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General properties of the spectrum of complex scaled Hamiltonians: The transition to two dimensions

H. Lehr* and C. A. Chatzidimitriou-Dreismann
I. N. Stranski-Institute for Physical and Theoretical Chemistry, Technical University of Berlin, Str. d. 17. Juni 112, D-0623 Berlin, Federal Republic of Germany

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In this paper we investigate the spectra of complex scaled two-dimensional Hamiltonians. More specifically, we compare the spectra of the two-dimensional Hamiltonians to those of underlying one-dimensional ones and find that phenomenologically the spectra also of nonseparable two-dimensional Hamiltonians can be understood as a direct sum of one-dimensional spectra. Moreover, certain parameters describing a string or string curve can be easily carried over to two dimensions. Furthermore, we address the connection to the emergence of coherent-dissipative structures and argue that no *specific* form of interaction is necessary for the latter, since in almost every case enough eigenvalues are available to fulfill the necessary quantization conditions.

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I. INTRODUCTION

In two recent papers [1,2] we have investigated the resonant part of the spectrum of one-dimensional Hamiltonians via the WKB approximation and the complex scaling method [3–8]; the original references are [9–11]. In order to facilitate the following discussion we will briefly restate the terminology, the concepts, and the main points of [1] and [2]. For reasons that will be clear later on, we are less interested in the set of discrete (complex) eigenvalues (i.e., the string), but more interested in the curve connecting these points: the string curve. The latter is defined most easily within the framework of the WKB — or phase integral — approximation [12], and has been given by Korsch earlier [13]

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

[t and t' are so-called transition points, i.e., points, where $q^2(z)$ is zero], where the functional form of $q(z)$ depends on the order of approximation used. In first order it is given by (we use atomic units throughout, so $\hbar = 1$)

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

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 [12]. The string curves represent a generalization of the strings, especially since certain parts that are of interest here are mass independent (see [1] for more information). Additionally, we argue that they are connected with the microcanonical unimolecular rate constant.

In Fig. 1 two typical string curves for one-dimensional double-barrier single-well potentials are depicted. Up to a certain point, which we called *detachment point*, the string curves stay very close to the real axis while after it they move rapidly away from the real axis. Then comes a portion of the string where the imaginary energy rises with real energy just as one would expect. From a certain point on, namely, the *localization threshold*, the situation is reversed. In Fig. 1(a) one sees that the imaginary energy grows with dropping real energy in a very smooth fashion. In Fig. 1(b), on the other hand, one sees a more complicated dependence of real and imaginary energies. We called the portion of the string up to the localization threshold the *regular* part of the string, while the portion following is called *irregular*. The irregular part of Fig. 1(a) is for obvious reasons called *smooth*, while that of Fig. 1(b) is called *wiggly* as is customary in the literature [13–18]. In [1] and [2] we showed that at the localization threshold the localization properties change: Before the localization threshold one has, as is to be expected, localization within the attractive region of the potential, while after it ("after" referring to quantum numbers higher than that of the localization threshold) localization is greatest *beneath* the barriers.

Furthermore, we introduced in [19] the concept of irreducible units of a potential. There and in [1] we showed that every potential can be decomposed into certain parts, which serve as generators for the spectrum, i.e. the complete discrete spectrum of the Hamiltonian can be expressed as

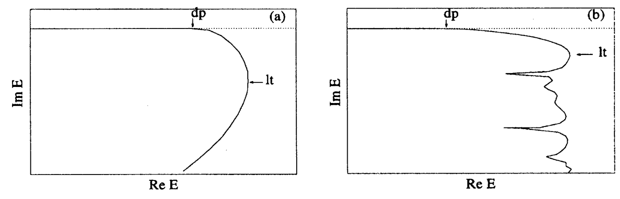

FIG. 1. Two of the most common string curves: (a) a smooth string curve and (b) a wiggly string curve. Indicated in the figure are the detachment point ("*dp*") and the localization threshold ("*lt*"). See the text for further details.

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*Present address: Deptartamento de Química Física, Martí i Franqués, 1, Universitat de Barcelona, E-08028 Barcelona, Spain.

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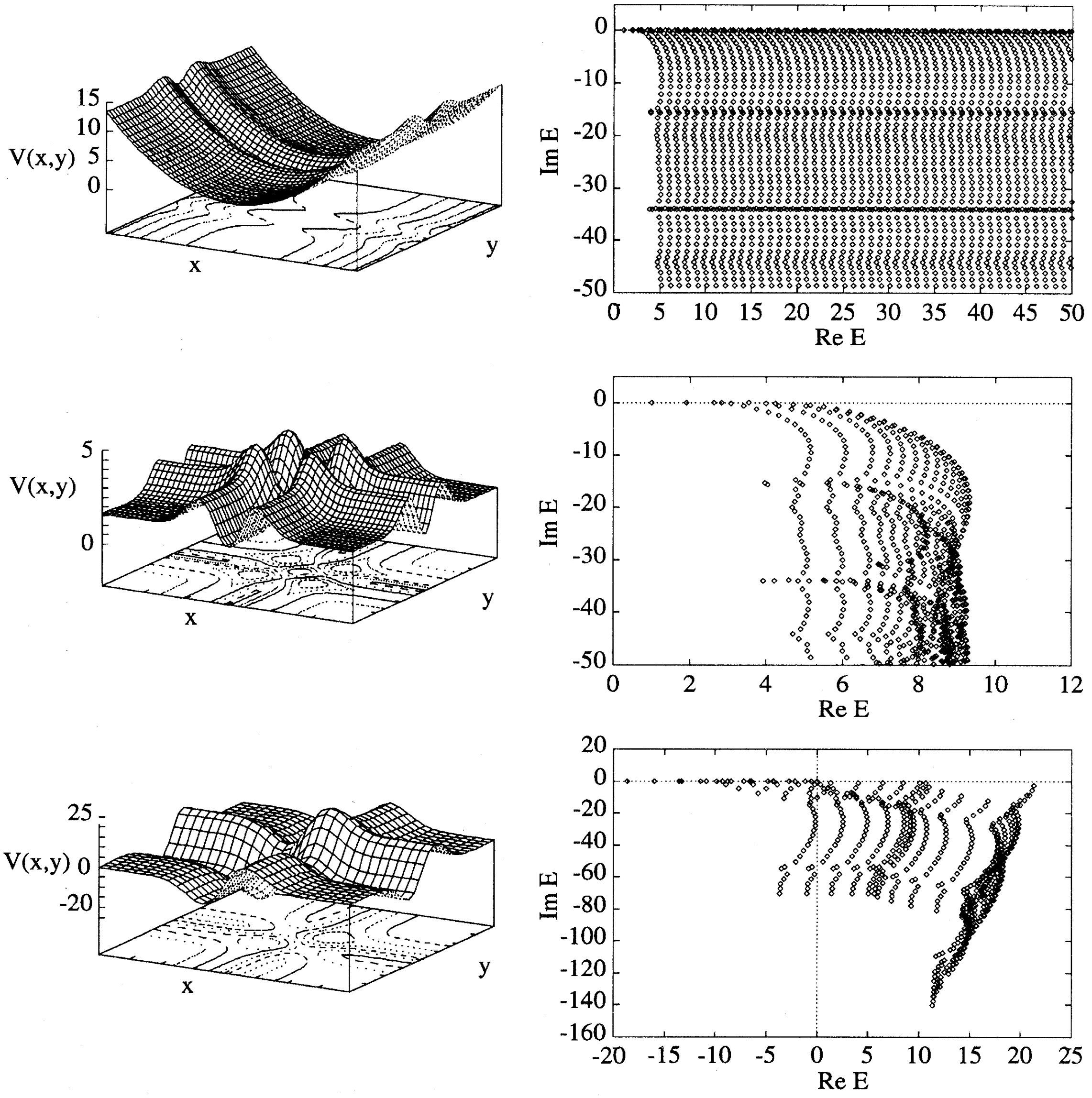

FIG. 2. Potentials (3)–(5) (from top to bottom) and details of the corresponding spectra. The intervals for the first potential are $-5 \leqslant x \leqslant 5$ and $-15 \leqslant y \leqslant 15$, for the second $-15 \leqslant x$, and $y \leqslant 15$, and for the last $-4 \leqslant x$ and $y \leqslant 4$. See the text for details. Atomic units are used here and in all the following figures.

$$\sigma_d = \bigcup_i \sigma_i,$$

where the σ_i are the discrete spectra of Hamiltonians corresponding to the irreducible units. There are only two different irreducible units, namely, a single well surrounded by barriers (of which one may be of infinite height) and a sole barrier. The former gives a string curve like those in Fig. 1 (the question of wiggly or smooth has been addressed in [1]), while the single barrier gives only an irregular part starting at the barrier height. The irreducible units may well overlap and so we may find, e.g., for a asymmetric double-barrier single-well potential (depending on the asymmetry) a so-called *composite* string (curve), i.e., one string curve with a regular and an irregular part and additionally an irregular part starting at the higher barrier height; we showed that the latter really is due only to the higher barrier and we concluded that such potentials are composed of two irreducible units. (For a pictorial representation see [1] and Fig. 2.)

The purpose of the present paper is twofold. First of all we wish to investigate what happens to the discrete spectra if we go to higher dimensions. Unfortunately, "higher" has to be read as "two" since the description is difficult enough already in two dimensions. Second, we wish to extend the "building block" principle of the one-dimensional spectra. Additionally, the spectra of higher-dimensional Hamiltonians are of great interest to us because of the connection to the theory of coherent dissipative structures. This theory deals with the emergence of quantum correlated structures in an otherwise disordered medium. Under special conditions, namely, that the spectrum of the relevant Hamiltonian exhibits a certain minimal number of eigenvalues whose real parts are equal and whose imaginary parts are equidistantly distributed in the complex energy plane, one can show [20] that the corresponding second-order (fermionic) density matrix exhibits (nondiagonalizable) Jordan blocks, which are the mathematical representation of the coherent dissipative structures. The theory has been successfully applied to many phenomena in physics, wherever quantum correlations (may) play a role. (For an introduction see the review [21] and furthermore [22–27].)

The question of concern to us now is to find out — using admittedly a somewhat simplistic ansatz — what conditions have to be met in order to find a distribution of eigenvalues like that mentioned above. So, apart from the interesting topic of determining resonant eigenvalues for one and two dimensions we have an additional interest in the general behavior of the eigenvalues under a change of, e.g., potential parameters or the analytic form of the potential. To this end, we start in one dimension and indeed one might say that there we are able to get a good idea of the behavior (see [1] and [2]). Then we turn to two dimensions in order to realize the differences from and the similarities to the one-dimensional case.

Numerical results have been obtained by the CSFGH method [28,29] in the one-dimensional case and by a method developed by us [30] based on a idea by Eckert [31] for two-dimensional problems. It might be appropriate to comment on some general features of such calculations in order to enable the reader to appreciate the results presented. One might say that the numerical spectrum we obtain consists of three contributions: the resonances, which are our main concern, the representation of the continuum and general numerical errors due to finite basis sets, and numerical integration of the numerical basis sets. Of these, those eigenvalues of the Hamiltonian matrix that represent continuum functions are the easiest to suppress. This is because we choose as a basis a set of resonant wave functions, which are in turn eigenfunctions of two arbitrarily chosen one-dimensional cuts through the potential surface. Those eigenfunctions naturally are solutions to a differential equation with a boundary condition that is incompatible with continuum solutions and therefore if the space of basis functions consists only of the former, we will not get a representation of the cut. If, on the other hand, we choose as a basis set a direct product of continuum solutions, we find the cut, but no resonances. Therefore in the figures that will be shown here, one will find no cut because we concentrated on finding resonances.

The group of continuum solutions together with that of the numerical artifacts is in any case more or less easy to distinguish from the group of resonances by the latter's property of being invariant, in the exact case, under a change of the angle θ, which is the angle of the complex rotation. Now, in the case of finite basis sets it is known that the complex eigenvalues exhibit so-called θ trajectories (see, e.g., [32]). The better the basis set, though, the less the eigenvalues depend on the angle. In our calculations the dependence must be very small considering the size of the basis-set and the numerical approximations involved. Nevertheless, there are always portions of the spectrum (especially in the vicinity of the cut) that are numerically very difficult to obtain with certitude. Therefore we do not introduce a cutoff of that sort: If the eigenvalue changes less than the cutoff under a rotation of, e.g., 0.1 rad, then we will call it stable, but instead we display in the main figures (Figs. 3 and 4) the numerical spectrum at two different angles in order to show graphically the effect of a change of θ. This means that wherever the diamonds ($\theta = 0.3$) and the pluses ($\theta = 0.4$) do not overlap, there is a certain uncertainty that we find resonances. Only where they "exactly" coincide can we talk justly of resonances.

Obviously, the quality of the results depends on the basis set chosen. The convenient property, though, of the method used here is that the basis set is determined directly by the problem, i.e., in one sense we have an optimal basis set. This is counterbalanced by the fact that we use a numerical basis set, i.e., we introduce errors by having to use a numerical integration scheme and by the finite accuracy of the numerical basis set. Nevertheless, this method seems to give the best results known to us in this context using the lowest number of basis functions.

II. TWO-DIMENSIONAL HAMILTONIANS: RESULTS

Before we start to investigate the transition from one to two dimensions, the appropriate choice of potentials should be discussed. Fortunately, our investigation in the one-dimensional case ([1,2]) showed that apart from the high quantum number behavior the concrete analytical form of the potential does not show any effect on the phenomenological form of the string curves. In other words, in [1] and [2] and also in [19], we investigated the spectrum of (a) polynomials, (b) polynomials times an exponential damping factor, (c) polynomials times a Gaussian damping factor, and (d) transcendent functions times an exponential and a Gaussian damping factor. In all cases we found the same general structure, if for a moment we neglect the irregular part (if any). Therefore, since in the two-dimensional case numerical limitations lead to the fact that we will be mainly considering the regular part (or even only part of that), the question of using or not using a Gaussian or an exponential damping factor is rather unimportant. Naturally, in the high quantum number limit, i.e., after the localization threshold, this changes the situation completely: In cases (a) and (d) above, the string curve does not even have a localization threshold (though for different reasons; see [1] and [19]) and therefore does not have an irregular part; in case (b) we find a smooth part and in (c) a wiggly irregular part. But again, since we cannot hope to describe string curves due to two-dimensional potentials to such an accuracy that the resonances position will be invariant under a substantial change in the angle θ, the general appearance of the part of the two-dimensional spectra under consideration will not depend on the particular choice of damping. Furthermore, we showed in [1] and [2] that the concepts introduced also do not depend on the specific choice of potential family, i.e., e.g., exponentially as well as Gaussian damped potentials both have a detachment point (even the same for the same height of the potential). Only the numerical values of, e.g., the localization threshold depend on that feature.

To this end we show in this paper only potentials with a Gaussian damping in order to more easily compare the following separable to the nonseparable potentials.

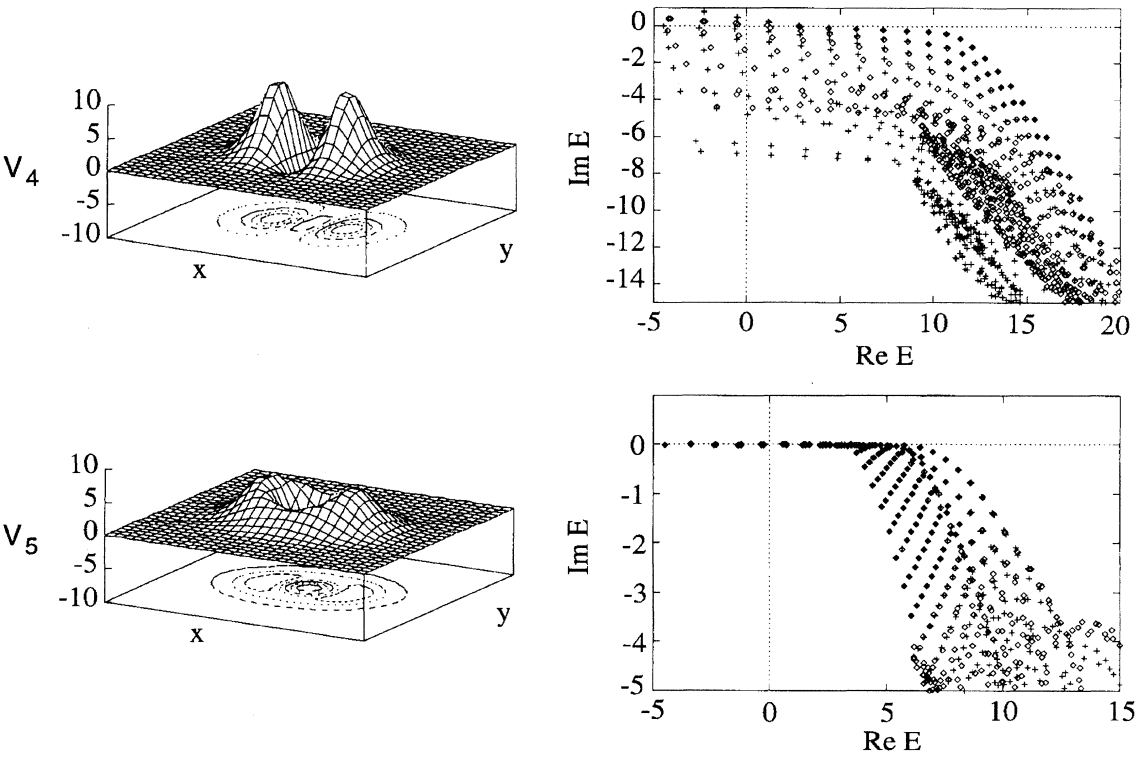

FIG. 3. Potentials and spectra for V_4 and V_5 from Eq. (6). The intervals shown here are for V_4 and V_5: $-4 \leq x$ and $y \leq 4$. For the parameters used see the text. Diamonds correspond to $\theta = 0.3$ and pluses to $\theta = 0.4$ rad.

It is instructive and important for the discussion later on to first look at the simplest two-dimensional Hamiltonians, namely, the separable ones. For this purpose we show in Fig. 2 parts of the spectra of complex scaled Hamiltonians corresponding to

$$V_1(x,y) = \tfrac{1}{2}x^2 + (\tfrac{1}{2}y^2 - 0.8)e^{-0.1y^2} + 0.8, \tag{3}$$

$$V_2(x,y) = (\tfrac{1}{2}x^2 - 0.8)e^{-0.1x^2} + (\tfrac{1}{2}y^2 - 0.8)e^{-0.1y^2} + 1.6, \tag{4}$$

$$V_3(x,y) = 25(xe^{-x^2} + ye^{-y^2}). \tag{5}$$

The first point worth noting is naturally the large number of resonances or strings. Quite opposite to the one-dimensional case, we have to accept that the single string almost never appears. Instead one finds a rather large number of strings that almost densely fill a certain portion of the complex energy plane. Apparently, going over to still higher dimensions will even "worsen" the situation: The density of the eigenvalues will greatly increase and therefore we will be able to find in a certain region of the energy plane eigenvalues almost everywhere. Specifically, we will be able to find more than one (even many) state with the same real energy but different lifetimes. This rather important point will be addressed later.

What about the concepts introduced earlier to describe strings or string curves? Apparently, the concept of a string curve must be reconsidered: Plotting the string curves of the above potentials would have resulted in a black area. Naturally, the main points would have been the same as in the one-dimensional case. As we showed there, the string curve above the detachment point at least up to the localization threshold (in the "smooth" case the whole string curve above the detachment point) is, to a very good approximation, mass independent. For every point of the string curve we can find a mass such that the corresponding Hamiltonian has an eigenvalue there. This is also true in the two-dimensional case, only that now we have an area to "choose" from. The detachment point can be carried over without any change in definition: it still corresponds to the smallest barrier height (see [1] and especially [2] for an investigation in the one-dimensional case). Observe that potential V_1 has a minimal barrier height that is identical to that of a cut at $x=0$, namely, 2.37 hartree, where we also find the detachment point in the two-dimensional case; see Fig. 2. Essentially the same is true for the other potentials. V_2 also has a minimal barrier height of 2.37 hartree (not to be easily observed in the figure, but obvious when considering the cut at $x=0$ or $y=0$) and a detachment point there. V_3 deserves a little more thought. Looking at a one-dimensional cut at about $x=0.8$, one finds a potential with one well and one barrier, which is shifted to negative energies. Therefore there exist particles with negative energy that can nevertheless escape to infinity. Analogous to the interpretation in the one-dimensional case, the lowest "barrier" corresponds here to the value that the potential is maximally shifted to negative energies because the particle can tunnel out there. (These poles in the third quadrant are not to be misinterpreted as virtual poles, they are regular resonances.)

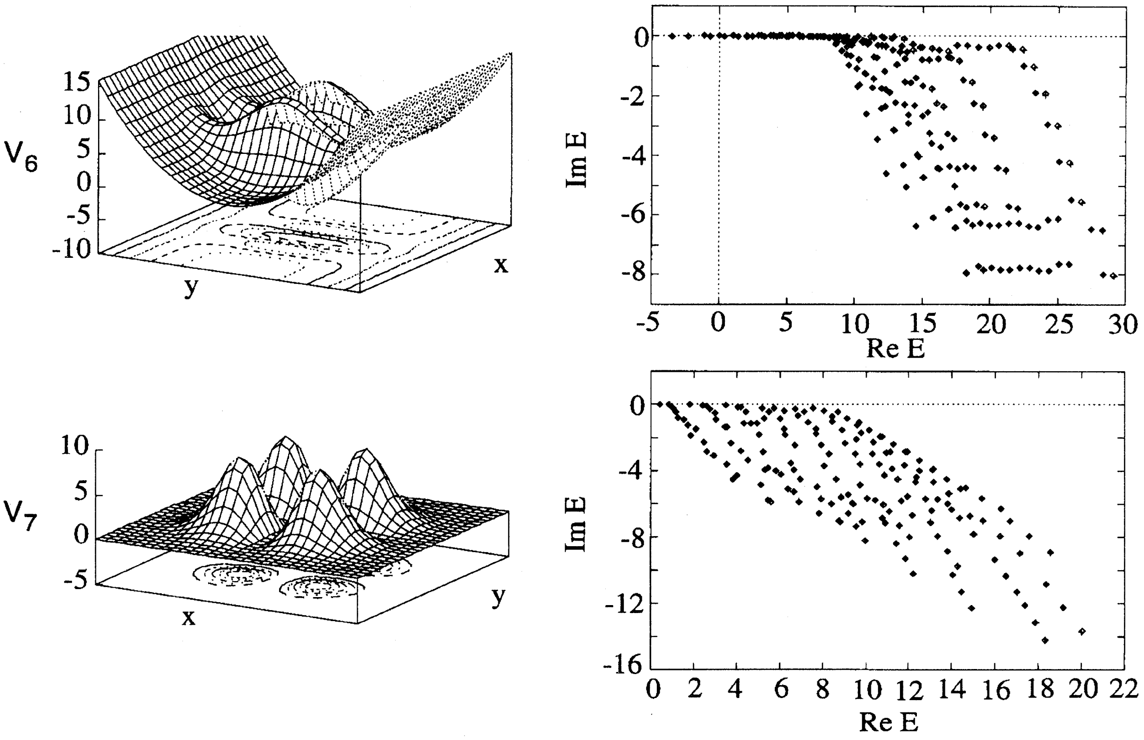

FIG. 4. Potentials and spectra for V_6 and V_7 from Eq. (6). The intervals shown here are for V_6 $-2.3 \leq x \leq 2.3$ and in the case of V_7 $-4 \leq x$ and $y \leq 4$. Note that V_6 is rotated by 90° in order to get a better view of it. For the parameters used see the text. Diamonds correspond to $\theta = 0.3$ and pluses to $\theta = 0.4$ radians.

The concept of a localization threshold is just as easily carried over to two dimensions. In the first example given, we do not naturally find any localization threshold because the potential tends to $+\infty$ along one coordinate. The same situation would have resulted from using any other polynomial, since we argued in [1] and especially [2] that such potentials do not have any localization threshold. In order to find a localization threshold in the two-dimensional case we obviously have to have a localization threshold along both one-dimensional cuts. The other two examples fulfill this condition and therefore we find that the "distance" between the strings diminishes and again we get a localization threshold. An interesting question in this context is whether a one-dimensional potential of height V_0 and depth V_u (we showed in 2 that the localization threshold depends on both parameters) has a higher or a lower real part of the localization threshold than a two-dimensional potential of maximal barrier height V_0 and maximal depth V_u. As an example we chose V_2, Eq. (4). First of all, it is of importance to keep the threshold at the same value in both one and two dimensions because, as shown also in [2], the localization threshold depends on V_0 and V_u both relatively and absolutely. The threshold for V_2 is 0.8 hartree and the barrier height is twice that of the one-dimensional potentials, namely, 4.74 hartree (i.e., 3.94 hartree above the threshold). The well depth is 0 hartree. Bearing this in mind we calculated the string curve of

$$V(x) \;=\; (1.15x^2 - 0.8)e^{-0.1x^2} + 0,$$

i.e., the parameter a (in front of x^2) was varied. Now it has been shown in [33] that the localization threshold depends, to a good approximation, linearly on this parameter. Using the method given in [2] for determining the localization threshold, we calculated a value of 10.08 hartree, which is factor 2.16 times the barrier height above the threshold. Looking at Fig. 2 one finds that this is slightly higher than the localization threshold of the two-dimensional potential, i.e. one gets a rough idea of the portion of the complex plane covered with resonances when looking at "effective" one-dimensional potentials in the sense of above. In this specific example the higher effective potential has a slightly higher localization threshold, but the difference is not significant enough to be interpreted quantitatively.

Let us now turn to nonseparable potentials to see whether we can expect a different kind of behavior for "truly" two-dimensional potentials. The examples we chose to give here are strings for the potentials

$$\begin{aligned} V_4(x,y) &= (35x^2 - 5.6)e^{-x^2-y^2}, & \mu &= 20 \\ V_5(x,y) &= [15(x^2+y^2) - 5.6]e^{-0.7x^2-1.1y^2}, & \mu &= 30 \\ V_6(x,y) &= (40x^2 - 5.6)e^{-x^2-y^2} + 3y^2, & \mu &= 10 \\ V_7(x,y) &= 30x^2y^2e^{-0.7x^2-0.7y^2}, & \mu &= 10, \end{aligned} \quad (6)$$

which are depicted together with the (numerical) spectra in Figs. 3 and 4. Additionally, we show in Figs. 5 and 6 the spectra at $\theta = 0.3$ rad together with the underlying one-dimensional spectra.

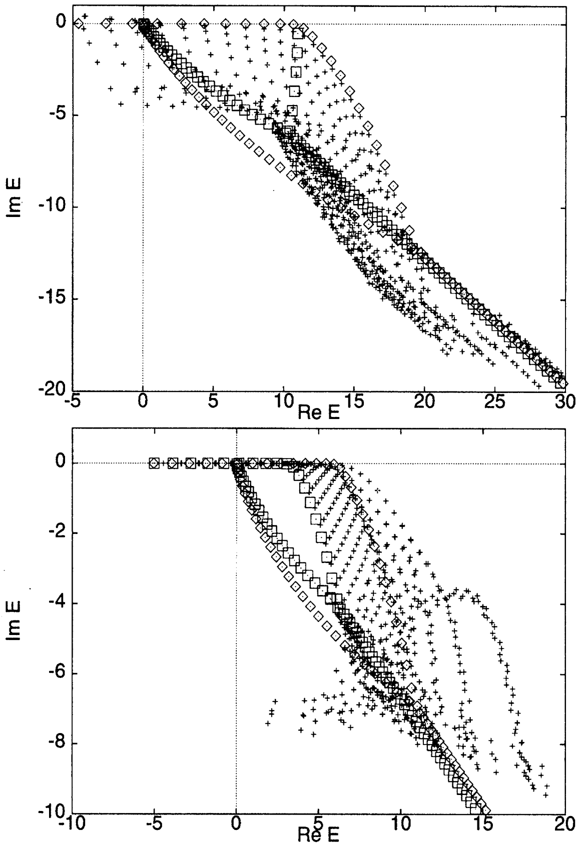

FIG. 5. Spectra of V_4 (top) and V_5 (bottom) for constant $\theta = 0.3$ rad together with the numerical one-dimensional spectra. Pluses stand for the two-dimensional spectrum, diamonds for the one-dimensional spectum in the x direction, and squares for the one-dimensional spectrum in the y direction. For explanations see the text.

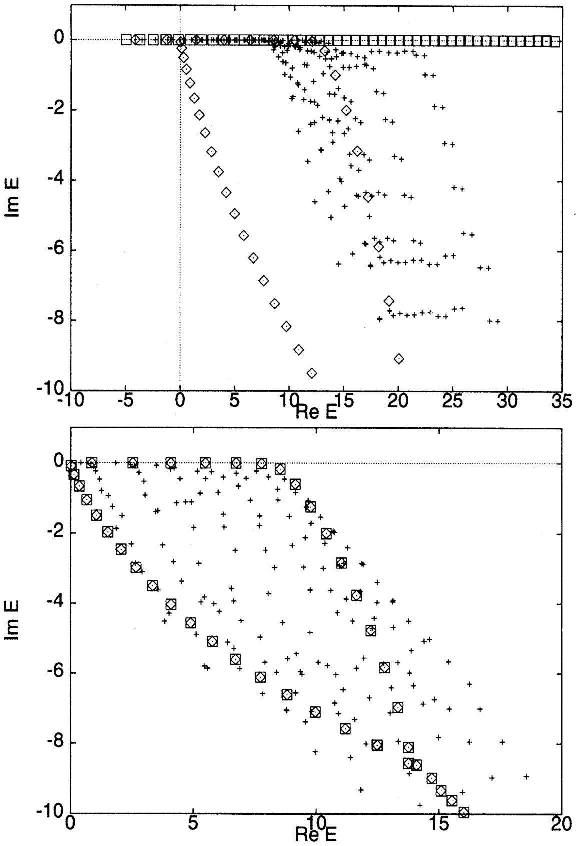

FIG. 6. Spectra of V_6 (top) and V_7 (bottom) for constant $\theta = 0.3$ rad together with the numerical one-dimensional spectra. Pluses stand for the two-dimensional spectrum, diamonds for the one-dimensional spectum in the x direction, and squares for the one-dimensional spectrum in the y direction. For explanations see the text.

For V_4 and V_5 we used 625 ($=25^2$) basis functions and for V_6 and V_7 we used 225 ($=15^2$), found by solving the one-dimensional problems keeping either x or y at a constant value. This value was chosen such that the "maximal" potential resulted, i.e., one with maximal depth and height. The one-dimensional problems were solved using the *complex scaled Fourier grid Hamiltonian* method [29] with a grid of 601 points. These were reduced to 201 (Gaussian) integration points and two-dimensional basis functions were formed by direct product of the sets of one-dimensional functions [30].

Turning now to V_4, a two-dimensional double barrier, one finds a number of slightly shifted strings that show the typical curvature. We expect this potential to have a localization threshold, although this point is not numerically accessible to us. The stability under rotation is, for the first strings, satisfactory but only from a real energy of about 7 hartree on. One reason for that is that the neighborhood to the cut and some of the points shown are not resonances in our sense because they are covered. Additionally, we know by experience that eigenvalues of simple Gaussian barriers are not particularly stable, much less so than that of other potentials. Since the solutions to one-dimensional problems directly enter the calculation, we are not surprised to find a lower stability. This effects also the determination of the detachment point, which in this case is not possible. But looking now at Fig. 5 we see that the two-dimensional strings are very similar to the one-dimensional one corresponding to $V_4(x,C)$; in fact, one may view the two-dimensional spectrum as consisting of strings of the latter type being shifted according to the eigenvalues of $V_4(C',y)$, i.e., the spectrum is *phenomenologically* the same as the one of a separable $V = V_4|_{y=C} + V_4|_{x=C'}$, a result that quite generally seems to be true. Additionally, the string corresponding to $V_4(x,C)$ is a upper limit for the strings of the two-dimensional potential; this also supports for the statement above. Let us stress that quite naturally this is only qualitative since, e.g., the strings are not shifted slightly to lower real energies, as would be the case for the separable potential mentioned above; but, as we are here more interested in a qualitative description, this is a minor point.

The potential V_5 differs from V_4 in that it does not enable barrierless tunneling; movement is restricted in every direction. The numerical stability is much better than in the former case; cf. Fig. 3. The stable regime extends to about $\mathrm{Im}(E) = -4$ hartree, which stems from the fact that only the lowest resonances are included in, the calculation. One observes rather clearly a detachment point at the expected energy (the lowest barrier height) and we observe again the typical curved strings, which again leads to the assumption that this potential will also have a localization threshold. Remarkable is that this spectrum also seems to consist of parallel shifted strings, but this time parallel to the imaginary energy axis. Figure 5 shows the reason for this behavior: One sees there that the strings belonging to the two-dimensional potential start above the lower string belonging to the one-dimensional potential $V(C',y)$. This is not very surprising since resonances below the lowest barrier height are very near the real energy axis and the detachment point of the two-dimensional potential and of that of dimension greater than one coincide. The first approximately ten strings are now shifted parallel to the imaginary energy axis; upon "crossing" the next string the pattern changes quite clearly. One can track this down to the following. A string can be decomposed into three parts, which have somewhat different properties: the part up to the detachment point, the part between the detachment point and the localization threshold, and the irregular part following the localization threshold. Returning now to the two-dimensional spectrum, one observes that resonances near the real energy axis are, to first order, composed of one-dimensional resonances, which are (both) below the detachment point. The ten strings mentioned now are due to one-dimensional functions of which one has an energy below and one an energy above their corresponding detachment point. The rest of the strings are the result of one-dimensional parts with energies above both barrier heights.

The other two examples are rather in line with the above statements. In the case of V_6 we find again a detachment point that corresponds to the lowest barrier height, which here is a local minimum *beneath* the barrier; see Fig. 4. As expected, the particles are "looking" for a minimal energy path to escape and lifetimes are drastically reduced when such a path is open. The spectrum consists of shifted strings more or less parallel to the imaginary energy axis, similar to V_1 of Fig. 2. That the strings stop at some real energy is here naturally caused by the finiteness of the basis set. We do not expect a localization threshold here because the potential is not bounded along one direction.

The picture we get from V_7 is very similar to that of V_2; see Figs. 4 and 2. We find again parallel shifted strings whose distance seems to get smaller if not as strong as in the case of V_2. But the structures are not as regular and a correlation between the one- and two-dimensional strings like in the case of V_4 and V_5 in the sense of maximum-minimum principle does not seem to be possible.

III. SUMMARY AND DISCUSSION

Some points can be learned from the above. First of all, one has to admit that because of the great number of resonances in the two-dimensional case, an investigation like in one dimension is beyond our possibilities. Calculating two-dimensional spectra of the quality shown or better is still a difficult task. As we know from experience, a crucial parameter in the stability of such calculations is the number of eigenvalues found. In one dimension we found that the number of representable complex discrete eigenvalues depends more or less only on the basis set size. Comparing now the numbers shown here with the typical number of eigenvalues in the one-dimensional case, one realizes the difficulties one has to face.

In spite of that, we hope to have convinced the reader that the concepts of detachment point and localization threshold can easily be extended to more than one dimension. We found, as in the one-dimensional case (see [2] for details), that the detachment point corresponds to the lowest "escape" possibility, i.e., the lowest barrier height. Furthermore, we showed that the strings belonging to nonseparable potentials are *phenomenologically* similar to those that correspond to separable potentials, i.e., one gets a good idea of the two-dimensional spectra when considering the spectra that belong to reasonable one-dimensional cuts of the potential. Insofar as we can extend the building block principle, we know what features the one-dimensional spectra will have and from that we can derive a qualitative picture of the two-dimensional spectra. There are of course special features connected with the non-separability, but for a *qualitative* discussion the above procedure is sufficient.

Let us now address the connection to the theory of coherent dissipative structures (for a somewhat detailed description see [21]). As mentioned, the formal representation of the correlated structures are Jordan blocks in the second-order density matrix, which can arise under specific conditions. The most important is that there is a (minimal) number of states with the same real energy and equidistant imaginary parts of the energy, i.e., for a coherent dissipative structure to emerge, we have to have a situation where we find for a given real energy (or rather within a certain real energy interval, which is given by the energy-time uncertainty relation) more than one resonant state.

The above condition now is rather difficult to fulfill in the one-dimensional case; the only reasonable candidates are the wiggly strings of Gaussian type of potentials [$V(x) = P(x)e^{-cx^2}$, where P is a polynomial]. In the two-dimensional case this situation is completely reversed. We have shown that in higher dimensions the number of resonances with almost the same real energy greatly increases. If one imagines now resonances for dimension 6, which is the dimension of the reduced second-order density matrix, one realizes that they will almost densely fill a certain portion of the complex energy plane. We conclude from this that the above condition does not request a specific interaction between the particles, but rather that for every potential we are able to find the situation requested. The authors are well aware of the rather qualitative character of this study, but nevertheless hope that it stimulates a discussion.

ACKNOWLEDGMENTS

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