Quantum exotic: A repulsive and bottomless confining potential

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Abstract

On a simple model $V(x,y) = A\,x^2 + B\,y^2 + C\,x^2y^2 + D\,(x^2y^4 + x^4y^2)$ we demonstrate that even in a classically repulsive regime (i.e., at couplings which make the potential decreasing to $-\infty$ in some directions) quantum mechanics may still support the purely discrete spectrum of bound states. In our example, there exists a critical boundary of this domain of stability where a further increase of repulsion causes an explosive escape of particles in infinity.

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1 Introduction

Hydrogen atom is one of the best known examples of a confinement of particles (electrons) in an attractive potential. Its discrete spectrum does not collapse – this is not perceived as as a paradox from the very early days of quantum mechanics [1]. The explanation is easily acceptable and goes back to the uncertainty principle. The stability of this atom in the origin may be well extended down to the inverse quadratic central attraction $V_{(v)}(r) \approx v/r^2$, $r \ll 1$ with a limited strength, $v > -1/4$ [2]. An unprotected fall of electrons to *this* singularity only takes place *beyond* the "natural" critical coupling $v = -1/4$. Its existence is not surprising – one simply re-accepts the safe classical intuition.

A scarcity of *non-central* examples of transition between confinement and its collapse is surprising and worrying. In more dimensions, our intuition may fail. In classical mechanics, a sign of warning comes from an unexpected emergence of chaos in the anisotropic Coulomb problem [3]. In two dimensions, the emergence of the classical chaos may serve as a guide to study of the quantum chaos [4]. This seems best illustrated by the elementary $\alpha \to 0$ limit of the quartic polynomial potential $V_{[\alpha]}(x, y) = x^2y^2 + \alpha\,(x^4 + y^4)$ which is bounded from below [5].

After quantization, the peculiar semi-bounded $\alpha \to 0$ extreme $V_{[0]}(x, y) = x^2y^2$ has re-attracted attention as an approximate model of a non-abelian field [6]. For this reason, the mathematical gap has quickly been filled. Several versions of the rigorous proof of the purely quantum confinement property at $\alpha = 0$ have been delivered by Simon [7]. A full parallel with the Coulombic stability has been re-established. On the basis of the Heisenberg uncertainty principle, each plane wave with energy $E > 0$ which tries to escape along an axis (say, x) in infinity proves unable to do so due to a decreasing width of its classically permitted narrow escape corridor $x^2\, y^2 \leq E$ with hyperbolic boundaries.

Many questions arise immediately: What are the limits of capacity of the narrow tubes to prevent the (classically permitted) asymptotical "constant speed" escape of quantum particles? What could be a decisive counter-acting mechanism? An acceleration by repulsion? Which "asymptotically bottomless" repulsive potentials could be interpreted as (say, two dimensional) asymptotical analogues of the above mentioned critical attraction $V_{(1/2)}(r) \approx -1/(2r)^2$? May a confinig two-dimensional quantum potential $V(x, y)$ be asymptotically unbounded from below at all?

In the present note, we intend to provide a few answers which, in all their incompleteness, do not seem entirely trivial. Even for polynomial forces in two dimensions, the abundance of couplings definitely hinders the classification. The semi-classical estimates of the number of bound states below a given energy may become (and often happen to be) meaningless. Still, we shall keep our mathematics virtually elementary and emphasize the underlying (and, sometimes, quite unexpected) physical consequences.

We shall pay attention just to a four-parametric family of particular sextic polynomial models

$$V_{(A,B,C,D)}(x, y) = A\, x^2 + B\, y^2 + C\, x^2 y^2 + D\, (x^2 y^4 + x^4 y^2), \qquad D > 0, \quad C \neq 0.$$

As we shall see, their special cases with a controllable and tuneable attraction to infinity may be called repulsive in plain language. In a way resembling the studies of the central attraction $V_{(-1/4\pm\varepsilon)}(r)$ we do not expect any immediate (and, even less, realistic) applicability of these repulsive forces. We just seek a connection between unusual asymptotics and a smooth transition between the confined and de-confined phase in non-central systems.

2 Analysis

2.1 Spectrum

In a preparatory step, let us abbreviate $\gamma = \sqrt{D} > 0$ and re-parametrize the couplings $C = 2\gamma\,(\alpha + \beta)$, $B = \alpha^2 - \gamma + \delta$ and $A = \beta^2 - \gamma + \delta$. Conversely, this defines the new parameters in terms of the old ones,

$$\alpha = \frac{C}{4\gamma} + \gamma\,\frac{A-B}{C}, \qquad \beta = \frac{C}{4\gamma} - \gamma\,\frac{A-B}{C}, \qquad \delta = A + \gamma - \alpha^2. \tag{1}$$

Such a change of notation simplifies our following key observation.

LEMMA. The spectrum of energies of the Hamiltonian

$$H_{(A,B,C,D)} = -\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} + V_{(A,B,C,D)}(x,y) \tag{2}$$

with the positive parameter $\delta > 0$ is discrete.

Proof. Firstly, let us notice that the assumption $C \neq 0$ is purely technical. Easily, the proof at some $C < 0$ would extend up to $C = 0$ since, due to the positive semi-definitness of x^2y^2, we may use the inequality $H_{(A,B,C,D)} \leq H_{(A,B,C+\varepsilon^2,D)}$. The discrete spectrum of its left-hand side implies the discrete form of the spectrum of the right-hand-side operator. In the second step, let us pick up a real (and, temporarily, freely variable) number $M > 1$ and split our Hamiltonian in two parts,

$$H_{(A,B,C,D)} = -\frac{1}{M}\frac{\partial^2}{\partial x^2} - \frac{1}{M}\frac{\partial^2}{\partial y^2} - \frac{M-1}{M}\frac{\partial^2}{\partial x^2} - \frac{M-1}{M}\frac{\partial^2}{\partial y^2} + V_{(A,B,C,D)}(x,y).$$

The well known estimate $-\frac{d^2}{dq^2} + \omega^2 q^2 \geq |\omega|$ of the harmonic-oscillator Hamiltonian may be recalled to imply

$$\frac{M-1}{M}\left(-\frac{\partial^2}{\partial x^2} + \frac{(\alpha+\gamma y^2)^2 M}{M-1}x^2\right) \geq \sqrt{\frac{M-1}{M}}\,|\alpha+\gamma y^2|$$

and

$$\frac{M-1}{M}\left(-\frac{\partial^2}{\partial y^2} + \frac{(\beta+\gamma x^2)^2 M}{M-1}y^2\right) \geq \sqrt{\frac{M-1}{M}}\,|\beta+\gamma x^2|.$$

We have $|\alpha+\gamma y^2| \geq \alpha+\gamma y^2$ and $|\beta+\gamma x^2| \geq \beta+\gamma x^2$ so that, irrespectively of the signs of α and β, we may conclude that

$$H_{(A,B,C,D)} \geq \sqrt{\frac{M-1}{M}}\,(\alpha+\beta) - \frac{1}{M}\frac{\partial^2}{\partial x^2} - \frac{1}{M}\frac{\partial^2}{\partial y^2} + \left[\left(\sqrt{\frac{M-1}{M}} - 1\right)\gamma + \delta\right](x^2+y^2). \tag{3}$$

As long as $\delta > 0$, the new couplings of the quadratic term remain positive for all the sufficiently large $M > M_{min}$. With any $M_{min} > 1$ such that

$$M_{min} + \sqrt{M_{min}(M_{min}-1)} \geq \frac{\gamma}{\delta}$$

our Hamiltonian $H_{(A,B,C,D)}$ becomes minorized by an ordinary separable harmonic oscillator. We may infer that it possesses the discrete spectrum only. QED.

Our LEMMA does not seem surprising. Indeed, whenever $\alpha^2 + \delta > \gamma$ and $\beta^2 + \delta > \gamma$, our potential $V_{(A,B,C,D)}(x,y)$ is minorized by its harmonic-oscillator part. Abruptly, the situation changes when we admit the negative values of A or B. The repulsivity constraint $A < 0$ (i.e., $\gamma - \alpha^2 > \delta > 0$) would induce an *accelerated* escape of a classical particle along the semi-axes $\pm x$. For $B < 0$ (i.e., $\gamma - \beta^2 > \delta > 0$) the escape would occur along $\pm y$. At both these conditions (i.e., for $\gamma - \max(\alpha^2, \beta^2) > \delta > 0$), the origin becomes a local maximum of $V_{(A,B,C,D)}(x, y)$. Our potential acquires a repulsive and bottomless form. At $\alpha = \beta = 0$, $\gamma = 1.1$ and $\delta = 0.1$ its shape is displayed in Figure 1.

2.2 The ground state energy

We have to notice that the escape tubes are very deep and not as narrow as one would expect. The area of the sections $V_{(A,B,C,D)}(x, y) = E$ remains infinite (!) at an arbitrary negative energy E. The shape of these sections resembles their quartic x^2y^2 predecessors with a steady narrowing proportional, say, to $1/x$ for $x \gg 1$. Still, in contrast to the positively semi-definite tubes in $V_{[0]}(x, y) \geq 0$, their present narrowing seems more than compensated by the quick downward fall of their bottom – this decrease is proportional to $-|A|\, x^2$ at $y = 0$, i.e. quadratic! With the same parameters as above, the situation is illustrated in Figure 2. In a broad interval of energies $2\sqrt{-E} \in (3, 9)$ the thinning of our escape sinks seems virtually negligible.

A flavour of a paradox strengthens with a subsequent observation that our only condition $\delta > 0$ of the impenetrability of sinks in LEMMA is in fact entirely independent of the signs of α and β. A reversal of these signs would change $C > 0$ into $C < 0$ and flip the *quartic*, asymptotically very strong part of our potential upside down, $(x^2y^2 > 0) \to (-x^2y^2 < 0)$. This is a significant change but it only shifts the energies. The lower estimate of the ground-state energies

$$E_{(g)} \geq \alpha + \beta \equiv \frac{C}{2\sqrt{D}} \tag{4}$$

holds for all the Hamiltonians (2) with $\delta > 0$.

For a proof, let us replace $M \in (1, \infty)$ by $\varepsilon = 1 - \sqrt{1 - 1/M} \in (0, 1)$. With the above inequality $-\frac{d^2}{dq^2} + \omega^2 q^2 \geq |\omega|$ applied to eq. (3) once more, this gives us the $\varepsilon-$dependent family of estimates

$$E_{(g)} \geq (\alpha + \beta)(1 - \varepsilon) + 2\sqrt{(\delta - \gamma\,\varepsilon)(2\varepsilon - \varepsilon^2)} \tag{5}$$

which confirms eq. (4) at any sufficiently small ε.

An improved estimate of $E(g)$ may be computed from eq. (5) at a right-hand-side maximum (achieved at an optimal value $\varepsilon_{(opt)}$). In the most interesting bottomless case with $\delta < \gamma$ we may denote $\delta/2\gamma = \rho^2 \in (0, 1/2)$, renormalize $\varepsilon = 2\rho^2\,\eta,\ \eta \in (0, 1)$ and put

$$E_{(g)} = (\alpha + \beta) + 2^{3/2}\,\delta\gamma^{-1/2} \max_{\eta \in (0,1)} W(\eta, \theta), \qquad \theta = -\text{Arsinh}\left[\sqrt{\frac{1}{2\gamma}}\ \left(\frac{\alpha + \beta}{2}\right)\right] \tag{6}$$

where $W(\eta, \theta) = \eta \sinh\theta + \sqrt{\eta(1 - \eta)(1 - \rho^2\,\eta)}$ and $\theta \in (-\infty, \infty)$.

A simplification occurs at $\theta = 0$ where the derivative of $W(\eta, 0)$ with respect to η vanishes at a unique root of an algebraic quadratic equation. We get a unique lower estimate of energies which is a decreasing function of the parameter $\rho^2 \in (0, 1/2)$,

$$\max_{\eta \in (0,1)} W(\eta, 0) = \sqrt{\frac{(F(\rho) + \rho^2)(F(\rho) + 1)}{(F(\rho) + \rho^2 + 1)^3}} \in \left(\frac{1}{\sqrt{3\sqrt{3}}}, \frac{1}{2}\right) = (0.43869\ldots, 0.5), \tag{7}$$

and $F(\rho) = \sqrt{1 - \rho^2 + \rho^4} \in (\sqrt{3}/2, 1)$.

At $\theta \neq 0$ a similar formula would contain a root of a biquadratic equation. A simple algorithm may be recommended instead. Its inspiration comes from an observation that in the interval $(0,1)$, the graph of the function $\sqrt{\eta(1-\eta)}$ is just an upper half of a circle. Its multiplication by the decreasing function $\sqrt{1-\rho^2\,\eta}$ only slightly deforms this shape. Its maximum moves down and to the left. An addition of a linear function gives the full graph of $W(\eta,\theta)$ as another very smooth deformation with the right end shifted up or down. Our idea is to approximate the decreasing factor $\sqrt{1-\rho^2\,\eta} \in (1/2,1)$ by a constant.

At an initial $n=0$ and with an extreme choice of $\eta=\eta_n=1$ we shall define $\sinh\,\theta_n = \sinh\,\theta/\sqrt{(1-\rho^2\,\eta_n)}$ and minorize

$$W(\eta,\theta) \geq W_n(\eta,\theta_n)\times\sqrt{1-\rho^2\,\eta_n}, \qquad \eta\leq\eta_n, \qquad W_n(\eta,\theta_n) = \eta\sinh\,\theta_n+\sqrt{\eta(1-\eta)}. \tag{8}$$

The (unique eligible) maximum of the simplified function $W_n(\eta,\theta_n)$ lies at the point $\eta_{n+1} = \exp\theta_n/(2\cosh\,\theta_n)$. Its value is easily found,

$$\max_{\eta\in(0,1)} W_n(\eta,\theta_n) = W_n(\eta_{n+1},\theta_n) = \frac{1+\exp 2\theta_n}{4\cosh\,\theta_n}. \tag{9}$$

and remains compatible with the minorization (8). Our approximate graph over-estimates the correct one for $\eta>\eta_{n+1}$ and under-estimates it for $\eta<\eta_{n+1}$. The true maximum must still lie to the left from its guess η_{n+1}. The validity of minorization (8) is preserved at $n+1$.

We may iterate the whole construction until a sufficient numerical precision is achieved. Table 1 samples its rate of convergence for $\sinh\,\theta=1$ and 2 at $\rho^2=0.4$.

3 Summary

In a weakly anharmonic regime (i.e., say, for $\alpha = \mathcal{O}(1) = \beta$ and small γ and δ) our estimate (4) looks very perturbative. The ground-state wavefunctions – perhaps, variational – may be expected to lie very close to the well known harmonic oscillator gaussians. The growth of γ does not change the picture too much. To our only surprize, the improved gaussian

$$\psi(x,y) = \exp\left(-\frac{\alpha}{2}\,x^2 - \frac{\beta}{2}\,y^2 - -\frac{\gamma}{2}\,x^2\,y^2\right) \tag{10}$$

becomes the *exact* ground-state wavefunction at $\delta = 0$.

A crisis comes when we try to diminish the coefficients α or β. The norm of $\psi(x,y)$ in eq. (10) starts growing and indicates a possible collapse of the system. Quickly, we re-establish the positivity of $\delta > 0$. Of no avail! The threat of collapse becomes unavoidable. The seemingly innocent condition $\delta = 0$ acquires its real physical significance as a point where the quantum impenetrability of our downward sinks is lost, at $\alpha = \beta = 0$ at least.

A deeper analysis of our LEMMA and its proof at any α and β recovers that after a change of sign of δ, our estimates start working in an opposite direction. In particular, deeply in our escape tubes, the *local* approximants of the bound-state energies move *downwards*. Quantum particles commence an accelerated motion and, after all, disappear in infinity. In our bottomless and, now, only a little bit more repulsive potential, the discrete spectrum of energies collapses down.

We may conclude that the apparent physical paradox of quantum confinement in the presence of an overall repulsion is clarified. It is resolved in full analogy with the central symmetric attraction $\approx v/r^2$. Beyond certain limit, the classical picture re-enters the scene. Nontrivial mathematics must be used. The present text revitalizes and generalizes the old Rellich's ideas [8] and their Simon's "sliced bread" rediscovery [7] to forces which are *not* bounded from below. In such a case we loose the safe "uncertainty principle" intuition (plane waves become accelerated). Our "asymptotically bottomless" forces require a more tricky treatment (basically, a local harmonic re-interpretation of transversal modes of the wavefunctions). Of course, such an analysis may be expected transferrable far beyond our particular sextic example.

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Figure captions

Figure 1. The negative half of potential $V_{(-1,-1,0,1.21)}(x,y)$.

Figure 2. The energy-dependence of boundaries $V_{(-1,-1,0,1.21)}(x,y) = E$ at (a) $E = -9/4$, (b) $E = -25/4$, (c) $E = -49/4$ and (d) $E = -81/4$.

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Table 1. Iterative determination of the lower energy estimates (6)

(a) for sinh $\theta = 1$ and

(b) for sinh $\theta = 2$.

	(a)		
iteration	η_n	θ_n	maximum
0	1.000	1.073	1.000
1	0.895	1.0464	1.14059
2	0.8902	1.04521	1.141076
3	0.889969	1.045154	1.1410952
4	0.8899577	1.0451516	1.14109612
0	0.889900	1.045138	1.141101
1	0.8899544	1.0451508	1.14109637
	(b)		
0	1.000	1.677	2.000
1	0.9663	1.66689	2.073945
2	0.965570	1.6666847	2.0739846
3	0.9655560	1.6666805	2.0739853
4	0.96555573	1.6666804	2.0739853
0	0.96555569	1.6666804	2.0739853
1	0.96555572	1.6666804	2.0739853