Double-well potentials and exact solvability[1]

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talk about harmonic oscillator twins

$$V(x) = V_{[d]}(x) = \begin{cases} (x-d)^2, & x > 0, \\ \\ (x+d)^2, & x < 0 \end{cases}$$

♡ curiosity in physics: never mentioned in the textbooks on quantum mechanics

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♡ motivation in math: relevant. i.a., in the Thom's catastrophe theory (TCT)

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♡ reference: MZ, Quant. Rep. 4 (2022) 309 (arXiv:1607.01297v2)

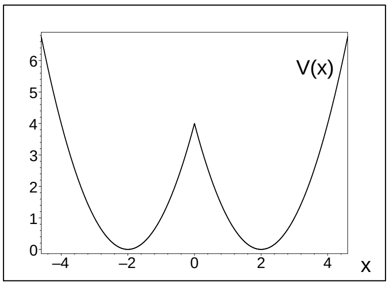

Figure 1: Double-well harmonic oscillator at $d = 2$.

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A. exact solvability: alternative definitions

$\diamondsuit$ main task: find $\boxed{\text{quantum bound states}}$ in 1D

> Schrödinger equadtion

$$-\frac{\mathrm{d}^2}{\mathrm{d}x^2}\,\psi_n(x) + V(x)\,\psi_n(x) = E_n\,\psi_n(x)\,, \qquad \psi_n(x) \in L^2(\mathbb{R})\,, \qquad n = 0, 1, \ldots$$

> if analytic $V(x)$ then Darboux/SUSY $\rightarrow$ ES (exact polynomial solvability)

> or QES (quasi-exact polynomial solvability)

> else: square-well, etc $\rightarrow$ $\boxed{\text{matching method}}$ $\rightarrow$ trigonometric formulae

♠ today: numerically inspired innovation

> standard 3D shooting method used in 1D

> idea (AHO, MZ 2016): 3D know-how ($V(x) = V(-x)$) + matching (at $x = 0$)

.

> simplification: use special functions → old concepts with new names emerge:

> NS (non-polynomial solvability)

> QNS (quasi-exact non-polynomial solvability)

> previous results: DW exponentials (Bessel functions), DW Morse (Gauss functions)

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B. elementary model

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1st question: where is our model relevant?

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answer: in a quantized TCT (p.t.o.)

♣ the Thom's classification of bifurcations

> the *classical* equilibria = minima of Lyapunov function, i.e., e.g., of

$$\boxed{V(x) = V^{(cusp)}(x, a, b) = x^4 + ax^2 + bx} \quad \text{which yields,}$$

in the $a - b$ plane, a spiked, cusp-shaped boundary between

> the single minimum regime (at $a > 0$) and the

> DW regime (at $a < 0$, with a not too large b)

> $\exists$ applications (e.g., Josephson junction between BECs – Goldberg et al, 2019)

> but not in the consequent quantum theory, due to tunneling

♠ in the quantized TCT

the general and universal Arnold-Lyapunov polynomial

$$V(x) = (x, a, b, c, \ldots) = x^{2k+2} + ax^{2k} + bx^{2k-1} + \ldots$$

was locally approximated by the DW-like HOs:

MZ., Arnolds potentials and quant. catastrophes, Ann. Phys. 413 (2020) 168050,

https://doi.org/10.1016/j.aop.2019.168050.

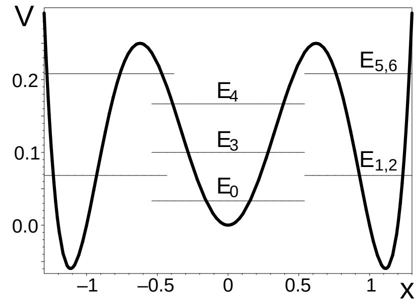

Figure 2: Quantum levels in the "butterfly" potential $V(x) = x^6 - 61/25\, x^4 + 36/25\, x^2$

✓ in detail:

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$>$ in the deep-well regime we approximate

$$V^{(cusp)}(R_\pm + \xi, a, b) = V^{(cusp)}(R_\pm, a, b) + \omega_\pm^2\, \xi^2 + \mathcal{O}(\xi^3) \qquad \text{by}$$

$$V(x, a, b) = \min\left[\omega_-^2\,(x - R_-)^2 + D_-\,,\, \omega_+^2\,(x - R_+)^2 + D_+\right]$$

$>$ then the quantum bifurcation occurs when $\omega_-^2 \approx \omega_+^2$ and $D_- \approx D_+$

$>$ *so that* in units s.t. $\omega = 1$ we get our model, $\boxed{V_{[d]} = x^2 - 2d\,|x| + d^2}$.

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2nd question: key merit of DW HO?

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answer: exact Jost solutions available!

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$>$ $\exists$ asymptotically correct (and known, confluent hypergeometric) $\boxed{\psi(x) \sim {}_1F_1}$

& user-friendly standard $\boxed{\text{NS}}$ matching rules:

$\diamondsuit$ consider parity: $\psi(x) = \psi(x, E, p) = (-1)^p\, \psi(-x, E, p)$ with $p = 0$ or $p = 1$

$\spadesuit$ normalize: $\lim_{x\to 0} \psi^{(+)}(x, E, 0) = \mathcal{N}_0 \neq 0\,,\qquad \lim_{x\to 0}(\psi_n^{(+)})'(x, E, 1) = \mathcal{N}_1 \neq 0$

$\clubsuit$ use b. c^s. <u>on half-line</u>: $\lim_{x\to 0}(\psi^{(+)})'(x, E, 0) = 0\,,\qquad \lim_{x\to 0} \psi^{(+)}(x, E, 1) = 0\,.$

& $\boxed{\text{the simplest QNS}}$ $N = 1$ single-well example: $d^{(QNS)} = -1$, $E = E_0^{(QNS)} = 3$,

$$\psi_0^{(QES)}(x) = \begin{cases} (1+x)\, e^{-\left(x^2/2+x\right)}, & x > 0, \\ (1-x)\, e^{-\left(x^2/2-x\right)}, & x < 0 \end{cases}$$

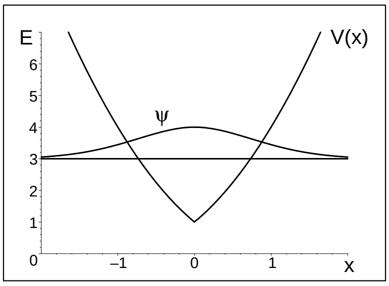

Figure 3: QNS ground state at $d = -1$.

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consequence: all NS & QNS by matching!

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C. non-polynomial quasi-exact states (the method)

♡ quartic QNS AHO model with $\boxed{\psi(x) = P(x)\, \exp W(x)}$

$$V^{(AHO)}(x) = \begin{cases} qx + rx^2 + sx^3 + x^4\,, & x < 0\,, \\ -qx + rx^2 - sx^3 + x^4\,, & x > 0\,, \end{cases}$$

> method = the matching of both of the $\boxed{\text{elementary ansatz}}$ branches at $x = 0$

> reference:

MZ, Symmetrized quartic polynomial oscillators and their partial exact solvability. Phys. Lett. A 380 (2016) 1414 - 1418 (doi: 10.1016/j.physleta.2016.02.035) (arXiv:1602.07088)

$\heartsuit$ the main trick: the branching of asymptotics (with $\tilde{a} = a$ and $\tilde{b} = b$),

$$W_{(non-analytic)}(x) = \begin{cases} W_{(left)}(x) = +x^3/3 + a\,x^2 + b\,x\,, & x < 0\,, \\ W_{(right)}(x) = -x^3/3 + \tilde{a}\,x^2 - \tilde{b}\,x\,, & x > 0\,. \end{cases}$$

® the $N = 2$ ansatz for $\psi^{(even)}(x)$ with $P_{(left)}(x,n) = (1 + ux + vx^2)$ yields

$>$ 2 WKB constraints, $-vs + 4\,av = 0\,, \quad 4\,a^2v + 4\,au - vr - us + 2\,bv = 0$,

$>$ obligatory linear coupling $q = q(a,b) = 4\,ab + 6$

$>$ obligatory energy $E = -p$, i.e., $E = E(a,b,v) = \frac{2\,u}{v} - 10\,a - b^2\,,$

$>$ plus the two matching constraints (P.T.O.)

> the two remaining equations are

$$4\,bv - q + 4\,ab + b^2 u + 2 + 6\,au - up = 0\,, \qquad 2\,a + 2\,bu + 2\,v - p + b^2 = 0\,.$$

> the first one offers the two eligible wave-function-coefficient roots

$$v = v_{\pm} = \frac{1}{4b}\left(-2\,ab + 2 \pm 2\,\sqrt{a^2 b^2 - 2\,ab + 1 - 2\,b^3}\right)$$

> the second one leaves the real value of $b \neq 0$ independently variable,

$$a = a_{\pm} = \frac{1}{20\,b}\left(-7\,b^3 - 8 \pm 3\,\sqrt{b^6 - 12\,b^3 + 16}\right)\,.$$

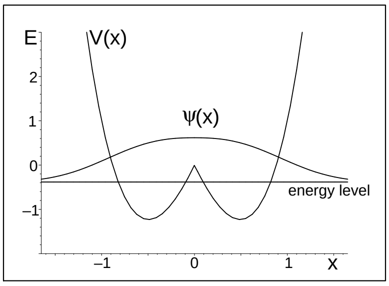

Figure 4: The QNS ground state in the $N = 2$ quartic potential at positive $b = 1$:

$$V_{\pm}(x) = \mp 3\ \left(1 + 1/\sqrt{5}\right) x + \left(2 + 9\ \left(-1 + 1/\sqrt{5}\right)^2 /4\right) x^2 \mp 3\ \left(-1 + 1/\sqrt{5}\right) x^3 + x^4$$

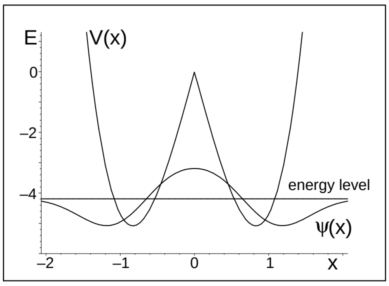

Figure 5: The second excited state at negative $b = -1$.

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♠ in the general case we get $N+1$ recurrences forming the linear eigenvalue problem

$$\begin{pmatrix} \mathcal{M}_{00} & \mathcal{M}_{01} & \mathcal{M}_{02} & 0 & \dots & 0 \\ \mathcal{M}_{10} & \mathcal{M}_{11} & \mathcal{M}_{12} & \mathcal{M}_{13} & \ddots & \vdots \\ 0 & \mathcal{M}_{21} & \mathcal{M}_{22} & \ddots & \ddots & 0 \\ 0 & \ddots & \ddots & \ddots & \mathcal{M}_{N-2N-1} & \mathcal{M}_{N-2N} \\ \vdots & \ddots & 0 & \mathcal{M}_{N-1N-2} & \mathcal{M}_{N-1N-1} & \mathcal{M}_{N-1N} \\ 0 & \dots & 0 & 0 & \mathcal{M}_{NN-1} & \mathcal{M}_{NN} \end{pmatrix} \begin{pmatrix} v_0 \\ v_1 \\ v_2 \\ \vdots \\ v_N \end{pmatrix} = p \begin{pmatrix} v_0 \\ v_1 \\ v_2 \\ \vdots \\ v_N \end{pmatrix}$$

with $E=-p$ and with matrix elements

$$\mathcal{M}_{k,k+2} = (k+1)(k+2)\,, \quad k = 0, 1, \ldots, N-2\,,$$

$$\mathcal{M}_{m,m+1} = 2\,b\,(m+1)\,, \quad \mathcal{M}_{m+1,m} = -2\,(N-m)\,, \quad m = 0, 1, \ldots, N-1$$

$$\mathcal{M}_{n,n} = 4\,a\,n + 2\,a + b^2\,, \quad n = 0, 1, \ldots, N$$

which are linear functions of parameters a and b.

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D. present model: two types of its solvability

§ preliminary remarks

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> even our $N = 1$ QNS ground-state wave function is clearly non-analytic at $x = 0$,

$$\frac{d^3}{dx^3}\psi_0^{(QNS)}\left(0^+\right) = 2\,, \quad \frac{d^3}{dx^3}\psi_0^{(QNS)}\left(0^-\right) = -2$$

> due to the parity symmetry, it is sufficient to consider just $x \geq 0$

> $\boxed{\exists \text{ both the NS solutions } (N = \infty) \text{ and the QNS states } (N < \infty)}$

§ preliminary remarks ctd.

> the exponential factor is fixed, containing the displacement parameter d,

$$\psi^{(QNS/NS)}\,(x,E) = e^{-x^2/2+d\,x} \times \sum_{k=0}^{N} a_k(E)\,x^k\,, \qquad x \geq 0\,, \qquad a_N \neq 0$$

> the parity-dependent energies $E_n^{(\pm)}$ are the roots of the matching rules

$$\psi_{(Jost)}(0,E^{(+)}) = 1\,, \quad \psi'_{(Jost)}(0,E^{(+)}) = 0$$

and

$$\psi_{(Jost)}(0,E^{(-)}) = 0\,, \quad \psi'_{(Jost)}(0,E^{(-)}) = 1\,.$$

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D.1. QNS solutions

♣ $N-$plet of relations between $N-1$ unknown coefficients $a_2,\, a_3,\, \ldots,\, a_N$ and $d^{(QNS)}$

$>$ $\boxed{N=0}$ and $E=1$:

$=$ odd case: solution cannot exist

$=$ even-parity solution only exists at $d=0$

$>$ $\boxed{N=1}$ and $E=3$: single constraint $2\,a_0+2\,d\,a_1=0$

$=$ odd case: only $d=0$

$=$ even case: the first nontrivial QNS solutions with $d=\pm 1$

summary: demand that $d\neq 0$ (skip trivial HO)

> $\boxed{N=2}$ and $E=5$: two relations

$$4a_0 + 2da_1 + 2a_2 = 0\,, \qquad 2a_1 + 4da_2 = 0\,.$$

= odd-parity: $d = d_\pm = \pm 1/\sqrt{2}$ and $a_2 = -d$.

= even-parity: $a_2 = 1/2$ and $d = \pm\sqrt{5/2}$.

> $\boxed{N=3}$, odd-parity: triplet of relations

$$2 + 2\,d\,a_2 + 3\,a_3 = 0, \quad d + a_2 = 0, \quad a_2 + 3\,d\,a_3 = 0$$

easy solution $a_3 = 1/3$, $d = \pm\sqrt{3/2}$ and $a_2 = -d$.

$>$ $\boxed{N=3}$, even-parity conditions

$$-2\,d\;+2\,d\,a_2+3\,a_3=0, \quad 3-d^2+a_2=0, \quad a_2+3\,d\,a_3=0$$

$>$ solution: quadruplet of eligible QNS shifts

$$d_{\pm,\pm}=\pm\sqrt{\frac{9\pm\sqrt{57}}{4}}\,.$$

every root defines the coefficients,

$$a_2=\frac{2d^2}{2d^2-1}\,, \qquad a_3=\frac{2d}{6d^2-3}\,.$$

✓ systematic approach

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> normalization conventions: $a_{N+1} = a_{N+2} = \ldots = 0$ and

$$\left\{ \begin{array}{llll} a_0 = 1\,, & a_1 = -d\,, & & \text{parity} = \text{even}\,, \\ a_0 = 0\,, & a_1 = 1\,, & a_2 = -d\,, & \text{parity} = \text{odd}\,. \end{array} \right.$$

> SE equivalent to linear recurrences

$$(E - 1 - 2n)\, a_n + 2d(n+1)\, a_{n+1} + (n+1)(n+2)\, a_{n+2} = 0\,, \qquad n = 0, 1, \ldots, N\,.$$

> the last, $n = N$ item fixes the energy, $E^{(QNS)} = 2N + 1$

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D.1.1. Even-parity problem

§ preliminary step (a)

> we will need the tridiagonal k by k matrices

$$\mathcal{P}^{(N,k)}(d) = \begin{pmatrix} d & 1 & 0 & 0 & \dots & 0 \\ 2N & 2d & 2 & 0 & \ddots & \vdots \\ 0 & 2N-2 & 4d & 6 & \ddots & 0 \\ 0 & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & 0 & 2(N-k+3) & 2(k-2)d & (k-1)(k-2) \\ 0 & \dots & 0 & 0 & 2(N-k+2) & 2(k-1)d \end{pmatrix}.$$

♡ result (a): QNS bound states with even parity

Theorem 1 *In terms of matrices $\mathcal{P}^{(N,k)}(d)$ the QNS wave-functions are known,*

$$a_k = a_k^{(N)} = \frac{(-1)^k}{k!(k-1)!} \det \mathcal{P}^{(N,k)}(d)\,, \quad k = (1, 2,)\, 3, 4, \ldots$$

Theorem 2 *The QNS constraint $a_{N+1}^{(N)} = 0$, i.e., the polynomial algebraic equation*

$$\det \mathcal{P}^{(N,N+1)}(d) = 0$$

defines the $N-$plet of the admissible values of the shift parameter $d = d^{(QNS)}$.

Table 1: QNS equations at the first few N.

1	$-2+2\,d^2$	$d+a_1=0$
2	$-5+2\,d^2$	$-1+2\,a_2=0$
3	$3-9\,d^2+2\,d^4$	$-8\,d+2\,d^3+3\,a_3=0$
4	$27-28\,d^2+4\,d^4$	$11-2\,d^2+12\,a_4=0$
5	$-15+75\,d^2-40\,d^4+4\,d^6$	$29\,d-19\,d^3+2\,d^5+15\,a_5=0$
$\vdots$	$\ldots$	$\ldots$

D.1.2. Odd-parity problem

§ preliminary step (b)

> we will need the tridiagonal k by k matrices

$$\mathcal{Q}^{(N,k)}(d) = \begin{pmatrix} 2d & 2 & 0 & \dots & 0 \\ 2N-2 & 4d & 6 & \ddots & \vdots \\ 0 & 2N-4 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & 2(k-1)d & k(k-1) \\ 0 & \dots & 0 & 2(N-k+1) & 2kd \end{pmatrix}.$$

♡ result (b): QNS bound states with odd parity

Theorem 3 *In terms of matrices $\mathcal{Q}^{(N,k)}(d)$ the QNS wave-functions are known,*

$$a_{k+1} = a^{(N)}_{k+1} = \frac{(-1)^k}{(k+1)!k!} \det \mathcal{Q}^{(N,k)}(d)\,, \quad k = 1, 2, \ldots$$

Theorem 4 *The QNS constraint $a^{(N)}_{N+1} = 0$, i.e., the polynomial algebraic equation*

$$\det \mathcal{Q}^{(N,N+1)}(d) = 0$$

defines the $N-$plet of the admissible values of the shift parameter $d = d^{(QNS)}$.

Table 2: QNS equations.

2	$-1 + 2\,d^2$	$d + a_2 = 0$
3	$-3 + 2\,d^2$	$-1 + 3\,a_3 = 0$
4	$3 - 12\,d^2 + 4\,d^4$	$-5\,d + 2\,d^3 + 6\,a_4 = 0$
5	$15 - 20\,d^2 + 4\,d^4$	$7 - 2\,d^2 + 30\,a_5 = 0$
$\vdots$	$\dots$	$\dots$

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D.2. NS solutions

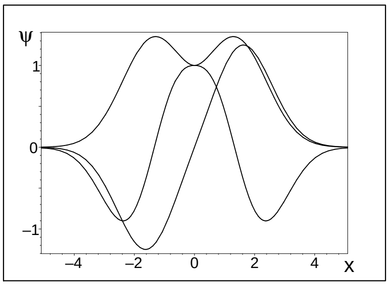

Figure 6: The first three double-well NS wave functions at non-QNS $d = 3/2$.

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D. 2. 1. the single well scenario

✓ single well in systematic approach

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> the change of variables with $d = -\mu^2 < 0$,

$$x - d = \sqrt{z} \in (-d, \infty)\,, \qquad \psi(x) = \exp(-z/2)\, w(z)\,.$$

> Kummer's equation with $a = (1-E)/4$ and $b = 1/2$,

$$z\frac{d^2 w(z)}{dz^2} + (b - z)\frac{d\,w(z)}{dz} - a\,w(z) = 0\,, \qquad z \in (\mu^4, \infty)$$

> no branch point,

$$w_{(even)}(z) = M(a,b,z) = \ {}_1F_1(a,b,z) =$$

$$= \sum_{s=0}^{\infty} \frac{(a)_s}{(b)_s\, s!} z^s = 1 + \frac{a}{b} z + \frac{a(a+1)}{b(b+1)2!} z^2 + \cdots$$

$$w_{(odd)}(z) = z^{1-b}\, M(a-b+1, 2-b, z)\,.$$

> asymptotic boundary condition,

$$w_{(physical)}(z) = U(a,b,z) = \frac{\Gamma(1-b)}{\Gamma(a-b+1)}\, M(a,b,z) +$$

$$+ \frac{\Gamma(b-1)}{\Gamma(a)} z^{1-b}\, M(a-b+1, 2-b, z)\ .$$

$>$ at $x \geq 0$,

$$\psi(x) = \psi(x, E) == \exp(-(x + \mu^2)^2/2) \; U\big((1 - E)/4, 1/2, (x + \mu^2)^2\big) \; .$$

$>$ numerical performance reflects our expectations

$=$ ground state pushed up to $E_0 = E_0(-\mu^2)$ with $E_0(-0.25) \approx 1.3349$ and $E_0(-1) = 3$

$=$ the second excitation moves from initial $E_2(0) = 5$ to $E_2(-1) \in (8.658, 8.659)$, etc.

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D. 2. 2. the double-well scenario

✓ double well with $d = \nu^2 > 0$ in systematic approach

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> the change of variables with a branch in $x - d = \pm\sqrt{z}$ under explicit control.

> initial boundary condition and oscillation theorem strategy with

$$\psi(x) = \psi(x, E) = C_1\, w_{(even)}[z(x)] + C_2\, w_{(odd)}[z(x)]\,.$$

> matching at $x = 0$ (i.e., at $z = \nu^4$) below the square-root branch.

Table 3: The shift-dependence of the ground-state energy.

shift d	0.00	0.25	0.50	0.75	1.00	1.50	2.00	∞
energy $E_0(d)$	1.00	0.76897	0.63553	0.59030	0.6189	0.80149	0.9514	1.00

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Table 4: The shift-dependence of the 1st-excited-state energy.

shift d	0.00	0.25	0.50	0.75	1.00	1.50	2.00	∞
energy $E_0(d)$	3.00	2.4839	2.0608	1.7247	1.4685	1.15748	1.0358	1.00

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Table 5: Shift-dependence of the 2nd-excited-state energy (at $d = 1$ the state is quasi-exact).

shift d	0.00	0.25	0.50	0.75	1.00	1.50	2.00	∞
energy $E_0(d)$	5.00	4.347	3.794	3.3447	3.00	2.649	2.735	3.00

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E. SUMMARY

talk about harmonic oscillator twins

$$V(x) = V_{[d]}(x) = \begin{cases} (x-d)^2, & x > 0, \\ (x+d)^2, & x < 0 \end{cases}$$

♡ curiosity in physics: never mentioned in the textbooks on quantum mechanics

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♡ motivation in math: relevant. i.a., in the Thom's catastrophe theory (TCT)

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♡ reference: MZ, Quant. Rep. 4 (2022) 309 (arXiv:1607.01297v2)

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THANKS FOR YOUR ATTENTION !

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SEE YOU ALL NEXT YEAR IN PRAGUE!