Double Well Potential: Perturbation Theory, Tunneling, WKB (beyond instantons)

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Outline

- One-dimensional Anharmonic Oscillator
- Double Well
- Perturbation Theory of Non-linealization Method
- Hydrogen in Magnetic Field

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$$\mathcal{H} \;=\; -\frac{d^2}{dx^2} \;+\; m^2x^2 + \; gx^4 \;, \qquad x \in R$$

- $m^2 \geq 0$ is anharmonic oscillator
- $m^2 < 0$ is double-well potential

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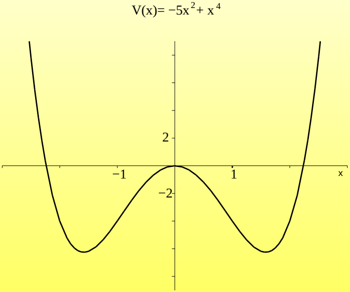

The double-well potential

Idea is to combine in a single approach:

- Perturbation Theory near the minimum of the potential

$$\Psi(x) = e^{-\alpha x^2}(1+\beta_1 x^2+\beta_2 x^3 \ldots)\ ,\ \alpha > 0 \qquad \text{(ground state)}$$

- correct WKB behavior at large distances (inside of the domain of applicability)
- Tunneling between classical minima

The art of interpolation ... it leads to a solution!
Solution: for any real x an eigenfunction is known with a certain relative accuracy $|\frac{\Psi_{approx}-\Psi_{exact}}{\Psi_{approx}}| \le \delta$

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What is known about eigenfunctions:

- For real $m^2, g \geq 0$ any eigenfunction $\Psi(x; m^2, g)$ is entire function in x
- Any eigenfunction has finitely many simple real zeros (the oscillation theorem)

and

infinitely many complex zeros situated on the imaginary axis

A Eremenko, A Gabrielov (Purdue), B Shapiro (Stockholm), 2008

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Main object to study is the **logarithmic derivative**

$$y \;=\; -\frac{\Psi'(x)}{\Psi(x)} \;=\; \varphi'(x) \quad , \; \Psi(x) = e^{-\varphi(x)}$$

here $\varphi(x)$ is the **phase**.

Riccati equation

$$y' - y^2 \; = \; E - \; m^2 x^2 \; - \; g x^4 \quad ,$$

In general, y is odd and

$$y \; = \; -\sum_{i=1}^{n} \frac{1}{x - x_i} \; + \; y_{reg}(x)$$

here x_i are nodes and $y_{reg}(0) = 0$.

Ground state: $n = 0$ *(no nodes),* $\qquad y = y_{reg}$

$\Rightarrow y$ has no singularities at real x and $y(0) = 0$.

♣ $y(x) = 0 -{>}$ extremes of $\Psi(x)$

If $m^2 \geq (m^2)_{crit}$, $\exists$ single maximum at $x = 0$

If $m^2 < (m^2)_{crit}$, $\exists$ two maxima and one minimum at $x = 0$

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Asymptotics

Asymptotics:

$$y_{reg} = g^{1/2}x|x| + \frac{m^2}{2g^{1/2}}\frac{|x|}{x} + \frac{n+1}{x} - \frac{4gE+m^4}{8g^{3/2}}\frac{1}{x|x|} - \frac{m^2}{2g}\frac{1}{x^3} + \dots$$

$$|x| \to \infty$$

$$y_{reg} = Ex + \frac{E^2-m^2}{3}x^3 + \frac{2E(E^2-m^2)-3g}{15}x^5 + \dots$$

$$|x| \to 0$$

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or, for phase

$$\varphi_{reg} \;=\; \frac{g^{1/2}x^2|x|}{3}+\frac{m^2}{2g^{1/2}}|x|+(n+1)\log|x|-\frac{4gE+m^4}{8g^{3/2}}\frac{1}{|x|}+\frac{m^2}{g}\frac{1}{x^2}+\ldots$$

$$|x|\to\infty$$

first two terms are H-J asymptotics (classical action), the third term also (but not its coeff) is defined by quadratic fluctuations

$$\varphi_{reg} \;=\; \frac{E}{2}x^2+\frac{E^2-m^2}{12}x^4+\frac{2E(E^2-m^2)-3g}{90}x^6+\ldots$$

$$|x|\to 0$$

It makes (physics) sense of pert theory at $m^2\geq 0$
(around a minimum of potential)

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Interpolation (ground state)

Let us interpolate perturbation theory at small distances and WKB asymptotics at large distances

$$\psi_0 \;=\; \frac{1}{\sqrt{1+c^2gx^2}}\,\exp\left\{-\frac{A+ax^2/2+bgx^4}{(D^2+gx^2)^{1/2}}\right\}$$

where A, a, b, c, D are free (variational) parameters

Very Rigid expression!

("hard" to modify)

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If we fix

$$b = \frac{1}{3} \quad , \quad a = \frac{D^2}{3} + m^2 \quad , \quad c = \frac{1}{D}$$

then

$$\psi_0 \;=\; \frac{1}{\sqrt{D^2+gx^2}} \exp\left\{-\frac{A+(D^2+3m^2)x^2/6+gx^4/3}{(D^2+gx^2)^{1/2}}\right\}$$

the **dominant** and the first **two subdominant** terms in the expansion of y at $|x| \to \infty$ are reproduced **exactly**
A, D *are still* **two** *free parameters which we can vary.*

Our approximation has no complex **zeroes** on imaginary $x-$axis but symmetrical branch cuts going along imaginary axis to $\pm i\infty$ (a meaning of square root)

If ψ_0 is taken as variational function then for **all** studied m^2 from -20 to $+20$ and $g = 2$
the variational energy reproduces 7 - 10 significant digits correctly!!

but the accuracy drops down at $m^2 < 0$ (from 10 at $m^2 = 0$ to 7 s.d. at $m^2 = -20$)

Can we fix it ?

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Perturbation Theory and Variational Method

Take a trial function $\psi_0(x)$ normalized to 1, then restore the potential V_0, energy E_0

$$\frac{\psi_0''(x)}{\psi_0(x)} \;=\; V_0 \;-\; E_0$$

and construct the Hamiltonian $H_0 = p^2 + V_0$.

Variational energy

$$\begin{aligned} E_{var} \;&=\; \int \psi_0 H \psi_0 = \underbrace{\int \psi_0 H_0\, \psi_0}_{=E_0} + \underbrace{\int \psi_0 \underbrace{(H - H_0)}_{V-V_0} \psi_0}_{=E_1} \\ &=\; E_0 + E_1 (V_1 = V - V_0) \end{aligned}$$

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- Variational energy can be considered as the first two terms in a perturbation theory,
  it seems natural to require a convergence of this PT series
- By calculation of next terms $E_2, E_3, \ldots$ one can evaluate an accuracy of variational calculation (i) and improve it iteratively (ii)
  (if the series is convergent, of course)

Our Perturbation Theory from Ψ_0 is definitely convergent
(perturbation is subordinate)

How to estimate the radius of convergency?

(end of remark)

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One more, physics property must be introduced into the approximation:

at $m^2 \to -\infty$ the barrier grows, tunneling between wells decreases, the wavefunction has **two maxima** (corresponding to two minima of the potential) and **one minimum** at origin which value tends to zero $\Rightarrow$

$$\psi_0 = \frac{1}{(D^2+gx^2)^{1/2}} \exp\left\{-\frac{A+(D^2+3m^2)x^2/6+gx^4/3}{(D^2+gx^2)^{1/2}}\right\} \times \cosh \frac{\alpha x}{(D^2+gx^2)^{1/2}}$$

(following the E.M. Lifschitz prescription, $\Psi_\pm = \Psi(x+\tilde{\alpha}) \pm \Psi(x-\tilde{\alpha})$)
in total, we have now three free parameters, A, D, α.

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More accurate:

- for $m^2 < 0$ the expansion of y at $x = 0$ does **not** make sense of Perturbation Theory expansion,
- it is expansion near *false* minimum (near maximum) potential.
- The expansion near potential minimum at $x_{min} = \pm\sqrt{\frac{m^2}{2g}}$ is well defined and it should be taken

It is that behind the Lifschitz prescription

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With this modification for all studied m^2 from -20 to $+20$ and at $g = 2$

the variational energy reproduces 9 - 11 significant digits

correctly!!

1-2 orders of magnitude improvement

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Perturbation Theory of *"Non-linealization"* Method
(*Logarithmic perturbation theory*)

Take Riccati equation instead of Schroedinger equation

$$y' - y^2 \ = \ E - V \ , \quad y = (\log \Psi)'$$

and develop PT there. If Ψ_0 is given, let

$$V \ = \ V_0 + \lambda V_1$$

where $V_0 = \Psi_0''/\Psi_0$, then perturbation theory

$$y = \sum \lambda^n y_n \ , \ E \ = \ \sum \lambda^n E_n$$

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For nth correction

$$\lambda^n \Big| \qquad {y'}_n - 2y_0 \cdot y_n = E_n - Q_n;$$

$$\begin{aligned} Q_1 &= V_1 \\ Q_n &= -\sum_{i=1}^{n-1} y_i \cdot y_{n-i} \ , \quad n = 2, 3, \ldots \end{aligned}$$

Multiply both sides by Ψ_0^2,

$$(\Psi_0^2 \ y_n)' = (E_n - Q_n)\, \Psi_0^2$$

Boundary condition: $|\Psi_0^2 \ y_n| \to 0$ at $|x| \to \infty$ (no particle current)

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$$E_n = \frac{\int_{-\infty}^{\infty} Q_n \Psi_0^2 \, dx}{\int_{-\infty}^{\infty} \Psi_0^2 \, dx}$$

$$y_n = \Psi_0^{-2} \int_{-\infty}^{x} (E_n - Q_n) \Psi_0^2 \, dx'$$

M. Price (1955), Ya.B. Zel'dovich (1956)

. . . Y.Aharonov-C.K.Au (1979), A.T. (1979) . . .

d = 1

ground-state

$$g = 2 \ , \ \ m^2 = 1$$

$$D = 4.33441$$

$$A = -9.23456$$

$$\alpha = 2.74573$$

$$* * *$$

$$E_{var} \ = \ 1.607541302594$$

$$\Delta E_{var} \ (\equiv \ E_2) \ = \ -1.2552 \times 10^{-10}$$

$$\tilde{E}_{var} = E_{var} + \Delta E_{var} \ = \ 1.607541302469$$

all digits are correct

the next correction E_3 is $\sim 10^{-14}$

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$$g = 2\ ,\ \ m^2 = -1$$

$$D = 4.059888$$

$$A = -12.4816$$

$$\alpha = 3.07041$$

$$* * *$$

$$E_{var} = 1.029560832093$$

$$\Delta E_{var} = -1.0382 \times 10^{-9}$$

$$\tilde{E}_{var} = E_{var} + \Delta E_{var} = 1.029560831054$$

all digits are correct

the next correction E_3 is $\sim 10^{-13}$

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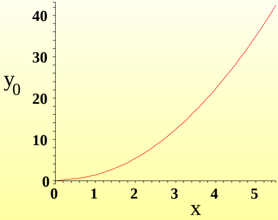
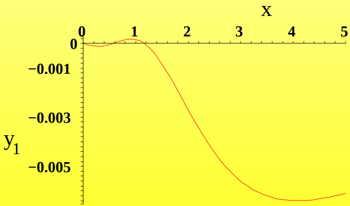


Logarithmic derivative y_0 as function of x for double-well potential with $m^2 = -1, g = 2$



The first correction y_1 for $m^2 = -1, g = 2$

Where $\frac{d^2\Psi}{dx^2}|_{x=0} = 0$? $\Longrightarrow$ When $E = 0$ (classical motion 'stops to feel' the presence of two minima)

$$E(m^2 = (m^2)_{crit} = -3.523390749, g = 2) \; = \; 0$$

- for $m^2 > (m^2)_{crit}$, $\frac{d^2\Psi}{dx^2}|_{x=0} < 0$
  (single-peak distribution)
  For $0 > m^2 > (m^2)_{crit}$ the potential is **double well** *one, but wavefunction is* **single peaked***, no memory about two minima, particle prefers to stay near unstable equilibrium point !*

- for $m^2 < (m^2)_{crit}$, $\frac{d^2\Psi}{dx^2}|_{x=0} < 0$
  (double-peak distribution) as it should be in WKB domain

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$$g = 2\ ,\ \ m^2 = -20$$

$$D = 6.765663$$

$$A = -286.6456$$

$$\alpha = 49.6136$$

$$* * *$$

$$E_{var} = -43.7793127$$

$$\Delta E_{var}\ (\equiv\ E_2) = -3.81 \times 10^{-6}$$

$$\tilde{E}_{var} = E_{var} + \Delta E_{var} = -43.7793165$$

all digits are correct

the next correction E_3 is $\sim 10^{-8}$

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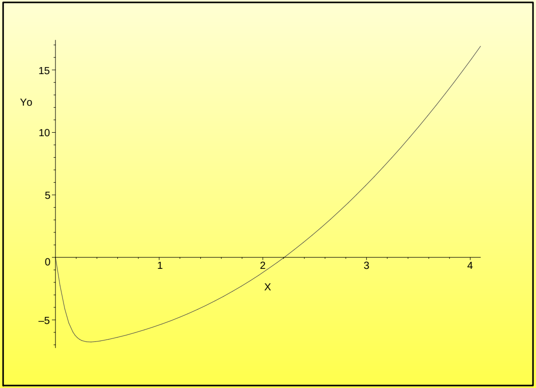

Logarithmic derivative y_0 as function of x for double-well potential $m^2 = -20, g = 2$

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First Excited State

Similar expansions for $|x| \to \infty$ and $x \to 0$ (with addition $-\log|x|$).

$$\psi_1 \;=\; \frac{1}{(D^2+gx^2)} \exp\left\{-\frac{A+(D^2+3m^2)x^2/6+gx^4/3}{(D^2+gx^2)^{1/2}}\right\} \times$$
$$\sinh \frac{\alpha x}{(D^2+gx^2)^{1/2}}$$

(following the E.M.Lifschitz presciption)

in total, we have **three** *free parameters,* A, D, α.

For all studied m^2 from -20 to +20 and $g=2$ the variational energy reproduces 9 - 11 significant digits **correctly**!!
(similar to the ground state)

$$g = 2\ ,\ \ m^2 = -20$$

$$D \ = \ 5.584375978$$

$$A \ = \ -246.643750$$

$$\alpha \ = \ 38.82768$$

$$* * *$$

$$E_{var} \ = \ -43.77931637$$

$$\Delta E_{var}\ (\equiv \ E_2) \ = \ -9.3618 \times 10^{-8}$$

$$\tilde{E}_{var} = E_{var} + \Delta E_{var} \ = \ -43.77931646$$

all digits are correct

the next correction E_3 is $\sim 10^{-10}$

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Energy Gap

$$\Delta E \;=\; E_{first\;\; excited\;\; state} \;-\; E_{ground\;\; state}$$

$$\Delta E \;=\; \frac{2^{11/4}}{\sqrt{\pi}}|m^2|^{5/4}e^{-\frac{\sqrt{2}|m^2|^{3/2}}{6}}\left(1-\frac{71}{12}\frac{1}{\sqrt{2}|m^2|^{3/2}}-\frac{6299}{288}\frac{1}{2|m^2|^3}+\ldots\right)$$

at $g = 2$

it is an asymptotic expansion ...

J Zinn-Justin et al, 1981-2001
E Shuryak et al, 1994 : $\frac{71}{12}$ - two loop contribution
$\frac{6299}{288}$ - is it three loop one ?
what about a next term, four-loop contribution?

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$$\star \quad g = 2\ ,\ \ m^2 = -20$$

$$\Delta E_{var} = 1.03282 \times 10^{-7}$$
$$\Delta E^{(1)}_{var} = 1.06529 \times 10^{-7}$$
$$\Delta E^{(2)}_{var} = 1.06525 \times 10^{-7}$$

$$one - instanton = 1.12154 \times 10^{-7} \qquad (5.3\%\ deviation)$$
$$one - instanton + correction = 1.06908 \times 10^{-7}\ (0.36\%\ deviation)$$
$$one - instanton + twocorrections = 1.06754 \times 10^{-7}\ (0.22\%\ deviation)$$

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(i) What about excited states ?

(ii) How to modify the function $\psi_{0,1}$?

$$\psi_0^{(n)} = \frac{P_n(x^2)}{(D^2+gx^2)^{n+1/2}} \exp\left\{-\frac{A+(D^2+3m^2)x^2/6+gx^4/3}{(D^2+gx^2)^{1/2}}\right\}$$

$$\cosh\frac{\alpha x}{(D^2+gx^2)^{1/2}} \equiv P_n(x^2)\tilde{\psi}_0^{(n)}$$

where P_n is a polynomial of nth degree with positive roots found through conditional minimization

$$(\psi_0^{(n)},\psi_0^{(\ell)}) = 0\ ,\ \ell = 0,1,2,...(n-1)$$

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and for negative parity states

$$\psi_1^{(n)} = \frac{P_n(x^2)}{(D^2+gx^2)^{n+1}} \exp\left\{-\frac{A+(D^2+3m^2)x^2/6+gx^4/3}{(D^2+gx^2)^{1/2}}\right\}$$

$$\sinh\frac{\alpha x}{(D^2+gx^2)^{1/2}} \equiv P_n(x^2)\tilde{\psi}_0^{(n)}$$

where P_n is a polynomial of nth degree with positive roots found through conditional minimization

$$(\psi_1^{(n)}, \psi_1^{(\ell)}) = 0\ ,\ \ell = 0, 1, 2, ...(n-1)$$

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(iii) How to find corrections to the excited states, to the functions $\psi_{0,1}^{(n)}$ *?* –

Perturbation Theory of *"Non-linealization"* Method, A.T. '79

If

$$V = V_0 + \lambda V_1$$

where $V_0 = \Psi_0''/\Psi_0$, then perturbation theory

$$\Psi = (P_n(x^2) + \lambda p_{n-1}^{(1)} + \ldots)\tilde{\psi}_0^{(n)} \exp(-\lambda\varphi_1 - \lambda^2\varphi_2 + \ldots) \ ,$$

$$E = \sum \lambda^n E_n$$

with constraint $p_{n-1}^{(1,2,\ldots)}$ are polynomials of $(n-1)$th degree

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Zeeman Effect on Hydrogen

$$\mathcal{H} \;=\; -\Delta \;-\frac{2}{r} + \gamma^2 \rho^2\ , \qquad x \in R^3$$

where $r = \sqrt{x^2+y^2+z^2}\ ,\ \rho = \sqrt{x^2+y^2}$ and γ magnetic field.
For Ground State:

$$(\nabla \cdot \vec{y}) - \vec{y}^2 \;=\; E - V \quad , \quad \vec{y} = \nabla \log \Psi$$

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For phase

$$\varphi \;=\; \frac{\gamma\rho^2}{2} + \ldots$$

$$|x| \to \infty$$

(no more terms are known so far!)
and

$$\varphi \;=\; r + a_{2,0} r^2 + a_{0,1}\rho^2 + a_{3,0} r^3 + a_{1,1} r\rho^2 + \ldots + a_{n,k} r^n (\rho^2)^k + \ldots$$

$$|x| \to 0$$

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Interpolation (ground state):

$$\psi_0 = \frac{1}{(D^2 + \alpha z^2 + 4\gamma^2\rho^2)^{1/2}}$$
$$\exp\left\{-\frac{A + ar + bz^2 + c\rho^2 + \gamma^2 r\rho^2}{(D^2 + \alpha z^2 + 4\gamma^2\rho^2)^{1/2}}\right\}$$

where A, a, b, c, D^2, α are variational parameters.

Relative accuracy in total energy for $\gamma = 0 - 1000$ is not less than 10^{-6}!

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HAPPY BIRTHDAY MISHA!

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