Double Well Potential: Perturbation Theory, Tunneling, WKB

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Outline

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

- $m^2 \geq 0$ is anharmonic oscillator
- $m^2 < 0$ is double-well potential (or Higgs, Lifschitz)

Idea is to combine in a single (approximate) wavefunction:

- Perturbation Theory near the minimum of the potential

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

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

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 real zeros (the oscillation theorem)

and

infinitely many complex zeros situated on the imaginary axis

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

Take the Schroedinger equation

$$\frac{\hbar^2}{2\mu}\,\frac{d^2\Psi}{dx^2} + (E - V)\Psi \ = \ 0$$

make a formal substitution

$$\Psi = e^{-\frac{\varphi}{\hbar}}$$

finally,

$$\hbar\,\frac{dy}{dx} - y^2 \ = \ 2\mu(E - V) \quad , \quad y = \frac{d\varphi}{dx}$$

the Bloch (or Riccati) equation.

Semiclassical expansion

$$y = y_0 + \hbar y_1 + \hbar^2 y_2 + \dots$$

$$y_0 = \pm(2\mu(E - V))^{1/2} = \pm p \quad , \quad y_1 = -\frac{1}{2}\log p \ , \ \text{etc}$$

Domain of applicability (naive)

$$\frac{\hbar y_1}{y_0} \ll 1$$

Definitely, it is applicable when $|p|$ is large ($x \to \infty$ for growing potentials)

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)*, $\quad y = y_{reg}$

$\Rightarrow y$ 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 $x = 0$

Asymptotics

Asymptotics:

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

$$|x| \to \infty$$

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

$$|x| \to 0$$

Asymptotics

or, for phase

$$\varphi \;=\; \frac{g^{1/2}x^2|x|}{3} + \frac{m^2}{2g^{1/2}}|x| + \log|x| - \frac{4gE+m^4}{8g^{3/2}}\frac{1}{|x|} + \frac{m^2}{g}\frac{1}{x^2} + \ldots$$

$$|x| \to \infty$$

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

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

$$|x| \to 0$$

Interpolation

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)

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 branch cuts going along imaginary axis to $\pm i\infty$.

If ψ_0 is taken a variational 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 with a decrease of $m^2 < 0$ (from 10 to 7 s.d.)

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

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

- Variational calculations 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)

One more, physical 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.

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

the variational energy reproduces 9 - 11 significant digits

correctly!!

Perturbation Theory of *"Non-linealization"* Method

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

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

For nth correction

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

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

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)

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

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

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

...Y.Aharonov (1979) ... A.T. (1979) ...

| d = 1
| ground-state

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

$$D = 4.33441$$

$$A = -9.23456$$

$$\alpha = 2.74573$$

$$* * *$$

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

$$\Delta E_{var} \ = \ -1.2552 \times 10^{-10}$$

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

all digits are correct
the next correction E_3 is of the order of 10^{-14}

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

$$D = 4.059888$$

$$A = -12.4816$$

$$\alpha = 3.07041$$

* * *

$$E_{var} = 1.029560832093$$

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

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

all digits are correct

the next correction E_3 is of the order of 10^{-13}

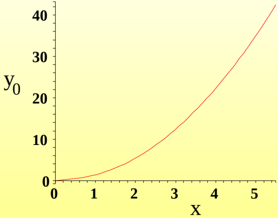

Figure: Logarithmic derivative y_0 as function of x for double-well potential with $m^2 = -1, g = 2$

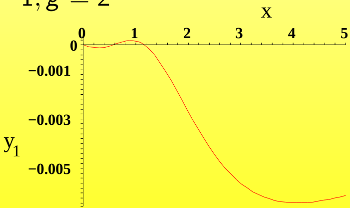

Figure: The first correction y_1 for $m^2 = -1, g = 2$

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

$$D = 6.765663$$

$$A = -286.6456$$

$$\alpha = 49.6136$$

$$* * *$$

$$E_{var} = -43.7793127$$

$$\Delta E_{var} = -3.81 \times 10^{-6}$$

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

all digits are correct
the next correction E_3 is of the order of 10^{-8}

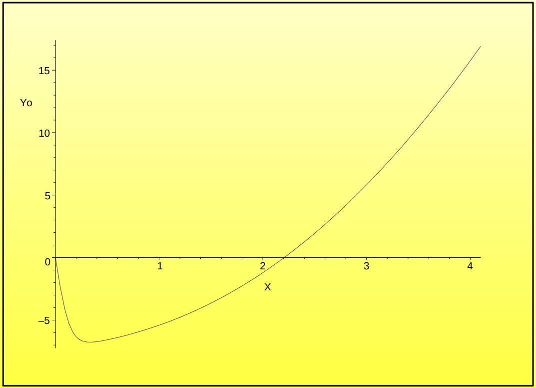

Figure: Logarithmic derivative y_0 as function of x for double-well potential $m^2 = -20, g = 2$

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

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)

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

$$D = 5.584375978$$

$$A = -246.643750$$

$$\alpha = 38.82768$$

* * *

$$E_{var} = -43.77931637$$

$$\Delta E_{var} = -9.3618 \times 10^{-8}$$

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

all digits are correct
the next correction E_3 is of the order of 10^{-10}

Energy Gap

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

$$\Delta E \;=\; \frac{2^{11/4}}{\sqrt{\pi}}|m^2|^{5/4}e^{-\frac{\sqrt{2}|m^2|^{3/2}}{6}}\left(1-\frac{71}{12}\frac{1}{\sqrt{2}|m^2|^{3/2}}-\frac{6299}{576}\frac{1}{|m^2|^3}+\ldots\right)$$

at $g = 2$

J Zinn-Justin et al , 2001

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

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

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

$$\star \quad g = 2\ ,\ \ m^2 = -10$$

$$\begin{aligned} \Delta E_{var} &= 0.033303855268 \\ \Delta E_{var}^{(1)} &= 0.033304504328 \\ \Delta E_{var}^{(2)} &= 0.033304503958 \end{aligned}$$

$$one - instanton = 0.03910369433 \qquad (17.4\%\ deviation)$$

$$one - instanton + correction = 0.03393024864\ (1.90\%\ deviation)$$

$$one - instanton + twocorrections = 0.03350261987\ (0.59\%\ deviation)$$

(i) What about excited states ?

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

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

where P_k is a polynomial of kth degree with positive roots found through conditional minimization

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

and for negative parity states

$$\psi_1^{(k)} = \frac{Q_k(x^2)}{(D^2+gx^2)^{k+1}} \exp\left\{-\frac{A+ax^2/2+gx^4/3}{(D^2+gx^2)^{1/2}}\right\}$$

$$\sinh \frac{\alpha x}{(D^2+gx^2)^{1/2}}$$

where Q_k is a polynomial of kth degree with positive roots found through conditional minimization

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

What about sextic oscillator?

$$\mathcal{H} \ = \ -\frac{d^2}{dx^2} \ + \ m^2x^2 + \ g_4x^4 + \ g_6x^6 \ , \qquad x \in R$$

If dimensionless number $q \equiv \frac{g_4^2}{4g_6^{3/2}} - \frac{m^2}{g_6^{1/2}} = 2n+3, n = 0, 1, 2, \ldots,$ the QES situation occurs, $(n+1)$ eigenstates are known exactly.

♠ For Ground State:

$$y' - y^2 \ = \ E - \ m^2x^2 \ - \ g_4x^4 - \ g_6x^6 \quad , \quad y(0) = 0$$

y has no simple poles at $x \in \mathbf{R}$.

Asymptotics:

$$y = g_6^{1/2} x^3 + \frac{g_4}{2g_6^{1/2}}\, x + \frac{1}{2}\Big(3 - q\Big)\, \frac{1}{x} -$$

$$\frac{1}{2g_6^{1/2}}\left[E + \frac{g_4}{2g_6^{1/2}}\Big(1 - q\Big)\right]\frac{1}{x^3} + \ \ldots \quad \text{at} \quad |x| \to \infty$$

There is no limit to the quartic osc case when g_6 tends to zero! Completely different expansion... But at small distances they are similar

$$y \ = \ Ex + \frac{E^2 - m^2}{3} x^3 + \frac{2E(E^2 - m^2) - 3g_4}{15} x^5 + \ldots \quad \text{at } |x| \to 0$$

Asymptotics:

$$\varphi = \frac{g_6^{1/2}}{4} x^4 + \frac{g_4}{4 g_6^{1/2}}\ x^2 + \frac{1}{2}\left(3 - q\right)\ \log x +$$

$$\frac{1}{4 g_6^{1/2}}\left[E + \frac{g_4}{2 g_6^{1/2}}\left(1 - q\right)\right]\frac{1}{x^2} + \ \ldots \quad \text{at} \quad |x| \to \infty$$

There is no limit to the quartic osc case when g_6 tends to zero!

For QES case $q = 3$ (no log term and all subsequent ones).

At small distances

$$\varphi \ = \ \frac{E}{2} x^2 + \frac{E^2 - m^2}{12} x^4 + \frac{2E(E^2 - m^2) - 3 g_4}{90} x^6 + \ldots \quad \text{at } |x| \to 0$$

Interpolation:

$$\psi_0 = \frac{1}{(D^2 + 2bx^2 + g_6 x^4)^{\frac{3-q}{8}}}$$
$$\exp\left\{-\frac{A + ax^2 + (g_4 + b)x^4/4 + g_6 x^6/4}{(D^2 + 2bx^2 + g_6 x^4)^{1/2}}\right\}$$

where A, a, b, D are variational parameters.

If $q = 3$ the potential is

$$V = (\frac{g_4^2}{4g_6} - 3\sqrt{g_6})x^2 + g_4 x^4 + g_6 x^6$$

and, finally,

$$\psi_0 \;=\; \exp\{-\frac{g_4}{4g_6^{1/2}}x^2 - \frac{g_6^{1/2}}{4}x^4\}$$

It is **quasi-exactly-solvable** case.

Depending on the parameters the sextic potential has one-, two- or three minima. The Lifschitz argument leads to

$$
\begin{aligned}
\psi_0 \;=\; & \frac{1}{(D^2+2bx^2+g_6x^4)^{\frac{3-q}{8}}} \\
\exp&\left\{-\frac{A+ax^2+(g_4+b)x^4/4+g_6x^6/4}{(D^2+2bx^2+g_6x^4)^{1/2}}\right\}\times \\
&\cosh\frac{\alpha x}{(D^2+2bx^2+g_6x^4)^{1/2}}\;+ \\
&\frac{B}{(\tilde{D}^2+2\tilde{b}x^2+g_6x^4)^{\frac{3-q}{8}}} \\
\exp&\left\{-\frac{\tilde{A}+\tilde{a}x^2+(g_4+\tilde{b})x^4/4+g_6x^6/4}{(\tilde{D}^2+2\tilde{b}x^2+g_6x^4)^{1/2}}\right\}
\end{aligned}
$$

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:

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

For phase

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

$$|x| \to \infty$$

and

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

$$|x| \to 0$$

Interpolation:

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

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

What about multidimensional quartic oscillator?

$$\mathcal{H} \;=\; -\Delta \;+\; m^2 \sum x_i^2 + \; g \left(\sum x_i^4 + \hat{c} \sum_{i \neq j} x_i^2 x_j^2 \right) \;\equiv -\Delta + V,$$

in $\quad x \in R^D$.
For Ground State:

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

Interpolation:

$$\psi_0 = \frac{1}{(d^2 + g\sum x_i^2)^{1/2}}$$

$$\exp\left\{ -\frac{A + a\sum x_i^2 + \ g\left(b\sum x_i^4 + c\sum_{i\neq j} x_i^2 x_j^2\right)}{(d^2 + g\sum x_i^2)^{1/2}} \right\}$$

where A, a, b, c, d are variational parameters.

$D = 2$ (A.T. 1988)

$D \to \infty$?