Outline

- One-dimensional Anharmonic Oscillator
- Double Well
- Perturbation Theory of Non-linealization Method
- Hydrogen in Magnetic Field
\[ \mathcal{H} = -\frac{d^2}{dx^2} + m^2 x^2 + gx^4, \quad x \in \mathbb{R} \]

- \( m^2 \geq 0 \) is anharmonic oscillator
- \( m^2 < 0 \) is double-well potential
The double-well potential

\[ V(x) = -5x^2 + x^4 \]
Idea is to combine in a single approach:

- Perturbation Theory near the minimum of the potential

\[ \psi(x) = e^{-\alpha x^2}(1 + \beta_1 x^2 + \beta_2 x^3 \ldots), \quad \alpha > 0 \] (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 
\[ \left| \frac{\psi_{\text{approx}} - \psi_{\text{exact}}}{\psi_{\text{approx}}} \right| \leq \delta \]
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
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

\[ y' - y^2 = E - m^2 x^2 - gx^4, \]

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), \( y = y_{reg} \)

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

\[ y(x) = 0 \rightarrow \text{extremes of } \Psi(x) \]

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

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

\[
y_{\text{reg}} = g^{1/2} |x| + \frac{m^2}{2g^{1/2}} \frac{|x|}{x} + \frac{n + 1}{x} - \frac{4gE + m^4}{8g^{3/2}} \frac{1}{x|x|} - \frac{m^2}{2g} \frac{1}{x^3} + \ldots
\]

\[|x| \to \infty\]

\[
y_{\text{reg}} = Ex + \frac{E^2 - m^2}{3} x^3 + \frac{2E(E^2 - m^2) - 3g}{15} x^5 + \ldots
\]

\[|x| \to 0\]
or, for phase

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

\(|x| \rightarrow \infty\)

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

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

\(|x| \rightarrow 0\)

It makes (physics) sense of pert theory at \(m^2 \geq 0\) (around a minimum of potential)
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 symmetrical branch cuts going along imaginary axis to \( \pm i\infty \)

(a meaning of square root)
If $\psi_0$ 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 ?
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

$$E_{\text{var}} = \int \psi_0 H \psi_0 = \int \psi_0 H_0 \psi_0 + \int \psi_0 (H - H_0) \psi_0$$

$$= E_0 + \int \psi_0 (H - H_0) \psi_0$$

$$= E_0 + E_1 (V_1 = V - V_0)$$
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 $\Psi_0$ is definitely convergent (perturbation is subordinate)

How to estimate the radius of convergency?

(end of remark)
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 \( \Rightarrow \)

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

(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, \( A, D, \alpha \).
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
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
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 \( \Psi_0 \) is given, let

\[ V = V_0 + \lambda V_1 \]

where \( V_0 = \psi''_0/\psi_0 \), then perturbation theory

\[ y = \sum \lambda^n y_n, \quad E = \sum \lambda^n E_n \]
For $n$th correction

$$\lambda^n \left| y'_n - 2y_0 \cdot y_n = E_n - Q_n; \right. $$

$$Q_1 = V_1$$

$$Q_n = -\sum_{i=1}^{n-1} y_i \cdot y_{n-i}, \quad n = 2, 3, \ldots$$

Multiply both sides by $\Psi_0^2$,

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

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)


d = 1

ground-state
\[ g = 2 \, , \, m^2 = 1 \]

\[ D = 4.33441 \]
\[ A = -9.23456 \]
\[ \alpha = 2.74573 \]

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\[ E_{\text{var}} = 1.607541302594 \]

\[ \Delta E_{\text{var}} \equiv E_2 = -1.2552 \times 10^{-10} \]

\[ \tilde{E}_{\text{var}} = E_{\text{var}} + \Delta E_{\text{var}} = 1.607541302469 \]

all digits are correct
the next correction \( E_3 \) is \( \sim 10^{-14} \)
\[ g = 2, \quad m^2 = -1 \]

\[ D = 4.059888 \]

\[ A = -12.4816 \]

\[ \alpha = 3.07041 \]

\[ * * * \]

\[ E_{\text{var}} = 1.029560832093 \]

\[ \Delta E_{\text{var}} = -1.0382 \times 10^{-9} \]

\[ \tilde{E}_{\text{var}} = E_{\text{var}} + \Delta E_{\text{var}} = 1.029560831054 \]

all digits are correct
the next correction \( E_3 \) is \( \sim 10^{-13} \)
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 \( \frac{d^2 \Psi}{dx^2}|_{x=0} = 0 \) ? \Rightarrow \text{When } E = 0 \text{ (classical motion ‘stops to feel’ the presence of two minima)}

\[
E(m^2 = (m^2)_{\text{crit}} = -3.523390749, g = 2) = 0
\]

- for \( m^2 > (m^2)_{\text{crit}} \), \( \frac{d^2 \Psi}{dx^2}|_{x=0} < 0 \)
  (single-peak distribution)
  \text{For } 0 > m^2 > (m^2)_{\text{crit}} \text{ 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 \( m^2 < (m^2)_{\text{crit}} \), \( \frac{d^2 \Psi}{dx^2}|_{x=0} < 0 \)
  (double-peak distribution) as it should be in WKB domain
\[ g = 2, \; m^2 = -20 \]

\[ D = 6.765663 \]

\[ A = -286.6456 \]

\[ \alpha = 49.6136 \]

\[ \ast \ast \ast \]

\[ E_{\text{var}} = -43.7793127 \]

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

\[ \tilde{E}_{\text{var}} = E_{\text{var}} + \Delta E_{\text{var}} = -43.7793165 \]

all digits are correct
the next correction \( E_3 \) is \( \sim 10^{-8} \)
Logarithmic derivative $y_0$ as function of $x$ for double-well potential $m^2 = -20, g = 2$
**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, $A, D, \alpha$. 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)
\[ g = 2 \, , \, m^2 = -20 \]

\[ D = 5.584375978 \]

\[ A = -246.643750 \]

\[ \alpha = 38.82768 \]

\[ * * * \]

\[ E_{\text{var}} = -43.77931637 \]

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

\[ \tilde{E}_{\text{var}} = E_{\text{var}} + \Delta E_{\text{var}} = -43.77931646 \]

all digits are correct

the next correction \( E_3 \) is \( \sim 10^{-10} \)
Energy Gap

\[ \Delta E = E_{\text{first excited state}} - E_{\text{ground state}} \]

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

at \( g = 2 \)

it is an asymptotic expansion ... 

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?
\[ g = 2, \ m^2 = -20 \]

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

\( \text{one} - \text{instanton} = 1.12154 \times 10^{-7} \quad (5.3\% \text{ deviation}) \)

\( \text{one} - \text{instanton} + \text{correction} = 1.06908 \times 10^{-7} \quad (0.36\% \text{ deviation}) \)

\( \text{one} - \text{instanton} + \text{twocorrections} = 1.06754 \times 10^{-7} \quad (0.22\% \text{ deviation}) \)
(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 $n$th degree with positive roots found through conditional minimization

\[(\psi_{0}^{(n)}, \psi_{0}^{(\ell)}) = 0, \quad \ell = 0, 1, 2, \ldots (n - 1)\]
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 \( n \)th degree with positive roots found through conditional minimization

\[ (\psi_1^{(n)}, \psi_1^{(\ell)}) = 0, \ \ell = 0, 1, 2, ...(n - 1) \]
(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 $p^{(1,2,\ldots)}_{n-1}$ are polynomials of $(n - 1)$th degree
Zeeman Effect on Hydrogen

\[ \mathcal{H} = -\Delta - \frac{2}{r} + \gamma^2 \rho^2, \quad x \in \mathbb{R}^3 \]

where \( r = \sqrt{x^2 + y^2 + z^2} \), \( \rho = \sqrt{x^2 + y^2} \) and \( \gamma \) magnetic field.

For Ground State:

\[ (\nabla \cdot \vec{y}) - \vec{y}^2 = E - V, \quad \vec{y} = \nabla \log \Psi \]
For phase

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

\[ |x| \to \infty \]

(no more terms are known so far!)

and

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

\[ |x| \to 0 \]
Interpolation (ground state):

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

where $A, a, b, c, D^2, \alpha$ are variational parameters.

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

Alexander Turbiner

Double Well
HAPPY BIRTHDAY MISHA!