expectation values of \( q \) and \( p \):

\[
\begin{align*}
\frac{d}{dt} \sigma_q(t) &= -\lambda \sigma_q(t) + \frac{1}{m} \sigma_p(t), \\
\frac{d}{dt} \sigma_p(t) &= -m\omega^2 \sigma_q(t) - \lambda \sigma_p(t).
\end{align*}
\]

(2.18)

(2.19)

However, for a complete description of the dynamics of a quantum system not only the first moments (expectation values) but also the second moments (variances and
covariances) are required. For two operators \( A, B \) the second moments are defined as

\[
\sigma_{AB} = \sigma_{BA} = \frac{1}{2} \text{Tr}(\rho(AB + BA)) - \text{Tr}(\rho A) \text{Tr}(\rho B).
\]  

(2.20)

If \( A = B \) then \( \sigma_{AA} \) is the variance of the operator \( A \), while for different operators \( \sigma_{AB} \) gives their covariance. The derivation of their time dependence is basically the same as for the first moments, the only difference being that instead of the operators \( q \) and \( p \) the operator products \( q^2 \), \( p^2 \) and \( pq \) are inserted into (2.8) and the commutators that have to be evaluated become a little bit more lengthy. To keep this part within reasonable boundaries, the explicit derivation will not be given here step-by-step. After the operator products are inserted into (2.8), their time dependence is obtained from (2.12) as

\[
\begin{align*}
\frac{d}{dt} \sigma_{qq}(t) & = -2\lambda \sigma_{qq}(t) + \frac{2}{m} \sigma_{pq}(t) + 2D_{qq}, \\
\frac{d}{dt} \sigma_{pp}(t) & = -2\lambda \sigma_{pp}(t) - 2m\omega^2 \sigma_{pq}(t) + 2D_{pp}, \\
\frac{d}{dt} \sigma_{pq}(t) & = -2\lambda \sigma_{pq}(t) - m\omega^2 \sigma_{qq}(t) + \frac{1}{m} \sigma_{pp}(t) + 2D_{pq}
\end{align*}
\]

(2.21)

where further abbreviations were introduced:

\[
D_{qq} = \frac{\hbar}{2} \sum_{j=1}^{2} |a_j|^2, \quad D_{pp} = \frac{\hbar}{2} \sum_{j=1}^{2} |b_j|^2, \quad D_{pq} = -\frac{\hbar}{2} \text{Re} \sum_{j=1}^{2} a_j^* b_j.
\]  

(2.22)

The constants defined above are called diffusion coefficients. They can play a decisive role in the dynamics of open systems, being directly related to preservation of crucial concepts such as the uncertainty relation or non-negativity of the density matrix, as will be discussed in more detail at a later point. The three coupled differential equations (2.21) can also be written in matrix form, which is convenient for their solution. By defining the matrices

\[
\sigma(t) = \begin{pmatrix} \sigma_{qq}(t) & \sigma_{pq}(t) \\ \sigma_{pq}(t) & \sigma_{pp}(t) \end{pmatrix}, \quad Y = \begin{pmatrix} -\lambda & 1/m \\ -m\omega^2 & -\lambda \end{pmatrix}, \quad D = \begin{pmatrix} D_{qq} & D_{pq} \\ D_{pq} & D_{pp} \end{pmatrix},
\]

(2.23)

an equivalent form of (2.21) is given by

\[
\frac{d}{dt} \sigma(t) = Y \sigma(t) + \sigma(t)Y^T + 2D.
\]  

(2.24)

With this and Eqs. (2.18), (2.19) the equations of motion are completed, and their solution is the next task to be accomplished. It should be mentioned that the presented derivation and the following solution of the above equations of motion was first introduced in Ref. [79] for the description of damping in deep inelastic collisions.
2.3.2 Solution

Let us first approach the equations of motion for the expectation values (2.18), (2.19). In general, two cases have to be considered, namely overdamped ($\lambda > \omega$) and underdamped ($\lambda < \omega$). As will be shown, only the second case is relevant for our study and hence the assumption $\lambda < \omega$ is made throughout. Since we are dealing with two first-order differential equations, two boundary conditions are required for a unique solution, that is, the initial values $\sigma_q^0 = \sigma_q(t = 0)$ and $\sigma_p^0 = \sigma_p(t = 0)$. Given those, the solutions can then be written in closed analytical form, which can be verified by simply inserting into the initial differential equation:

$$
\sigma_q(t) = e^{-\lambda t} \left( \cos(\omega t)\sigma_q^0 + \frac{1}{m\omega} \sin(\omega t)\sigma_p^0 \right), \quad (2.25)
$$

$$
\sigma_p(t) = e^{-\lambda t} \left( -m\omega \sin(\omega t)\sigma_q^0 + \cos(\omega t)\sigma_p^0 \right). \quad (2.26)
$$

As we see, the average momentum and position oscillate with the frequency $\omega$ around zero, and the amplitude decreases exponentially in time where $\lambda$ is the damping constant. This picture is very similar to the one known from classical mechanics and shows that the choice of the Lindblad operators was indeed meaningful.

The solution of the equations of motion for the second moments can also be found analytically by making the following ansatz for the matrix equation (2.24):

$$
\sigma(t) = e^{tY} \left( \sigma^0 - \sigma^\infty \right) \left( e^{tY} \right)^T + \sigma^\infty. \quad (2.27)
$$

Here, $\sigma^0$ denotes the initial covariance matrix (i.e. it contains the values $\sigma_{qq}(t = 0)$, $\sigma_{pp}(t = 0)$ and $\sigma_{pq}(t = 0)$) and $\sigma^\infty$ its asymptote. The matrix $e^{tY}$ is found by diagonalizing $Y$:

$$
e^{tY} = e^{-\lambda t} \left( \begin{array}{cc}
\cos(\omega t) & \frac{1}{m\omega} \sin(\omega t) \\
-m\omega \sin(\omega t) & \cos(\omega t)
\end{array} \right). \quad (2.28)
$$

The asymptotic values $\sigma_{qq}(\infty)$, $\sigma_{pp}(\infty)$ and $\sigma_{pq}(\infty)$ can be determined from the diffusion coefficients if the ansatz (2.27) is inserted back into the differential equation (2.24), which leads to the condition

$$
Y \sigma^\infty + \sigma^\infty Y^T = -2D. \quad (2.29)
$$

Now, both sides of the above equation are symmetrical $2 \times 2$ matrices and hence it can be rewritten as a system of three linear equations for the elements of $\sigma^\infty$. By explicitly writing out the sum of the matrix products on the left hand side, we arrive at

$$
\begin{pmatrix}
D_{qq} \\
D_{pp} \\
D_{pq}
\end{pmatrix} = \begin{pmatrix}
\lambda & 0 & -\frac{1}{m} \\
0 & \lambda & m\omega^2 \\
\frac{m\omega^2}{2} & -\frac{1}{2m} & \lambda
\end{pmatrix} \begin{pmatrix}
\sigma_{qq}(\infty) \\
\sigma_{pp}(\infty) \\
\sigma_{pq}(\infty)
\end{pmatrix} \quad (2.30)
$$
which can be solved for the elements of $\sigma^\infty$:

$$\sigma_{qq}(\infty) = \frac{(m\omega)^2(2\lambda^2 + \omega^2)D_{qq} + \omega^2D_{pp} + 2m\omega^2\lambda D_{pq}}{2(m\omega)^2\lambda(\lambda^2 + \omega^2)},$$

$$\sigma_{pp}(\infty) = \frac{(m\omega)^2\omega^2D_{qq} + (2\lambda^2 + \omega^2)D_{pp} - 2m\omega^2\lambda D_{pq}}{2\lambda(\lambda^2 + \omega^2)},$$

$$\sigma_{pq}(\infty) = \frac{-\lambda(m\omega)^2D_{qq} + \lambda D_{pp} + 2m\lambda^2 D_{pq}}{2m\lambda(\lambda^2 + \omega^2)},$$

(2.31)

So far, it was assumed that the phenomenological diffusion coefficients defined in (2.22) are explicitly known. However, a proper choice of the latter is a very fundamental problem in quantum diffusion equations, and there is a considerable amount of papers in which their influence on the dynamics and conditions that have to be imposed on them were thoroughly studied [55, 80-82]. Thus, only a very brief discussion will be given here.

The definitions of the phenomenological friction constant (2.15) and the diffusion coefficients (2.22) directly imply the conditions

$$D_{qq} > 0, \quad D_{pp} > 0, \quad D_{qq}D_{pp} - D_{pq}^2 \geq \lambda^2\hbar^2/4,$$

(2.32)

where the last condition follows from the Cauchy-Schwarz inequality. Apart from their mathematical necessity, these conditions also contain a deep physical meaning. In fact, it can be shown that the non-negativity of the density matrix is preserved for all times only if these fundamental constraints are satisfied. They are also closely related to the generalized uncertainty relation (given by the determinant of the matrix $\sigma(t)$ defined in (2.23)) which for any time $t$ reads

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

(2.33)

A set of diffusion coefficients that obeys (2.32) is often called 'quantum mechanical'. Also master equations with diffusion coefficients that do not fulfill the constraint have been used. Such diffusion coefficients are usually referred to as 'classical' because the quantum nature of the system is violated. Nevertheless, physically meaningful results can be extracted also from such diffusion coefficients under certain conditions. A rather common (though, as pointed out in Ref. [72], somewhat contradictory) approach to determine the diffusion coefficients is to postulate an asymptotic state, i.e. the asymptotic variances and covariances become an input parameter and the diffusion coefficients are determined from the latter. For example, if a harmonic oscillator coupled to a reservoir at some thermodynamical temperature $T$ is assumed to approach an asymptotic Gibbs state

$$\rho(\infty) = \frac{e^{-H/k_B T}}{\text{Tr}(e^{-H/k_B T})},$$

(2.34)
where $k_B$ is the Boltzmann constant, the temperature dependent diffusion coefficients are

\[
\begin{align*}
D_{qq} & = \frac{\hbar \lambda}{2m\omega} \coth \left( \frac{\hbar \omega}{2k_B T} \right), \\
D_{pp} & = \frac{\hbar \lambda m \omega}{2} \coth \left( \frac{\hbar \omega}{2k_B T} \right), \\
D_{pq} & = 0.
\end{align*}
\]

In the high temperature limit, these expressions simplify to

\[
D_{qq} = \frac{\lambda k_B T}{m \omega^2}, \quad D_{pp} = m k_B T \lambda, \quad D_{pq} = 0.
\] (2.36)

In the limit $T \to 0$, however, the diffusion coefficients do not depend on temperature:

\[
D_{qq} = \frac{\hbar \lambda}{2m\omega}, \quad D_{pp} = \frac{1}{2} \hbar \lambda m \omega, \quad D_{pq} = 0.
\] (2.37)

Moreover, the last set of coefficients has the advantage that it is fully determined by the phenomenological friction constant $\lambda$ (note that the fundamental constraint (2.32) is fulfilled) and is, therefore, very well suited for the investigation intended here. After inserting this set into (2.31), the asymptotic variances and covariance simplify to

\[
\begin{align*}
\sigma_{qq}(\infty) & = \frac{\hbar}{2m\omega}, \\
\sigma_{pp}(\infty) & = \frac{\hbar m \omega}{2}, \\
\sigma_{pq}(\infty) & = 0.
\end{align*}
\] (2.38)

As we see, the asymptotic state has 'minimal uncertainty', i.e. the generalized uncertainty relation (2.33) becomes an equality:

\[
\sigma_{qq}(\infty) \sigma_{pp}(\infty) - \sigma_{pq}^2(\infty) = \hbar^2/4.
\] (2.39)

There is much more that could be said about the role and different choices of diffusion coefficients. This discussion, however, is beyond the scope of this thesis, and more details can be found in the previously mentioned references. To sum up, the solutions (2.25), (2.26), (2.27) completely determine the dynamics of the system considered here, and with the chosen set of diffusion coefficients (2.37), $\lambda$ is the only phenomenological constant that the dynamics contains.
2.4 The model potential

2.4.1 Required conditions

As just shown, the Lindblad equation for the harmonic oscillator is exactly analytically solvable. This is a big advantage which can be exploited. If we consider a model potential which, in a certain region, coincides with a harmonic oscillator but also contains resonances, the following picture can be adopted: The time evolution of, for example, an initial Gaussian wave packet in this model potential can be numerically calculated \textit{ab initio}, i.e. by solving the time dependent Schrödinger equation, and compared to reduced Lindblad dynamics for a harmonic oscillator within the region where both potentials coincide. The crucial point is that, in the Lindblad case, a harmonic oscillator potential can be used because the dissipative effect of resonances is virtually accounted for by Lindblad operators, that is, simply by the fact that the time evolution is governed by the Lindblad equation. From this comparison, information about the emerging phenomenological constants can be extracted. Thus, the model potential has to fulfill the following conditions:

- It has to coincide with a harmonic oscillator potential in a certain region
- Resonances need to be present
- It should be given as a closed analytical expression

The last requirement is necessary if one wants to work with B-Splines and complex rotation in order to determine the positions of bound and resonant states and the widths of the latter. A model potential which satisfies the conditions listed above can be implemented by multiplying a harmonic oscillator potential with a smooth exponential cutoff which leads to a barrier:

\[ U_m(q) = U_h(q) \left( 1 - \frac{1}{1 + \exp(-(q - q_B)/\tau)} \right) \]

(2.40)

where

\[ U_h(q) = \frac{1}{2} m \omega^2 (q - q_0)^2 - U_0. \]

(2.41)

The parameter \( \tau \) 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 gives approximately the position of the barrier). The constant shift in coordinate \( (q_0) \) and energy \( (U_0) \) is just a trivial coordinate transformation which does not influence the equations of motion and was introduced simply for convenience. For a better illustration, the model potential is shown in figure 2.1 together with a harmonic oscillator potential. The region in which the comparison of the dynamics is to be made is given by \( q \leq q_B \). For this purpose, the physical states (bound and resonant) of the model potential have to be determined.
Figure 2.1: Model potential vs. harmonic oscillator potential

The model potential $U_m$ (2.40) (solid line) shown together with a harmonic oscillator potential $U_h$ (2.41) (dashed line) for $m = 1.0$, $\omega = 3.9$, $q_0 = 1.833$, $q_B = 3.35$, $U_0 = 7.0$, $\tau = 0.19$ (all quantities are given in atomic units).

2.4.2 Determination of bound and resonant states

The basic procedure of combining complex rotation with a B-Splines representation was already described in the first part of the thesis. It can be applied to the model Hamiltonian

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

(2.42)

in exactly the same way as to the Coulomb Hamiltonian, the only difference being that the model potential cannot be represented as a finite power series (1.17) in $q$. Still, complex rotation can be implemented but instead of simply multiplying the potential terms proportional to $q^n$ in the Hamiltonian matrix with $\exp(i\theta)$ (which was possible for the Coulomb Hamiltonian) one can compute the real and imaginary parts of the complex rotated potential $U_m(q\exp(i\theta))$ and multiply the imaginary part with $i$ when setting up the complex symmetric Hamiltonian matrix. The latter one is then diagonalized to yield the desired eigenvalues, which are shown in table 2.1 for the parameters as listed in the caption of figure 2.1. The two bound states lie close to the analytically known positions of an ideal harmonic oscillator and their distance approximately equals $\hbar\omega$: $E_1 = \hbar\omega/2 - U_0 = -5.05$, $E_2 = 3\hbar\omega/2 - U_0 = -1.15$, $\Delta E = 3.89$, $\hbar\omega = 3.9$ (here and in the following atomic units are used). 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. If one considers a wave packet centered in the region $0 < q < q_B$ in the model potential with a rather low energy expectation value (i.e. the overlap with the bound states is high), then the dissipative interaction arising from the tunneling of the high-energy components through the barrier will be dominated by the lowest resonance only, and one can expect the contribution from the second resonance, which lies above the barrier, to be very small (this will be also verified explicitly at a later point). Hence already the second resonance is not relevant for the present study. For this reason, further resonances that were found at even higher energies are not listed in the table.

### 2.5 Comparison of the dynamics

Let us now consider a typical Gaussian one-dimensional wave packet of the form

$$
\psi(q, t = 0) = \frac{1}{(2\pi\sigma_{qq}^0)^{1/4}} \exp \left( -\frac{1}{4\sigma_{qq}^0}(q - \sigma_q^0)^2 + \frac{i}{\hbar} \frac{\sigma_p^0}{2} \right) \tag{2.43}
$$

as the initial state. In the coordinate representation given above, $\sigma_q^0$ gives the position around which the wave packet is centered (i.e. it is the coordinate expectation value) and, similarly, $\sigma_p^0$ is the momentum expectation value. The initial spread in position space, $\sigma_{qq}^0$, also determines the initial spread in momentum space, $\sigma_{pp}^0$, as

$$
\sigma_{pp}^0 = \hbar^2 / (4\sigma_{qq}^0), \tag{2.44}
$$

which can be easily shown by means of a Fourier transformation. The idea is to propagate this wave packet in time in two ways, in the model potential using the Schrödinger equation and in the harmonic oscillator potential using the Lindblad equation. In the latter case, however, it is actually enough to propagate the probability density $|\psi(q)|^2$ (or $|\psi(p)|^2$, respectively) in order to extract information about the observables. This is due to the fact that, as is well known, in a potential

<table>
<thead>
<tr>
<th>State</th>
<th>Re($E$)</th>
<th>$-\text{Im}(E) = \Gamma/2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bound</td>
<td>-5.045</td>
<td></td>
</tr>
<tr>
<td>Bound</td>
<td>-1.155</td>
<td></td>
</tr>
<tr>
<td>Resonance</td>
<td>2.62</td>
<td>$3.3 \times 10^{-2}$</td>
</tr>
<tr>
<td>Resonance</td>
<td>6.21</td>
<td>0.44</td>
</tr>
</tbody>
</table>
2.5. Comparison of the dynamics

which is quadratic in $q$ and $p$, an initial Gaussian wave packet remains Gaussian for all times. For Lindblad dynamics, this is also explicitly shown for a wave packet as given in (2.43) in e.g. [57,67,68]. This means that for any time $t$ the first and second moments ($\sigma_q(t), \sigma_p(t), \sigma_{qq}(t)$ and so on) are simply given by (2.25),(2.26),(2.27), which can be inserted directly in $|\psi(q)|^2$ ($|\psi(p)|^2$) to obtain the probability density at the time $t$. So, once the Lindblad equations of motion, as given in the previous part, are solved, the form of the wave packet is known for all times.

The unitary propagation of the above wave packet in the model potential requires numerical treatment. Also here, a B-Splines expansion turns out to be an efficient tool. First, a box of sufficient size is imposed in which the knot points are distributed. Then, the time-independent Schrödinger equation for the model Hamiltonian (2.42) is solved in this box, yielding the box energies $\epsilon_j$ and the box eigenstates $\varphi_j$. The latter ones are obtained in terms of B-Splines as

$$\varphi_j(q) = \sum_i c_i^j B_i(q). \quad \tag{2.45}$$

Since the Hamiltonian of the system is time independent, the time propagation is straight forward: It is enough to expand the initial wave packet in the box eigenstates,

$$\psi(q, t = 0) = \sum_k d_k \varphi_k(q), \quad d_k = \langle \varphi_k | \psi(t = 0) \rangle, \quad \tag{2.46}$$

so that the wave function for any time $t$ is given by

$$\psi(q, t) = \sum_k d_k \varphi_k(q) \exp(-i\epsilon_k t/\hbar) \quad \tag{2.47}$$

and hence full information about the system for all times is provided. The next question is which quantities, obtained from the two approaches, are suitable to be compared. This is discussed in the following subsection.

2.5.1 Population and energy content

It is well known that, in the presence of a resonance caused by a potential barrier, the population of the system will decay exponentially (due to tunneling through the barrier) and the width of the resonance gives the decay rate. However, if also bound states are present, the population of the latter ones is stable and gives therefore the asymptotic total population. Applying this to our particular model potential, it is therefore meaningful to define the total norm contained in the region of interest as

$$P(t) = \int_{-\infty}^{q_{\text{BB}}} |\psi(q, t)|^2 dq, \quad \tag{2.48}$$
while the population of the two present bound states (cf. table 2.1) is given by

$$P_B = |d_1|^2 + |d_2|^2\tag{2.49}$$

with the coefficients $d_1, d_2$ from the expansion (2.46). If we consider the initial wave packet to be centered at rest ($\sigma_p^0 = 0$) around the potential minimum ($\sigma_q^0 = q_0$) and choose a moderate initial spread $\sigma_q^0$, the initial norm in the region of interest will be very close to unity (e.g. $P(t = 0) = 0.9987$ for $\sigma_q^0 = 0.25$ in the following illustrative calculations and the deviation from unity is most likely caused by the numerics). Therefore, the previously described exponential decay of the norm, converging towards the bound state population (which is, for the given initial wave packet, $P_B = 0.947$), should behave as

$$P(t) = (1 - P_B)e^{-\Gamma t} + P_B,\tag{2.50}$$

where $\Gamma$ is the width of the lowest resonance (table 2.1). Comparing this expectation with the explicit calculation, i.e. propagating $\psi(q,t=0)$ in time as described before and then numerically evaluating the integral in (2.48), indeed yields a very good agreement, as shown in figure 2 in paper II. There is a very small deviation at the beginning, which can be understood if one recalls that the initial state is a wave packet and, even if centered around 0 in momentum space, still has small high energetic components which are classically allowed outside the barrier. Hence, these components can leave the region $q < q_B$ without tunneling and cause a slight deviation from the exponential decay (2.50). Still, the overall agreement is convincing and also verifies the previously made statement that the decay is totally dominated by the lowest resonance only. However, although the time behavior of the population clearly illustrates the dissipative character of the system, it is not a suitable quantity to be compared to Lindblad dynamics, because the latter one is norm conserving. As shown in subsection 2.3.2, the asymptotic state of a harmonic oscillator is centered around the potential minimum ($\sigma_q(\infty) = q_0$) and has average momentum $\sigma_p(\infty) = 0$ and second moments as given in (2.38). Since, as already mentioned, the Gaussian form is preserved for all times in a harmonic oscillator potential, the final population within the Lindblad dynamics $P_L$ in the region $q < q_B$ can even be expressed analytically:

\[
P_L = \frac{1}{\sqrt{2\pi\sigma_{qq}(\infty)}} \int_{-\infty}^{q_B} \exp\left(-\frac{1}{2\sigma_{qq}(\infty)}(q - q_0)^2\right) dq = \frac{1}{\sqrt{2\pi\sigma_{qq}(\infty)}} \int_{-\infty}^{q_B-q_0} \exp\left(-\frac{1}{2\sigma_{qq}(\infty)}s^2\right) ds = \frac{1}{\sqrt{2\pi\sigma_{qq}(\infty)}} \left[ \int_{-\infty}^{0} \exp\left(-\frac{1}{2\sigma_{qq}(\infty)}s^2\right) ds + \int_{0}^{q_B-q_0} \exp\left(-\frac{1}{2\sigma_{qq}(\infty)}s^2\right) ds \right].\tag{2.51}\]
2.5. Comparison of the dynamics

The first term in this expression simply gives 1/2, which follows directly from the Gaussian integral

$$\int_{-\infty}^{0} \exp(-as^2) \, ds = \frac{1}{2} \sqrt{\frac{\pi}{a}}, \quad a > 0. \quad (2.52)$$

The second term can be written in terms of the error function

$$\operatorname{erf}(z) = \frac{2}{\sqrt{\pi}} \int_{0}^{z} \exp(-s^2) \, ds \quad \text{(note: } \operatorname{erf}(\infty) = 1) \quad (2.53)$$

as follows:

$$P_L = \frac{1}{2} + \frac{1}{\sqrt{2\pi} \sigma_{qq}(\infty)} \int_0^\mu \exp\left(-\frac{1}{2\sigma_{qq}(\infty)} s^2\right) \, ds$$

$$= \frac{1}{2} + \frac{1}{\sqrt{\pi}} \int_0^\mu \exp(-u^2) \, du, \quad \mu = \frac{q_B - q_0}{\sqrt{2\sigma_{qq}(\infty)}}, \quad (2.54)$$

and, by inserting the definition,

$$P_L = \frac{1}{2} + \frac{1}{2} \operatorname{erf}\left(\frac{q_B - q_0}{\sqrt{2\sigma_{qq}(\infty)}}\right). \quad (2.55)$$

If we now insert the used values for $q_0, q_B, m, \omega$ (as $\sigma_{qq}(\infty) = 1/(2m\omega)$ in atomic units) in this expression, the numerical result is, as expected,

$$P_L = \frac{1}{2} + 0.4999887 \approx 1. \quad (2.56)$$

However, a quantity which is not conserved within Lindblad dynamics is the energy expectation value. Therefore, it appears to be more suitable for a comparison to the time evolution in the model potential. The question is whether a corresponding expression can also be defined for the model Hamiltonian. The "normal" definition for a quantum system restricted to some area $A < q < B$ in position space with a Hermitian Hamiltonian $H$ is given by

$$\frac{1}{N} \int_A^B \psi^*(q) H \psi(q) \, dq = E_H = \frac{1}{N} \int_A^B (H \psi(q))^* \psi(q) \, dq, \quad N = \int_A^B |\psi(q)|^2 \, dq, \quad (2.57)$$

where $\psi$ a the wave function of the system. However, simply copying this definition leads to a complex energy expectation value for the case studied here: Although the box states in which the wave function is expanded are orthogonal with respect to the scalar product

$$\int_{-\infty}^{+\infty} \varphi_j^*(q) \varphi_k(q) \, dq = \delta_{jk}, \quad (2.58)$$
this relation does not hold if the integration is taken only from \(-\infty\) to \(q_B\). Hence, if the expansion in box states is inserted in the analog of the definition (2.57) for our model system, the last term in the expression

\[
\int_{-\infty}^{q_B} \psi^*(q, t) H_m \psi(q, t) = \sum_k |d_k|^2 \epsilon_k \int_{-\infty}^{q_B} |\varphi_k(q)|^2 \, dq \\
+ \sum_{k \neq j} d_j^* d_k \epsilon_k e^{i(\epsilon_j - \epsilon_k) t / h} \int_{-\infty}^{q_B} \varphi_j^*(q) \varphi_k(q) \, dq
\]

(2.59)
does not vanish, which leads to complexity. This can be avoided if, instead of copying the definition (2.57), the latter one is first rewritten as

\[
E_H = \frac{1}{2N} \left( \int_A^B \psi^*(q) H \psi(q) + \int_A^B (H \psi(q))^* \psi(q) \, dq \right). \quad (2.60)
\]

Now, the analog of the above expression will always be real because it is the sum of two terms which are each others complex conjugates. This leads to the following definition for the expectation value of the energy content in the region \(q < q_B\):

\[
\langle E \rangle(t) = \frac{1}{2P(t)} \int_{-\infty}^{q_B} (\psi^*(q, t) H_m \psi(q, t) + (H_m \psi(q, t))^* \psi(q, t)) \, dq \\
= \frac{1}{2P(t)} \int_{-\infty}^{q_B} (\psi^*(q, t) H_m \psi(q, t) + \text{h.c.}) \, dq \\
= \frac{1}{P(t)} \text{Re} \left( \int_{-\infty}^{q_B} \psi^*(q, t) H_m \psi(q, t) \, dq \right), \quad (2.61)
\]

where \(P(t)\) is defined in Eq. (2.48). What can be said about its time evolution? The intial and the asymptotic values can be guessed: The former one should be very close to the energy expectation value of a Gaussian wave packet in a harmonic oscillator, since the initial wave packet is almost completely located in the region \(q < q_B\) where the model potential coincides with a harmonic oscillator. This analytical value, for a wave packet as given in (2.43), reads

\[
E_0 = \frac{1}{2m} \left( \sigma_{pp}^0 + (\sigma_p^0)^2 \right) + \frac{1}{2} m \omega^2 \left( \sigma_{qq}^0 + (\sigma_q^0)^2 \right), \quad (2.62)
\]

which, for the used parameters, becomes \(E_0 - U_0 = -4.60\) (here the constant energy shift \(U_0\) is included). An explicit numerical calculation of \(\langle E \rangle(t = 0)\) from Eq. (2.61) gives \(\langle E \rangle(t = 0) = -4.61\), confirming the guess. As for the asymptotic value, one expects convergence towards the energy initially contained in the two bound states which is given by

\[
E_\infty = \frac{|d_1|^2 \epsilon_1 + |d_2|^2 \epsilon_2}{|d_1|^2 + |d_2|^2} = \frac{|d_1|^2 \epsilon_1 + |d_2|^2 \epsilon_2}{P_B}, \quad (2.63)
\]
2.5. Comparison of the dynamics

which is also confirmed by explicit calculation ($E_\infty = -5.03$ vs. $\langle E \rangle(t \to \infty) = -5.04$). To describe the overall time evolution, $\langle E \rangle(t)$ is calculated for several times $t$ and the results are very well described by qualitatively the same exponential behavior as the probability density, i.e.

$$\langle E \rangle(t) = (E_0 - U_0 - E_\infty)e^{-\Gamma t} + E_\infty. \quad (2.64)$$

The comparison between the explicitly calculated time evolution and the exponential decay given above is shown in figure 3 in paper II. As in the previously described norm loss, there is a slight deviation at the beginning, which can be explained by the same arguments (small high-energetic components which are classically allowed outside the region $q < q_B$). Now, with the energy dissipation in the model potential being known (2.64), the only thing left to do is to derive the corresponding expression for a harmonic oscillator within the Lindblad theory in order to be able to make the intended comparison.

2.5.2 Main conclusion

The initial energy expectation value of a Gaussian wave packet in a harmonic oscillator was already given in Eq. (2.62). This can be verified either by explicitly evaluating

$$E_0 = \int_{-\infty}^{\infty} \psi^*(q, t = 0)H\psi(q, t = 0) \, dq \quad (2.65)$$

(with $H$ as given in Eq. (2.10)) or simply by recalling the relation between the energy expectation value and the expectation values of $p^2$ (denoted by $\langle p^2 \rangle$) and $q^2$ (denoted by $\langle q^2 \rangle$ respectively) for a harmonic oscillator:

$$E_0 = \frac{1}{2m} \langle p^2 \rangle(t = 0) + \frac{1}{2}m\omega^2 \langle q^2 \rangle(t = 0). \quad (2.66)$$

Then the relation (2.62) follows directly from the definitions of $\sigma_q, \sigma_{qq}, \sigma_p, \sigma_{pp}$ since

$$\langle q^2 \rangle = \sigma_q^2 + \sigma_{qq}, \quad \langle p^2 \rangle = \sigma_p^2 + \sigma_{pp}. \quad (2.67)$$

However, since the initial Gaussian form is preserved for all times in a harmonic oscillator potential, the energy expectation value within Lindblad dynamics at any time follows directly from the initial equation (2.62):

$$E_L(t) = \frac{1}{2m}(\sigma_{pp}(t) + \sigma_p(t)^2) + \frac{1}{2}m\omega^2(\sigma_{qq}(t) + \sigma_q(t)^2). \quad (2.68)$$

Here, the time evolution of $\sigma_q(t), \sigma_{qq}(t), \sigma_p(t), \sigma_{pp}(t)$ is given by the previously obtained solutions of the Lindblad equation for the first two moments. For the
particular case studied here, i.e. a wave packet at rest centered in the potential minimum with no initial covariance \(\sigma_{pq}^0 = 0\), the time evolution of the covariance matrix (2.27) reduces to

\[
\sigma(t) = e^{-2\lambda} \left( \begin{array}{cc} \cos(\omega t) & \frac{1}{m\omega} \sin(\omega t) \\ -m\omega \sin(\omega t) & \cos(\omega t) \end{array} \right) \left( \begin{array}{cc} \sigma_{pp}^0 - \hbar/(2m\omega) & 0 \\ 0 & \sigma_{qq}^0 - \hbar m\omega/2 \end{array} \right) \\
\times \left( \begin{array}{cc} \cos(\omega t) & -m\omega \sin(\omega t) \\ \frac{1}{m\omega} \sin(\omega t) & \cos(\omega t) \end{array} \right) + \left( \begin{array}{cc} \hbar/(2m\omega) & 0 \\ 0 & \hbar m\omega/2 \end{array} \right)
\]

(2.69)

where the asymptotic values of \(\sigma_{qq}, \sigma_{pp}, \sigma_{pq}\) from Eq. (2.38) were inserted. Evaluating the matrix products we arrive at

\[
\sigma_{qq}(t) = e^{-2\lambda} \left[ \cos^2(\omega t) \left( \sigma_{qq}^0 - \frac{\hbar}{2m\omega} \right) + \frac{1}{(m\omega)^2} \sin^2(\omega t) \left( \sigma_{pp}^0 - \frac{\hbar m\omega}{2} \right) \right] + \frac{\hbar}{2m\omega},
\]

\[
\sigma_{pp}(t) = e^{-2\lambda} \left[ (m\omega)^2 \sin^2(\omega t) \left( \sigma_{qq}^0 - \frac{\hbar}{2m\omega} \right) + \cos^2(\omega t) \left( \sigma_{pp}^0 - \frac{\hbar m\omega}{2} \right) \right] + \frac{\hbar m\omega}{2}.
\]

(2.70)

Inserting this into (2.68), one obtains, after a few algebraic simplifications, the following result (where now also the constant shift \(U_0\) is included):

\[
E_L(t) = \left( E_0 - \frac{\hbar \omega}{2} \right) e^{-2\lambda} + \frac{\hbar \omega}{2} - U_0.
\]

(2.71)

This looks quite similar to the time evolution in the model potential (2.64). In fact, if the following condition is fulfilled,

\[
E_\infty \approx \frac{\hbar \omega}{2} - U_0,
\]

(2.72)

(which is true in our case: \(E_\infty = -5.03\) vs. \(\hbar \omega/2 - U_0 = -5.05\)), both \(\langle E(t)\rangle\) and \(E_L(t)\) show exactly the same time dependence if the phenomenological friction constant \(\lambda\) and the resonance width \(\Gamma\) obey the relation

\[
\lambda = \frac{\Gamma}{2}.
\]

(2.73)

This comparison allows us to formulate the main result:

**To describe the dissipative effect of a resonance by Lindblad operators of the form (2.9), a suitable choice for the phenomenological friction constant (2.15) is given by the half width of the resonance.**

Such a conclusion may sound very general. There are, however, several limitations which are discussed below. Although the heuristic nature of the phenomenological constants is partly resolved by the obtained relation (2.73), the latter turns out to be sufficiently valid only under certain conditions.
2.6 Summary and discussion of the second chapter

To obtain information about the phenomenological constants that emerge from the Lindblad operators in a Markovian master equation, a particular case of an open quantum system was studied in which the coupling to the continuum via a resonance (resulting from a potential barrier) leads to an exponential decay both of the population and the energy content due to tunneling through the barrier. The dynamics of an initially Gaussian wave packet in this model potential was compared to the non-unitary time evolution of the same wave packet in a harmonic oscillator potential within the Lindblad equation, so that virtually the dissipative effect of the resonance is simulated by Lindblad operators. From this, a connection of the phenomenological friction constant to the resonance width could be found.

Explicitly, the obtained relation (2.73) was derived from the time dependence of the energy expectation value, i.e. by comparing Eqs. (2.64) and (2.71). In order for it to hold, the first necessary condition is the approximate equality of the asymptotic values (2.72). It can be shown analytically that, for a Gaussian wave packet in a harmonic oscillator with Lindblad operators of the form (2.9), the asymptotic energy expectation value is always (i.e. for any initial conditions) given by the oscillator ground state energy \( E_L(\infty) = \hbar \omega / 2 \). The asymptotic energy expectation value in the model potential, however, strongly depends on the overlap of the initial wave packet with the bound states, as can be seen from Eq. (2.63). The obtained approximate equality is therefore only valid for low-energetic wave packets, which presents quite a significant restriction. It should be noted that it was the choice of the initial conditions of the wave packet (to be centered around the potential minimum with no average initial momentum) that ensured the validity of (2.72). Furthermore, not only the asymptotic values but also the exponential behavior itself that was found here depends on the initial conditions. As shown in figures 2 and 3 in paper II, there is a slight deviation from the exponential decay (Eqs. (2.50) and (2.64)) due to the presence of high energetic components which are classically allowed to pass the barrier. Now, if the wave packet mainly consisted of such components, a large part would leave the region \( q < q_B \) very fast and only the remaining low-energetic part will decay exponentially. Consequently, the agreement with the Lindblad time evolution becomes worse. Another related aspect is the presence of several resonances. While in the present study the decay was dominated by the lowest resonance only and all others could be completely disregarded, this may no longer be possible at higher energies. In that case, extensions of the model to more than one phenomenological constant can be necessary.

Also, it is worth mentioning that the model potential treated here is rather simple. In real physical applications, one may be confronted with more difficult ones and hence even a local approximation by a harmonic oscillator (in order to apply the Lindblad equation) can be questionable. In this case, other forms of Lindblad
operators than (2.9) may be a better choice, eventually leading to a different set of phenomenological constants in the equations of motion. Altogether, it can be concluded 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 (2.15) appear, the relation (2.73) can still be adopted at least as a first guess, especially if no other more elaborated alternatives are available.
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Bibliography


Paper I

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Possibility of resonant capture of antiprotons by highly charged hydrogenlike ions

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Abstract. Recently, an experimental setup was proposed by Lapierre et al (in Physics with ultra slow antiproton beams, AIP Conference Proceedings, edited by Y. Yamazaki and M. Wada (2005), vol. 793, p. 361) which would allow antiprotons and highly charged ions to collide repeatedly in an electron beam ion trap (EBIT) due to a nested trap configuration. As mentioned by the authors, such a setup may open the possibility to study antiproton capture into well-defined states through a resonant process which involves simultaneous electron excitation. In the present work, we give some theoretical estimations of the feasibility of that process.

PACS. 36.10.-k Exotic atoms and molecules (containing mesons, antiprotons and other unusual particles) – 32.80.Zb Autoionization

1 Introduction

Exotic atoms are fascinating systems where the parameters determining the properties of ordinary matter can be tuned and investigated in completely new regimes. As a consequence these systems can often be used as test benches for fundamental constants and symmetries. For example, the studies of metastable states in antiprotonic Helium recently lead to a new and much improved value for the electron-antiproton mass ratio [1]. That value can be translated to a determination of the proton-antiproton mass ratio, i.e. to a test of CPT symmetry. The antiprotonic systems studied so far [2–15] are produced when antiprotons are stopped in liquids or gases. A slow antiproton can then replace one of the atomic (A) electrons (occupying the main quantum number \( n_e \)) through the process

\[
A + \bar{p} \rightarrow A^+ \bar{p} + e, \quad \text{where it will enter into a state with main quantum number } n \approx n_e \sqrt{\mu_p/\mu_e}.
\]

With the planned Facility for Low-Energy Antiproton and Ion Research (FLAIR) at GSI, Germany, cooled antiprotonic beams of an intensity many orders of magnitude larger than available today will be provided. This might open new possibilities for the production of antiprotonic exotic systems. As mentioned in [16], the nested trap configuration of the electron beam ion trap at the Max Planck Institute in Heidelberg, Germany (HD-EBIT) would eventually, if combined with an antiproton source of sufficient intensity, allow to search for a process that can be seen as the antiprotonic analogon of the resonant process of dielectronic recombination. If, in an antiproton-ion collision, the energy of the antiproton \( \epsilon_p \) is tuned such that the resonant condition is fulfilled, a target electron can be excited and a doubly excited electron-antiproton state may form

\[
A^{q+} + \bar{p} \rightarrow [A^q \bar{p}]^{**} \quad (1)
\]

where \( q \) is the charge of the ion \( A \). The doubly excited electron-antiproton state can subsequently decay by electron, antiproton or photon emission, and the different decay rates will essentially determine the cross section for antiprotonic capture. This process would, if probable enough, provide an excellent possibility for high precision spectroscopy of antiprotonic ions, since the capture occurs in a well defined state that can be controlled by tuning the collision energy. In this work, we aim to investigate the formation and decay channels of such a state in order to obtain a theoretical estimation of its feasibility. For simplicity, we restrict ourselves to collisions with highly charged hydrogenlike ions with the electron being in the ground state.

The present article is structured as follows. In section 2, we schematically describe possible decay channels for resonant antiproton capture and present a way to estimate the cross section. The computational methods are given in section 3 and some illustrative calculations for an example ion are shown in section 4. In the last section, the validity and restrictions on the chosen approach are discussed, followed by some concluding remarks. Atomic units are used throughout unless stated otherwise.

2 Theory

2.1 Decay channels

The doubly excited state \([A^{q+} \bar{p}]^{**}(nl\prime)(n\prime l\prime)\bar{p}\) formed in the collision (1) is lying above the ground state of \( A^{q+} \). We
2.2 Estimation of the cross section

In dielectronic recombination calculations it is common to describe the strength of an isolated resonance by a Lorentz profile as in e.g. [18, 19]:

\[ \sigma(\epsilon) = \frac{1}{\pi} \frac{\Gamma/2}{(E_d - E_i - \epsilon)^2 + \Gamma^2/4}, \]  

(6)

where \( E_d \) is the energy of the doubly excited state, \( E_i \) the initial energy of the target ion (simply given by the 1s orbital energy in our case) and \( \epsilon \) the positive energy of the incoming particle. This description is known to be adequate for resonances with a width much smaller than the distance from the nearest threshold. Clearly, the profile has its maximum at \( \epsilon = E_d - E_i \). The width of the doubly excited state is denoted by \( \Gamma \) and \( S \) is the recombination strength of the process, i.e. the integrated cross section

\[ S = \int \sigma(\epsilon) d\epsilon. \]  

(7)

Since the described mechanism for antiprotonic capture is very similar to dielectronic recombination, there is no reason to abandon this picture. Some modifications, however, are indeed necessary. For dielectronic recombination, the recombination strength can be expressed through the autoionization rate \( A_a \) and the total radiative rate \( A_r \) (i.e. the sum over all possible radiative channels) and is proportional to \( S \sim A_a A_r/(A_a + A_r) \) because the emission of a photon is the only possible stabilization channel and the particles are indistinguishable. Furthermore, if the rates differ by some orders of magnitude, the faster one can be neglected in the fraction and \( S \) is simply proportional to the slowest rate (this is often the case in light systems, where \( S \sim A_r \)). In the present case we have to differentiate between antiproton, Eq. (2), and electron emission, Eq. (3), and since the electron emission provides an additional stabilization channel it should be included in the expression for \( S \), which with all factors reads

\[ S = \frac{\hbar^3 \pi^2}{2 \mu_p (E_d - E_i)} g_d A_a \sum A_{\text{stab}}. \]  

(8)

Here, the sum over all stabilization channels, \( \sum A_{\text{stab}} \), includes now the total radiative rate and the rate for all electron emission channels and \( A_e \) is the antiproton ejection rate which corresponds to autoionization in dielectronic recombination. The weight factors \( g_d \) and \( g_i \) stand for the multiplicity of the doubly excited state and of the initial ion respectively. We can conclude that for a quantitative treatment of the process the calculations of the rates of the different decay channels is indispensable.

3 Computational methods

Essentially, one has to calculate the positions and widths of the resonances as well as the radiative transition rates. The widths occur due to the coupling to the continuum through the electron-antiproton interaction and can be determined together with their positions by means of complex rotation. The radiative rates can be obtained within the dipole approximation, as briefly described below.

3.1 Complex rotation

The technique of complex rotation has proven to be a powerful tool for the description of resonances in atomic systems during the last decades. It has also recently been applied to antiprotonic helium [20]. Its advantage, obtained by rotating the Hamiltonian eigenvalue problem into the complex plane, is that it allows a simultaneous calculation of the positions, \( E_r \), and the widths, \( \Gamma \), of the resonances from the complex eigenvalues, \( E \), of the complex symmetric Hamiltonian matrix

\[ E = E_r - i\Gamma/2. \]  

(9)

The non-relativistic three-body Hamiltonian of the system in the center of mass frame reads

\[ H = \frac{p_e^2}{2\mu_e} + \frac{p_\bar{p}^2}{2\mu_\bar{p}} + \frac{P_e \cdot P_\bar{p}}{m_N} - \frac{e^2}{4\pi\epsilon_0} \left( \frac{Z}{r_e} + \frac{Z}{r_\bar{p}} - \frac{1}{r_\bar{e}} \right), \]  

(10)

where \( Z \) is the nuclear charge, \( \mu_e \) and \( \mu_\bar{p} \) denote the reduced masses of the electron and antiproton (and \( m_N \) the
mass of the nucleus, \( r_e \) and \( r_p \) their distance to the nucleus and \( r_{12} = |r_e - r_p| \) the distance between them. The kinetic energy of the nucleus is accounted for through the use of reduced masses in the first two terms and the inclusion of the term \( \mathbf{p}_e \cdot \mathbf{p}_p/m_N \), referred to as mass polarization in the following.

We set up the Hamiltonian matrix in a basis of hydrogenlike product wave functions

\[
|\phi_{ab}^{(S\ell\pi)} = |\{n_a n_b n_{\ell b}\} S \ell \pi],
\]

where \( S \) is the total spin, \( L \) is the total angular momentum and \( \pi \) is the parity. The one-particle hydrogenlike orbitals can be obtained efficiently through B-Splines, which are piecewise polynomial functions defined on a given set of points, referred to as a knot sequence, distributed in a certain interval. B-Splines have several desirable properties [21] and are widely used in physical applications (see e.g. [22] for an overview). The solutions to the hydrogenlike one-particle Hamiltonian,

\[
h(r) = \frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial r^2} + \frac{l(l+1)\hbar^2}{2\mu r^2} - \frac{Ze^2}{4\pi\epsilon_0 r}, \quad (12)
\]

are expanded as

\[
P_{nl}(r) = \sum_i c_i B_i(r), \quad (13)
\]

where the coefficients \( c_i \) are obtained by solving the eigenvalue equation given by the projection of the Hamiltonian in Eq. (12) onto the B-Spline set. Complex scaling of the radial coordinate \( r \rightarrow r \exp(i\theta) \) with a real rotation angle \( 0 \leq \theta \leq \pi/4 \) is introduced in Eq. (12) by multiplying the kinetic energy term with \( \exp(-2i\theta) \) and the potential energy term with \( \exp(-i\theta) \).

The two-particle Hamiltonian (10) can be written as

\[
H = h_e + h_p + h_{12}, \quad (14)
\]

where \( h_e \) and \( h_p \) have the form as in Eq. (12) (with \( r = r_e, r_p, \mu = \mu_e, \mu_p \)) and

\[
h_{12} = \frac{\mathbf{p}_e \cdot \mathbf{p}_p}{m_N} + \frac{e^2}{4\pi\epsilon_0 r_{12}} \quad (15)
\]

where the contributions to the kinetic and potential energy are scaled as before. Now each matrix element of \( H \) in the basis (11) can be calculated, yielding a complex symmetric Hamiltonian matrix. After diagonalization, the energies of the resonances are obtained in the form given in (9). The whole procedure follows closely that of Refs. [23, 24].

### 3.2 Radiative transitions

We use the first order perturbation approach in the dipole approximation where the radiative rate \( A_r \) for a transition from an initial state \( |\psi_i\rangle \) to a final state \( |\psi_f\rangle \) is in first order given by

\[
A_r = \frac{1}{4\pi\epsilon_0} \frac{4}{3\hbar^4} \left( \frac{\Delta E}{e} \right)^3 |\langle \psi_f | E_1 | \psi_i \rangle|^2. \quad (16)
\]

### Fig. 1.

(Color online) Calculated structure of the electron-antiproton resonances in hydrogenlike Calcium at fixed total angular momentum \( L = 12 \) (This choice will be motivated in section 4.1). The dashed lines indicate resonances arising from contributions with \( n_e = 2 \), while solid lines denote resonances from higher electronic states \( (n_e = 3, 4) \). The numbers 44, 45, 48, 49 are the main quantum numbers of the contributing one-particle antiprotonic orbitals \( n_p \). The 1s threshold of Ca\(^{19+}\) is at -200 a.u.

Here, \( \Delta E \) is the energy difference between the initial and the final state and \( E_1 \) is the dipole transition operator. The final state \( |\psi_f\rangle \) is approximated by a product state of the antiprotonic and electronic one-particle orbitals. For a highly charged ion this gives sufficient accuracy. Even in light exotic systems such as antiprotonic Helium this approximation can be used [25], although corrections to the energy clearly become more important [26].

### 4 Illustrative calculations

As an illustration, we will investigate a few chosen resonances in a collision of antiprotons with a medium heavy hydrogenlike ion, Ca\(^{19+}\). The high charge simplifies the calculations, since the correlation between the electron and the antiproton is rather weak in this case. (This does not hold for very light systems - antiprotonic Helium shows strong molecular features where e.g. a Born-Oppenheimer treatment is suitable [27]). On the other hand, the ion is light enough so that a non-relativistic treatment is meaningful. The decisive quantity for the process studied here is, as will be shown later, the capture rate into the doubly excited state which to a first approximation is independent of nuclear charge. The results presented can thus be generalized to neighboring ions, at least for a qualitative picture. The calculated structure of the positions of the resonances for a total angular momentum of \( L = 12 \)
(see below) is schematically shown in figure 1. All resonances arising from the \( n_e = 2, n_p = 48 \) configurations lie below the 1s threshold, apart from one. The latter one, however, lies very close to the threshold. Such resonances are known to be very hard to describe numerically, and no reliable results for the width were obtained in this work. The resonances arising from the \( n_e = 3, n_p = 45 \) and \( n_e = 4, n_p = 44 \) configurations lie very densely and could not be resolved properly. The isolated resonance approach (6) may not be valid in this case. Further, if the aim is to be able to control which state the antiproton is captured into an isolated resonance is more appropriate. Thus, we focus on resonances with their main contribution from the \( n_e = 2, n_p = 49 \) configurations in the following illustrative calculations.

4.1 Angular momentum dependence and validation

The described combination of complex rotation with B-Splines and subsequent diagonalization of the complex matrix (also known as complex scaled configuration interaction CSCI) has already been applied to multiply excited electronic states (see e.g. [24]). However, when applying the same method to doubly excited electron-antiproton states one is confronted with some practical difficulties due to the fast oscillations of the high-n antiprotonic states and the different extensions of the antiprotonic and the electronic wave functions. To handle this situation we work with different knot sequences for the two particles. The number of knot points \( N_k \) used for the electronic functions is \( N_k = 45 \) with a box size of 2.0 a.u. and \( N_k = 275, 325 \) for the antiprotonic functions with a box size of 0.2 a.u. The electronic knot sequence is linear in the beginning and exponential further out. This is a scheme that is well tested. The distance between the knots in the antiprotonic sequence is on the other hand slowly and steadily increasing to obtain roughly the same number of knots between the nodes in the \( n = 49 \) states for the full extension of the wave function. The needed number of B-Splines is estimated through comparison of the numerically calculated energies of the relevant hydrogenlike one-particle orbitals with the analytical values, that is, \( N_k \) is increased until a sufficiently good agreement is achieved. For example, the analytical value of the antiprotonic \( n = 49 \) orbital is \( E = -149.1940989 \) a.u., and the numerically obtained values are \( E = -149.194087 \) a.u. (with \( N_k = 275 \)) and \( E = -149.1940855 \) a.u. (with \( N_k = 325 \)).

In order to further check the method for numerical stability, we calculate some relevant quantities with analytical wave functions and compare those with the corresponding result obtained with our method. This also allows us to analyze the role of the total angular momentum, as will be discussed below.

As the next step in the validation procedure we calculate the antiproton ejection rate for a single product state in the framework of the Fermi Golden Rule and compare with the one obtained with complex rotation. In the framework of the former, a decay rate \( \Gamma \) (or the corresponding width \( \Gamma = \hbar A \)) for a transition from an initial state \( |\psi_i\rangle \) to a final state \( |\psi_f\rangle \) caused by an interaction \( U \) is given by

\[
\Gamma = 2\pi \rho |\langle \psi_f | U | \psi_i \rangle|^2,\tag{17}
\]

where \( \rho \) denotes the density of states. For the antiproton emission from a doubly excited electron-antiproton state, \( U \) can be approximated by the Coulomb interaction between the particles \( (U = (r_{12})^{-1}) \) in atomic units. For further simplification, we represent the final state by a single product wave function of the electronic 1s orbital and the antiprotonic regular Coulomb function with an energy \( \epsilon \) and angular momentum \( L \) which is also the total angular momentum of the system

\[
|\psi_f\rangle = |\{1s \epsilon L\} L\rangle.\tag{18}
\]

The initial doubly excited state can be represented in the basis (11), and since the total spin and parity are unaffected by the Coulomb interaction we can write

\[
|\psi_i\rangle = \sum_{a,b} c_{ab} |\{n_a l_a n_b l_b\} L\rangle \tag{19}
\]

where \( a, b \) run over all fixed parity combinations for which \( l_a \) and \( l_b \) can be coupled to \( L \). The main contribution will come from the dominating basis functions (with \( n_a = 2 \) and \( n_b = 49 \)), that is, from the matrix elements of the form

\[
\langle \{1s \epsilon L\} L | (r_{12})^{-1} | \{2s 49 L\} L \rangle, \tag{20}
\]

\[
\langle \{1s \epsilon L\} L | (r_{12})^{-1} | \{2p 49 L \pm 1\} L \rangle.
\]

They can be explicitly written as

\[
\langle \{n_a l_a \epsilon l_b \} L | (r_{12})^{-1} | \{n_c l_c n_d l_d\} L \rangle = \sum_{k=0}^{\infty} R^k (1)^{l_a + l_c + L} \left\{ l_a \parallel l_c | \langle l_a || C^k || l_c \rangle \langle l_b || C^k || l_d \rangle \right\}.
\]
where we introduced the standard notation for Wigner 6j-symbols and reduced matrix elements between spherical tensor operators $C^k$ [28], representing the angular part, while $R^k$ stands for the radial part of the integral

$$R^k = \int dr_1 dr_2 P_{n_1 l_1}(r_1) F_{r_2}^k(r_2) \frac{r_2^k}{r_2} P_{n_2 l_2}(r_2)$$

where we denote the Coulomb wave with energy $\epsilon$ and angular momentum $l_b$ by $F_{r_2}^k$ and by $P_{n_1 l_1}$ the bound state reduced radial wave function, which are all known analytically. For a stable implementation of Coulomb functions, Barnett’s algorithm was used [29]. To investigate the angular momentum dependence we restrict ourselves to the first matrix element in (20) with $l_a = l_c = 0$ and $l_b = l_d = L$ (see (21)). Here, the angular part equals unity and only the $k = 0$ term in the sum contributes. The results of the calculation are shown in figure 2. It turns out that the squared matrix element is indeed very sensitive to the total angular momentum and can vary by several orders of magnitude (similar behaviour is also found for the other matrix elements listed in (20)). If we also account for the multiplicity, the recombination strength (8) is proportional to $g_4 A_4$ and has its maximum around $L = 12$. This motivates our choice of angular momentum (cf. caption of figure 1).

We can now compare the transition rate calculated with Fermi Golden Rule and analytical wave functions for a single product state with the width obtained as the imaginary part of the complex scaled second-order energy contribution, which should be identical. We look thus for the equality

$$\pi |\langle \{1s e 12\} 12 | \{2s 49 12\} 12 \rangle|^2 = \left| \sum_{\epsilon} \text{Im} \left[ \frac{\langle \{1s e 12\} 12 | \{2s 49 12\} 12 \rangle|^2}{E_\epsilon^2 + E_\epsilon^0 49,12 - E_\epsilon^1} \right] r \rightarrow 0 \exp(i\theta) \right|$$

The sum on the right hand side runs over the whole spectrum of the antiprotonic radial functions $\epsilon$ (with the corresponding energies $E_\epsilon$) generated with B-Splines and $N$ is the number of the states included (which is limited by the chosen B-Spline parameters). The energy $\epsilon$ of the Coulomb wave on the left hand side equals the term $\epsilon = E_\epsilon^2 + E_\epsilon^0 49,12 - E_\epsilon^1 = 0.812$ a.u. that appears in the denominator on the right hand side. Note however that the energies $E_\epsilon$ are complex and thus the condition $\epsilon \neq E_\epsilon$ holds for all $\epsilon$ in (23). As shown in figure 3 agreement is achieved for a sufficient number of included configurations (the relative difference between the analytical value and the converged result is about $10^{-4}$). A similarly good agreement is found also for the other matrix elements. However, one should keep in mind that the results given so far do not even approximately give the true antiproton ejection rate since we considered only one particular basis state instead of a coherent sum. Nevertheless, the scaling with respect to total angular momentum could be investigated and the numerical accuracy was tested.

**Fig. 3.** Convergence of expression (23) as a function of the number of included states $N$ (here $N_{\text{max}}=316$) for the matrix element $A = \pi |\langle \{1s e 12\} 12 | \{2s 49 12\} 12 \rangle|^2$. All values are given in atomic units.

### 4.2 Rates

The number of configurations that can be included in a full CSCI calculation in practice is, of course, limited by the computational resources and the basis set needs to be truncated in some way. After performing some convergence tests, the following configuration have been used. We restricted the angular symmetries to $\{s, L\}$ and $\{p, L \pm 1\}$, while the maximum number of antiprotonic orbitals is limited by the used B-Splines parameters as $N_k - k - 2 = 316$ where $N_k = 325$ is the number of knot points used and $k = 7$ the order of the B-Splines. The same restriction applies to the number of electronic orbitals, for the representation of which $N_k = 45$ knotpoints were used and hence $N_{\text{max}} = 36$. However, to keep the size of the matrix to be diagonalized within reasonable boundaries we truncated the antiprotonic basis further. For a correct representation of the antiprotonic emission channel and the bound part we included the maximum number of antiprotonic states in the configurations with the electronic $1s$, $2s$ and $2p$ orbitals, while for the remaining electronic orbitals only 114 antiprotonic orbitals were used. This was found to be sufficient for convergence (cf. also figure 3) and yields a matrix size of about $10^4 \times 10^4$.

As indicated in Eq. (8), not only the total width but also the antiproton ejection rate and electronic Auger rate have to be calculated distinctly in order to obtain the recombination strength. Both processes, however, arise from the electron-antiproton interaction, and it is not trivial to separate them. An approximate separation can be achieved by excluding configurations which form a certain decay channel, and as a check for consistency one can compare the sum of the hereby estimated partial widths with the obtained total width. In order to exclude Auger electron emission, only antiprotonic orbitals with $n \geq 44$ were included, so that the system becomes virtually stable against electron emission because of the absence of low lying antiprotonic states. On the other hand, to isolate the electron emission channel the low lying antiprotonic states
should definitely be included, while now all configurations involving the electronic 1s orbital are excluded so that the system is virtually stable against emission of the antiproton. All calculations were performed with and without the mass polarization term to investigate its significance. The results are shown in table 1.

It is found that the antiproton ejection rate of the highest 2-49 resonance is very low and could not be resolved properly in the present calculation. The result after including mass polarization is below the achieved numerical accuracy and is therefore not given in the table. The other two resonances, however, are broader and can be described rather well. The effect of the mass polarization term is clearly visible and should not be neglected even for rather heavy nuclei. The reason is of course that even compared to the large mass of a heavy nucleus the mass of the antiproton is not negligible. The second and third resonance also show good consistency in the distinct description of the channels since the sum of the antiproton and electron emission widths agrees rather well with the obtained total width. The observed difference arises most likely due to interference effects between the channels, underlining the approximative nature of an independent treatment.

To calculate the radiative rates, we will exploit the fact that in the expansion in the basis (11) the doubly excited states are almost completely determined by only a few basis states, namely those with \( n_e = 2, l_e = s, p \) and \( n_p = 49, l_p = 11, 12, 13 \). Thus, to apply the approach described in section 4.2 we explicitly consider the matrix element that appears in (16). For a transformation of the form \( \langle \{ n l n' l' \} L_i \rangle \to \langle \{ n l n' l' \} L_f \rangle \) it reads

\[
A_r = \frac{e^2}{4 \pi \epsilon_0} \frac{3h}{\hbar c} \left( \frac{\Delta E}{c} \right)^3 (2L_f + 1) \times \left( \int P_{n'l'}(r) \rho_{n'l'}(r) dr \right)^2 \left( \frac{L_f}{l'} \frac{1}{1} \frac{L_i}{l'} \right)^2 \langle l' || c || l' \rangle^2.
\]

Compared to electronic radiative transitions, the antiprotonic ones are found to be several orders of magnitude slower. The reason is the small energy difference between the levels for small changes in the main quantum number \( n \) (\( A_r \sim (\Delta E)^3 \)). For big changes in \( n \), on the other hand, the transitions are suppressed by the fact that the initial and final wave functions have almost no overlap. We can therefore safely neglect the antiprotonic radiative transitions in the following. Because of dipole selection rules, only the basis states that include the electronic 2p orbital contribute (i.e. the basis states \{\{2p 49 11\}12, \{\{2p 49 13\}13\} \}), while no contribution arises from the basis state \{\{2s 49 12\}12\}. We obtain distinct rates for radiative stabilization into the final product states \{\{1s 49 11\}11 (\( \Delta L = -1 \)-transition) and \{\{1s 49 13\}13 (\( \Delta L = +1 \)-transition) by inserting the relevant quantum numbers in Eq. (24) and multiplying the result with the squared expansion coefficient that corresponds to the contributing basis state. The results are shown together with the coefficients in table 2 where the total radiative stabilization rate is approximated by the sum of both partial rates. As one can see from comparison with table 1, the electronic radiative rates are about two orders of magnitude larger than the ones for antiproton and electron ejection.

### Table 2. Partial half widths for electronic radiative transitions into the final states \{\{1s 49 11\}11 (\( \Delta L = -1 \)) and \{\{1s 49 13\}13 (\( \Delta L = +1 \)) and total radiative half widths of the 2-49 resonances from table 1, given in atomic units (\( a_0 = a \cdot 10^{6} \)). The coefficients from the expansion of the doubly excited states in the basis (11) correspond to the basis states \{\{2s 49 12\}12 (c1), \{\{2p 49 11\}12 (c2) and \{\{2p 49 13\}12 (c3).

<table>
<thead>
<tr>
<th>Without mass-pol.</th>
<th>Res. I</th>
<th>Res. II</th>
<th>Res. III</th>
</tr>
</thead>
<tbody>
<tr>
<td>Position</td>
<td>-195.586</td>
<td>-194.786</td>
<td>-193.628</td>
</tr>
<tr>
<td>( \Gamma / 2(\tilde{p}) )</td>
<td>7.4[-5]</td>
<td>8.8[-6]</td>
<td>2.0[-5]</td>
</tr>
<tr>
<td>( \sum (\Gamma / 2(\tilde{p}, e)) )</td>
<td>4.5[-5]</td>
<td>9.2[-6]</td>
<td>2.8[-5]</td>
</tr>
<tr>
<td>( \Gamma / 2(\tilde{p} \pi) )</td>
<td>5.8[-5]</td>
<td>9.5[-6]</td>
<td>3.0[-5]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>With mass-pol.</th>
<th>Res. I</th>
<th>Res. II</th>
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</tr>
</thead>
<tbody>
<tr>
<td>Position</td>
<td>-195.586</td>
<td>-194.786</td>
<td>-193.628</td>
</tr>
<tr>
<td>( \Gamma / 2(e) )</td>
<td>6.2[-5]</td>
<td>8.5[-6]</td>
<td>1.3[-5]</td>
</tr>
<tr>
<td>( \sum (\Gamma / 2(\tilde{p}, e)) )</td>
<td>1.9[-5]</td>
<td>5.0[-5]</td>
<td></td>
</tr>
<tr>
<td>( \Gamma / 2(\tilde{p} \pi) )</td>
<td>7.8[-5]</td>
<td>1.9[-5]</td>
<td>5.3[-5]</td>
</tr>
</tbody>
</table>

4.3 Recombination strength and cross section

The calculated rates can now be used to estimate the recombination strength (S). Since the antiproton ejection width of the 2-49 resonance at \(-195.586 \) a.u. could not be resolved clearly, we will focus on the other two resonances at \(-194.786 \) a.u. (Res. II) and \(-193.628 \) a.u. (Res. III). For the chosen example, the multiplicity of the initial ion with the electron being in the 1s state is \( g_e = 2 \) due to spin, while the multiplicity of the doubly excited state \( d \) is given by its total angular momentum \( L_d = 12 \) and 4 possible spin couplings to \( g_d = 4 \cdot (2L_d + 1) = 100 \). Since the radiative transitions turned out to be by far the fastest, the stabilization fraction \( F_\text{s} = \sum A_{\text{stab}} / (A_\text{e} + \sum A_{\text{stab}}) \) approximately equals unity \( (F_\text{s} = 0.98 \) for Res. II and \( F_\text{s} = 0.96 \) for Res. III), and the inclusion of the electronic Auger rate changes the result by only about one percent. Furthermore, we see that as long as radiative stabilization dominates (which is the case for large \( Z \)), a very precise calculation of radiative rates is not necessary since they cancel in the expression for the recombination strength. The only quantity that needs to be determined to a rather
high accuracy is the antiproton ejection rate since the recombination strength is proportional to the latter. The expression for the strength can be written as

\[ S = \left( \frac{\hbar^2}{m_e} \right) \xi \]

where \( \xi \) is a dimensionless quantity

\[ \xi = \frac{\pi^2}{2(p_\pi/m_e)} \frac{g_d}{g_s} F_s \]

and with \( \hbar^2/m_e = 7.62 \cdot 10^{-16} \text{eV cm}^2 \) we obtain \( S_{II} = 7.1 \cdot 10^{-22} \text{eV cm}^2 \) for Res. II and \( S_{III} = 11.7 \cdot 10^{-22} \text{eV cm}^2 \) for Res. III. The Lorentz shaped cross section profile (6) for Res. II, shown in figure 4, has its maximum at 7.56 kbar at 0.14 keV. Similarly, the peak for Res. III reaches its maximum of 14.06 kbar at 0.17 keV. The widths of both resonances are much smaller then the energy distance between them and thus they can be treated as isolated to a good approximation.

5 Discussion and concluding remarks

To estimate the feasibility of resonant antiproton capture by electron excitation in highly charged ions, we adopted a theoretical approach which is based on the one often used in calculations on dielectronic recombination. The choice is motivated by the similarity of the processes. We performed illustrative calculations for a few resonances in hydrogenlike \( \text{Ca}^{19+} \) and found the cross section to be about a few kilobarn in the 0.1-0.2 keV region. The stabilization of the intermediate doubly excited electron-antiproton states is dominated by electronic radiative transitions.

The question is now how the obtained results should be interpreted with regard to the feasibility of the process in general. In principle, the calculated recombination strengths are of the same order as found in dielectronic recombination calculations and measurements, see e.g. Ref. [30] on lithiumlike beryllium or [31] for \( \text{He}^+ \) where the calculated strengths lie in the region \( 1 \leq S \leq 25 \cdot 10^{-22} \text{eV cm}^2 \). Therefore, an experimental observation of the process described in the present work does not seem impossible. Another question is whether the results can be used to draw conclusions also about ions in other charge states. The antiproton ejection rate (which is, as mentioned before, the decisive quantity) is independent of \( Z \) to a first approximation, and hence the qualitative picture is also valid for neighboring ions. However, the radiative rate scales as \( Z^4 \) which means that for lighter ions the stabilization fraction \( F_s \) can be significantly smaller than one and hence the cross section decreases. Also the electron-antiproton correlation becomes more and more significant as \( Z \) decreases. For significantly higher nuclear charge, on the other hand, relativistic effects can play a role.

Finally, there is another aspect that should be discussed. In antiproton-ion collisions, capture can also occur through a non-resonant process if an initially bound electron is scattered into the continuum:

\[ \bar{p} + A^{q+} \rightarrow [\bar{p}A^{(q+1)+}] + e. \]

This process has no counterpart in electron-ion recombination since in that case the number of bound electrons would be conserved. The process has been studied by Cohen for several singly charged ions [32] and by Sakimoto for \( \text{He}^+ \) [33]. The cross sections they provide are relatively large, about \( \sim 0.2 \alpha_0^2 \) or \( \sim 5 \text{Mbarn} \) for a center of mass energy of 1 a.u. Note though that this is the total cross section summed over all angular momenta and over all final states of the captured antiproton, while the present calculations consider the capture into a specific quantum state. This non-resonant process is indistinguishable from the resonant process where the doubly excited state decays by electron emission. Ref. [33] finds in fact that this type of resonances gives a larger contribution than the pure direct process. This might be because the considered impact energy is such that many resonances (Rydberg series) overlap in energy and can be populated, compare e.g. the energy region of the (3-45) and (4-44) resonances in figure 1. If the purpose is to control into which state the antiproton is captured such a resonance dense region is not an optimal choice. In highly charged ions where the energy difference between different \( n \)-manifolds is larger it might be easier to avoid them. A related question is that of energy difference between different \( n \)-manifolds.\[ \Delta n = 6 \] and the degree of antiproton excitation the situation can be very different. The antiproton ejection rate (which is, as mentioned before, the decisive quantity) is independent of \( Z \) to a first approximation, and hence the qualitative picture is also valid for neighboring ions. However, the radiative rate scales as \( Z^4 \) which means that for lighter ions the stabilization fraction \( F_s \) can be significantly smaller than one and hence the cross section decreases. Also the electron-antiproton correlation becomes more and more significant as \( Z \) decreases. For significantly higher nuclear charge, on the other hand, relativistic effects can play a role.

In conclusion, we may say that from this first theoretical estimate the exotic dielectronic-like process of resonant antiproton capture in highly charged ions does not seem to be completely out of reach.
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Paper II

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.

PACS numbers: 03.65.−w, 03.65.Yz, 03.65.Xp

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 $\rho$. Among those, the Markovian master equation derived by Lindblad [27] presents the most general form:

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

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

where $\omega$ 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:

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

The parameter $\tau$ 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
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

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

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

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

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,

$$H = -\frac{\hbar^2}{2m} \frac{d^2}{dq^2} + U(q),$$

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

$$E = E_r - i\Gamma/2,$$

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.

<table>
<thead>
<tr>
<th>State</th>
<th>$\text{Re}(E)$</th>
<th>$\text{Im}(E) = \Gamma/2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bound</td>
<td>−5.045</td>
<td>−</td>
</tr>
<tr>
<td>Bound</td>
<td>−1.155</td>
<td>−</td>
</tr>
<tr>
<td>Resonance</td>
<td>2.62</td>
<td>$3.3 \times 10^{-2}$</td>
</tr>
<tr>
<td>Resonance</td>
<td>6.21</td>
<td>0.44</td>
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</tbody>
</table>

Eigenvectors of the complex Hamiltonian matrix, but their imaginary parts vanish. Continuum energies are rotated by the angle $2\theta$, 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 $\psi_j = \sum c_i B_i$). By solving the resulting generalized eigenvalue equation $H\mathbf{c} = E\mathbf{B}\mathbf{c}$, (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

$$\frac{dA}{dt} = \frac{i}{\hbar} [H, A] + \frac{1}{2\hbar} \sum_j (V_j^\dagger [A, V_j] + [V_j^\dagger, A] V_j),$$

(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

\[
V_j = a_j p + b_j q, \quad V_j^\dagger = a_j^* p + b_j^* q, \quad j = 1, 2, \tag{10}
\]

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

\[
\sigma_q = \text{Tr}(\rho q), \quad \sigma_p = \text{Tr}(\rho p). \tag{11}
\]

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

\[
\lambda = -\text{Im} \sum_{j=1}^2 a_j^* b_j, \tag{12}
\]

can be written in the following form:

\[
\begin{align*}
\frac{d}{dt} \sigma_q(t) &= -\lambda \sigma_q(t) + \frac{1}{m} \sigma_p(t), \tag{13a} \\
\frac{d}{dt} \sigma_p(t) &= -m\omega^2 \sigma_q(t) - \lambda \sigma_p(t). \tag{13b}
\end{align*}
\]

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

\[
\begin{align*}
\sigma_q(t) &= e^{-\lambda t} \left( \cos(\omega t)\sigma_q^0 + \frac{1}{m\omega} \sin(\omega t)\sigma_p^0 \right), \tag{14a} \\
\sigma_p(t) &= e^{-\lambda t} \left( -m\omega \sin(\omega t)\sigma_q^0 + \cos(\omega t)\sigma_p^0 \right). \tag{14b}
\end{align*}
\]

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

\[
\sigma_{AB} = \sigma_{BA} = \frac{1}{2} \text{Tr}(\rho(AB + BA)) - \text{Tr}(\rho A)\text{Tr}(\rho B). \tag{15}
\]

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 \(\sigma_p\) and \(\sigma_q\), respectively), and their covariance \(\sigma_{pq}\). To write these equations in a compact form, it is convenient to define the symmetrical covariance matrix:

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

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

\[
\sigma_{qq}(t)\sigma_{pp}(t) - \sigma_{pq}^2(t) \geq \hbar^2/4. \tag{17}
\]

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

\[
\frac{d}{dt} \sigma(t) = Y \sigma(t) + \sigma(t)Y^T + 2D, \tag{18}
\]

where \(Y\) is a matrix of commutators.
where we used the abbreviations
\[ Y = \begin{pmatrix} -\lambda & 1/m \\ -m\omega^2 & -\lambda \end{pmatrix}, \quad D = \begin{pmatrix} D_{qq} & D_{pq} \\ D_{pq} & D_{pp} \end{pmatrix}. \]

The elements of $D$ are usually called ‘diffusion coefficients’ and are defined as
\[ D_{qq} = \frac{\hbar}{2} \sum_{j=1}^{2} |a_j|^2, \quad D_{pp} = \frac{\hbar}{2} \sum_{j=1}^{2} |b_j|^2, \quad D_{pq} = -\frac{\hbar}{2} \text{Re} \sum_{j=1}^{2} a_j^* b_j. \]

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
\[ D_{qq} > 0, \quad D_{pp} > 0, \quad D_{qq}D_{pp} - D_{pq}^2 \geq \frac{\lambda^2\hbar^2}{4}, \]
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]:
\[ D_{qq} = \frac{\hbar \lambda}{2m\omega}, \quad D_{pp} = \frac{1}{2}\hbar \lambda m\omega, \quad D_{pq} = 0. \]

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 $\lambda$ 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,
\[ \sigma(t) = e^{tY} (\sigma^0 - \sigma^\infty)(e^{tY})^T + \sigma^\infty, \]
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
\[ Y\sigma^\infty + \sigma^\infty Y^T = -2D. \]

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 $\sigma^\infty$. The result is
\[ \begin{align*}
\sigma_{qq}(\infty) &= \frac{(m\omega)^2(2\lambda^2 + \omega^2)D_{qq} + \omega^2D_{pp} + 2m\omega^2\lambda D_{pq}}{2(m\omega)^2\lambda(\lambda^2 + \omega^2)}, \\
\sigma_{pp}(\infty) &= \frac{(m\omega)^2\omega^2D_{qq} + (2\lambda^2 + \omega^2)D_{pp} - 2m\omega^2\lambda D_{pq}}{2\lambda(\lambda^2 + \omega^2)}, \\
\sigma_{pq}(\infty) &= \frac{-\lambda(m\omega)^2D_{qq} + \lambda D_{pp} + 2m\lambda^2D_{pq}}{2m\lambda(\lambda^2 + \omega^2)}. 
\end{align*} \]
Inserting the diffusion coefficients (22) in the above expressions, the asymptotic values can be shown to simplify to
\[
\sigma_{qq}(\infty) = \frac{\hbar}{2m\omega}, \quad \sigma_{pp}(\infty) = \frac{\hbar m\omega}{2}, \quad \sigma_{pq}(\infty) = 0.
\] (26)

The exponential of the matrix that appears in (23) is found by diagonalizing \( Y \):
\[
e^{tY} = e^{-\lambda t} \left( \begin{array}{cc}
\cos(\omega t) & \frac{1}{m\omega} \sin(\omega t) \\
-m\omega \sin(\omega t) & \cos(\omega t)
\end{array} \right).
\] (27)

Hence, the time evolution of the first and second moments of the open quantum system is fully determined by (14a), (14b) and (23) (provided given initial conditions \( \sigma_{0q}, \sigma_{0p} \) and \( \sigma_{0} \) which, however, do not influence the asymptotic values), and contains \( \lambda \) 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
\[
\psi(q, t = 0) = \frac{1}{(2\pi \sigma_{0qq})^{1/4}} \exp \left( -\frac{1}{4\sigma_{0p}^2} (q - \sigma_{0q})^2 + \frac{i}{\hbar} q \sigma_{0p} \right),
\] (28)

which is centered around \( \sigma_{0q} \) in \( q \)-space with the initial spread \( \sigma_{0qq} \), and \( \sigma_{0p} \) is the momentum expectation value. By means of a Fourier transformation it can also be shown that the initial spread in \( p \)-space, \( \sigma_{0p} \), is given by the initial spread in \( q \)-space as \( \sigma_{0pp} = \frac{\hbar^2}{4\sigma_{0qq}} \). 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 (14a), (14b) 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 \( \epsilon_j \) and the box eigenfunctions \( \varphi_j \) in terms of B-splines:
\[
\varphi_j(q) = \sum_i c_i^j B_i(q).
\] (29)

In the following step, the initial wavefunction (28) is expanded in the box eigenstates as
\[
\psi(q, t = 0) = \sum_k d_k \varphi_k(q), \quad d_k = \langle \varphi_k | \psi(t = 0) \rangle,
\] (30)

and thus the wavefunction for any time \( t \) is obtained as a solution of the time-dependent Schrödinger equation:
\[
\psi(q, t) = \sum_k d_k \varphi_k(q) \exp(-i\epsilon_k t/\hbar).
\] (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. \( q \leq q_R \). 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, \( \sigma_{0p} = 0, \sigma_{0q} = q_0 \). We define the norm \( P \) contained in the region of interest as
\[
P(t) = \int_{-\infty}^{q_R} |\psi(q, t)|^2 dq.
\] (32)
and with a moderate choice of $\sigma_0^{ij}$ the initial norm is very close to unity (e.g., $P(t = 0) = 0.9987$ for $\sigma_0^{ij} = 0.25$ 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

$$P_B = |d_1|^2 + |d_2|^2,$$

(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

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

(34)

a very good agreement is achieved for $\alpha = \Gamma$, where $\Gamma$ 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:

$$\langle E \rangle(t) = \frac{1}{P(t)} \text{Re} \left( \int_{-\infty}^{\infty} \psi^*(q,t) H_m \psi(q,t) dq \right),$$

(35)

which will be discussed below.

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

$$\int_{-\infty}^{\infty} \psi_j^*(q) \psi_k(q) dq = \delta_{jk}.$$  

(36)
They are, however, not orthogonal if the integration is taken only from \(-\infty\) to \(q_B\). Hence, the expression 
\[
\int_{-\infty}^{q_B} \psi^*(q, t)H_m\psi(q, t) \, dq
\]
is, in general, complex since the last term in the equation below does not vanish:
\[
\int_{-\infty}^{q_B} \psi^*(q, t)H_m\psi(q, t) = \sum_k |d_k|^2 |\varphi_k(q)|^2 + \sum_{k \neq j} d_k^* d_j e^{i(\epsilon_j - \epsilon_k)t/\hbar} \int_{-\infty}^{q_B} \psi_k^*(q)\psi_j(q) \, dq.
\]
(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, \(\psi\),
\[
\frac{1}{N} \int \psi^* H \psi = E_H = \frac{1}{N} \int (H\psi)^* \psi, \quad N = \int |\psi|^2,
\]
so that it can also be written as
\[
E_H = \frac{1}{2N} \left( \int \psi^* H \psi + \int (H\psi)^* \psi \right).
\]
(39)

Going back to our case, the analogue of the above expression is
\[
\langle E \rangle(t) = \frac{1}{2P(t)} \int_{-\infty}^{q_B} (\psi^*(q, t)H_m\psi(q, t) + (H_m\psi(q, t))^*\psi(q, t)) \, dq
\]
\[
= \frac{1}{2P(t)} \int_{-\infty}^{q_B} (\psi^*(q, t)H_m\psi(q, t) + \text{h.c.}) \, dq
\]
\[
= \frac{1}{P(t)} \Re \left( \int_{-\infty}^{q_B} \psi^*(q, t)H_m\psi(q, t) \, dq \right),
\]
(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
\[
E_0 = \frac{1}{2m} \left( \frac{\sigma_{pp}^0 + \sigma_{qq}^0}{4\sigma_{pp}^0} \right) + \frac{1}{2} m \omega^2 \left( \frac{\sigma_{pp}^0 + \sigma_{qq}^0}{4\sigma_{pp}^0} \right),
\]
(41)

where \(\sigma_{pp}^0 = \hbar^2 / (4\sigma_{qq}^0)\). 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
\[
E_\infty = \frac{|d_1|^2 \epsilon_1 + |d_2|^2 \epsilon_2}{|d_1|^2 + |d_2|^2},
\]
(42)

which is also rather well confirmed by the calculation (\(E_\infty = -5.03\) versus \(\langle E \rangle(t \rightarrow \infty) = -5.04\)). The calculated overall time evolution of \(\langle E \rangle\) suggests a fit with a function of the same form as in (34), i.e.
\[
\langle E \rangle(t) = (E_0 - U_0 - E_\infty) e^{-\beta t} + E_\infty,
\]
(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

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

(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 ($\sigma_{pq}^0 = 0$), expression (44) can be analytically shown to simplify to

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

(45)

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

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

(46)

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

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

(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 $\sigma_p^0$ 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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