Polynomial potentials and coupled quantum dots
in two and three dimensions

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Abstract

Polynomial potentials \( V(x) = x^4 + \mathcal{O}(x^2) \) and \( V(x) = x^6 + \mathcal{O}(x^4) \) were introduced, in the Thom’s purely geometric classification of bifurcations, as the benchmark models of the so called cusp catastrophes and of the so called butterfly catastrophes, respectively. Due to their asymptotically confining property, these two potentials are exceptional, viz., able to serve similar purposes even after quantization, in the presence of tunneling. In this paper the idea is generalized to apply also to quantum systems in two and three dimensions. Two related technical obstacles are addressed, both connected with the non-separability of the underlying partial differential Schrödinger equations.

The first one [viz., the necessity of a non-numerical localization of the extremes (i.e., of the minima and maxima) of \( V(x, y, \ldots) \)] is resolved via an ad hoc reparametrization of the coupling constants. The second one [viz., the necessity of explicit construction of the low lying bound states \( \psi(x, y, \ldots) \)] is circumvented by the restriction of attention to the dynamical regime in which the individual minima of \( V(x, y, \ldots) \) are well separated, with the potential being locally approximated by the harmonic oscillator wells simulating a coupled system of quantum dots (a.k.a. an artificial molecule). Subsequently it is argued that the measurable characteristics (and, in particular, the topologically protected probability-density distributions) could bifurcate in specific evolution scenarios called relocalization catastrophes.
1 Introduction

The current progress in nanotechnologies leads to multiple innovations and challenges encountered in the condensed matter physics and optics as well as in their numerous applications, say, in material science [1] or in informatics [2]. *Pars pro toto* let us mention here, for illustration, the very recent success in the experimental preparation of isolated tunable quantum dots and of their interacting multiplets exhibiting, often, various not quite expected phenomenological features and properties [3, 4].

Initially, the best suited candidates for the theoretical explanation and description of properties of the quantum dot systems *alias* artificial or macroscopic atoms [5] and/or quantum-dot molecules [6] appeared to be the one-, two- or three-dimensional square wells. Although the typical size of the systems themselves is given in nanometers, their energy levels still happened to be discrete and described by Schrödinger equation [7]. For theoreticians as well as experimentalists, a source of certain doubt still lied in the non-analyticity of the discrete, rectangular square-well potentials $V(x)$, $V(x, y)$ or $V(x, y, z)$. At the same time, most of the ambitious replacements of these discontinuous toy-model functions by some more realistic and smoother shapes led to the bound-state wave functions and energies given in a purely numerical form.

In recent paper [8] we revealed that between the square-well and the brute-force numerical extremes there may exist a broad grey zone in which the potentials may be chosen in a specific, mathematically friendlier polynomial form while the states themselves can be obtained in a partially non-numerical but still fairly reliable perturbation-approximation form. In our present paper we intend to outline an extension of such an idea from the one-dimensional systems of Ref. [8] to several $D-$dimensional scenarios where $D = 2$ or $D = 3$.

A concise introduction to the field of description of the quantum dot molecules in $D$ dimensions by analytic potentials will be given in section 2. We will describe there the path of extension of the approach and methods of Ref. [8] beyond $D = 1$. In section 3 we then pick up the first nontrivial polynomials of order $2N + 2 = 4$ and provide the details of suitable quantum-dot-molecular models and of the geometry of the related $D = 2$ potentials (in subsection 3.1) and of the analogous $D = 3$ potentials (in subsection 3.2). The next class of potentials with maximal power $2N + 2 = 6$ will subsequently be studied in sections 4 and 5 with the respective choices of $D = 2$ and of $D = 3$. Our results may finally be found discussed and summarized in the last two sections 6 and 7.
2 Polynomial potentials in classical and quantum physics

2.1 Partial differential Schrödinger equations

Phenomenological models of planar or spatial quantum systems are usually defined via a suitable local potential \( V \) and via the respective partial differential Schrödinger equation

\[
\left[ -\frac{\hbar^2}{2\mu_x} \frac{d^2}{dx^2} - \frac{\hbar^2}{2\mu_y} \frac{d^2}{dy^2} + V(x, y) \right] \psi_m(x, y) = E_m \psi_m(x, y), \quad m = 0, 1, \ldots
\]  

or

\[
\left[ -\frac{\hbar^2}{2\mu_x} \frac{d^2}{dx^2} - \frac{\hbar^2}{2\mu_y} \frac{d^2}{dy^2} - \frac{\hbar^2}{2\mu_z} \frac{d^2}{dz^2} + V(x, y, z) \right] \psi_n(x, y, z) = E_n \psi_n(x, y, z), \quad n = 0, 1, \ldots
\]

A conflict may then emerge between the needs of phenomenology (where the realistic potential may be strongly subject-dependent and far from elementary) and the costs of the solution. Those physicists who are interested in the predictions of the measurable properties of the spectra of energies (and/or of the other measurable quantities) are willing to accept any cost, even when a complicated, brute-force numerical method had to be used. In the theory-oriented circles, the costs tend to be lowered. In the literature this is reflected by a disproportionate occurrence of analytic models which are separable and solvable in closed form.

We believe that at least a partial weakening of the conflict might be provided by the analytic models which only remain separable and solvable approximately. In this spirit we will require a strong form of analyticity in the sense that the potentials in Eqs. (1) and (2) (etc) would be just polynomials (of any even order \( 2N + 2 \geq 4 \)) in the \( D \)-plet of the real spatial coordinates \( x, y, \ldots \). This being said, we will also require that

\[
V(x, y, \ldots) = (x^2 + y^2 + \ldots)^{N+1} + \mathcal{O}[(x^2 + y^2 + \ldots)^N],
\]

i.e., that our partial differential Schrödinger equation still remains separable at large distances. For the sake of definiteness we will only consider here the first few simplest even-parity polynomials \( V(x, y, \ldots) \) with \( 2N + 2 \leq 6 \) and with \( D \leq 3 \).

2.2 One-dimensional cusp and butterfly catastrophes

In a broader area of physics the technical advantages of working with polynomial potentials \( V(x, y, \ldots) \) emerge not only in the bound-state theory of quantum mechanics (where the analyticity of potentials leads to an enormous simplification of perturbation-expansion techniques of solving Schrödinger equations [9]) but also in the qualitative considerations in classical mechanics and optics. In the latter setting people usually recall the phenomenology of bifurcations.
in the generic classical dynamical systems where deep role can be attributed to general $D = 1$ polynomials $V(x)$. In the form presented by Arnold [10], the mathematical form of the latter classical-physics idea inspired also our recent paper [8]. We revealed and described there certain quantum-mechanical $D = 1$ analogues of the classical bifurcations. Our present paper can be read as an explicit, constructive extension of the $D = 1$ results of paper [8] to the first two higher spatial dimensions $D = 2$ and $D = 3$.

As indicated in review [11], one of the most widely known qualitative classifications of the parametric dependence of stationary equilibria and of their bifurcations in a generic classical dynamical system is due to René Thom [12]. In his terminology, different configurations of possible bifurcations carry dedicated names of a “fold catastrophe”, of a “cusp catastrophe”, etc. In every one of these arrangements the eligible equilibria were identified with the minima or maxima of certain benchmark polynomials $V(x, y, \ldots)$, also known, in this context, as Lyapunov functions [13]. For example, one of the most popular bifurcation patterns called “cusp” has been assigned, in this scheme, the one-dimensional quartic-polynomial Lyapunov function

$$V^{[cusp]}(x) = x^4 + ax^2 + bx.$$  

The superscripted name “cusp” refers to the cusped-shaped curve which separates the two regions supporting one and two stable classical equilibria (i.e., minima of $V^{[cusp]}(x)$) in the $a - b$ plane of parameters.

In our paper [8] we pointed out that at least a part of the classical theory could be perceived as a semiclassical limit of its quantum-mechanical extension. Every polynomial Lyapunov function (sampled by Eq. (4)) could then play the role of a potential. In loc. cit. we emphasized, in parallel, that besides the limited number of the candidates taken from the Thom’s list, it makes good sense to extend this list in a way recommended by Arnold [10], i.e., to the infinite family of polynomials of arbitrary degree.

In fact, this degree had to be even because due to the emergence of quantum tunneling we had to omit all of the Thom’s asymptotically decreasing (i.e., non-confining) benchmark potentials (like, e.g., $V^{[fold]}(x) = x^3 + ax$, etc) as unstable. In fact, it appeared rather unfortunate that out of the Thom’s list of seven basic benchmarks $V(x)$ or $V(x, y)$ we couldn’t accept any Thom’s sample of the $D = 2$ Lyapunov function. Even at $D = 1$ we were only left with the cusp of Eq. (4) and with the only other, so called butterfly Lyapunov function

$$V^{[butterfly]}(x) = x^6 + ax^4 + bx^3 + cx^2 + dx.$$  

In this way, we also included the Arnold’s higher-degree polynomials. Otherwise, the number of optional parameters would remain too restricted.
According to the brief subsequent comment [14] the main weakness of paper [8] was that in spite of its quantum, genuinely non-geometric and deeply operator-theoretic nature, its results remained restricted to the most elementary one-dimensional class of toy models. In what follows, we intend to fill the gap. We will consider just the cusp and butterfly quantum potentials $V(x)$, but we will extend the results of Ref. [8] and cover both the two- and three-dimensional generalized scenarios.

2.3 Asymptotically separable polynomial potentials

In conventional Schrödinger equations the mass-dependence constants $\Lambda_j = \hbar^2 / 2\mu_j$ may be treated as a $D$-plet of variable phenomenological parameters. This would open the way to the study of the semiclassical limit where these constants are small, $\Lambda_j \approx 0$. Under this assumption one reveals that the low-lying energy levels $E_0, E_1, \ldots$ converge to the same value which is equal to the absolute minimum $V(X,Y,\ldots)$ of the potential at $x = X$, $y = Y$, etc. In this sense the semiclassical limit mediates a connection between quantum mechanics and, say, the Thom’s [12] classical theory describing equilibria and the bifurcations alias catastrophes in non-quantum dynamical systems (see also the thorough dedicated reviews [15]).

The latter observation motivated our quantum-mechanical $D = 1$ study [8]. Potentials were chosen there, for the sake of simplicity, in the form of the Arnold’s [10] even-parity polynomials $V(x) = x^{2N+2} + O(x^{2N})$ of any degree $2N + 2$. We pointed out that in spite of the emergence of tunneling at non-vanishing $\Lambda_j \neq 0$, the Thom’s classical catastrophes characterized by an abrupt change of the observable features of the system after a minor change of the parameters can find certain analogues in the genuine quantum context.

In the opposite, ultra-quantum limit with large $\Lambda_j \to \infty$ the distance between the minimum $V(X,Y,\ldots)$ and the ground-state energy $E_0$ (as well as between $E_0$ and $E_1$, etc) happens to grow. The shape of the potential remains relevant even far from the origin. This observation forces one to eliminate the odd-degree polynomials (like $V^{[fold]}(x) = x^3 + ax$, etc) from the Thom’s list as unstable and unacceptable after quantization.

We will only consider the reality-reflecting dimensions $D = 2$ and $D = 3$ in what follows. Moreover, we will simplify our task by admitting just Schrödinger equations which are asymptotically separable. This will be achieved via constraint [3]. Such an additional simplification is purely formal because we will not use the asymptotic separability of Schrödinger equations, treating constraint [3] merely as a means of elimination of qualitatively less essential coupling constants.

The dynamics-modifying role of at least some of these omitted constants may be transferred to the mass terms $\Lambda_j$. Having clarified their direct role of mediators of the classical and/or ultra-
quantum limits, we shall skip this analysis, and we shall keep all of the mass terms \( \Lambda_j \) equal to one in what follows.

## 3 Cusp potentials in more than one dimension

Paper [16] should be cited here as offering one of the pioneering studies of the one-dimensional Schrödinger equation in which the role of the potential is played by the elementary \( D = 1 \) version of the cusp Lyapunov function. The authors performed, in particular, a detailed analysis of the localization and delocalization of the probability distributions. The paper strongly motivated also our present analysis of the possibilities of a qualitative understanding of the \( D = 2 \) and \( D = 3 \) Schrödinger equations containing the generalized potentials of the cusp type.

The apparently purely numerical, non-separable partial-differential nature of such a schematic bound state project redirected, presumably, attention of may interested researchers to the study of the full-fledged, realistic quantum systems in which the cusp-catastrophic phenomena only re-emerged as a consequence of their constructive analysis. For an illustration of this trend let us only recall the very recent study [17] in which the term “quantum catastrophe” has been attributed to an open quantum system (sampled by a Josephson junction made of two Bose-Einstein condensates) in which the authors apply the Thom’s concepts of the fold and cusp catastrophes to the caustics in the number-difference probability distribution.

In this context our present study of the \( D = 2 \) and \( D = 3 \) models looks, and is, rather naive. One has to emphasize that the above-mentioned direction of considerations (cf. also, in this respect, [18, 19]) really represents just one of many innovative applications of the classical Thom’s theory.

### 3.1 Two dimensions

Two-parametric cusp-type, asymptotically separable potential

\[
V^{[cusp]}(x, y) = r^4 - 2 \alpha^2 x^2 - 2 \beta^2 y^2, \quad r^2 = r^2(x, y) = x^2 + y^2
\]  

with, say, \( \alpha^2 > \beta^2 \) has its real extremes (or, more precisely, the points of stationarity – if any) at the roots \((X, Y)\) of the following coupled pair of polynomial equations

\[
\partial_X V^{[cusp]}(X, Y) = 4X(R^2 - \alpha^2) = 0, \quad \partial_Y V^{[cusp]}(X, Y) = 4Y(R^2 - \beta^2) = 0
\]

where we abbreviated \( R^2 = R^2(X, Y) = X^2 + Y^2 \). On this background it is now rather lengthy but entirely straightforward to reveal and prove that the local points of stationarity occur at
\((X, Y) = (0, 0)\) (this is a local or absolute maximum at the origin), at \((X, Y) = (0, \pm \beta)\) (two local saddle points located off the origin), and at \((X, Y) = (\pm \alpha, 0)\) (the other two local or absolute minima off the origin – see Fig. 1 for an illustrative example).

![Figure 1: \(V(x, y) \leq 0\) part of potential (6) with the two equal minima \(V(\pm \alpha, 0) = -\alpha^4\) and with the two equal saddle-point values \(V(\pm \beta, 0) = -\beta^4\) at parameters \(\alpha = 1.4\) and \(\beta = 1\).](image)

Near both of the non-central local or absolute minima we may re-arrange our polynomial potential yielding the exact, terminating Taylor series,

\[
V^{[\text{cusp}]}(x, y) = -\alpha^4 + 4 \alpha^2 (x \mp \alpha)^2 + 2 (\alpha^2 - \beta^2) y^2 \pm 4 \alpha (x \mp \alpha)^3 \pm 4 \alpha y^2 (x \mp \alpha) + (x \mp \alpha)^4 + 2 y^2 (x \mp \alpha)^2 + y^4.
\]

As long as we assumed that \(\alpha^2 > \beta^2\) we may immediately conclude that these extremes in fact represent the two absolute minima of the potential. We may also notice that during the tentative decrease of \(\alpha^2\) to its boundary value \(\beta^2\) (i.e., during a transition to the rotationally invariant and exactly separable, continuous-spectrum-supporting Mexican-hat limit of the potential) the leading-order approximation of the low lying discrete spectrum generated by the locally dominant harmonic-oscillator well loses its precision because the well itself becomes too much protruded and less and less confining along the \(y\)-axis.
3.2 Three dimensions

At $D = 3$ the positions $(X, Y, Z)$ of the real points of stationarity of the asymptotically separable quartic potential

$$V^{[\text{cusp}]}(x, y, z) = r^4 - 2 \alpha^2 x^2 - 2 \beta^2 y^2 - 2 \gamma^2 z^2,$$

will vary with the triplet of parameters such that, say, $\alpha^2 > \beta^2 > \gamma^2$. These positions will be determined by the three coupled polynomial equations

$$\begin{align*}
\partial_X V^{[\text{cusp}]}(X, Y, Z) &= 4 X (R^2 - \alpha^2) = 0, \\
\partial_Y V^{[\text{cusp}]}(X, Y, Z) &= 4 Y (R^2 - \beta^2) = 0, \\
\partial_Z V^{[\text{cusp}]}(X, Y, Z) &= 4 Z (R^2 - \gamma^2) = 0
\end{align*}$$

where we abbreviated $X^2 + Y^2 + Z^2 = R^2(X, Y, Z) = R^2$.

| (X,Y,Z)  | V(X,Y,Z) |
|----------|----------|
| 1 (0,0,0) | (central local maximum) 0 |
| 2 (0,0,±γ) | (two saddle points) −γ^4 |
| 3 (0,±β,0) | (two saddle points) −β^4 |
| 4 (±α,0,0) | (two absolute minima) −α^4 |

Table 1: Points of stationarity of potential

In a small vicinity of every stationarity point the potential may be replaced again by its respective leading-order approximation. Thus, near the origin, i.e., near the local maximum at $(X, Y, Z) = (0, 0, 0)$ we reveal, in its small vicinity, an inverted-cup shape,

$$V(x, y, z) \approx -2 \alpha^2 x^2 - 2 \beta^2 y^2 - 2 \gamma^2 z^2.$$  

(9)

Near another stationary point $(X, Y, Z) = (±\alpha, 0, 0))$ we discover a pair of absolute minima,

$$V(x, y, z) \approx -\alpha^4 + 4 \alpha^2 (x \mp \alpha)^2 + (-2 \beta^2 + 2 \alpha^2) y^2 + (-2 \gamma^2 + 2 \alpha^2) z^2.$$  

(10)

In this approximation, due to the emergent separability and exact solvability of the reduced model, the numerical construction of the low-lying bound states may be replaced by the leading-order closed formulae followed, if needed, by the perturbation-theory evaluation of corrections (these exercises are left to the reader).
At the other two stationary-point candidates \((X, Y, Z) = (0, \pm \beta, 0)\) and \((X, Y, Z) = (0, 0, \pm \gamma)\) we obtain the respective local approximations

\[
V(x, y, z) \approx -\beta^4 + (2 \gamma^2 - 2 \alpha^2) x^2 + 4 \gamma^2 (y \mp \beta)^2 + (2 \beta^2 - 2 \gamma^2) z^2
\]

and

\[
V(x, y, z) \approx -\gamma^4 + (2 \gamma^2 - 2 \alpha^2) x^2 + (2 \gamma^2 - 2 \beta^2) y^2 + 4 \gamma^2 (z \mp \gamma)^2 ,
\]

i.e., the saddle-point behavior. The list is complete. The situation is summarized in Table 1.

One could also characterize the global shapes of the potentials by displaying the pictures of their separate \(x = 0\) or \(y = 0\) or \(z = 0\) sections. Clearly, the simplicity of the model makes such an illustration redundant. Moreover, the resulting pictures would all look precisely like Fig. 1 above.

4 Butterfly potential in two dimensions

In [8] we considered the first nontrivial confining \(D = 1\) potential \([5]\) in a spatially symmetric special case with \(b = d = 0\). We choose negative \(a = -3(\alpha^2 + \beta^2)\) together with positive \(c = 3\alpha^2\gamma^2\) where \(\gamma^2 = \gamma^2(\alpha, \beta) = \alpha^2 + 2 \beta^2\). This enabled us to guarantee that our one-dimensional potential \(V^{[\text{butterfly}]}(x)\) had a triple-well shape admitting the three well-separated local minima (mimicking quantum dots) such that \(V(x) = 0\) vanished at \(x = 0\) and such that \(V(\pm \gamma) = (\alpha^2 - \beta^2)\gamma^4\) could have both signs. Now we intend to introduce an analogue of this model at \(D = 2\).

4.1 Basic features

In the context of quantum physics we are interested in the identification of the situation in which a small change of parameter would cause a “relocalization catastrophe”, i.e., an abrupt jump from the single-centered measurable probability density localized near the origin to the topologically different quantum state with the two-centered probability density localized far from the origin.

At \(D = 2\), having the same quantum-dot-related motivation as at \(D = 1\), the five-parametric two-dimensional sextic-polynomial potential

\[
V^{[\text{butterfly}]}(x, y) = r^6 - 3 a x^4 - 3 u x^2 y^2 - 3 b y^4 + 3 c x^2 + 3 d y^2 , \quad r^2 = r^2(x, y) = x^2 + y^2
\]

will be considered with positive \(a, \ b, \ c\) and \(d\), and with a real \(u\).

First of all we will have to find the real extremes of the potential if any. Along the same lines as above the coordinates \((X, Y)\) of these extremes must satisfy the following two coupled polynomial equations

\[
\partial_X V^{[\text{butterfly}]}(X, Y) = 6X (R^4 - 2a X^2 - u Y^2 + c) = 0 ,
\]
\[ \partial Y V^{[butterfly]}(X,Y) = 6Y (R^4 - u X^2 - 2b Y^2 + d) = 0. \] (15)

The trivial central extreme at \((X,Y) = (0,0)\) is a local minimum because whenever \(x\) and \(y\) remain sufficiently small we can simply reorder and truncate,

\[ V^{[butterfly]}(x,y) = 3c x^2 + 3 d y^2 + 3a x^4 + 3u x^2y^2 + 3by^4 + r^6 \approx 3c x^2 + 3d y^2. \] (16)

We easily identify the four off-central extremes with \((X,Y) = (0, \pm Y)\) and

\[ Y^2 = b \pm \sqrt{b^2 - d} \] (17)

plus, similarly, the other four extremes with \((X,Y) = (\pm X, 0)\) where

\[ X^2 = a \pm \sqrt{a^2 - c}. \] (18)

In the light of the latter formulae it makes sense to reparametrize the couplings,

\[ a = \alpha_x^2 + \beta_x^2, \quad c = \alpha_x^2(\alpha_x^2 + 2\beta_x^2) = \alpha_x^2\gamma_x^2, \] (19)

\[ b = \alpha_y^2 + \beta_y^2, \quad d = \alpha_y^2(\alpha_y^2 + 2\beta_y^2) = \alpha_y^2\gamma_y^2. \] (20)

A complete parallel emerges with the one-dimensional case. The reparametrization yields the following, most elementary parameter-interpretation formulae

\[ X^2 = \alpha_x^2 < X^2 = \gamma_x^2 \] (21)

and

\[ Y^2 = \alpha_y^2 < Y^2 = \gamma_y^2. \] (22)

Considering just the real points of stationarity (having an elementary geometric interpretation and being localized along the coordinate axes) one reveals a one-to-one correspondence between the guarantees of their reality at \(D = 2\) and at \(D = 1\).

4.2 Points of stationarity off the coordinate axes

What remains to be discussed is the localization of the \(D = 2\) points of stationarity which do not lie on one of the coordinate axes. Under the assumption \(X \neq 0 \neq Y\) these points must be sought as the roots of the set of equations

\[ R^4 - u R^2 + c = (2a - u) X^2, \quad R^4 - u R^2 + d = (2b - u) Y^2. \] (23)
Figure 2: The low-lying part of potential (13) in the \((x - y)\)-symmetric five-deep-dots regime, with \(V(x, y) < 7.5\), \(\alpha_{x,y} = 1\), \(\gamma_{x,y} = 1.9\) and with \(u = -16/3\).

These two relations may be reinterpreted as the respective definitions of \(X^2\) and \(Y^2\) in terms of an unknown quantity \(R^2\). The condition of compatibility \(X^2 + Y^2 = R^2\) is to be added at the end. This yields the exactly solvable quadratic equation for \(R^2\) leading to the two closed-form roots

\[ R^2 = R_{\pm}^2(u) = \frac{uz(u) + 1 \pm \sqrt{uz(u) + 1}^2 - 4z(u)w(u)}}{2z(u)} \]  

where we abbreviated

\[ w(u) = \frac{c}{2a - u} + \frac{d}{2b - u}, \quad z(u) = \frac{1}{2a - u} + \frac{1}{2b - u}. \]  

It is rather straightforward to sample the variability of descriptive features of our asymptotically circular (i.e., asymptotically separable) model. At the positive and large values of \(u\), indeed, both of our above-mentioned auxiliary functions \(w(u)\) and \(z(u)\) are small and negative. In such a dynamical regime the parameters \(R_{\pm}(u)\) defined by formula (24) cannot be real so that we only have to consider the real stationary points such that \(X = 0\) or \(Y = 0\) or \(X = Y = 0\). The corresponding shape of the potential is then sampled in Figure 2. We choose there the values of parameters \(\alpha_x = \alpha_y = 1\), \(\gamma_x = \gamma_y = 1.9\) and a fairly large \(|u|\). In such an arrangement the potential still has the standard and expected single local minimum in the origin. This is accompanied by the four absolute minima which are perceivably deeper and mutually well separated. We may conclude that after transition from one to two dimensions the shape of the butterfly-inspired sextic polynomial potentials becomes richer and more flexible than a priori expected.
An exhaustive qualitative classification and discussion of our fully general five-parametric model would be too long. Even any non-exhaustive, illustrative description of the details of the parametric dependence of the bound states lies beyond the scope of our present study. Still, its fairly detailed outline considering a few most elementary special cases of potential (13) containing just three independent parameters and possessing a triplet of minima separated by pronounced barriers is under preparation at present [14].

5 Butterfly potential in three dimensions

5.1 Points of stationarity on coordinate axes

In three dimensions let us abbreviate 
\[ r^2 = r^2(x, y, z) = x^2 + y^2 + z^2 \]
and consider the following nine-parametric family of potentials
\[
V^{[butterfly]}(x, y, z) = r^6 - 3 a x^4 - 3 b y^4 - 3 c z^4 - 3 u x^2 y^2 - 3 v x^2 z^2 - 3 w y^2 z^2 + 3 p x^2 + 3 q y^2 + 3 s z^2 .
\]
(26)

We assume that \( p, q \) and \( s \) are positive so that we recognize, immediately, the existence of a local minimum at \((x, y, z) = (X, Y, Z) = (0, 0, 0)\). Indeed, near this point we have, in the leading-order approximation,
\[
V^{[butterfly]}(x, y, z) \approx 3 p x^2 + 3 q y^2 + 3 s z^2 .
\]
(27)

The search for the other minima, maxima or saddle points of our sixth-degree polynomial of three variables (26) may proceed in a way paralleling our preceding constructions. First, we differentiate
\[
\partial_X V^{[butterfly]}(X, Y, Z) = 6 X (R^4 - 2 a X^2 - u Y^2 - v Z^2 + p) ,
\]
\[
\partial_Y V^{[butterfly]}(X, Y, Z) = 6 Y (R^4 - 2 b Y^2 - u X^2 - w Z^2 + q) ,
\]
\[
\partial_Z V^{[butterfly]}(X, Y, Z) = 6 Z (R^4 - 2 c Z^2 - v X^2 - w Y^2 + s)
\]
and reparametrize the couplings,
\[
a = \alpha_x^2 + \beta_x^2 , \quad p = \alpha_x^2 (\alpha_x^2 + 2 \beta_x^2 ) = \alpha_x^2 \gamma_x^2 ,
\]
\[
b = \alpha_y^2 + \beta_y^2 , \quad q = \alpha_y^2 (\alpha_y^2 + 2 \beta_y^2 ) = \alpha_y^2 \gamma_y^2 ,
\]
\[
c = \alpha_z^2 + \beta_z^2 , \quad s = \alpha_z^2 (\alpha_z^2 + 2 \beta_z^2 ) = \alpha_z^2 \gamma_z^2 .
\]

This identifies those stationary points which lie on one of the coordinate axes. Their location and some properties are sampled in Table 2.
Table 2: Points of stationarity of potential (26) along coordinate axes. Parameters and their differences are assumed partially ordered, with $\gamma_2^2 > \gamma_y^2 > \gamma_z^2$ and $\alpha_2^2 - \beta_2^2 < \alpha_y^2 - \beta_y^2 < \alpha_z^2 - \beta_z^2 < 0$.

| (X,Y,Z)       | V(X,Y,Z)       |
|---------------|----------------|
| 1 (0,0,0)     | (single central local minimum) 0 |
| 2 (0,0,±α_z)  | (two saddle points) $\alpha_z^4(\alpha_z^2 + 3 \beta_z^2)$ |
| 3 (0,±α_y,0)  | (two saddle points) $\alpha_y^4(\alpha_y^2 + 3 \beta_y^2)$ |
| 4 (±α_x,0,0)  | (two saddle points) $\alpha_x^4(\alpha_x^2 + 3 \beta_x^2)$ |
| 5 (0,0,±γ_z)  | (saddle points or local minima) $(\alpha_z^2 - \beta_z^2)\gamma_z^4$ |
| 6 (0,±γ_y,0)  | (saddle points or local minima) $(\alpha_y^2 - \beta_y^2)\gamma_y^4$ |
| 7 (±γ_x,0,0)  | (saddle points or absolute minima) $(\alpha_x^2 - \beta_x^2)\gamma_x^4$ |

5.2 Points of stationarity off the coordinate axes

Off the coordinate axes the family of points of stationarity $(X,Y,Z)$ may be separated into the three perpendicular-plane subfamilies (such that $X = 0$ but $Y \neq 0 \neq Z$, etc) and the fourth, bulk space subfamily with all of the stationary-point coordinates $X, Y$, and $Z$ non-vanishing. In the former three cases the answers represented by the closed-form roots of a quadratic algebraic equation remain fully analogous to their $D = 2$ predecessors (in fact, the $Z = 0$ root is given precisely by Eq. (24) above). In the last, bulk-space case the real triplet of quantities $(X,Y,Z)$ (if any) must coincide with the roots of the reduced coupled algebraic equations

\[
R^4 - 2AX^2 - uY^2 - vZ^2 + p = 0,
\]

(28)

\[
R^4 - 2BY^2 - uX^2 - wZ^2 + q = 0,
\]

(29)

\[
R^4 - 2CZ^2 - vX^2 - wY^2 + s = 0.
\]

(30)

After transition from $D = 2$ to $D = 3$ the process of the solution of these equations does not change too much. In a preparatory step we may again temporarily treat the symbol $R^4$ as an arbitrarily variable real parameter. Relations (28) – (30) may be then re-read as the linear algebraic set

\[
\begin{bmatrix}
2a & u & v \\
u & 2b & w \\
v & w & 2c
\end{bmatrix}
\begin{bmatrix}
X^2 \\
Y^2 \\
Z^2
\end{bmatrix}
= \begin{bmatrix}
R^4 + p \\
R^4 + q \\
R^4 + s
\end{bmatrix}.
\]

(31)

These equations are solvable via an elementary matrix inversion determining quantities $X^2$, $Y^2$ and $Z^2$ as linear functions of our auxiliary parameter $R^4$. The insertion of the resulting definitions
$X^2 = X^2(R^4)$, $Y^2 = Y^2(R^4)$ and $Z^2 = Z^2(R^4)$ in the constraint $R^2 = X^2 + Y^2 + Z^2$ finally yields quadratic equation

$$R^2 = X^2(R^4) + Y^2(R^4) + Z^2(R^4)$$

(32)

for unknown $R^2$ as well as the two explicit forms $R^2_{\pm}$ of its root.

6 Discussion

Even in the latter, butterfly model at $D = 3$, the exhaustive analysis of the domains of parameters in which the roots $R$ are real and positive would be lengthy but still straightforward. In particular, the shape of the potential will stay characterized, in the most interesting scenarios, by the presence of several pronounced local minima of the depths under our control. They would be mutually separated by barriers so that the low-lying states would be localized near absolute minimum or minima.

Naturally, all of these observations would be supported by the corresponding closed formulae. At the same time, one has to pay main attention to the special cases in which these formulae simplify. Thus, in a way promoted in our methodical guide [8], one should pay particular attention to the most user-friendly cases in which the parameters are large, $\alpha^{2}_{x,y,z} \gg 1$ as well as $\beta^{2}_{x,y,z} \gg 1$. Indeed, precisely in this dynamical regime our potentials happen to exhibit the phenomenologically most interesting shapes as sampled in Fig. 2. Let us now describe and discuss a few samples of these simplified scenarios in more detail.

6.1 The case of small $u$, $v$ and $w$

The simplifications of mathematics caused by the use of the large parameters $\alpha$ and $\beta$ can be sought along the lines outlined in section 3.1 above. New complications arise due to the three parameters $u$, $v$ and $w$ which need not be positive. Fortunately, the inversion in Eq. (31) becomes trivial whenever their size is negligible. The explicit simplified form of our quadratic Eq. (32) then reads

$$(ab + ac + bc) R^4 - 2abc R^2 + sab + qac + pbc = 0.$$ 

(33)

In the isotropic limit $\alpha_x = \alpha_y = \alpha_z = \alpha$ and $\beta_x = \beta_y = \beta_z = \beta$, for example, we get the roots

$$R^2_{\pm} = \frac{1}{3} \left( \alpha^2 + \beta^2 \pm \sqrt{\beta^4 - 8 \alpha^2 (\alpha^2 + 2\beta^2)} \right).$$

(34)

We arrive at the following criterion guaranteeing the reality (i.e., the existence) of the points of stationarity.
Lemma 1 Both roots (34) are (simultaneously) real and positive if and only if the ratio \( \xi = \alpha/\beta \) is small enough, such that \( \xi^2 (2 + \xi^2) \leq 1/8 \), i.e., such that \( \xi \leq \frac{1}{2} \sqrt{-4 + 3\sqrt{2}} \approx 0.2462928572 \).

6.2 The case of large \( u, v \) or \( w \)

In the opposite extreme with a scale parameter \( \lambda \gg 1 \) such that \( \alpha_{x,y,z} = O(\lambda) \) and \( \beta_{x,y,z} = O(\lambda) \) while \( |u| = O(\lambda^2) \) or \( |v| = O(\lambda^2) \) or \( |w| = O(\lambda^2) \) we may omit the other, newly subdominant terms from Eq. (31) and obtain its simplified version

\[
\begin{bmatrix}
0 & u & v \\
u & 0 & w \\
v & w & 0
\end{bmatrix}
\begin{bmatrix}
X^2 \\
Y^2 \\
Z^2
\end{bmatrix}
= \begin{bmatrix}
R^4 + p \\
R^4 + q \\
R^4 + s
\end{bmatrix}
\] (35)

with the \( R^4 \)-parametrized solution

\[
\begin{bmatrix}
X^2(R^4) \\
Y^2(R^4) \\
Z^2(R^4)
\end{bmatrix}
= \frac{1}{2uvw}
\begin{bmatrix}
-w^2 & vw & uw \\
vw & -v^2 & vu \\
uw & vu & -u^2
\end{bmatrix}
\begin{bmatrix}
R^4 + p \\
R^4 + q \\
R^4 + s
\end{bmatrix}.
\] (36)

Reconstruction rule (32) then leads to quadratic equation

\[
(-w^2 + 2vw + 2uw - v^2 + 2vu - u^2)R^4 - 2uvwR^2 -
-pw^2 + qvw + suw + puv - v^2q + svu + puv + qvu - su^2 = 0.
\] (37)

Formula for its roots \( R^2_\pm \) is elementary but lengthy to print. Fortunately, in the isotropic limit with \( u = v = w \) it remains compact and transparent,

\[
R^2_\pm = \frac{1}{3} u \pm \sqrt{u^2 - 3p - 3q - 3s}.
\] (38)

As long as the values of \( p, q \) and \( s \) are assumed large and positive, we arrive at another elementary criterion guaranteeing the existence of the points of stationarity lying off the coordinate axes.

Lemma 2 Solution (in fact, both roots) (38) remains real and positive (i.e., acceptable) if and only if the value of \( u \) is positive and, moreover, sufficiently large,

\[
u = v = w \geq \sqrt{3(p + q + s)} = O(\lambda^2).
\] (39)
6.3 Experimental aspects

A key descriptive feature of the present $D = 2$ and $D = 3$ polynomial potentials $V(x, y, \ldots)$ is a nontrivial though still constructive and controllable variability of the dominance of the subsets of their local minima. This implies that at a fixed set of parameters the bound state densities reflecting the dominance form a topologically protected feature of the system. At the same time, we saw that along certain parameter-subdomain boundaries this protection may be made fragile via a comparatively very small change of the parameters.

This is one of the not entirely obvious manifestations of certain incomplete qualitative parallels between the Thom’s classical classification of catastrophes where there is, by definition, no tunneling, and its present quantum-theoretical analogue in which the tunneling is, naturally, present and allowed. In fact, the control of the intensity of the tunneling is only one of the aspects of the possible measurable features of the systems which would be sufficiently well described by one of the present polynomial potentials. The phenomenon may be suppressed via a heightening and/or broadening of the barriers. Along these lines one could really expect an enhancement of our understanding of “the confinement of 2D electrons in customizable potentials” [4], etc.

Another, more specific experimental benefit may be seen in the smoothness of the shapes of the polynomial potentials which we sampled above. Indeed, such potentials might fit the realistic shapes of quantum dots much better than the discontinuous square wells. After all, the sets of quantum dots are quite difficult to prepare. Typically, quoting again the words of Ref. [4], this has been achieved by “using a low-temperature scanning tunneling microscope” as a microscopic drilling tool which may “create and directly image a new type of coupled quantum dot system in graphene”.

Even in our present, most elementary polynomial-potential models we revealed a fairly high sensitivity of their shapes and spectra to the parameters. For this reason it seem really challenging to search for the abrupt probability-redistribution transitions called “relocalization catastrophes”, with a perceivable phenomenological appeal. In a longer perspective the latter transitions may be expected to be exploited, e.g., in the quantum versions of the information processing.

Once we restrict attention again just to our most complicated $D = 3$ polynomial potential (26) we may really confirm that whenever some of the relevant parameters become large (forming a regime of particular interest), the explicit determination of the positions of all of the local minima of $V(x, y, z)$ happened to be fairly user-friendly, i.e., as straightforward as at $D = 2$. We saw that the analogy with the $D = 2$ predecessor survived also in the vicinity of all of the local extremes, minima or maxima. With good precision, the shape of the potential remained approximately equal there to a separable, exactly solvable harmonic-oscillator well. As a consequence of such an apparently purely technical observation, a non-numerical, closed-formula access has been open not
only to the low-lying energies $E_0, E_1, \ldots$ but also, more importantly, to the dominant components of the density distributions $|\psi_0|, |\psi_1|, \ldots$. Indeed, as long as one knows the parameter-dependence of the latter low-lying harmonic-oscillator states locally, i.e., near every (i.e., not necessarily just absolute) minimum, one can determine the critical values of parameters at which the dominance gets transferred from an “old” absolute minimum or minima to the “new” set of the topologically different ones.

The latter, quantum-tunneling-related process of an abrupt change of dominance was given the name of relocalization catastrophe in [8]. Several schematic $D = 1$ illustrations of the experimentally observable change of the subdomain were presented there in detail. In our present upgraded, $D > 1$ models the mathematics of the construction (i.e., of the search for the crossings of the locally dominant would-be ground states $E_0$) remained the same.

What appeared to be new and different is the rich more-dimensional structure of the domain $\mathcal{D}$ as well as of its subdomains $\mathcal{D}_i$ which are characterized by the specific, different lists of the dominant (i.e., absolute) minima of $V(x,y,z)$. From the quantum-world perspective, a move between any two parametric subdomains $\mathcal{D}_A$ and $\mathcal{D}_B$ alters the depths of the minima and is accompanied by the (avoided) crossings of the respective candidates $E_0^{(A)}$ and $E_0^{(B)}$ for the global ground state energy.

Naturally, the phenomenological wealth of the models should be kept in balance with the intuitive transparency of the formulae. If achieved, the predictions of the abrupt changes of the probability density distributions could really open a new branch of the theory, especially if one manages to localize the quantum-catastrophic boundaries between the separate, topology-protected subdomains in the space of parameters $\mathcal{D}$. In parallel, this might also prove deeply satisfactory from the experimentalist’s point of view.

7 Summary

In all of our present cusp ($N = 1$) and butterfly ($N = 2$) models in dimensions $D = 2$ and $D = 3$ we were able to specify the admissible, well-behaved domains of parameters inside which the qualitative structure and behavior of the low-lying spectra of bound-state energies and wave functions was “regular”, approximately separable and fairly well approximated by the closed, harmonic-oscillator-type formulae. Naturally, whenever we tried to move closer to the “prohibited” boundaries of these domains, we observed the loss of reliability of our approximations. This made our basically non-numerical polynomial-interaction picture of the related physical reality consistent.

We kept in mind that due to the non-separability of our partial differential Schrödinger equa-
tions an intuitive insight in some global features of the system might be misleading. Typically, for potentials admitting the existence of multiple local minima it may be difficult to localize the abrupt changes of the topological structure of probability densities $\{|\psi_m(x, y)|\}$ or $\{|\psi_m(x, y, z)|\}$, especially when they happen to be caused by a minor variation of the coupling constants. This was the key problem which we addressed.

We were inspired by the observation that in $D > 1$ dimensions and in the case of non-separable phenomenological potentials a way of circumventing technical obstacles is most often sought in the restriction of attention to the models which are separable [20]. In our present paper we weakened such a pragmatic constraint. We only assumed the form of separability which emerges far from the origin, asymptotically (cf. Eq. (3)).

For the sake of brevity we also considered just the first few nontrivial non-separable-interaction scenarios. We assumed that $D = 2$ and $D = 3$ and that $V \approx r^4$ or $V \approx r^6$ at the very large distances from the origin, i.e., at $|r| \gg 1$. We admitted the general polynomial forms of the potentials while requiring that these functions of coordinates were oscillatory. In the low-energy regime such a strategy was rewarded by the not quite expected approximate separability and approximative local solvability of Schrödinger equations.

Marginally, let us add that our choice of models led, serendipitously, also to a few interesting mathematical benefits. The first one reflects our analyticity assumptions and consists in the user-friendly nature of description of the shape of the potentials in question. Another benefit is connected with the assumption of the locally pronounced nature of the individual potential valleys and barriers. As its byproduct we obtained the models of artificial molecules which proved tractable, in a fairly good approximation, non-numerically.

Summarizing, after the present transition from elementary $D = 1$ to higher dimensions $D = 2$ and $D = 3$ we have to appreciate the survival of the transparency of the resulting approximate non-numerical formulae. This is certainly opening the way toward several practical applications, especially in the brand new context of quantum catastrophes. In this context our constructions of the low-lying quantum bound states may be expected to prove useful and instructive, especially due to their phenomenologically promising multi-quantum-dot nature.
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