The WKB approximation

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Friday 1st December, 2017

QM-Seminar, Prof. Georg Wolschin, University Heidelberg

Table of contents

History

WKB = Wentzel, Kramers, Brillouin in 1926

+Jeffreys (In 1923)? ⇒ WBK, BWK, WKBJ, JWKB and BWKJ ...

The classical WKB approximation

The idea

- Schrödinger equation

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V)\psi = 0$$

The idea

- Schrödinger equation

$$\frac{d^2\psi}{dx^2} + k(x)^2\psi = 0$$

The idea

- Schrödinger equation

$$\frac{d^2\psi}{dx^2} + k(x)^2\psi = 0$$

- Substitution

$$k(x) = \sqrt{\frac{2m}{\hbar^2}(E - V)} \qquad \text{if} \quad \mathrm{E > V(x)}$$
$$k(x) = i\sqrt{\frac{2m}{\hbar^2}(V - E)} = i\kappa(x) \qquad \text{if} \quad \mathrm{E < V(x)}$$

The idea

- Schrödinger equation

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- Solution

$$k = k_0 \quad \Rightarrow \quad \psi(x) = \exp(\pm i k_0 x)$$

$$k = k(x) \quad \Rightarrow \quad \text{In general no analytical solutions}$$

The idea

- Schrödinger equation

$$\frac{d^2\psi}{dx^2} + k(x)^2\psi = 0$$

- What if k varies very solwly? $k'(x) \ll 1$
  We expect solutions in this form

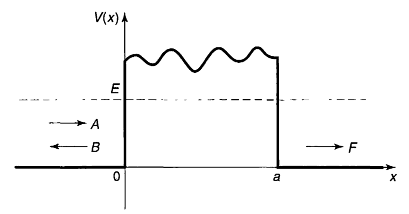
$$\exp(\pm i k_0 x) \Rightarrow \exp\Big[\pm i \int k(x) dx \Big]$$

- Does this new "solution" satisfies the Schrödinger equation?

Tunneling

Potential barrier

Potential Barrier



D. Griffiths, *Introduction to Quantum Mechanics*

$$\psi_1 = Ae^{ikx} + Be^{-ikx} \qquad x < 0$$

$$\psi_2 \approx \frac{C}{\sqrt{\kappa(x)}} e^{\int_0^x \kappa(t)dt} + \frac{D}{\sqrt{\kappa(x)}} e^{-\int_0^x \kappa(t)dt} \qquad 0 \leq x \leq a$$

$$\psi_3 = Fe^{ikx} \qquad x > a$$

Transmission probability

$$\psi_1 = Ae^{ikx} + Be^{-ikx} \qquad x < 0$$

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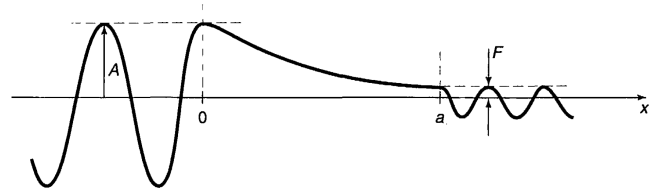
How does the transmission probability look like?

Expectation: Continuous + Decreasing



Qualitative structure of the wave function of the alpha decay

D. Griffiths, *Introduction to Quantum Mechanics*

Transmission probability

$$\psi_1 = Ae^{ikx} + Be^{-ikx} \qquad x < 0$$

$$\psi_2 \approx \frac{C}{\sqrt{\kappa(x)}} e^{\int_0^x \kappa(t)dt} + \frac{D}{\sqrt{\kappa(x)}} e^{-\int_0^x \kappa(t)dt} \qquad 0 \leq x \leq a$$

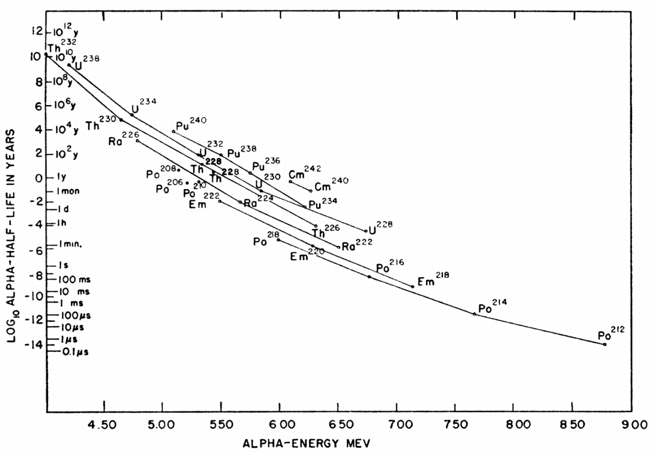
$$\psi_3 = Fe^{ikx} \qquad x > a$$

How does the transmission probability look like?
Expectation: Continuous + Decreasing

$$\Rightarrow T = \frac{|F|^2}{|A|^2} \propto \exp\left[-2 \int_0^a \kappa(t)dt) \right]$$

Example: Alpha decay

Transmission probability

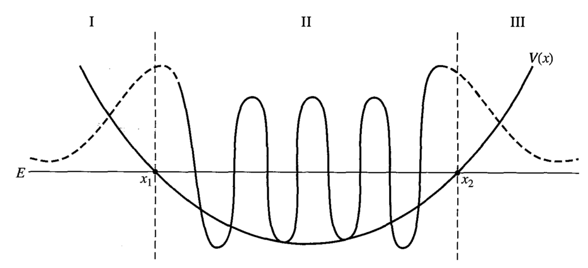


Logarithm of the lifetime versus energy

I. Perlman, A. Ghiorso, and G. Seaborg, "Relation between half-life and energy in alpha-decay"

The connection formula

At the turning point



Schematic diagram of the WKB solution

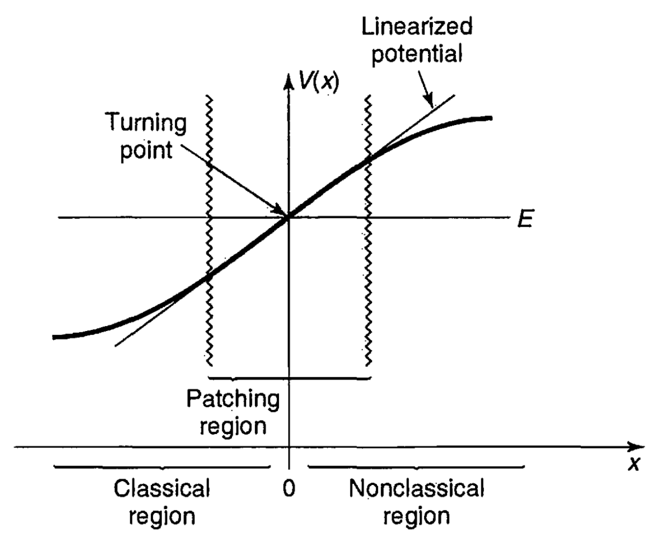
J. J. Sakurai, *Modern Quantum mechanics*

$$\psi(x) = \begin{cases} \frac{1}{\sqrt{\kappa(x)}} A e^{\int_0^x \kappa(t)dt} \\ \frac{1}{\sqrt{k(x)}} B e^{i\int_x^0 k(t)dt} + \frac{1}{\sqrt{k(x)}} C e^{-i\int_x^0 k(t)dt} \\ \frac{1}{\sqrt{\kappa(x)}} D e^{-\int_0^x \kappa(t)dt} \end{cases}$$

We want ONE solution over all three regions

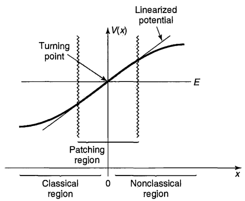
$\Rightarrow$ Relation between the coefficients

At the turning point



Approximation at the turning point
D. Griffiths, *Introduction to Quantum Mechanics*

At the turning point



General WKB solutions of both sides

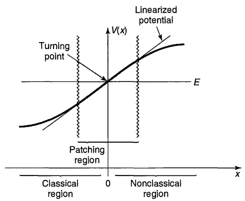
$$\psi(x) = \begin{cases} \frac{1}{\sqrt{k(x)}} B e^{i\int_x^0 k(t)dt} + \frac{1}{\sqrt{k(x)}} C e^{-i\int_x^0 k(t)dt} \\ \frac{1}{\sqrt{\kappa(x)}} D e^{-\int_0^x \kappa(t)dt} \end{cases}$$

- Approximated Schrödinger equation at the turning point

$$\frac{d^2\psi}{dz^2} - z\psi = 0$$

$$z = \alpha x \quad \text{and} \quad \alpha = \left[\frac{2\mathrm{m}}{\hbar^2}\mathrm{V}'(0)\right]^{\frac{1}{3}} > 0$$

At the turning point



General WKB solutions of both sides

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- Approximated Schrödinger equation at the turning point

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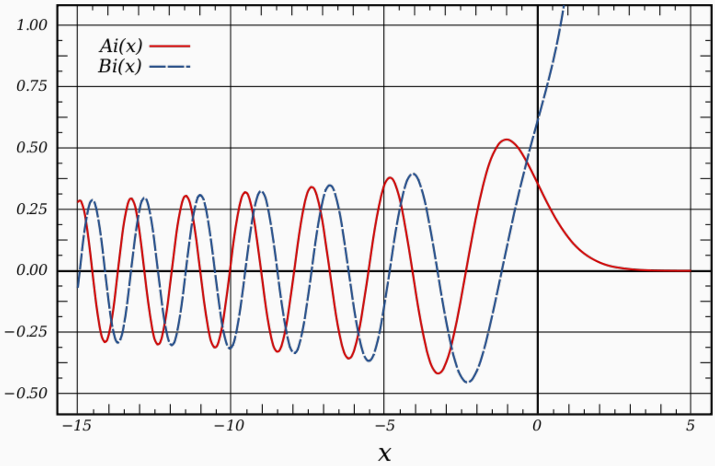
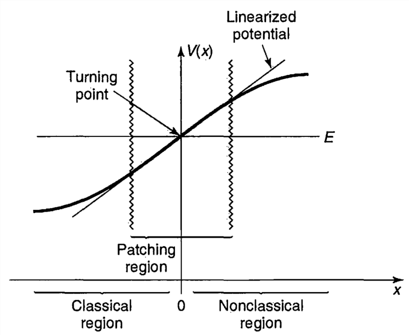
- Exact solution to this potential $\Rightarrow$ Airy function

At the turning point



Airy functions
from Wikipedia "Airy function"

At the turning point



To find out the relation between B, C and D:

- Using WKB to solve the Schrödinger equation with the linear potential
- Comparing it with the asymptotic behaviour of the Airy functions.

$$\psi(x) = \begin{cases} \frac{1}{\sqrt{k(x)}} B e^{i\int_x^0 k(t)dt} + \frac{1}{\sqrt{k(x)}} C e^{-i\int_x^0 k(t)dt} \\ \frac{1}{\sqrt{\kappa(x)}} D e^{-\int_0^x \kappa(t)dt} \end{cases}$$

Comparing the coefficients

- Schrödinger equation

$$\frac{d^2\psi}{dz^2} - z\psi = 0 \quad \text{with} \quad \mathrm{z} = \alpha \mathrm{x} \quad \text{and} \quad \alpha = \left[\frac{2\mathrm{m}}{\hbar^2}\mathrm{V}'(0)\right]^{\frac{1}{3}} > 0$$

Comparing the coefficients

- Schrödinger equation

$$\frac{d^2\psi}{dz^2} - z\psi = 0 \quad \text{with} \quad \mathrm{z} = \alpha \mathrm{x} \quad \text{and} \quad \alpha = \left[\frac{2\mathrm{m}}{\hbar^2}\mathrm{V}'(0)\right]^{\frac{1}{3}} > 0$$

- WKB $x > 0$

$$\psi(x)_{WKB} = \frac{D}{\alpha^{3/4}x^{1/4}} \exp\left[-\frac{2}{3}(\alpha x)^{\frac{3}{2}}\right]$$

- Airy function $x \gg 1$

$$\psi(x)_{Airy} \approx \frac{a}{2\sqrt{\pi}(\alpha x)^{1/4}} \exp\left[-\frac{2}{3}(\alpha x)^{\frac{3}{2}}\right] + \frac{b}{2\sqrt{\pi}(\alpha x)^{1/4}} \exp\left[\frac{2}{3}(\alpha x)^{\frac{3}{2}}\right]$$

Comparing the coefficients

- Schrödinger equation

$$\frac{d^2\psi}{dz^2} - z\psi = 0 \quad \text{with} \quad \mathrm{z} = \alpha \mathrm{x} \quad \text{and} \quad \alpha = \left[\frac{2\mathrm{m}}{\hbar^2}\mathrm{V}'(0)\right]^{\frac{1}{3}} > 0$$

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- Result

$$\frac{D}{\sqrt{\alpha}} = \frac{a}{2\sqrt{\pi}} \quad ; \quad \mathrm{b} = 0$$

Comparing the coefficients

- WKB $x < 0$

$$\psi(x)_{WKB} = \frac{1}{\alpha^{3/4}(-x)^{1/4}}\left\{B\exp\left[i\frac{2}{3}(-\alpha x)^{\frac{3}{2}}\right]+C\exp\left[-i\frac{2}{3}(-\alpha x)^{\frac{3}{2}}\right]\right\}$$

- Airy function $x \ll -1$

$$\psi(x)_{Airy} = \frac{a}{\sqrt{\pi}(-\alpha x)^{1/4}}\frac{1}{2i}\left\{\exp\left[i\frac{\pi}{4}+i\frac{2}{3}(-\alpha x)^{\frac{3}{2}}\right] - \exp\left[-i\frac{\pi}{4}-i\frac{2}{3}(-\alpha x)^{\frac{3}{2}}\right]\right\}$$

Comparing the coefficients

- WKB $x < 0$

$$\psi(x)_{WKB} = \frac{1}{\alpha^{3/4}(-x)^{1/4}}\left\{B\exp\left[i\frac{2}{3}(-\alpha x)^{\frac{3}{2}}\right]+C\exp\left[-i\frac{2}{3}(-\alpha x)^{\frac{3}{2}}\right]\right\}$$

- Airy function $x \ll -1$

$$\psi(x)_{Airy} = \frac{a}{\sqrt{\pi}(-\alpha x)^{1/4}}\frac{1}{2i}\left\{\exp\left[i\frac{\pi}{4}+i\frac{2}{3}(-\alpha x)^{\frac{3}{2}}\right]\right.$$
$$\left.-\exp\left[-i\frac{\pi}{4}-i\frac{2}{3}(-\alpha x)^{\frac{3}{2}}\right]\right\}$$

- Result

$$\frac{B}{\sqrt{\alpha}} = \frac{a}{2i\sqrt{\pi}}e^{i\pi/4} \qquad \frac{C}{\sqrt{\alpha}} = -\frac{a}{2i\sqrt{\pi}}e^{-i\pi/4}$$

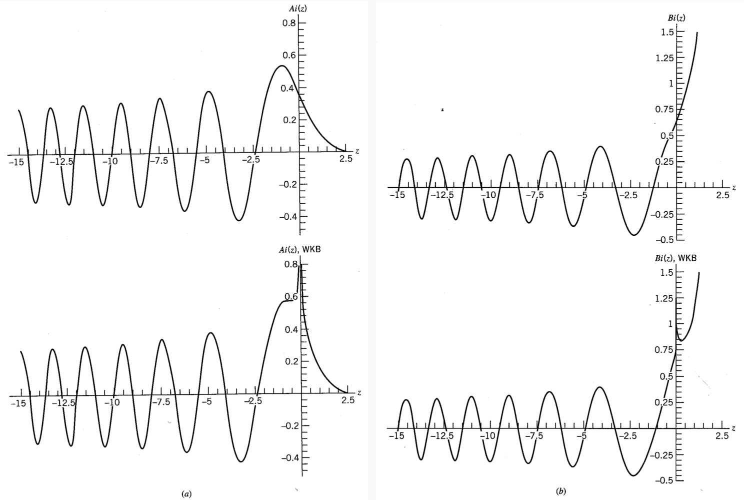
Comparing the coefficients

$$\psi(x) = \begin{cases} \frac{1}{\sqrt{k(x)}} B e^{i \int_x^0 k(t)dt} + C e^{-i \int_x^0 k(t)dt} \\ \frac{1}{\sqrt{\kappa(x)}} D e^{-\int_0^x \kappa(t)dt} \end{cases}$$

- Final result: The connection formulas

$$B = -ie^{i\pi/4} \cdot D$$
$$C = -ie^{-i\pi/4} \cdot D$$

Comparing the coefficients



Comparing the exact solution of the Airy function and the WKB approximated solution E. Merzbacher, *Quantum mechanics*

New development & Applications

Application on quantum field theory

Cosmological particle production and the precision of the WKB approximation

Sergei Winitzki
Department of Physics, Ludwig-Maximilians University, 80333 Munich, Germany
(Dated: February 7, 2008)

Particle production by slow-changing gravitational fields is usually described using quantum field theory in curved spacetime. Calculations require a definition of the vacuum state, which can be given using the adiabatic (WKB) approximation. I investigate the best attainable precision of the resulting approximate definition of the particle number. The standard WKB ansatz yields a divergent asymptotic series in the adiabatic parameter. I derive a novel formula for the optimal number of terms in that series and demonstrate that the error of the optimally truncated WKB series is exponentially small. This precision is still insufficient to describe particle production from vacuum, which is typically also exponentially small. An adequately precise approximation can be found by improving the WKB ansatz through perturbation theory. I show quantitatively that the fundamentally unavoidable imprecision in the definition of particle number in a time-dependent background is equal to the particle production expected to occur during that epoch. The results are illustrated by analytic and numerical examples.

Content of the article

- Under the assumption of an expanding universe:
  Vaccum defined at $t_0 \neq$ Vaccum defined at t_1
  $\Rightarrow$ particle production
- WKB can be applied to the Klein Gordon equation to calculate the particle production
- Problem:
  First order WKB: No reasonable result
  Higher order WKB: Divergent after n_{max}
- Improvement:
  Pertubation of the coefficients $\Rightarrow$ convergent
  Estimating the error term of higher order WKB

Particle production in expanding universe

- Field quantisation using a mode expansion

$$\hat{\chi}(t,x) = \int \frac{d^3\mathbf{k}}{(2\pi)^{3/2}} \frac{1}{\sqrt{2}} \left(\hat{a}_k e^{i\mathbf{k}\cdot\mathbf{x}} v_k(t) + H.e. \right)$$

- The mode functions $v_k(t)$ are complex-valued solutions of

$$v_k'' + \left(k^2 + m^2 - \frac{a''}{a} \right) v_k = 0$$

- The vacuum state $|0\rangle$ is defined by $\hat{a}_k |0\rangle = 0$ for all $\mathbf{k}$
  $v_{k,a}(t)$ is the vacuum defined at $t = t_0$
  $v_{k,b}(t)$ is the vacuum defined at $t = t_1$
  Particle production: $v_{k,b}(t_1) \neq v_{k,a}(t_1) = U(t_1, t_0) v_{k,a}(t_0)$

Particle production in expanding universe

- Rewriting the Klein Gordon equation

$$\epsilon^2 v_k'' + \omega_k^2(t) v_k = 0$$

- In a flat minkowski space time:

$$\omega = \mathrm{const} \quad \mathrm{and} \quad \mathrm{v_k} \propto \mathrm{e}^{-\mathrm{i}\omega_\mathrm{k}\mathrm{t}/\epsilon}$$

- In expanding universe (treated as curved space in QFT):

$$V_{WKB}(t) = \frac{\sqrt{\epsilon}}{\sqrt{\omega(t)}} \exp\Big(- \frac{i}{\epsilon} \int^t \omega(t')dt' \Big)$$

- We can use WKB to define $v_a(t_0)$ and $v_b(t_1)$

Particle production in expanding universe

- Goal: Calculating the particle number density $|\beta|^2$ with

$$\beta = \frac{v_a'(t_1)v_b(t_1) - v_a(t_1)v_b'(t_1)}{2i}$$

- Need $v_a'(t_1)$
- Applying first order WKB again?
  Result: No particle production $\Rightarrow$ Contradiction
- Requiring higher order WKB

Higher orders of WKB approximation

- Equation

$$\epsilon^2 \frac{d^2\psi}{dt^2} + \omega(t)^2\psi = 0$$

- Assumption (W and B real functions)

$$\psi(x) = \exp\left[\pm i \int W(t) + iB(t)dt\right] \qquad W(t) \approx \omega(t)$$

- Substituting in the equation

$$\dot{B} - B^2 = \omega^2 - W^2$$
$$\dot{W} - 2WB = 0$$

Higher orders of WKB approximation

- Equation

$$\epsilon^2 \frac{d^2\psi}{dt^2} + \omega(t)^2\psi = 0$$

- Assumption (W and B real functions)

$$\psi(x) = \exp\Big[\pm i \int W(t) + iB(t)dt\Big] \qquad W(t) \approx \omega(t)$$

- Substituting in the equation

$$B = \frac{\dot{W}}{2W}$$
$$W = \sqrt{\omega^2 - \epsilon\Big(\frac{\ddot{W}}{2W} - \frac{3\dot{W}^2}{4W^2}\Big)}$$

Higher orders of WKB approximation

- Substituting B in, we have

$$\psi(t) = \frac{1}{\sqrt{W(t)}} \exp\Big[\pm i \int W(t)dt \Big]$$

with

$$W = \sqrt{\omega^2 - \epsilon\big(\frac{\ddot{W}}{2W} - \frac{3\dot{W}^2}{4W^2}\big)}$$

- How can we solve W?

Higher orders of WKB approximation

- Substituting B in, we have

$$\psi(t) = \frac{1}{\sqrt{W(t)}} \exp\Big[\pm i \int W(t) dt\Big]$$

with

$$W = \sqrt{\omega^2 - \epsilon\Big(\frac{\ddot{W}}{2W} - \frac{3\dot{W}^2}{4W^2}\Big)}$$

- Assuming W has the following power series expansion:

$$W(t) = \omega + \epsilon S_1(t) + \epsilon^2 S_2(t) + \cdots \qquad (*)$$

- Substituting $(*)$ in the function
  Solve it by collecting terms with equal powers of ϵ iteratively

Higher orders of WKB approximation

Solution of higher order WKB

$$W(t) = \omega - \varepsilon\left(\frac{1}{4}\frac{\ddot{\omega}}{\omega^2} - \frac{3}{8}\frac{\dot{\omega}^2}{\omega^3}\right)$$
$$+\varepsilon^2\left(\frac{1}{16}\frac{\omega^{(4)}}{\omega^4} - \frac{5}{8}\frac{\dddot{\omega}\dot{\omega}}{\omega^5} - \frac{13}{32}\frac{\ddot{\omega}^2}{\omega^5} + \frac{99}{32}\frac{\ddot{\omega}\dot{\omega}^2}{\omega^6} - \frac{297}{128}\frac{\dot{\omega}^3}{\omega^7}\right) + \ldots$$

Higher orders of WKB approximation

- Solution in the form:

$$W(t) = \omega + \epsilon S_1(t) + \epsilon^2 S_2(t) + \cdots$$

Problem:

- Estimation of the series

$$|S_n| \propto \left(\frac{\epsilon}{2\omega(t)}\right)^{2n} \frac{(2n)!}{|t - t_1|^{2n+1}}$$

Divergent !!

- The estimated order n_* which gives the best accuracy

$$n_* \propto \epsilon^{-1}\omega(t)|t - t_1|$$

$$S_* \propto \frac{1}{\sqrt{n_*}} exp(-2n_*)$$

Improvement of WKB approximation

- Classical WKB approximation

$$x(t) = C_1 X_+(t) + C_2 X_-(t) \quad \text{with} \quad \mathrm{X}_\mp = \frac{1}{\sqrt{\omega(\mathrm{t})}} \exp\left[\pm \mathrm{i} \int_{\mathrm{t}_0}^{\mathrm{t}} \omega(\mathrm{t}')\mathrm{dt}'\right]$$

- Perturbation of the coefficients

$$x(t) = p(t) X_+(t) + q(t) X_-(t)$$

Improvement of WKB approximation

- Classical WKB approximation

$$x(t) = C_1 X_+(t) + C_2 X_-(t) \quad \text{with} \quad \mathrm{X}_\mp = \frac{1}{\sqrt{\omega(\mathrm{t})}} \exp\left[\pm \mathrm{i} \int_{\mathrm{t}_0}^{\mathrm{t}} \omega(\mathrm{t}')\mathrm{d}\mathrm{t}'\right]$$

- Perturbation of the coefficients

$$x(t) = p(t) X_+(t) + q(t) X_-(t)$$

- Two degrees of freedeom $\Rightarrow$ another constraint

$$\frac{dx(t)}{dt} = i\omega(t)\Big[-p(t)X_+(t) + q(t)X_-(t)\Big]$$

- Solving $p(t)$ and $q(t)$, represented as series of X_+ and X_-

Improvement of WKB approximation

- Representing $p(t)$ and $q(t)$ by X_+ and X_-

$$p(t) = 1 + \frac{1}{2}\int_{t_0}^{t} \frac{\dot{\omega}X_-}{\omega X_+} q(t')dt'$$

$$q(t) = \frac{1}{2}\int_{t_0}^{t} \frac{\dot{\omega}X_+}{\omega X_-} p(t')dt'$$

- Repeting the successive procedure

$$p(t) = 1 + \sum_{n=1}^{\infty} u_{2n}(t) \qquad u_{2n}(t) = \frac{1}{2}\int_{t_0}^{t} \frac{\dot{\omega}X_-}{\omega X_+} u_{2n-1}dt'$$

$$q(t) = \sum_{n=1}^{\infty} u_{2n-1}(t) \qquad u_{2n+1}(t) = \frac{1}{2}\int_{t_0}^{t} \frac{\dot{\omega}X_+}{\omega X_-} u_{2n}dt'$$

- Bremer series (convergent)

$$x(t) = X_+ + \Sigma_{n=1}^{\infty}(u_{2n-1}X_- + u_{2n}X_+)$$

Precision of the WKB series

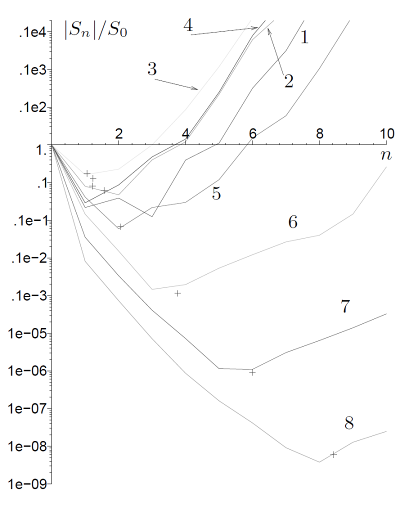
- Goal: Estimating the precision of WKB series
- Procedure
  - Representing the exact solution $x(t)$ by Bremer series
  - Comparing it with the WKB series
- Optimal order

$$n_{max} = min_{t_i} \left| \int_{t_0}^{t_i} \omega(t) dt \right|$$

- Error of optimally truncated WKB series

$$\frac{1}{\sqrt{n_{max}}} \exp(-2n_{max})$$

Precision of the WKB series



$$\omega(t) = \omega_0\left(1 + A\tanh\frac{t}{T}\right)$$

$$n_{max} \approx w_0|t_0|(1 \pm A)$$

Magnitudes of first 10 terms S_n, $n = 1, 2, \cdots, 10$, of the WKB series for $\omega(t)$ and different values of t_0. Crosses indicate the error estimates.

W. Winitzki, "Cosmological particle production and the precision of the WKB approximation" 2008

Four steps of doing approximation

1. Assuming a general form of the solution ($e^{iu(x')}$)
2. Substituting in the equation (Schrödinger equation)
3. Solving the variables or functions
4. Estimating the error

Thank you !