General properties of the spectrum of complex scaled Hamiltonians: Detachment point and localization threshold

H. Lehr and C. A. Chatzidimitriou-Dreismann
I. N. Stranski-Institute for Physical and Theoretical Chemistry, Technical University of Berlin, Strasse d. 17 Juni 112, D-10623 Berlin, Federal Republic of Germany
(Received 21 October 1994)

In this paper we concentrate on the most prominent points describing string curves: the detachment point and the localization threshold. We show that the detachment point is identical to the potential height for symmetric potentials and to the lowest barrier height in the general asymmetric case. Furthermore, we show that the existence of a detachment point is due to spectral concentration at the barrier top. Concerning the localization threshold, we show that the localization properties alter drastically at this point; the classical mechanism of a particle being trapped between potential barriers breaks down at this point. We then derive a condition for the existence of the localization threshold in the framework of the Wenzel-Kramers-Brillouin method and consider the dependence of the localization threshold on physical potential parameters; it is shown that there is no simple correspondence of the localization threshold to such parameters, since the localization threshold also depends on the explicit analytical form of the potential.

PACS number(s): 34.10.+x, 03.65.Nk, 11.55.Fv, 11.55.Bq

I. INTRODUCTION

In a recent publication [1], we started a discussion on the phenomenological description of string curves of complex scaled (one-dimensional) Hamiltonians (for an introduction to complex scaling, see, e.g., [2–7]; the original references are [8–10]). By a string curve we mean the set of poles connected by a suitable curve, not just the set of poles. The definition can be grasped most easily in the framework of the Wenzel-Kramers-Brillouin (WKB) — or phase integral — approximation [11], which was given by Korsch earlier [12],

$$\mathfrak{N} \equiv \frac{1}{\pi}\int_t^{t'} q(z)\,dz - \frac{1}{2} \in \mathbb{R}, \tag{1}$$

where the functional form of $q(z)$ depends on the order of approximation used. In the first order it is given by (we are using atomic units throughout, so $\hbar = 1$)

$$q(z) = \sqrt{2\mu[E - V(z)]}, \tag{2}$$

where E is complex (for physical reasons $\mathrm{Im}(E) \leq 0$) and $V(z)$ is the analytical continuation of the potential into the complex plane (μ is the mass of the system). Higher order approximations can be found using either higher order WKB approximations or the phase integral method [11]. The function $\mathfrak{N}$ coincides with the quantum number when it is an integer; it has been called "quantum number function" [12]. We refrain from using this term because the possibility of extending the quantum number operator to real or even complex values is uncertain. At those points, i.e., where $\mathfrak{N}$ is an integer, Eq. (1) reduces to the (generalized) Bohr-Sommerfeld formula

$$\int_t^{t'} q(z)\,dz = \pi\left(n + \frac{1}{2}\right). \tag{3}$$

Some comments concerning Eq. (1) seem appropriate: First of all, the integral extends from one so-called *transition point* t to another point t'. (Transition points are points in the complex plane where $q^2(z)$ is zero; see Fig. 1.) In the case of a symmetric potential, one may alternatively use zero as the lower and t' as the upper limit (a factor of 2 has to be included, naturally). Second, the formula is trivially applicable only when no more than a pair of transition points is relevant. In terms of the general description of strings, one can say the following: Eq. (1) is applicable above the *detachment point* and, in the case of a wiggly irregular part, up to the *localization threshold*, if t' is chosen to be identical to t_2 of Fig. 1. The terms detachment point and localization threshold have been introduced in Ref. [1]. In order to facilitate the discussion we briefly repeat the terminology here. In Fig. 2, two typical strings for double barrier single well potentials are depicted. Up to a certain point that we call the *detachment point*, the strings stay very close to the real axis, while after that point they move rapidly away from it. It is one of the purposes of the present paper to "prove" this statement. Beyond the detachment point comes a portion of the string where the imaginary energy grows with increasing real energy, just as one would expect. From a certain point on, namely, the *localization threshold*, the situation is reversed. In Fig. 2(a) one sees that the imaginary energy grows with decreasing real energy in a very smooth fashion. In Fig. 2(b), on the other hand, one sees a more complicated interdependence of real and imaginary energy. We call the portion of the string up to the localization threshold the *regular* part of the string, while the one following it is called *irregular*. The irregular part of Fig. 2(a) is, for obvious reasons, called *smooth*, while that of Fig. 2(b) is called *wiggly*, as is customary in the literature [12–17]. It is one of the main objectives of this paper to show that at the localization threshold the localization properties change:

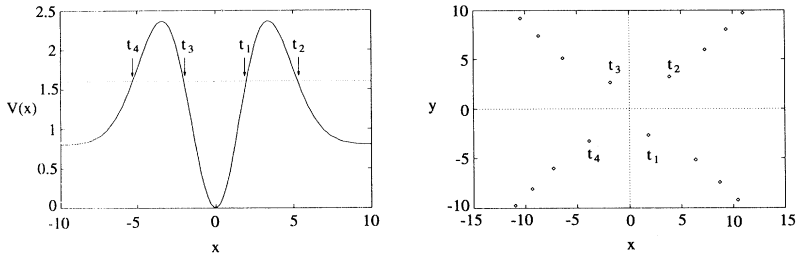

FIG. 1. A typical double barrier potential and the distribution of the transition points. In the left-hand part of the figure one sees the potential together with the four classical turning points labeled $t_1 - t_4$ for a real energy below the barrier height. On the right-hand side part of the complex z plane is depicted. The points correspond to zeroes of the function q^2 for a complex eigenenergy of the potential with real part above the barrier height. One observes that the transition points have moved now into the complex plane. Note also that there are additional zeroes, which have no analogue on the real axis.

Before the localization threshold, one has — as is to be expected — localization within the attractive region of the potential, while after it ("after" refers to quantum numbers higher than that of the localization threshold) localization is greatest *beneath* the barriers. We suspect that those eigenvalues correspond to retarded backscattering; cf. Sec. III.

So, to return to the discussion of Eq. (1), it is appropriate to mention the following: The string curve (*not* the individual poles) is mass independent above the detachment point and — for wiggly types of string — up to the localization threshold, as we showed in Ref. [1]. For smooth types the whole string is mass independent above the detachment point. This is consistent with the WKB analysis, as can be seen from the following. It is obvious that Eq. (1) or (3) predicts zero imaginary parts for real parts of the energy below the potential height, i.e., when t' is chosen to be t_1. Therefore, the application of Eq. (1) or (3) is invalid below the detachment point; this is a well known fact in WKB theory. One knows that — whenever the transition points are connected by Stokes' lines [on which $q(z)dz$ is purely imaginary] — one has to use a more general formula,

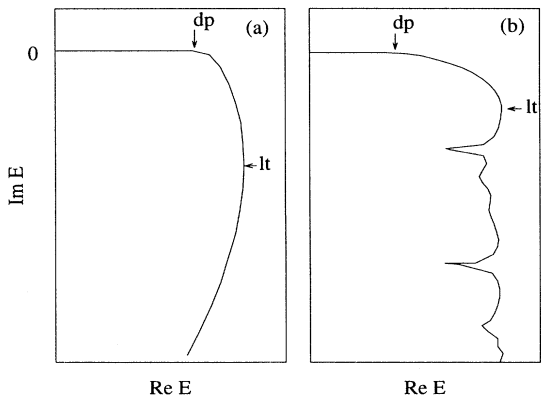

FIG. 2. Two of the most common string curves. (a) shows a smooth string curve, while (b) shows a wiggly string curve. Indicated in the figure are the detachment point (dp) and the localization threshold (lt). See text for further details.

$$\mathfrak{N} \equiv \frac{1}{\pi}\alpha - \frac{1}{2\pi}\left[\epsilon - \epsilon\ln(-\epsilon)\right] + \frac{i}{2\pi}\ln\left[\frac{\sqrt{2\pi}\exp(\frac{1}{2}\pi\epsilon)}{\Gamma(\frac{1}{2} - i\epsilon)}\right] - \frac{1}{2}, \tag{4}$$

(Γ denotes the Γ function) where, for symmetric potentials,

$$\alpha = \int_0^{t_1} q(z)\,dz$$

and

$$\pi\epsilon = -i\int_{t_1}^{t_2} q(z)\,dz$$

(see again Fig. 1 for a definition of t_1 and t_2). This formula has been derived by Connor [18] and used to determine energies and lifetimes of resonances [19,20]. As one can see from Eq. (4), the function $\mathfrak{N}$ depends not only on the integral inside the attractive region of the potential, but also on the integral over the barrier. Therefore, for the energy even below the detachment point, the solution to this equation yields complex numbers quite different from Eq. (1) or (3). One also observes that the condition $\mathrm{Im}\mathfrak{N} = 0$ is now a function of mass also, just as is observed in calculations (not of WKB type) using, e.g., the Fourier grid Hamiltonian method [21,22] or direct numerical integration [23–25].

For a wiggly string above the localization threshold, Andersson [26] has shown that in order to obtain results consistent with those of direct numerical integration (and other methods not using the WKB approximation) obtained first by Rittby, Elander, and Brändas [14], one has to include more than one transition point (more than one pair if one disregards symmetry of the potential). He therefore ended a long discussion about the existence of wiggles, which had been started by Korsch, Laurent, and Möhlenkamp [13], who doubted the results of Rittby, Elander, and Brändas. Korsch included in his WKB calculation only one pair of transition points and consequently found a smooth string. In our terms his findings can be explained in the following manner:

The correct wiggly part of the string is mass dependent, while a smooth irregular part is not. He used essentially Eq. (1), which is obviously mass independent, and therefore found a smooth string. Now, upon inclusion of more than one transition point, Eq. (1) for a symmetric potential reads

$$\mathfrak{N} = \ln\left(\sum_{r=1}^{N} e^{4i\alpha_{0r}}\right) \in \mathbb{R}, \tag{5}$$

with

$$\alpha_{0r} = \int_0^{t_r} q(z)\,dz \tag{6}$$

where N is the number of the relevant transition points t_r in the first quadrant of the complex z plane. Equation (5) simply follows from the outgoing wave boundary condition embedded in the WKB formalism [17,26].

Another word on the selection of the relevant transition points is in order. Below the potential height V_0 the choice is obvious: For a double barrier potential all four transition points have to be included. For energies above V_0 one gets correct results when using (for symmetric potentials) the transition point that lies in the first quadrant of the complex plane. This point corresponds — speaking analogously — on the real axis to the *outer* transition point. The "inside" transition points (that are important solely for bound states) completely lose importance. This is also true for the "outer" ones at the localization threshold. Andersson has shown that soon after the localization threshold, the correct results can be obtained using the next (few) transition points only. It should be noted that the latter have no analogue on the real axis. To give an example of the above described behavior, we show in Table I imaginary parts of integrals α_{ij} for $V(x) = (ax^2 + bx)e^{-x^2}$ $(a = 9.9467, b = 3.7300, \mu = 70.0)$. This potential is asymmetric and, following [1], therefore has a composite string curve with two irregular parts, of which one begins at the higher barrier height. One sees from the table that the resonances below the lower barrier top can be understood (approximately) by searching $\mathrm{Im}\alpha_{31} = 0$ (these are the innermost turning points). Then we are in a region where the real part of the energy is above one of the barrier heights but below the other. Consequently, approximations to the correct eigenvalues are found by including the next turning point on *this side*, i.e., t_4. An analoguos situation comes about, when we cross the higher potential height. Eigenvalues above that can be described by a simple Bohr-Sommerfeld formula using the outermost turning points. The second irregular part, on the other hand, since — as we argued in [1] (see also [27]) — it corresponds to a different irreducible unit of the potential, is found by looking at $\mathrm{Im}\alpha_{12}$, i.e., the integral over the higher barrier. In this context our general description of string curves in the WKB framework might also be of interest [1]. One sees from this that in the different parts of the string curve different turning points have to be considered relevant.

After these preliminary remarks, we now proceed in Sec. II to deal with the detachment point. Section III considers the localization threshold, and in Sec. IV we summarize our findings.

II. THE DETACHMENT POINT

As we have described above and in Ref. [1], the pole string corresponding to a double barrier potential stays

TABLE I. The first 17 resonances of the asymmetric potential $V(x) = (ax^2 + bx)e^{-x^2}$ $(a = 9.9467, b = 3.7300, \mu = 70.0)$ calculated using the complex scaled Fourier grid Hamiltonian (CSFGH) method [22] with basis set size 701 and $-6 \geq x \geq 6$. Also shown are the imaginary parts of integrals α_{ij} for different i and j. The lower barrier height is 2.367 and the higher 5.084 hartree. The two separated resonances m=16 and 17 belong to the additional irregular part (see [1] for an extensive discussion). Eigenvalue 13 cannot be interpreted using a simple Bohr-Sommerfeld formula; here a more general ansatz has to be used. The parameter m does not represent a quantum number. The numbering of the turning points follows Fig. 1. To facilitate the discussion, α_{ij}'s being close to zero are in boldface type.

m	Re(E)	Im(E)	Imα_{31}	Imα_{41}	Imα_{12}	Imα_{42}
1	0.4335	-0.0000	**-0.0000**	-3.1388	5.7881	2.6493
2	0.9175	-0.0000	**-0.0000**	-1.4705	4.0219	2.5514
3	1.3722	-0.0000	**-0.0000**	-8.5835	-20.4931	-29.0771
4	1.7920	-0.0000	**-0.0000**	-4.7808	-21.7472	-26.5280
5	2.1631	-0.0010	**-0.0092**	-1.6591	-19.8470	-21.5064
6	2.4560	-0.0397	-0.7496	**-0.0478**	-17.5734	-17.6213
7	2.7362	-0.1747	-2.8786	**0.0019**	-15.4660	-15.4642
8	3.0497	-0.3502	-5.2572	**-0.0030**	-13.1691	-13.1724
9	3.3862	-0.5442	-7.7360	**-0.0031**	-10.7702	-10.7732
10	3.7451	-0.7480	-10.3023	**-0.0015**	-8.2835	-8.2851
11	4.1289	-0.9546	-12.9610	**0.0009**	-5.7044	-5.7034
12	4.5430	-1.1579	-15.7351	**0.0038**	-3.0121	-3.0083
13	4.9892	-1.2806	-18.1722	0.4180	-0.2466	0.1714
14	5.0578	-1.4371	-19.4074	-0.3120	0.2428	**-0.0692**
15	5.2500	-1.7470	-22.0030	-1.5563	1.5527	**-0.0035**
16	5.0794	-0.2613	-11.6332	7.1934	**-0.0121**	7.1812
17	5.0617	-0.7841	-15.2491	3.5793	**-0.0120**	3.5673

very close to the real axis below a certain value that we called *detachment point*. In fact, this is valid for every potential that provides an attractive region plus adjacent barriers, i.e., also for potentials that have single barriers or a wall (barrier of infinite height) on one side in addition to a well. In short, there must be simply a possibility of localization. If this is not the case (e.g., for simple Gaussian barriers) there are no complex eigenvalues below the detachment point; the latter coincides in those cases with the localization threshold [1].

The question that naturally arises in this context is whether the detachment of the string from the real axis is a continuous process. If not, one may with good reason find a "point" where the string detaches.

An instructive quantity here is the second derivative of the imaginary part of the energy with respect to real energy. Some words of explanation may be appropriate: What we search for is a point where the string detaches, i.e., a point beyond which the imaginary part of the energy grows much more rapidly than below it. Therefore, the first derivative with respect to real energy should exhibit a different slope of the "curve" below and above the detachment point. This again means that we should find a very characteristic behavior around this point in the second derivative: Either the slope changes discontinuously, in which case we will find a peak, or the transition is continuous but not differentiable, which will give a discontinuous transition in the second derivative (just as in the derivative of $|x|$). In Fig. 3 we show the second derivative approximated by

$$\frac{d^2\mathrm{Im}(E_n)}{d[\mathrm{Re}(E_n)]^2} \approx \frac{\mathrm{Im}(E_{n+2}) - 2\,\mathrm{Im}(E_{n+1}) + \mathrm{Im}(E_n)}{\mathrm{Re}(E_{n+2} - E_{n+1})\mathrm{Re}(E_{n+1} - E_n)} \quad (7)$$

for three different masses for the potential

$$V(x) = \left(\frac{1}{2}x^2 - J\right)e^{-\alpha x^2} + J \quad (8)$$

(with $J = 0.8$ and $\alpha = 0.1$), which has been used extensively in the literature [13–15,26,28,29]. We have chosen rather high masses in order to get a denser set of eigenvalues around the detachment point. Please observe that the value of 2.36 Hartree is exactly the height of the potential above the threshold. We found basically the same result, namely, identical values of detachment point and V_0 for every (symmetric) potential that we checked. To give at least an example, we have chosen three different potentials from three different families, namely,

$$V_1(x) = -x^3 + ax^2 \quad \text{with} \quad a = 2.5188,\ \mu = 150.0,$$
$$V_2(x) = bx^2 \cdot e^{-\alpha x} \quad \text{with} \quad b = 4.3733,\ \alpha = 1.0,\ \mu = 60.0,$$
$$V_3(x) = (\tfrac{1}{2}x^2 - J)e^{-\beta x^2} + J$$
$$\text{with} \quad J = 0.8,\ \beta = 0.1,\ \mu = 100.0. \quad (9)$$

(Please note that polynomial potentials such as $V_1(x)$ are not dilatation analytic in the strict sense, so the theorems underlying complex scaling [8–10] do not apply. Nevertheless, it is known that potentials of this type can have stable complex eigenvalues and we have recently given support to the fact that one can indeed identify them as resonances [30].) All of the above have one thing in common: The potential height above V_0 is at 2.367 43 Hartree. Apart from keeping this constant, we have tried to change everything else. So $V_1(x)$ has a threshold at $-\infty$ (see, however, [30]), while that of $V_2(x)$ is at zero and that of $V_3(x)$ is at 0.8 hartree. The analytical form is completely different, the masses (although they do not have any influence) are different and same is true for other parameters such as barrier thickness, etc. As must be concluded from Fig. 4, they nevertheless have the same detachment point, which in turn is identical to V_0. So we conclude that for symmetric potentials the detachment point is identical to the height of the potential above the threshold.

Let us turn now to the question of asymmetric potentials. As one might suspect — especially after the last

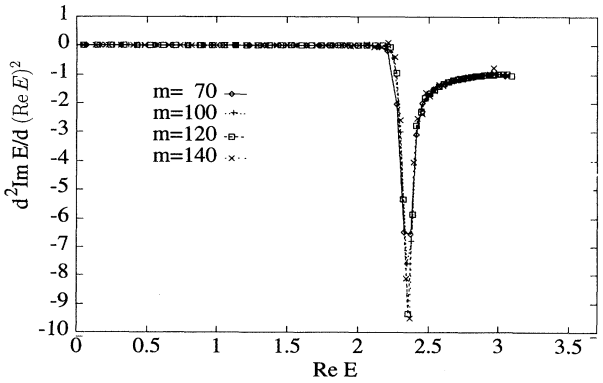

FIG. 3. The second derivative of the imaginary part of the energy with respect to the real part for the potential $V(x) = (0.5x^2 - 0.8)e^{-0.1x^2} + 0.8$. Masses were 70, 100, 120, and 140 a.u., basis set size 701, and $-25 < x < 25$. One observes very clearly a peak at the barrier height of 2.3674 hartree.

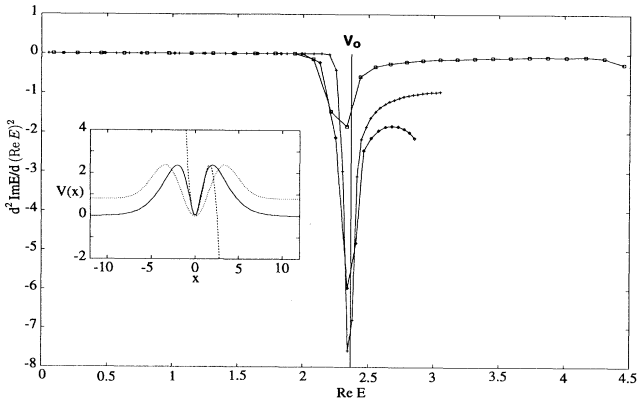

FIG. 4. The second derivative of the imaginary part of the energy with respect to the real part as in Fig. 3. This time, for three different potentials (9) (squares, diamonds, and pluses for $V_1 - V_3$). In spite of the differences between the potentials (they only have the barrier height in common), one observes only one peak for all three at exactly the position of the barrier height.

paragraph — the detachment point here is identical to the *lowest* of the relevant barriers. As proof, we show in Fig. 5 the second derivative of the imaginary part of the energy with respect to real energy of two different asymmetric potentials, namely,

$$V_4(x) = -x^4 + ax^2 + bx$$

$$\text{with } a = 3.4740, b = 0.50, \mu = 150.0, \tag{10}$$

$$V_5(x) = a\left(4x^2 - bx\right) e^{-x^2}$$

$$\text{with } a = 2.4867, b = 1.50, \mu = 200.0.$$

As one sees easily from the figure, the detachment point again correlates perfectly with the lower one of the barrier heights (2.367 43 hartree). In fact (cf. Fig. 5) the second derivative really has two peaks, namely, one at the lower and one at the other barrier height. Please note that we have calculated the second derivative within *one* string, i.e., we have explicitly neglected the eigenvalues of the second irregular part starting at the potential height of the higher barrier; for a general discussion see [1].

As we remarked earlier [1], it is our strong belief that the string represents the specific unimolecular microcanonical rate constant. This gives — in this context — a good way to extract the barrier height(s) from experimental data. Obviously, when plotting the second derivative of the rate constant with respect to energy it should give pronounced peak(s) at the barrier height.

In order to find out why the second derivative of the imaginary part of the energy has a peak at V_0, it is most instructive to look at the WKB results. Conner has shown [18] that for $|\mathrm{Im}(E)| \ll \mathrm{Re}(E)$ the half width $\Gamma = -2\,\mathrm{Im}(E)$ can be expressed as

$$\Gamma_n = \left|\frac{\omega_n}{2\pi} \ln\left(1 + e^{2\pi\varepsilon}\right)\right|, \tag{11}$$

where

$$\omega_n^{-1} = 2\mu \int_0^{t_1} \frac{1}{q(z)}\, dz \tag{12}$$

is the WKB approximation to the density of states within the well and

$$\varepsilon = \begin{cases} \left|\int_{t_1}^{t_2} q(z)\, dz\right|, & E_n < V_0 \\ -\left|\int_{t_1}^{t_2} q(z)\, dz\right|, & E_n > V_0 \end{cases} \tag{13}$$

is the integral "over the barrier." It can be shown numerically that this approximation gives rather good results for (real) energies even above V_0 [31]. Please note that (a) only real energies are used in the above formulas and (b) Eq. (11) was originally intended to be used at the resonances' (real) energies only. With that application in mind, generalizing Eq. (11) to continuous energies (and, consequently, dropping the index n), we find as second derivative

$$\frac{\partial^2\Gamma}{\partial E^2} = \frac{1}{2\pi}\left\{\frac{\partial^2\omega}{\partial E^2}\ln T + \left(\frac{2}{T}\frac{\partial\omega}{\partial E} - \frac{\omega}{T^2}\right)\frac{\partial T}{\partial E} + \frac{\omega}{T}\frac{\partial^2 T}{\partial E^2}\right\}, \tag{14}$$

where $T = 1 + \exp(2\pi\varepsilon)$. The piecewise definition of ε guarantees that it will be continuous and continuously differentiable. In fact, ε is almost linear. The density ω^{-1} rises very strongly at V_0. In Fig. 6 we show the density of states of $V(x) = (0.5x^2 - 0.8)e^{-0.1x^2} + 0.8$ in the WKB approximation and evaluated via

$$\omega^{-1} \approx \tfrac{1}{2}\,|E_{i+1} - E_{i-1}|$$

with the correct energy eigenvalues. Note the good agreement, especially below V_0, and note also that although agreement is worse above V_0, the form predicted by WKB is semiquantitatively correct. By inspecting Fig. 6, one

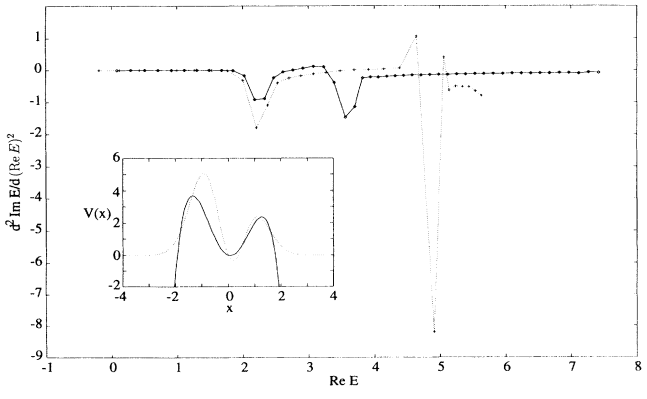

FIG. 5. Plot analogous to Fig. 4 for the asymmetric potentials (10). Besides the expected peak at the lower barrier (2.367 43 hartree) one finds an additional peak at the higher barrier heights.

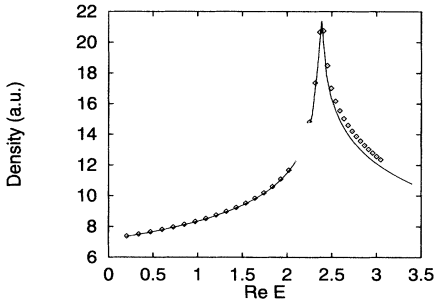

FIG. 6. Density of eigenvalues for $V(x) = (0.5x^2 - 0.8)e^{-0.1x^2} + 0.8$ and $\mu = 60$ a.u. with a peak around the potential height of 2.36 hartree. This indicates that there is indeed a detachment *point* and not a smooth transition. The solid line is the result of a WKB calculation evaluating Eq. (12) using *real* energies. The agreement is good throughout, although it necessarily diminishes for higher energies.

can see that the cusp, which shows in the density, will be the reason for the pole in the second derivative of Γ with respect to energy. This means that the effect of finding a detachment *point* — as opposed to a continuous process of detaching — is really due to a spectral concentration at the potential height V_0.

Let us note in passing another interesting point that can be understood by looking at the WKB approximation: The number of resonances below the potential height depends on the *total* potential height (height minus depth) and — trivially — on the mass. In other words, the number of resonances below V_0 is constant, if one changes the height and the depth in such a way that the total height remains constant (the positions of the maxima naturally also have to be conserved, so that the "box" will be of comparable size). Naturally, this is true only within one potential family, i.e., for potentials that exhibit the same "localization ability." In Table II we list the number of resonances with energy up to V_0 for constant mass (μ= 25 a.u.) and potentials with different ratios of height to depth. As can be seen there, this number is approximately constant over a large range of ratios $|V_0/V_u|$. This shows, among other things, that resonances do not behave any differently from bound state eigenvalues.

Within the framework of WKB, this is quite obvious. The number of resonances below the barrier height V_0 for a symmetric potential is given by

$$N(E \leq V_0) = \text{int}\,[\Re(E = V_0)] = 2\ \text{int}\left(\int_0^{t_1(V_0)} q(z, E = V_0)\, dz\right), \quad (15)$$

where it is understood that one approaches V_0 from below (for energies higher than V_0 the above integral is purely imaginary, so the definition has to be changed). The integral on the right-hand side depends on the difference between E and V_0 (and on the mass). Therefore, if one keeps the total height constant, the integral on the right-hand side — and therefore the number of resonant eigenvalues below V_0 — will be approximately constant. While in principle the sheer dependence on the difference between E and $V(x)$ is not correct (e.g., the correct transmission coefficient depends on both the energy and the difference $E - V_0$), in this case the WKB results are in good agreement with the correct ones.

III. THE LOCALIZATION PROPERTIES

The next important point in the description of pole string curves is the localization threshold. As we mentioned earlier, the localization properties of the eigenstates change significantly at this point. To illustrate this fact, let us show an example, where we calculated the wave functions corresponding to states with quantum numbers below, at, and above the localization threshold for the potential $V(x) = (0.5x^2 - 0.8)e^{-0.1x^2} + 0.8$; see Fig. 7. A short remark regarding the figure: We depict there the absolute square of complex scaled wave functions at $\theta = 0.75$. Although the eigensolutions depend on the opening angle, the general pattern is qualitatively constant after reaching the minimum angle. Moreover, we have normalized the depicted solutions but used the incorrect form of the scalar product, namely,

$$\int_{-\infty}^{+\infty} [\psi(\eta x)]^* \psi(\eta x)\, \eta\, dx = 1$$

instead of the correct form,

$$\int_{-\infty}^{+\infty} [\psi(\eta^* x)]^* \psi(\eta x)\, \eta\, dx = 1 \quad (16)$$

(for a discussion of the scalar product to be used under complex scaling, see, e.g., [32] and also [33]). The reason for doing this was simply that normalizing in this way gives moduli of the same order of magnitude so that comparison is greatly facilitated. Additionally, here we are only interested in the qualitative localization patterns and these are independent of the above two scalar products.

One expects of a (quasi)bound state that it is localized within the attractive part of the potential or, rather, between the barriers, since our physical picture of such states is that they are trapped for a certain (including infinite) time by the target. Therefore, it is mandatory that states corresponding to this physical picture be localized mostly between, say, $-x_{max}$ and x_{max} for a symmetric double barrier, where x_{max} denotes the position of the barrier maxima. While we find that this is true for all states below the localization threshold, the pattern of localization shifts significantly (see Fig. 7) around the localization threshold to maximal localization beneath the barrier maxima. This means that the physical mechanism leading to the complex eigenvalues changes here.

TABLE II. Number N of eigenvalues (bound states and resonances) below the barrier height for some members of the family $V(x) = a(0.5x^2 - b)\exp(-cx^2)$ (mass 25 a.u.). V_u denotes the well depth, V_0 the barrier height. The last values drop out a little, but it is to be considered that for that value of b almost no barrier exists.

a	b	c	V_u	V_0	$V_t = V_0 - V_u$	$\lvert V_0/V_u\rvert$	N
70.00000	0.08	1.00000	-5.60	10.972	16.57	1.9593	11
63.34796	0.15	1.16279	-9.50	7.070	16.57	0.7440	11
53.99588	0.25	1.51515	-13.50	3.073	16.57	0.2277	11
49.42716	0.30	1.78571	-14.83	1.744	16.57	0.1176	10
40.69989	0.40	2.77778	-16.28	0.292	16.57	0.0179	10
33.14027	0.50	6.25000	-16.57	0.002	16.57	0.0001	8

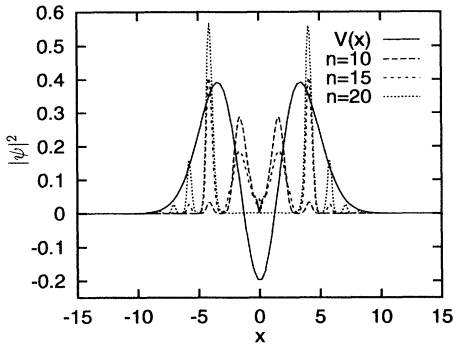

FIG. 7. The absolute square $|\psi|^2$ of selected wave functions of $V(x) = (0.5x^2 - 0.8)e^{-0.1x^2} + 0.8$ ($\mu = 1$) plus the potential itself (scaled by a factor of $1/6$). The quantum number $n = 10$ is equivalent to an energy below the localization threshold, $n = 15$ is at the localization threshold and $n = 20$ corresponds to an energy above the localization threshold. As can be seen in the figure, the localization pattern changes drastically from being localized within the well to being localized beneath the barriers. Please note that the localization pattern is quite independent of the angle θ. For graphical reasons the wave functions are normalized in the standard $\mathcal{L}^2$ way instead of using the (correct) complex-scaling way of Eq. (16).

Below the localization threshold we have "classical" tunneling as described above. Above the localization threshold we find a new mechanism; its true nature is hidden, though. We assume — as a working hypothesis — that those states correspond to retarded backscattered ones. This assumption is based on the observation that single barriers such as Gaussian barriers $\propto \exp(-cx^2)$ show no regular, but only an irregular, string curve. Since the only reason for giving complex eigenvalues for such potentials can be the above mentioned retarded backscattering, we adopted our hypothesis (which, by the way, is by no means crucial for our work). We have no proof of that, though. Clearly, the static picture is not sufficient here to characterize these states in a convincing manner. A detailed dynamical study might shed some light on the nature of these states. Nevertheless, it is clear that these states behave very differently from those of the regular part of the string and that the change occurs at the localization threshold (which is naturally the reason for our labeling it by this term).

Now after having shown that the physical mechanism leading to the complex eigenvalues changes at the localization threshold, we are now able to attack the following questions.

(a) Does a string curve corresponding to a potential always have a localization threshold? In other words, can we give a condition where a string curve will have a localization threshold?

(b) On which potential parameters does the localization threshold depend? Are we able — as in the case of the detachment point — to determine the localization threshold by using only physical potential parameters such as height, depth, width/mass, etc.?

The starting point for answering these question was the semiclassical WKB approximation, which we had already used successfully to determine whether a string curve will be smooth or wiggly [1]. As has been mentioned above, for a description of the part of the string curve that is of relevance here, it is sufficient to use a simple Bohr-Sommerfeld formula such as Eq. (1). The string curve is then described to within the error of the WKB method by requesting

$$\mathrm{Im}\alpha_{02} = \mathrm{Im}\left(\int_0^{t_2} q(z)dz\right) = 0,$$

where t_2 is the first transition point in the first quadrant of the complex z plane; see Fig. 1. (In the case of smooth string curves, the above condition describes the whole string curve above the detachment point.) If we now look at the string curve as a function $\mathrm{Re}E(\mathrm{Im}E)$, looking for the localization threshold is equivalent to finding a maximum of this function, i.e., we are looking for an $\mathrm{Im}E$ in the fourth quadrant of the complex energy plane for which

$$\frac{d\,\mathrm{Re}E}{d\,\mathrm{Im}E} = 0$$

holds. (The restriction to the fourth quadrant of the complex energy plane is not crucial for the following reason: As we showed, the detachment point is identical to the potential height above the threshold; by adding a constant to the threshold we can always shift the detachment point to a positive real energy. As the localization threshold is now always greater than or maximally equal to the detachment point, it suffices to search for a maximum in the fourth quadrant of the energy plane.) Therefore, we form the expression $d\,\mathrm{Im}\alpha/d\,\mathrm{Im}E$ and set the above terms to zero. In principle, we should also show that the function $\mathrm{Im}\alpha$ is complex differentiable by verifying the Cauchy-Riemann differential equation, but since this operation is elementary and lengthy, we omit it here.

Let the first transition point have the coordinates $(a + ib)$ and the second $(a' + ib')$ with $a' > a$ and $b > b'$. Since q has no singularities within this interval we can choose our integration contour to be $y = mx + b$ as long as we do not cross a cut, which is no restriction between adjacent transition points. We then have

$$\alpha = \int_{a+ib}^{a'+ib'} q[x + iy]\, d(x + iy)$$

$$\Longrightarrow \mathrm{Im}(\alpha) = \int_a^{a'} \mathrm{Im}q[x(1 + im) + ib] + m\,\mathrm{Re}q[x(1 + im) + ib]\, dx.$$

Because of the assumed symmetry of the potential, we have a symmetric integration interval and therefore can evaluate the above integral with lower limit $(0 + i0)$. (The following can easily be extended to the more general asymmetric case. For reasons of simplicity in notation, though, we refrain from formulating it.) It then follows that

$$0 = 2\,\mathrm{Im}\alpha_{02} \longrightarrow 0 = 2\,\frac{\partial\,\mathrm{Im}\alpha_{02}}{\partial\,\mathrm{Im}E},$$

from which we get

$$
\begin{aligned}
0 &= \frac{\partial \,\mathrm{Im}\alpha_{02}}{\partial \,\mathrm{Im}E} \\
&= \frac{\partial}{\partial \,\mathrm{Im}E}\int_0^{a'} \mathrm{Im}q[x(1+im)] + m\,\mathrm{Re}q[x(1+im)]\,dx \\
&= (\mathrm{Im}q[a'+ib'] + m\,\mathrm{Re}q[a'+ib'])\,\frac{\partial a'}{\partial \mathrm{Im}E} \\
&\quad + \int_0^{a'} \frac{\partial}{\partial \,\mathrm{Im}E}\Big(\mathrm{Im}q[x(1+im)] \\
&\quad + m\,\mathrm{Re}q[x(1+im)]\Big)\,dx.
\end{aligned}
$$

Now, $q[a'+ib']$ is, by definition of the transition point, zero, so that the first term of the last equation vanishes. Now we have

$$
\frac{\partial \,\mathrm{Re}q}{\partial \,\mathrm{Im}E} = \sqrt{\frac{\mu}{2}}\,\frac{\partial}{\partial \,\mathrm{Im}E}\,(\sqrt{E-V}+\sqrt{E-V}^{*}), \tag{17}
$$

$$
\frac{\partial \mathrm{Im}q}{\partial \,\mathrm{Im}E} = -i\sqrt{\frac{\mu}{2}}\,\frac{\partial}{\partial \,\mathrm{Im}E}\,(\sqrt{E-V}-\sqrt{E-V}^{*}). \tag{18}
$$

For the function $\sqrt{E-V}^{*}$ one finds, by explicit computation or by using the Schwarz reflection theorem,

$$
\sqrt{E-V}^{*} = \left(\sqrt{|E-V|}e^{i\phi/2}\right)^{*} = \sqrt{(E-V)^{*}}
$$

such that from (17) it follows that

$$
\frac{\partial \,\mathrm{Re}q}{\partial \,\mathrm{Im}E} = \sqrt{\frac{\mu}{2}}\left(\frac{\frac{d\,\mathrm{Re}E}{d\,\mathrm{Im}E}+i}{\sqrt{(E-V)}} + \frac{\frac{d\,\mathrm{Re}E}{d\,\mathrm{Im}E}-i}{\sqrt{(E-V)^{*}}}\right)
$$

and a similar expression from (18),

$$
\frac{\partial \,\mathrm{Im}q}{\partial \,\mathrm{Im}E} = -i\sqrt{\frac{\mu}{2}}\left(\frac{\frac{d\,\mathrm{Re}E}{d\,\mathrm{Im}E}+i}{\sqrt{(E-V)}} - \frac{\frac{d\,\mathrm{Re}E}{d\,\mathrm{Im}E}-i}{\sqrt{(E-V)^{*}}}\right).
$$

Putting at zero the derivatives of the real part of the energy with respect to the imaginary part, we get

$$
\frac{\partial \,\mathrm{Re}q}{\partial \,\mathrm{Im}E} = \frac{\mathrm{Im}q}{|q|^2},
$$

$$
\frac{\partial \,\mathrm{Im}q}{\partial \,\mathrm{Im}E} = \frac{\mathrm{Re}q}{|q|^2}.
$$

Since m is a parameter within the integral, it follows that

$$
\begin{aligned}
0 &= \int_0^{a'} \frac{\partial}{\partial \,\mathrm{Im}E}\{\mathrm{Im}q[x(1+im)] + m\,\mathrm{Re}q[x(1+im)]\}\,dx \\
&= \int_0^{a'} \frac{\mathrm{Re}q[x(1+im)]}{|q|^2} + m\frac{\mathrm{Im}q[x(1+im)]}{|q|^2}\,dx
\end{aligned} \tag{19}
$$

which means that the localization threshold is given by

$$
\begin{aligned}
&\int_0^{a'} \mathrm{Im}q[x(1+im)] + m\,\mathrm{Re}q[x(1+im)]\,dx \\
&= \int_0^{a'} \frac{\mathrm{Re}q[x(1+im)]}{|q|^2} + m\frac{\mathrm{Im}q[x(1+im)]}{|q|^2}\,dx = 0.
\end{aligned} \tag{20}
$$

As an example, we show these lines along with the spectrum of a Hamiltonian with $V(x) = 7.5e^{-x}$ in Fig. 8.

With the above condition (20) we are now able to give a condition for the existence of a localization threshold, because of the following: Very generally, it holds that $\int \mathrm{Im}(q) \le 0$ (analogously, $\int \mathrm{Re}(q) \ge 0$) and since $1/|q|^2$ is a positive function, it is also true that $\int \mathrm{Im}(q)/|q|^2 < 0$. This means that we can always write

$$
\int_0^{a'} \frac{\mathrm{Re}q[x(1+im)]}{|q|^2}\,dx = C_1\int_0^{a'} \mathrm{Re}q[x(1+im)]\,dx,
$$

$$
\int_0^{a'} \frac{\mathrm{Im}q[x(1+im)]}{|q|^2}\,dx = C_2\int_0^{a'} \mathrm{Im}q[x(1+im)]\,dx,
$$

with $C_1, C_2 \ge 0$. Let us now assume that the first part of condition (20) is fulfilled, so that we are on the string curve. Then, trivially

$$
\int_0^{a'} \mathrm{Im}q[x(1+im)]\,dx = -m\int_0^{a'} \mathrm{Re}q[x(1+im)]\,dx.
$$

The second part now reads

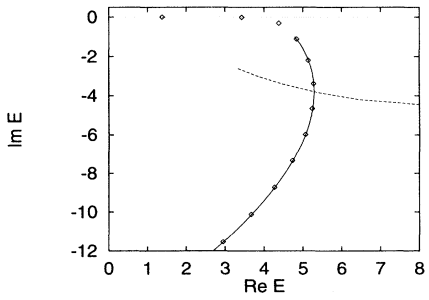

FIG. 8. Part of the string curve (solid line) for the potential $V(x) = 7.5x^2e^{-x}$ together with the resonances for $\mu = 1$. Additionally, the curve (19) (dashed line) is depicted. The point where the two lines cross is identical to the localization threshold.

$$
\begin{aligned}
0 &= \int_0^{a'} \frac{\mathrm{Re}q[x(1+im)]}{|q|^2} + m\int_0^{a'} \frac{\mathrm{Im}q[x(1+im)]}{|q|^2}\,dx \\
&= C_1 \int_0^{a'} \mathrm{Re}q[x(1+im)]\,dx + mC_2 \int_0^{a'} \mathrm{Im}q[x(1+im)]\,dx \\
&= C_1 \int_0^{a'} \mathrm{Re}q[x(1+im)]\,dx - m^2 C_2 \int_0^{a'} \mathrm{Re}q[x(1+im)]\,dx, \\
0 &= C_1 - m^2 C_2,
\end{aligned}
$$

since we may well assume that $\int_0^{a'} \mathrm{Re}q[x(1+im)]\,dx$ is not zero. Therefore, we get

$$
m = \sqrt{\frac{C_1}{C_2}} = \left(\frac{\int_0^{a'} \frac{\mathrm{Re}q[x(1+im)]}{|q|^2}\,dx \int_0^{a'} \mathrm{Im}q[x(1+im)]\,dx}{\int_0^{a'} \frac{\mathrm{Im}q[x(1+im)]}{|q|^2}\,dx \int_0^{a'} \mathrm{Re}q[x(1+im)]\,dx} \right)^{1/2}, \tag{21}
$$

which is naturally to be read as a condition, i.e., there is one and only one point $E = E_r + iE_i$ where the above holds. Now one observes that the rhs of Eq. (21) fulfills the inequality

$$
0 \le \left(\frac{\int_0^{a'} \frac{\mathrm{Re}q[x(1+im)]}{|q|^2}\,dx \int_0^{a'} \mathrm{Im}q[x(1+im)]\,dx}{\int_0^{a'} \frac{\mathrm{Im}q[x(1+im)]}{|q|^2}\,dx \int_0^{a'} \mathrm{Re}q[x(1+im)]\,dx} \right)^{1/2} \le 1, \tag{22}
$$

since the function $1/|q|$ has a singularity at a' and grows in this direction like $1/x$. Now, since with our choice of the phase the argument of q^2 is between $[-\pi, \pi]$ and since the phase is necessarily proportional to $-x$, we find for

$$
\int_0^{a'} \frac{\mathrm{Re}q[x(1+im)]}{|q|^2}\,dx = \int_0^{a'} \frac{\cos(\frac{\phi}{2})}{|q|}dx,
$$

$$
\int_0^{a'} \frac{\mathrm{Im}q[x(1+im)]}{|q|^2}\,dx = \int_0^{a'} \frac{\sin(\frac{\phi}{2})}{|q|}dx,
$$

that $\sin(\frac{\phi}{2})$ has a positive slope at the pole in $1/|q|$, i.e., tends to -1, while the cosine term tends to zero. From this follows very generally that

$$
C_2 \ge C_1.
$$

The above inequality (22) can now be interpreted in the following way: *Let m be chosen such that*

$$
0 = \int_0^{a'} \mathrm{Im}q[x(1+im)] + m\,\mathrm{Re}q[x(1+im)]\,dx.
$$

If, now, this m ever gets larger than unity, there must have been a point $E = E_r + iE_i$, *where also*

$$
0 = \int_0^{a'} \frac{\mathrm{Re}q[x(1+im)]}{|q|^2} + m\frac{\mathrm{Im}q[x(1+im)]}{|q|^2}\,dx
$$

was true. The string curve $\mathrm{Im}(\alpha_{02}) = 0$ *belonging to V has then — looked upon as a function* $\mathrm{Re}E\,(\mathrm{Im}E)$ *— had a maximum and therefore there exists a localization threshold.*

If m stays smaller than unity on the string curve, then a localization threshold does not necessarily exist. This is the case, e.g., for potentials of the type $V(x) = -x^4 + ax^2$, for which even

$$
\int_0^{a'} \frac{\mathrm{Re}q[x(1+im)]}{|q|^2} + m\frac{\mathrm{Im}q[x(1+im)]}{|q|^2}\,dx > 0 \tag{23}
$$

is true for all energies whose imaginary part is finite. As an example, we show in Fig. 9 the lhs of the above equation as a function of the imaginary part of the energy for selected values of the real energy. For this type of potential the relevant WKB integral can even be solved analytically [34]; the analytic solution also does not show any trace of a localization threshold.

In fact, we found for all polynomial potentials that Eq. (23) holds, so that we dare to say that such potentials do not have a localization threshold. This is supported by analyzing the situation in terms of localization. As we showed above, the localization properties change drastically when crossing the localization threshold. The considered polynomial potentials, however, have at least one side where they tend to $-\infty$. This means now that there is a forced localization such that $\langle\psi \mid H\psi\rangle$ can stay finite.

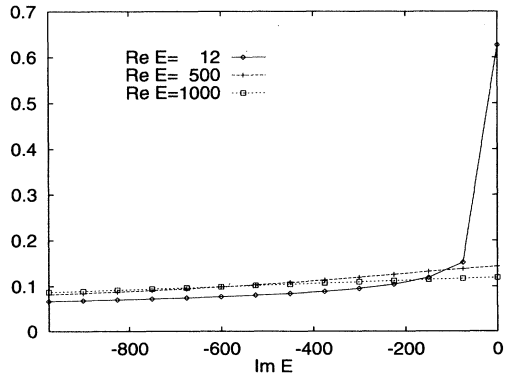

FIG. 9. Lhs of Eq. (23) as a function of the imaginary part of the energy for different real parts (in a.u.). The potential used here was $V(x) = -x^4 + ax^2$ ($a = 6.624$). Real energy of 12 a.u. corresponds to the barrier height. As one can see from the figure, the depicted function is positive even for very large values of $|E|$ so that a localization threshold is impossible.

With the above analysis we reduced the question of the localization threshold to the slope m (these slopes between adjacent transition points also played a major role in the question of a wiggly or smooth irregular part; see [1]). Therefore, certain dependencies of the localization threshold on the parameters can very easily be understood by the dependency of the slope on these parameters. For example, it is obvious that the localization threshold will be shifted to smaller $|E|$ if the potential height is diminished. First, the slope m is raised for a given energy if one lowers the potential height. Second, this is also physically clear, since if one lowers the potential height, one diminishes the "localization strength" and therefore the point where localization properties change must lie at lower energies.

On the other hand, m depends on both the depth of the potential at $x = 0$ and the height at $x = x_{max}$. Therefore, we cannot expect that the localization threshold stays invariant if one changes either. This is documented in Fig. 10. In the left-hand part of the figure we depict the dependency of the localization threshold on the potential height, while keeping constant the depth for the potential $V(x) = (ax^2 - 0.8)e^{-0.1x^2}$. Please note that this plot is doubly logarithmic. One observes a clearly nonlinear behavior for small values of the potential height, while for larger values the dependency is to a very good approximation linear. (For comparison we added a straight line to the figure, whose slope naturally is unity in doubly logarithmic scales.) In the right part of the figure we show the dependency on the depth of the potential well. While the real part of the localization threshold does not change that drastically with the depth (a change of factor 10 maximally doubles the real part, while changing the height by the same amount shifts the localization threshold to a value that is 20 times higher), the change cannot be neglected.

The localization threshold also depends on the fraction of the potential above and below the threshold, i.e. when altering V_0 (barrier height) and V_u (well depth), while keeping the total height $V_t = V_0 - V_u$ constant, the localization threshold changes. (See also Figs. 12 – 17 in Ref. [1] to see the dependency of the localization threshold on different parameters.)

The dependency of the slope m and, therefore, of the localization threshold is rather complex and, moreover, a determination of the latter only in terms of physical potential parameters such as height, depth, mass/thickness, etc. is certainly ruled out because the zeroes of $E - V$ and therefore m also depend on the analytic form of the potential. Assume, for example, that we have a potential of the form $V(x) = P(x)e^{Q(x)}$, where both P and Q are suitable polynomials (P may also be of order zero). It then shows that raising the order of either P or Q, while keeping the potential height constant (to have a constant detachment point, so we can compare the results) shifts the localization threshold to both higher ReE and ImE (and, therefore, to higher $|E|$). Even keeping constant other parameters such as $\int V(x)dx$ does not change the situation. This is immediately clear, because one observes the following. Let, e.g., $V_n(x) = a'x^n e^{-cx}$ and the height of the reference potential $n = 2, c = 1$ be $V_2(x_{max}) = 4ae^{-2}$. Then we find for a' the expression

$$a' = 4a \left(\frac{c}{n}\right)^n e^{n-2}.$$

Since we have to keep constant the potential height, this restricts the family V_n to

$$V_n(x) = \frac{4a}{n^n} e^{n-2}(cx)^n e^{-cx},$$

so that we are left with a single free parameter c. But changing this parameter is equivalent to a real dilatation (or a change in the mass of the system) and therefore all the V_n for one n have identical string curves above the detachment point (only string curves; naturally, the strings are different). Keeping constant the potential height and depth very generally and not only in this specific example places us in the situation where only real dilatations of the potential are still possible and, therefore, independent of how we determine the parameter c [e.g., through $\int V_n(x)dx = \int V_2(x)dx$] we always get the same string curve and the same localization threshold. Turning this statement around, we might say that the localization threshold is independent of the thickness of a barrier or the width of the well, if changed in the above sense.

In Fig. 11(a) we show parts of the string curves of the potentials V_n for $n = 2, 4, 6$. As a reference, we used the potential proposed by Bain, *et al.* [35]: $V(x) = 7.5x^2e^{-x}$. Please observe the following two points. First, raising the

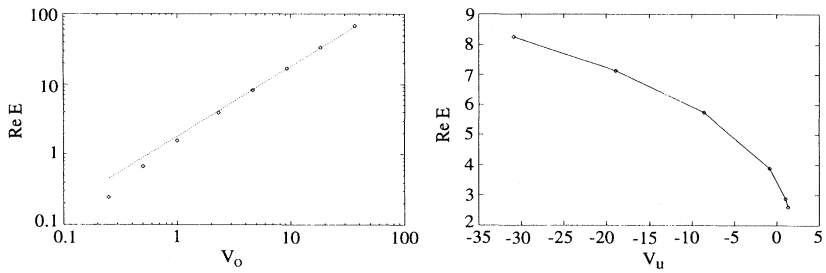

FIG. 10. Dependence of the real part of the localization threshold on the potential height while keeping the well depth constant (left-hand side of the figure) and on the well depth, while keeping the potential height constant (right-right side). The left part is a doubly logarithmic plot and we have added for comparison a straight line Re$(E) = mV_0$ with the slope $m = 1.8$.

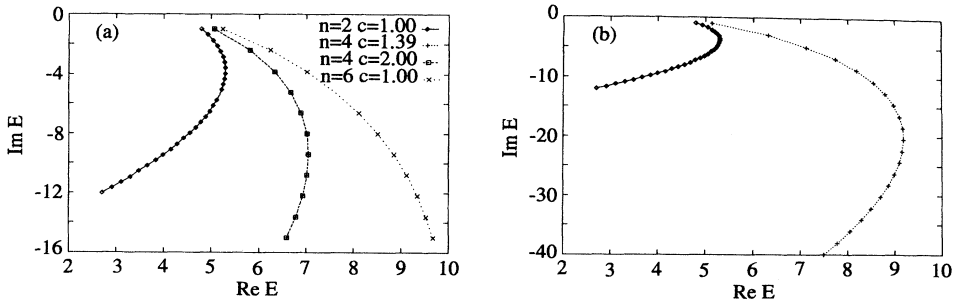

FIG. 11. (a) shows parts of the string curves of the family $V_n(x)$ defined in the text for $n = 2, 4, 6$. For $n = 4$, string curves for two choices of c are shown; the string curves are strictly identical. (b) shows parts of the string curves for $V(x) = 7.5x^2e^{-x}$ (diamonds) and $V(x) = 1.10346x^2e^{-0.1x^2}$ (pluses). One observes that the localization threshold depends on both the order of the polynomial in front of the exponential and of the polynomial in the exponential in the sense that it is shifted to both higher ReE and ImE if the orders are raised. The points in the figure do not represent resonances.

order of $P(x)$ in the above nomenclature shifts the localization threshold to higher $|E|$. Second, the two string curves for $n = 4$ are strictly identical. The same shift is found if raising the order of $Q(x)$, as can be seen from Fig. 11(b). There we show parts of the string curves of $V(x) = 7.5x^2e^{-x}$ and $V(x) = 1.103\,46x^2e^{-0.1x^2}$, which have once more the potential height in common. Again the potential with the higher order definitely has a higher localization threshold.

In conclusion, we might say that the localization threshold depends on potential height and depth (relative *and* absolute), but not on mass/thickness. Additionally, the localization threshold depends on the specific analytic form of the potential, we can therefore not hope to describe it by physical potential parameters only.

IV. SUMMARY

This contribution has two main purposes: First, we wanted to deepen the discussion about string curves and second, we wanted to "prove" earlier statements from [1]. We concentrated here on the two most prominent points that serve to describe string curves: the detachment point and the localization threshold.

For the first we showed that, in short, it is equal to the potential height in the symmetric case. In the asymmetric case we observe two peaks in the second derivative of the imaginary energy with respect to the real part of the energy. The detachment point is then identical to the height of the lower barrier. There is no need to include more cases in this discussion, since we showed earlier [1] that one string curve corresponds to one and only one irreducible unit of the potential. Since there are only two irreducible units, namely, a sole barrier and a barrier-well combination (of which one barrier can be of zero, finite, or infinite height), there are only two general cases. In the case of a single barrier, localization threshold and detachment point coincide and both are identical to the barrier height. The case of an (asymmetric) barrier-well combination has been addressed above.

Furthermore, we showed that, treating the problem semiclassically, one finds that in fact the density of states is the real cause for the existence of a detachment *point*. We found that there is a spectral concentration at V_0, which induces, therefore, a peak in the density, which again gives rise to a singularity in the above derivative, Eqs. (7) and (14), respectively.

In addition we gave another example of the fact that bound states and resonances really can be understood as one concept. As is known, the number of bound states in a potential well can be approximated by knowing the depth and width of the corresponding well. Generalizing, we showed that the number of resonances including bound states (which we understand as resonances with infinite lifetime) is constant if one keeps the total height (as a generalization of the former depth) and the width constant.

The next topic of concern was the localization threshold. First of all, we showed that the part of the string curve before the localization threshold (the regular part) and the one after it (the irregular part) show very distinct localization properties of the corresponding eigensolutions of the complex scaled Schrödinger equation. Solutions out of the set of poles belonging to the regular part of the string (curve) can be correlated with the classical picture of particles being trapped in the attractive part of the potential: the localization is concentrated between the barrier maxima. But around the localization threshold, localization shifts in the direction of the barriers and after the localization threshold, the particles are localized mostly beneath the barriers; localization within the attractive part of the potential is negligible. This points to a different physical mechanism underlying those eigenvalues; its true nature, however, is still undetermined.

We were able to give, in the framework of the WKB theory, a condition for the existence of the localization threshold. Specifically, we showed that whenever the slope between the first transition points in the first and third quadrants (t_4 and t_2 in the nomenclature of Fig. 1) are chosen such that

$$0 = \int_0^{a'} \mathrm{Im}q[x(1+im)] + m\,\mathrm{Re}q[x(1+im)]\,dx$$

exceeds the value 1, then there has to have been a localization threshold. Therefore, localization threshold and m are deeply connected; m_{02}, as one might call it because we were looking at the path $\mathrm{Im}\alpha_{02} = 0$, which describes the relevant part of the string curve to within the error of the WKB method, is "responsible" for the localization threshold, while m_{24}, as we showed in an earlier paper [1], governs the question of whether the irregular part of the string curve is smooth or wiggly. Polynomial potentials seem to have no localization threshold, because they fulfill

$$\int_0^{a'} \frac{\mathrm{Re}q[x(1+im)]}{|q|^2} + m\frac{\mathrm{Im}q[x(1+im)]}{|q|^2}\,dx > 0,$$

which is contradictory to having a localization threshold. We argued that the fact that such potentials tend to $-\infty$ at least on one side leads to a "nonnormal" localization of the wave function and therefore not to a localization threshold. (The only exception known to us is the simple inverted parabolic barrier, which has equidistant poles in the complex plane with real energy exactly that of the barrier height.)

The localization threshold has a very complex dependence on the physical potential parameters; only mass/thickness can be excluded from the discussion because, as we showed in [1], the string curve in the relevant part does not depend on the mass (and mass and thickness are unitarily equivalent; cf., e.g., [1]). Additionally, the localization threshold depends on the specific analytical form of the potential involved, which is much more serious. For potentials of the type $V(x) = P(x)e^{Q(x)}$ (P, Q are polynomials; the order of P may also be zero), the localization threshold shifts to both higher $\mathrm{Re}E$ and $\mathrm{Im}E$ if raising either order. While the dependence on the order of Q is much more drastic, the one on the order of P is far from being negligible.

ACKNOWLEDGMENTS

It is a pleasure to thank Erkki Brändas (Uppsala) for many insightful discussions. This work was supported in part by the Fonds der Chemischen Industrie (Frankfurt am Main).

[1] H. Lehr and C. Chatzidimitriou-Dreismann, Phys. Rev. A **50**, 2347 (1994).
[2] P. Löwdin, Adv. Quantum Chem. **19**, 87 (1988).
[3] B. Junker, Adv. At. Mol. Spec. **18**, 207 (1982).
[4] *Resonances: The Unifying Route Towards the Formulation of Dynamical Processes*, edited by E. Brändas and N. Elander, Lecture Notes in Physics Vol. 325 (Springer-Verlag, Berlin, 1989).
[5] *Resonances — Models and Phenomena*, edited by S. Albeverio, L.S. Ferreira, and L. Streit, Lecture Notes in Physics Vol. 211 (Springer-Verlag, Berlin, 1984).
[6] Int. J. Quantum Chem. **14**, No. 4 (1978).
[7] Int. J. Quantum Chem. **31**, No. 5 (1987).
[8] J. Aguilar and J. Combes, Commun. Math. Phys. **22**, 269 (1971).
[9] E. Balslev and J. Combes, Commun. Math. Phys. **22**, 280 (1971).
[10] B. Simon, Ann. Math. **97**, 247 (1973).
[11] N. Fröman and P. Fröman, in *Forty More Years of Ramifications: Spectral Asymptotics and its Applications*, edited by S.A. Fulling and F.J. Narcowich, Discourses in Mathematics and its Applications, Vol. 1 (Texas A&M University, College Station, 1992), pp. 121–159.
[12] H. Korsch, in *Resonances — Models and Phenomena*, (Ref. [5]), pp. 217–234.
[13] J. Korsch, H. Laurent, and R. Möhlenkamp, Phys. Rev. A **26**, 1802 (1982).
[14] M. Rittby, N. Elander, and E. Brändas, Mol. Phys. **45**, 553 (1982).
[15] M. Rittby, N. Elander, and E. Brändas, Phys. Rev. A **26**, 1804 (1982).
[16] M. Rittby, N. Elander, and E. Brändas, Phys. Rev. A **24**, 1636 (1981).
[17] N. Andersson (unpublished).
[18] J. Connor, Mol. Phys. **25**, 1469 (1973).
[19] J. Connor and A. Smith, Chem. Phys. Lett. **88**, 559 (1982).
[20] J. Connor and A. Smith, J. Chem. Phys. **78**, 6161 (1983).
[21] C. Marston and G. Balint-Kurti, J. Chem. Phys. **91**, 3571 (1989).
[22] S.-I. Chu, Chem. Phys. Lett. **167**, 155 (1990).
[23] B. Johnson, J. Chem. Phys. **69**, 4678 (1978).
[24] B. Johnson, J. Chem. Phys. **67**, 4086 (1977).
[25] B. Johnson, J. Comp. Phys. **13**, 445 (1973).
[26] N. Andersson, Int. J. Quantum Chem. **46**, 375 (1993).
[27] H. Lehr, C.A. Chatzidimitriou-Dreismann, and E. Brändas, Phys. Scr. **49**, 528 (1994).
[28] N. Moiseyev, P.R. Certain, and F. Weinhold, Mol. Phys. **36**, 1613 (1978).
[29] H. Korsch, H. Laurent, and R. Möhlenkamp, J. Phys. B **15**, 1 (1982).
[30] H. Lehr and C. Chatzidimitriou-Dreismann, Chem. Phys. Lett. **201**, 278 (1993).
[31] B. Böhmer, H. Lehr, and C.A. Chatzidimitriou-Dreismann (unpublished).
[32] N. Elander and E. Brändas, in *Resonances: The Unifying Route Towards the Formulation of Dynamical Processes*, edited by E. Brändas and N. Elander, Lecture Notes in Physics Vol. 325 (Springer-Verlag, Berlin, 1989), pp. 541–552.
[33] A. Scrinzi and N. Elander, J. Chem. Phys. **98**, 3866 (1993).
[34] J. Caballero Carretero and A. Martin Sánchez, J. Math. Phys. **28**, 636 (1987).
[35] R. Bain, J.N. Bardsley, B.R. Junker, and C. Sukumar, J. Phys. B **7**, 2189 (1974).