CC

IAEA LIBRARY
SUB 9479
IC/94/68

INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

CERN LIBRARIES, GENEVA

P00023041

ON THE (DE)-STABILIZATION OF QUANTUM MECHANICAL BINDING BY POTENTIAL BARRIERS

H. Hogreve

INTERNATIONAL
ATOMIC ENERGY
AGENCY

UNITED NATIONS
EDUCATIONAL,
SCIENTIFIC
AND CULTURAL
ORGANIZATION

MIRAMARE-TRIESTE

International Atomic Energy Agency
and
United Nations Educational Scientific and Cultural Organization
INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

ON THE (DE-)STABILIZATION OF QUANTUM MECHANICAL BINDING BY POTENTIAL BARRIERS

H. Hogreve
International Centre for Theoretical Physics, Trieste, Italy.

Abstract

Stabilization and destabilization effects caused by adding or rising a potential barrier are studied for a simple one-dimensional quantum system. Calculating the motion of the corresponding S -matrix poles for varying barrier width and height, this reveals the scenario for the transition between bound, virtual and resonance states. Our results show that the presence of a barrier leads to nonanalyticity of the ground state with respect to the involved coupling constants. Furthermore, for increasing barrier width the size of the virtual regime shrinks drastically, so that it might be hardly detectable in many practical situations.

MIRAMARE-TRIESTE
April 1994

Quantum Hamiltonians of the form $H(\lambda) = -d^2/dr^2 + V(r; \lambda)$ acting in $L^2(\mathbb{R}^+)$ and describing motion on the half-line $\mathbb{R}^+$ are commonly encountered after separation of multidimensional systems. Here V denotes a parameter dependent effective potential that we assume to be decomposable as $V(r; \lambda) = V_1(r) + V_2(r; \lambda)$ where V_2 represents a potential barrier, viz. $V_2(r; \lambda) = \lambda V_2(r; 0) \geq 0$ with $\limsup_{r \rightarrow \infty} V_2(r; \lambda) = 0$. If $V_2(r; \lambda)$ is sufficiently regular in r (including the endpoints $\lim_{r \rightarrow 0}$ and $\lim_{r \rightarrow \infty}$), then appropriate boundary conditions lead to a self-adjoint realization of H whose continuous spectrum is unchanged by the presence of the barrier, $\sigma_{\text{ess}}(H(\lambda)) = \sigma_{\text{ess}}(H(0))$, for all finite values $0 \leq \lambda < \infty$ of the coupling constant λ . Furthermore, let us suppose that the potential V_1 supports a bound state with energy $E(\lambda = 0) < 0$ and a nonvoid continuous spectrum, $\sigma_{\text{ess}}(H) \neq \emptyset$, where for convenience we shift the energy scale such that the threshold is placed at zero, i.e. $E_{\text{thr}} = \inf \sigma_{\text{ess}}(H) = \limsup_{r \rightarrow \infty} V_1(r) = 0$. Then, starting from 0, increasing λ is tantamount to rising the potential barrier, and – if classical theory were applicable – intuition would predict a stronger binding due to an enhanced confinement of the particle. However, since V_2 is nonnegative, quantum mechanically it is clear that increasing λ decreases the binding energy $|E(\lambda)|$. In fact, as long as $E \in \sigma_d(H)$, the Feynman - Hellmann theorem gives $E(\lambda_1) < E(\lambda_2)$ for $\lambda_1 < \lambda_2$. The fate of the bound state as $E(\lambda)$ approaches E_{thr} , yet, is a priori less clear. Assuming $E(0)$ close enough to E_{thr} , one may expect that for λ sufficiently large (but $\lambda < \infty$) the bound state is absorbed into the continuum, and, in some way, turned into a resonance. Obviously this is a destabilizing effect of the barrier. On the other hand, usually one also attributes the "creation" of some additional resonance levels (as e.g. $\mathcal{E}$ in Fig.1) to barriers. These higher lying levels are not necessarily the result of decayed bound states. Nevertheless, similar as those other resonance states they embody a metastable configuration of the system where initially the particle is quasibound, but finally escapes via tunneling through the barrier. These additionally induced quasibound states represent a stabilizing effect of the barrier.

Motivated by various concrete physical situations, as for instance the shape of Born - Oppenheimer potential energy curves for (multiply) positively charged diatomic molecular

ions [1,2] or the metastability of highly excited noble gas clusters [3], our aim here is to investigate in some detail the transitions between bound and resonance states that result from changing the barrier parameters. The general mechanism of analogous transitions was discussed previously in the context of the so-called "threshold behaviour" [4,5]. In particular, if $V \in C_0^\infty(\mathbb{R}^3)$ and if $E(\mu)$ is a (nondegenerate) eigenvalue of $H(\mu) = -\nabla^2 + \mu V$ that tends to zero as $\mu \downarrow \mu_0$, it was rigorously proved by Klaus and Simon [4] that either (A) $E(\mu) = O((\mu - \mu_0)^2)$ and 0 is not an eigenvalue of $H(\mu_0)$, but $E(\mu)$ can be analytically continued for $\mu \leq \mu_0$ and for $\mu > \mu_0$ the bound state turns into a virtual state; or (B) $E(\mu) = O(\mu - \mu_0)$ and 0 is an eigenvalue of $H(\mu_0)$; in this case, $E(\mu)$ is not analytic at $\mu = \mu_0$ since simultaneously a virtual state approaches 0 as $\mu \downarrow \mu_0$, colliding with the bound state at $\mu = \mu_0$ and producing a resonance pair for $\mu < \mu_0$. If in addition V is purely attractive, $V \leq 0$, then Klaus and Simon proved that the ground state E_1 always falls into class (A) and that $E_1(\mu) < 0$ is analytic on $0 < \mu < \infty$.

In this study we adopt the definition of virtual (or "antibound") states as being associated with real poles on the second ("unphysical") E -sheet of the S -matrix for H , whereas resonance states are associated with nonreal complex poles of $S(E)$. Mimicking arguments of Ref. [6], for the situation considered below it is possible to demonstrate rigorously the equivalence of bound state poles of $S(E)$ (i.e. real negative poles on the first sheet) with negative eigenvalues of the Hamiltonian H . Thus we have the disjoint decomposition of the set of S -poles

$$\mathcal{P}_S = \{E \in \mathbb{C} \mid S(k^2) \text{ has a pole at } E = k^2\} = \mathcal{P}_S^b \dot{\cup} \mathcal{P}_S^v \dot{\cup} \mathcal{P}_S^r \quad (1)$$

into the sets of bound, virtual, and resonance state poles, $\mathcal{P}_S^b = \{E^b \in \mathcal{P}_S \mid E^b \in \mathbb{R}_0^-, \exists \psi \in L^2(\mathbb{R}^+) : H\psi = E\psi\}$, $\mathcal{P}_S^r = \{E^r \in \mathcal{P}_S \mid E^r \in \mathbb{C} \setminus \mathbb{R}\}$, $\mathcal{P}_S^v = \mathcal{P}_S \setminus (\mathcal{P}_S^b \cup \mathcal{P}_S^r)$. For a discussion of the experimental significance of virtual and resonance states we refer to the textbooks by Newton [5] and Böhmer [6].

To avoid unnecessary technical complications, we study the arising (de)stabilization

effects on the simple one-dimensional model of a square well with barrier (cf. Fig.1), viz.

$$V(r; \gamma, \lambda, \Delta) = V_1(r; \gamma) + V_2(r; \lambda, \Delta) \quad (2)$$

where

$$V_1(r; \gamma) = \begin{cases} -\gamma, & r \in I_1 \\ 0, & r \in \mathbb{R} \setminus I_1 \end{cases} \quad \text{and} \quad V_2(r; \lambda, \Delta) = \begin{cases} \lambda, & r \in I_2 \\ 0, & r \in \mathbb{R} \setminus I_2 \end{cases} \quad (3)$$

and where we set $I_1 = [0, r_1)$, $I_2 = [r_1, r_2)$, $I_3 = [r_2, \infty)$. Thus the well depth is given by γ (by scaling arguments we can restrict our attention to unit length $r_1 = 1$), the barrier height by λ , and the barrier width by $\Delta = r_2 - r_1$. Imposing Dirichlet boundary conditions at $r = 0$, the Hamiltonian $H(\gamma, \lambda, \Delta) = -d^2/dr^2 + V(\cdot; \gamma, \lambda, \Delta)$ becomes a symmetric operator and a self-adjoint extension can be constructed on a certain domain $\mathcal{D}(H)$ [9]. Apart from rendering H not dilation analytic, the nonsmoothness of V has no influence on the effects discussed in the sequel. On the other hand, the simple form of V allows explicit expressions for the involved S -matrix and the pole conditions (that are, unfortunately, more complicated than those for a square well without barrier [8]).

Setting $E = k^2$ with $k \in \mathbb{C}$, the Schrödinger equation for H becomes

$$\left(\frac{d^2}{dr^2} - V(r) + k^2 \right) \psi(r) = 0. \quad (4)$$

Fundamental systems of solutions of Eq.(4) are given by $\{u_j^+, u_j^-\}$ where $u_j^\pm(r) = \exp(\pm i k_j r)$ and $k_1^2 = k^2 + \gamma$, $k_2^2 = k^2 - \lambda$, $k_3 = k$. Note that on I_3 the functions $u_3^\pm$ are identical to the so-called "irregular solutions" $f_\pm(k; r)$ [5]. The remaining part of $f_\pm(k; r)$ on $I_1 \cup I_2$ is obtained by matching with linear combinations of $u_j^\pm$ at r_j , $j = 1, 2$, in such a way that $f_\pm$ and its derivatives become continuous, $f_\pm \in C^1(\mathbb{R}^+)$. This leads to the Jost functions

$$\begin{aligned} \mathcal{F}_\pm(k) &:= f_\pm(k; 0) = \\ &= [(\cos k_1 \mp i k k_1^{-1} \sin k_1) \cos k_2 \Delta - (k_1 k_2^{-1} \sin k_1 \pm i k k_2^{-1} \cos k_1) \sin k_2 \Delta] e^{\pm i k} \end{aligned} \quad (5)$$

and thus to an explicit S -matrix $S(k) = \mathcal{F}(k)_- / \mathcal{F}_+(k)$. From Eq.(5) it is clear that $\mathcal{F}_\pm$ and therefore also S depend on k_1 and k_2 as even functions; hence branching singularities

for $S(k)$ are excluded and the only possible singularities of $S(k)$ are poles determined by $\mathcal{F}_+(k) = 0$. Furthermore, since $\bar{S}(k) = S(-\bar{k})$, resonance poles come in pairs and pole searching can be restricted to e.g. the region $\text{Re}(k) \geq 0$. Straightforward manipulations recast the condition $\mathcal{F}_+(k) = 0$ into

$$(k_1 + k_2)^2(k_1 \cos k_1 - i k_2 \sin k_2) - \gamma(k_1 \cos k_1 + i k_2 \sin k_2)e^{2ik_2\Delta} = 0 \quad (6)$$

with $k_1 = \sqrt{k^2 + \gamma}$, $k_2 = \sqrt{k^2 - \lambda}$. Finally, separating real and imaginary parts turns Eq.(6) into a system of transcendental equations (that reduces to a single equation if there is no barrier) for the two unknowns $\text{Re}(E)$ and $\text{Im}(E)$. To solve this system numerically, we devised a kind of two-dimensional bracketing procedure. Below, we shall restrict our considerations to the motion of S -poles on the sheets of the energy surface (an extended discussion covering also the pole trajectories on the k -plane can be found in Ref.[10]). More specifically, the main questions that will concern us here are: (i) To which extent does the general transition scenario outlined above continues to hold for variations of the barrier parameters λ and Δ ? (ii) In particular, does the ground state still plays its special role in having no transitions to a resonance state? (iii) Are there some universal stabilization schemes of resonance states for increasing barriers? In question (iii) we mean by stabilization of resonances $E \in \mathcal{P}_S^r$ a decreasing imaginary part $|\text{Im}(E)|$ as function of the barrier parameters. Such a definition is suggested by the interpretation of $|\text{Im}(E)|$ as being inversely proportional to the lifetime of the considered resonance.

Turning first to questions (i) and (ii), one might expect an affirmative answer to (i), since the same type of arguments employed in Ref.[4] remain valid if applied to operators of the form $H_0 + V_2(\lambda, \Delta)$ (at least for smooth potentials) but where $H_0 = -\nabla^2$ is replaced by $H_0 = -\nabla^2 + V_1(\gamma)$ with $V_1 \leq 0$. However, since the nonpositivity of the potential was essential for those special properties of the ground state proved by Klaus and Simon, doubts on (ii) seem to be justified. In Fig.2 we consider the destabilization of the ground $n = 1$ and of the first excited state $n = 2$ with $\gamma = 5$ and $\gamma = 28$, respectively, for various barrier widths. Indeed, for the ground as for the excited state we find three different

regimes in λ . If $\lambda \in [0, \lambda_{bv}^c]$, i.e. in the first regime, the barrier being below its critical height $\lambda_{bv}^c(\gamma, \Delta; n)$, the exposed poles represent bound states whose energies are plotted as solid lines in Fig.2. If $\lambda > 0$ in this regime, we found for both states always a (bound, virtual)-pole pair, although in Fig.2 we only include its bound state part. At λ_{bv}^c , the bound state energies are passing through the branch point $E = 0$ (that is actually not a pole of S because at $E = 0$ also the nominator $\mathcal{F}_-$ of S vanishes, cf. [8]) and then continue on the negative real axis of the second sheet as virtual state energies. In this virtual regime, $\lambda \in (\lambda_{bv}^c, \lambda_{vr}^c]$, we have a (virtual, virtual)-pole pair whose energies are always negative and approaching each other for growing λ ; in particular, the energy of the decayed bound state decreases monotonically. This is most clearly seen in the magnifications of the energy curves displayed for $\Delta = 0.5$ in the inserts of Fig.2, where the virtual energies on the second sheet are represented by dash-dotted lines. For $\lambda = \lambda_{vr}^c$, both virtual energy poles are colliding at an $E_n(\lambda_{vr}^c)$ still on the negative real axis. When the barrier height exceeds the critical value $\lambda_{vr}^c(\gamma, \Delta; n)$ (but remains finite), we are in the regime of resonance states characterized by (resonance, resonance)-pole pairs with complex E values. In Fig.2 we depict the real parts $\text{Re}(E)$ of the poles $E \in \mathcal{P}_S^r$ as dashed curves and their imaginary parts $\text{Im}(E)$ as dotted lines (the "capture state" [7] counterparts of E located symmetrically on the the upper half-plane of the second sheet are not shown). Starting always at zero for $\lambda = \lambda_{vr}^c$, for λ just above λ_{vr}^c the imaginary energies $\text{Im}(E)$ decrease more or less distinctly (depending on the barrier width) before this tendency is reversed and the $\text{Im}(E)$ approach zero as $\lambda \rightarrow \infty$. This implies that also in the resonance regime the destabilization effect of the barrier persists until the barrier has achieved a certain height; raising λ further results in a stabilization of the state in the sense defined above. The real parts $\text{Re}(E)$ of the resonance energies start at negative values where they match continuously the collided virtual energies at λ_{vr}^c (indicated by dots in Fig.2); then the $\text{Re}(E)$ increase monotonically with λ (at least for those states included in Fig.2; cf. however Fig.5) with approximately the same speed as the bound state energies before. As a consequence of this behaviour a somewhat counterintuitive picture emerges, namely for λ in a small vicinity above λ_{vr}^c

the corresponding $\text{Re}(E)$ level is negative and must be drawn below the threshold energy $E_{\text{thr}} = 0$ in Fig.1.

Fixing the barrier height λ but varying instead the width Δ leads to the same transition sequence bound $\rightarrow$ virtual $\rightarrow$ resonance as found for increasing λ . For the corresponding trajectories of the resonance poles we refer to Fig.3. Also in this case the $\text{Im}(E)$ pass through a minimum that becomes deeper and is shifted towards smaller Δ for increasing heights λ . In particular for larger λ , as the barrier becomes wider, both, $\text{Re}(E)$ and $\text{Im}(E)$ tend rather rapidly to their asymptotic values, $E_n(\gamma + \lambda)$ and 0, respectively (here $E(\gamma + \lambda)$ denotes the n th energy level for the square well Hamiltonian with potential $V(r; \gamma + \lambda, 0, 0)$). Obviously $\text{Re}(E)$ and $\text{Im}(E)$ depend more sensitively on Δ than on λ , a property becoming even more pronounced in semiclassical situations. This can likewise be inferred from the boundary curves for larger Δ in Fig.4 where (λ, Δ) -stability portraits are displayed for the $n = 1, 2$ states. As a consequence, already for moderate barrier widths the computational detection of the virtual regime may become a difficult task. The tinniness of the virtual regime must also be the reason that no virtual energies were observed in the transitions of vibronic levels during the deformation of molecular potential energy curves [1].

Fig.5 depicts complex resonance pole trajectories as λ increases from 0 to ∞ , i.e. interpolates between the situations of a finite and infinite square well. In the latter case, the Hamiltonian is decoupled, $H = H_{\text{in}} \oplus H_{\text{out}}$, with the inner Hamiltonian H_{in} describing the infinite well and the outer one H_{out} a free motion on $[1 + \Delta, \infty)$. Since H_{in} has only pure point spectrum $\sigma(H_{\text{in}}) = \{(n\pi)^2 - \gamma \mid n \in \mathbb{N}\}$ and H_{out} only continuous spectrum $\sigma(H_{\text{out}}) = \mathbb{R}_0^+$, for $\lambda = \infty$ all resonances died out and all pole trajectories have to end up on the real axis of the first sheet. Displayed in Fig.5 are six low-lying states, some of the trajectories for the lowest n being not included due to their smallness on the scale of Fig.5. Among those resonances shown, two trajectories have apparently no starting points. More precisely, for $n = 3, 6$ if $\gamma = 5$ or $n = 4, 6$ if $\gamma = 28$, the $\text{Im}(E) \rightarrow -\infty$ on the second sheet as $\lambda \rightarrow 0$. These resonances are obviously created by the barrier and usually termed

"barrier top resonances" (at least for sufficient barrier height when they are close to the real axis). Contrasting the situation without well, where for growing barrier height the $\text{Re}(E)$ of such resonances also increases without limit [8], here for $\lambda \rightarrow \infty$ the respective trajectories tend to the corresponding energy levels of the infinite well. Although the local shape of the trajectories in Fig.5 looks rather nonuniform (note, for instance, the initial decrease of $\text{Re}(E)$ with λ for some curves), on a larger scale one can recognize common characteristics. Starting with $\lambda = 0$, after an initial region with possibly decreasing $\text{Im}(E)$, the trajectories pass through a region of rapid increase of $\text{Im}(E)$ until they reach a kind of plateau. In this plateau region, the curves being not too far away from the real axis, now the real parts $\text{Re}(E)$ grow further while the $\text{Im}(E)$ tend more slowly towards zero. A final region is entered when the $\text{Im}(E)$ are very close to the real axis and is characterized by an even slower decay of the $\text{Im}(E)$. This crude classification for the trajectories implies a corresponding one for the stability behaviour, i.e. for rising barrier height an initial region of possible destabilization is followed by three regions of fast, moderate and slow stabilization of the resonance states. Note that there is no correlation between these regions and a "trapping" of the resonance level behind the barrier, i.e. there is no faster stabilization if $\text{Re}(E(\lambda)) < \lambda$.

As mentioned above, Klaus and Simon [4] proved the behaviour $E(\mu) = O((\mu - \mu_0)^2)$ as $\mu \downarrow \mu_0$ for their case (A) of a transition bound $\rightarrow$ virtual at μ_0 . Similarly, in our situation we observe $E(\lambda) = O((\lambda - \lambda_{\text{bv}}^c)^2)$ if $\lambda \rightarrow \lambda_{\text{bv}}^c$ (from any side) and Δ remains fixed. For $\lambda \uparrow \lambda_{\text{vr}}^c$ and constant Δ we obtain $E(\lambda) = O(\lambda - \lambda_{\text{vr}}^c)$. If $\lambda \rightarrow \infty$, then $\text{Re}(E(\lambda)) - E(\infty) = O(\lambda^{-1})$ and $\text{Im}(E(\lambda)) = O(\lambda^{-1})$ where $E(\infty)$ stands for the corresponding energy level in $\sigma(H_{\text{in}})$. Keeping λ fixed and varying Δ , for $\Delta \rightarrow \infty$ the square well limits are approached exponentially in Δ ; otherwise the behaviour around the transition points Δ_{bv}^c and Δ_{vr}^c is completely analogous to the corresponding λ -transitions. These approach speeds can be extracted from our numerical data and can also be confirmed by lengthly but straightforward expansions of Eq.(6) around the transition points [10].

Finally, let us summarize those aspects of our findings that are most relevant to the

questions (i) - (iii) posed before.

(i) If for $\lambda = 0$ the energy of any (ground or excited) bound state is close enough to the threshold E_{thr} , then for increasing $\lambda \in [0, \infty)$ this state passes through the transition sequence bound $\rightarrow$ virtual $\rightarrow$ resonance. Such a process was also seen for a model consisting of an attractive (Dirac) δ interaction in front of a step potential [12], but differs from the case of barriers caused by a centrifugal term $U_\ell(r) = \ell(\ell + 1)r^{-2}$ with $\ell > 0$ where the virtual regime is completely absent from the transition sequence [4,5,11]. In contrast to our results for $\ell = 0$, the $\ell > 0$ barriers induce a direct transition bound $\rightarrow$ resonance when a (bound, virtual)-pole pair collides at E_{thr} [5]. However, both situations $\ell = 0$ and $\ell > 0$ are not directly comparable since for $\ell > 0$ the domain of the Hamiltonian is no longer identical to the one for $\ell = 0$. Indeed, the r^{-2} singularity of U_ℓ requires different boundary conditions at $r = 0$ to produce a self-adjoint Hamiltonian. Moreover, the r^{-1} tail of U_ℓ for $r \rightarrow \infty$ allows bound states at the threshold E_{thr} . Recalling another important outcome of our computations, viz. the observed drastic diminution of the virtual regime for widening barriers, obviously the $\ell > 0$ barriers do succeed in what finite barriers could never achieve, i.e. in shrinking the virtual regime to zero.

(ii) The special role of the ground state in having never a resonance transition for purely attractive potentials is eliminated by the presence of barriers. If $V_2 > 0$, the transition sequence of the ground state looks like all the other ones: For $\lambda \in [0, \lambda_{\text{bv}}^c)$, it enjoys a (bound, virtual)-pole pair turning into a (virtual, virtual)-pair for $\lambda > \lambda_{\text{bv}}^c$ and afterwards into a (resonance, resonance)-pair if $\lambda_{\text{vr}}^c < \lambda < \infty$. Hence, if the potential contains barriers, in general the ground state energy is no more an analytic function of λ (and thus theorem 2.3 of Ref.[4] cannot be extended to such V). This fact may be of interest for related analyticity questions, as e.g. the analyticity of the ground state of the three-dimensional square well (originally pointed out by Stillinger [13]) opposed to the singularity of the ground state energy of the atomic helium Hamiltonian $-\nabla_1^2 - \nabla_2^2 - r_1^{-1} - r_2^{-1} + \lambda|r_1 - r_2|^{-1}$ studied by Baker *et al* [14] (note that $|r_1 - r_2|^{-1}$ is actually a kind of barrier term).

(iii) As a consequence of the Feynman - Hellmann theorem, for increasing λ all bound

states are destabilized because their binding energies decrease. If already for $\lambda = 0$ the binding energy is sufficiently small, a more drastic destabilization follows via the transition sequences described above. Virtual states are destabilized by moving their poles farther away from E_{thr} . In the resonance regime, if a resonance pole is "born" at λ_{vr}^c , then for λ slightly above λ_{vr}^c this resonance is also destabilized due to an initial increase of $|\text{Im}(E)|$. For (further) growing λ and for the other resonances, depending on the respective portion of the pole trajectory (determined by the actual λ), either a rapid, moderate, or slow stabilization occurs. Another kind of stabilization effect results from additional ("barrier top") resonances as soon as a barrier is added. The ultimate step of stabilization for all resonances is reached in the limit $\lambda \rightarrow \infty$ where their poles converge to the respective energy levels of the infinite square well. Analogous transitions and (de)stabilization phenomena (but with an enhanced parameter sensitivity) can be observed for variations of the barrier width Δ . Moreover, tracking down the behaviour of the S -pole trajectories, we encountered situations not covered by standard text book pictures, as for resonances for which $\text{Re}(E)$ (including its surrounding "uncertainty width" $\text{Im}(E)$) lies below the threshold E_{thr} .

Although here we restricted our analysis to variations of barrier parameters for fixed well depths, it is equally interesting – from a more general [15] as well as from a physical [1] point of view – to explore systems where simultaneously the well depth and barrier height (or width) change, or, for fixed barriers, the well depth $-\gamma$ is raised from negative to positive values. This, however, goes beyond the scope of the present study and will be discussed in Ref.[10].

Acknowledgments

Clarifying questions by Dr. H. Schlereth, Trieste, hints by Dr. W. Knop, Zürich, and by Dr. H. Zewdie, Addis Abeba, for improving the graphics, and the kind hospitality of Professor Abdus Salam, the scientific and staff members of the CM section of the ICTP, the IAEA and UNESCO are gratefully acknowledged.

References

- [1] J. Ackermann and H. Hogreve, J. Phys. B **25** (1992) 4069; H. Hogreve, J. Chem. Phys. **98** (1993) 5579
- [2] H. Hogreve, J. Chem. Phys. **96** (1991) 3010; J. Ackermann and H. Hogreve, Chem. Phys. Lett. **202** (1993) 23
- [3] E.E. Ferguson, C.R. Albertoni, R. Kuhn, Z.Y. Chen, R.G. Keesee, and A.W. Castleman, J. Chem. Phys. **88** (1988) 6335; C.R. Albertoni, A.W. Castleman, and E.E. Ferguson, Chem. Phys. Lett. **157** (1989) 159
- [4] M. Klaus and B.Simon, Ann. Phys. (N.Y.) **130** (1980) 251
- [5] R.G. Newton, Scattering theory of waves and particles, 2nd edition, Springer, New York, 1982
- [6] M. Reed and B. Simon, Methods of Modern Mathematical Physics III, Scattering Theory, Academic Press, New York, 1979
- [7] A. Böhm, Quantum mechanics, Springer, New York, 1979
- [8] H.M. Nussenzveig, Nucl. Phys. **11** (1959) 499; H.M. Nussenzveig, Causality and dispersion relations, Academic Press, New York, 1972
- [9] K. Jörgens and F. Rellich Eigenwerttheorie gewöhnlicher Differentialgleichungen, Springer, Berlin, 1976
- [10] H. Hogreve, (to be submitted)
- [11] A.O. Barut and F. Calogero, Phys. Rev. **128** (1962) 1383; C.G. Bollini and J.J. Giambiagi, Nuovo Cimento **28** (1963) 341; P. Kraus and C.J. Pearson, Nuovo Cimento **28** (1963) 500; Y.M. Lomsadze, I.V. Khimich, and J.M. Shuba, Nucl. Phys. **67** (1965) 631
- [12] P.J. Hofstee, H.G.Muller, and A.Tip, J. Phys. A **22** (1989) 2667
- [13] F.H. Stillinger, Phys. Rev. A **15** (1977) 806
- [14] D.E. Freund, B.D. Huxtable and J.D. Morgan III, Phys. Rev. A **29** (1984) 9801
- [15] P. Duclos, A global approach to the location of quantum resonances, p.39 - 53 in: Operator calculus and spectral theory, eds. M.Demuth, B.Grams, B.W.Schulze, Birkhäuser, Basel, 1992

Figure captions

- Fig.1** Potential of the considered model consisting of a (unit) well with coupling constant γ and a barrier of width Δ with coupling constant λ .
- Fig.2** Energy poles of the S -matrix determined by Eq.(6) for three different barrier widths $\Delta = 0.3, 0.5$, and 1.0 . Solid curves indicate real energies corresponding to bound states (viz. the ground state $n = 1$ for $\gamma = 5$ and the first excited state $n = 2$ for $\gamma = 28$) or virtual states. Real parts of complex poles are plotted as dashed lines, imaginary parts as dotted curves. The inserts magnify those regions for the $\Delta = 0.5$ curves where the transition from a bound to a virtual (dashed dotted lines) and finally to a resonance pole occurs. Magnifications of the corresponding transition regions for the $\Delta = 0.3$ and 1.0 curves look similar.
- Fig.3** Resonance energy poles of the S -matrix on the second sheet of the E -surface for various λ as a function of the barrier width Δ . As in Fig.2, the $\text{Re}(E)$ are represented by dashed, the $\text{Im}(E)$ by dotted curves. Again, the curves for $\gamma = 5$ emerge from the ground state $n = 1$, and those for $\gamma = 28$ from the first excited state $n = 2$.
- Fig.4** Stability portrait (in doubly logarithmic scale) on the (Δ, λ) -parameter plane for the ground state (if $\gamma = 5$) and first excited state (if $\gamma = 28$). The tiny region between the curves corresponds to the regime of virtual states.
- Fig.5** Curves of resonance poles of the S -matrix on the second sheet of the E -surface for λ varying from 0 to ∞ . Dashed curves indicate "barrier top" resonances. The added symbols signify different λ values: $\bullet \lambda = 0$; $\circ \lambda = 10$; $\diamond \lambda = 50$; $\square \lambda = 100$; $\times \lambda = \infty$.

Fig.1

Fig.2

Fig.3

Fig.4

Fig.5