Landau Method for potentials with soft singularities

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Landau Method

Gives matrix elements in 1D QM:

$$\mathcal{A} = \langle N|\hat{x}|0\rangle = \lim_{j\to 0} \langle N|\hat{x}\cdot \overbrace{\exp(-j\hat{x}/\hbar)}^{\text{regulator}}|0\rangle = \lim_{j\to 0}\int_{\mathbb{R}} x e^{-jx/\hbar}\psi_N(x)\psi_0(x)dx$$

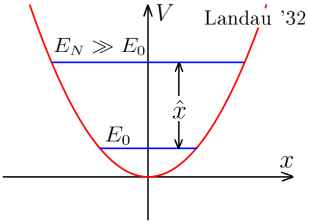
1. Decompose $\psi_N = \underbrace{\psi_N^+}_{''p>0''} + \underbrace{\psi_N^-}_{''p<0''} = 2\mathrm{Re}\,\psi_N^+$ on real axis
2. Deform integration contour into upper-half plane ($\psi_N^+ \to 0$)
3. Substitute semiclassical expressions for wavefunctions:

$$\psi_N^+ \propto \exp\left(\frac{i}{\hbar}\int_{a_N}^{x} p_N dx\right), \quad \psi_0 \propto \exp\left(-\frac{i}{\hbar}\int_{a_0}^{x} p_0 dx\right)$$

4. $ip_N(x) - ip_0(x) - j = 0 \Rightarrow x_*(j) \in \mathbb{C}$ – saddle point.

   $x_*(j\to 0) \to$ singularity: $\boxed{V(x_*) = \infty}$

5. Saddle-point integration $\Rightarrow \mathcal{A} \propto \lim_{j\to 0}\mathrm{Re}\exp\left(\frac{i}{\hbar}\int_{a_N}^{x_*} p_N dx - \frac{i}{\hbar}\int_{a_0}^{x_*} p_0 dx - \frac{jx_*}{\hbar}\right)$



Example: anharmonic oscillator

Consider anharmonic oscillator with a potential

$$V(x) = \frac{x^2}{2} + \frac{\lambda x^4}{4}$$

$$\mathcal{A} = \mathrm{const} \cdot \hbar^0 \cdot \mathrm{e}^{-W_L}(1 + \mathcal{O}(\hbar))$$

$$W_L = \underbrace{-\frac{1}{\hbar}\int\limits_{a_N}^{\infty} |p_N| dx + \frac{1}{\hbar}\int\limits_{a_0}^{\infty} |p_0| dx}_{\text{Landau integral}}$$

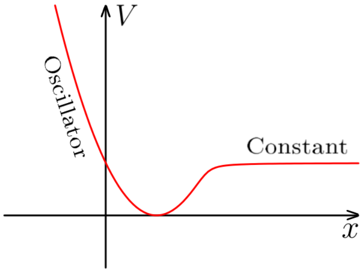
- $\boxed{x = \infty}$ – singularity point of the potential $V(x)$
- **Question: What if we consider potentials such that $V(x) \neq \infty$ at the singularity point?**

For example, potentials with soft (i.e. branch point) singularities

Model and motivation

$$V(x) = \frac{\omega^2}{2}\left[\sqrt{(x-x_0)^2+a^2} - x\right]^2$$

- Has two branch point singularities in the complex plane: $x_s = x_0 + ia$ and $\bar{x}_s$
- $V(x_s) = \frac{\omega^2 x_s^2}{2} \neq \infty$
- Exactly solvable in the limit $a \to 0$



Singularity is no longer a saddle point at $j \to 0$, because

$$\underbrace{\sqrt{2E_N - 2V(x_s)}}_{p_N(x_s)} \neq \underbrace{\sqrt{2E_0 - 2V(x_s)}}_{p_0(x_s)}$$

$$\Downarrow$$

Generalization of Landau Method needed

Exact WKB

$$\boxed{\hbar^2\Psi'' + p^2(x)\Psi = 0;\ -p^2(x) = U_0 + \lambda\sqrt{x}}\qquad p(x) = \sqrt{2V(x) - 2E}$$

Theorem: $\Psi(x)$ is analytic on two-sheeted Riemann surface – **Proven**

- $\Psi(x) = c_+\Psi_+(x) + c_-\Psi_-(x)$
- $\Psi_\pm(x)$=Borel sum $\underbrace{\left[p^{-1/2}(x)\cdot\exp\left(\pm i\hbar^{-1}\int^x p(x)dx\right) + \text{corrections in } \hbar\right]}_{\text{semiclassical asymptotic series}}$
- $\Psi(x)$ Borel summable $\Leftrightarrow x \notin$ Stokes line, i.e. $\mathrm{Im}\left(i\hbar^{-1}\int_{x_0}^{x} p(x)dx\right) \neq 0$ $\quad x_0$ – origin of Stokes line
- Otherwise, if $\mathrm{Re}\left(\pm i\hbar^{-1}\int_{x_0}^{x} p(x)dx\right) > 0 \Leftrightarrow \Psi_\pm(x)$ is not Borel summable $\Leftrightarrow c_\pm$ jumps
- **Theorem** $\Rightarrow$ All Stokes lines $\in$ Riemann surface

Stokes lines in $\sqrt{x}$ potential

$\Psi(x) = c_+\Psi_+(x) + c_-\Psi_-(x)$

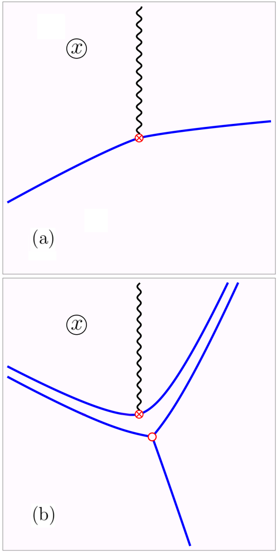
- Turning point $\Rightarrow$ 3 Stokes lines ($c_\pm \to c_\pm + ic_\mp$)
- Singularity point $x = 0 \Rightarrow$ additional Stokes lines

Derivation of $c_\pm$ jumps

1. Born expansion in λ: $\Psi_\pm = \Psi_\pm^{(0)} + \lambda\Psi_\pm^{(1)} + \mathcal{O}(\lambda^2)$
2. $$\Psi_+ = \mathrm{e}^{\frac{\sqrt{U_0}x}{\hbar}}\left[1+\lambda\left(\frac{A}{\hbar}x^{3/2}+B\sqrt{x}\underbrace{\sum_{n=0}^{\infty}\left(\frac{3A\hbar}{2x}\right)^n\Gamma(n-1/2)}_{\text{incomplete gamma-function}}\right)+\mathcal{O}(\lambda^2)\right]$$
3. $\mathcal{B}(t) = \sum_{n=0}^{\infty} t^n \frac{\Gamma(n-1/2)}{n!} = -2\sqrt{\pi}\sqrt{1-t}$ – singular at $t = 1$!

$$\left.\begin{aligned} c_- &\to c_- \pm \frac{i\lambda}{4U_0^{5/4}}\sqrt{\frac{\pi\hbar}{2}}c_+(1+\mathcal{O}(\lambda\sqrt{\hbar})) \\ c_+ &\to c_+ \pm \frac{\lambda}{4U_0^{5/4}}\sqrt{\frac{\pi\hbar}{2}}c_-(1+\mathcal{O}(\lambda\sqrt{\hbar})) \end{aligned}\right\}$$

Answer
(Confirmed by *Y. Takei '95*)



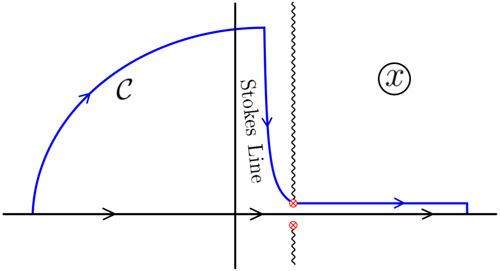
Contour Deformation

$$V(x) = \frac{\omega^2}{2}\left[\sqrt{(x-x_0)^2+a^2} - x\right]^2$$

$$\mathcal{A} = \langle N|\hat{x}|0\rangle = \int_{\mathbb{R}} \psi_N x \psi_0 dx = 2\mathrm{Re}\left(\int_{\mathbb{R}} \psi_N^+ x \psi_0 dx\right)$$

- Deform $\mathbb{R}$ into contour $\mathcal{C}$
- On $\mathcal{C}$: $\psi_N^+ \approx \frac{C_N}{2\sqrt{p_N}} \exp\left(\frac{i}{\hbar}\int_{a_N}^{x} p_N dx + \frac{i\pi}{4}\right)$

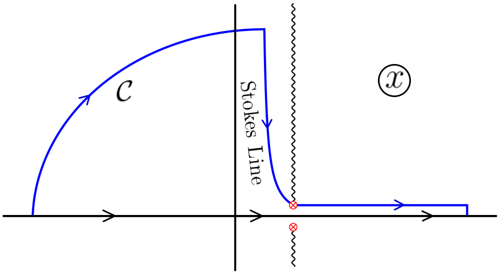
  $\psi_0 \approx \frac{C_0}{2\sqrt{p_0}} \exp\left(-\frac{i}{\hbar}\int_{a_0}^{x} p_0 dx - \frac{i\pi}{4}\right)$ $\quad a_N$ – turning point
- $\mathcal{A} \propto \mathrm{Re}\left(\int_{\mathcal{C}} \frac{x}{\sqrt{p_0 p_N}} e^{W(x)}\right)$; $W(x) = \frac{i}{\hbar}\int_{a_N}^{x} p_N\, dx - \frac{i}{\hbar}\int_{a_0}^{x} p_0\, dx$
- Statement: $\mathrm{Re}\, W(x)$ on the contour $\mathcal{C}$ is maximal at the singularity point $x = x_s$ $\Leftrightarrow$ integral is saturated at $x \approx x_s$



Integral saturation

$$W(x) = \frac{i}{\hbar}\int_{a_N}^{x} p_N\,dx - \frac{i}{\hbar}\int_{a_0}^{x} p_0\,dx$$

- Integral over the arc vanishes ($p_N - p_0 \sim i\frac{E_N - E_0}{2\omega x}$ as $x \to -\infty$)
- 1) On Stokes line ψ_N^+ decays fastest
  2) ψ_0 grows slower $\Rightarrow$ on Stokes line segment
  $\mathrm{Re}\, W(x)$ is maximal at $x = x_s$



- On horizontal segment $V(x) \approx \overbrace{V(x_s) = \frac{\omega^2 x_s^2}{2}}^{\text{for small } a} \Rightarrow$

$$\frac{1}{\sqrt{2}}\mathrm{Im}(p_N - p_0) \approx \sqrt{V(x_s) - E_0} - \sqrt{V(x_s) - E_N} > 0$$

Statement is proven!

But there is one problem: semiclassics breaks down at $x \approx x_s$!

$$\Downarrow$$

Born expansion is needed

$$V(x \approx x_s) = V(x_s) + \underbrace{\beta\sqrt{x - x_s}}_{\text{perturbation}} + \mathcal{O}(x - x_s)$$

$$x - x_s = \hbar\chi, \quad \chi = \mathcal{O}(1)$$

$$\underbrace{\begin{aligned}\psi^-_{0,\,pert} &= A_0 e^{-\chi\varkappa_0^{(s)}}\left(1 + a_0\beta\hbar^{1/2}\chi^{3/2} + b_0\beta\hbar^{1/2}e^{2\chi\varkappa_0^{(s)}}\Gamma\left(\tfrac{3}{2},\, 2\varkappa_0^{(s)}\chi\right) + \mathcal{O}(\beta^2\hbar)\right)\\ \psi^+_{N,\,pert} &= A_N e^{\chi\varkappa_N^{(s)}}\left(1 + a_N\beta\hbar^{1/2}\chi^{3/2} + b_N\beta\hbar^{1/2}e^{-2\chi\varkappa_0^{(s)}}\Gamma\left(\frac{3}{2},\, e^{i\pi}2\varkappa_N^{(s)}\chi\right) + \mathcal{O}(\beta^2\hbar)\right)\end{aligned}}_{\text{glue with semiclassical solutions in region } \chi\sim a\hbar^{-1/3} \Leftrightarrow x - x_s \sim a\hbar^{2/3}}$$

Gluing: $A_0 A_N = \frac{iC_0 C_N}{4\sqrt{\varkappa_0^{(s)}\varkappa_N^{(s)}}} e^{W_s}$; $\quad W_s \equiv W(x_s) = \frac{i}{\hbar}\int\limits_{a_N}^{x_s} p_N\, dx - \frac{i}{\hbar}\int\limits_{a_0}^{x_s} p_0\, dx$, $\quad \overbrace{\varkappa_N^{(s)} = \sqrt{2V(x_s) - 2E_N}}^{\text{Euclidean momentum at } x = x_s}$

Matrix Elements evaluation

1. Take integral in the vicinity of the x_s
2. $\mathcal{A} = 2\hbar \mathrm{Re}\Big(\int_{\mathcal{C}} (\underbrace{x_s}_{\langle N|x_s|0\rangle = 0} + \hbar\chi)\psi^{+}_{N,\,pert}\psi^{-}_{0,\,pert}\,d\chi\Big) = 2\hbar^2 \mathrm{Re}\Big(\int_{\mathcal{C}} \psi^{+}_{N,\,pert}\chi\psi^{-}_{0,\,pert}\,d\chi\Big)$
3. Note: **this integral cannot be evaluated by saddle-point method (unlike in original Landau Method)!**

Answer

$$\mathcal{A} = \mathrm{Re}\Big(\hbar^{9/4} P(E_N)\exp(\tilde{W}_s + i\phi(E_N))\Big)$$

$\tilde{W}_s = W_s + \frac{i}{\hbar}\int_{a_0}^{x_*} p_0\,dx = W_s - \underbrace{1/4 \cdot \ln \hbar}_{\hbar^{5/2} \to \hbar^{9/4}} + f(x_0, a, \omega)$ – better for numerical test; $\underbrace{x_* = \frac{1}{2}(x_0 + a^2/x_0)}_{V(x_*) = 0}$

Full Answer

$$\mathcal{A} = 2\mathrm{Re}\left(\frac{\hbar^{9/4}\omega^2 a x_s}{(-A\varkappa_N^{(s)})^{1/2}E_N^2}\left(\frac{\omega_0\omega_N^2}{\pi \mathrm{e}^2}\right)^{1/4}\mathrm{e}^{g(\tilde{a})}\mathrm{e}^{\tilde{W}_s}\right)$$

- $A = a(\varkappa_N^{(s)} - \varkappa_0^{(s)})$
- $\tilde{a} \equiv a/x_0, \quad \tilde{E}_N \equiv E_N/\omega^2 x_0^2; \quad \underbrace{\omega_N = \frac{2\omega}{1 + \frac{\tilde{a}^2}{(1-2\tilde{E}_N)^{3/2}}}}_{\text{angular frequency}}$
- $g(\tilde{a}) = \frac{\omega_0}{4\omega}(1 + i\tilde{a} - \tilde{a}^2 \ln \tilde{a} - i\pi/2)$

$$\tilde{W}_s = \frac{\omega x_0^2}{2\hbar}\left[\frac{1}{2}(1+3i\tilde{a})(\tilde{\varkappa}_N^{(s)} - 1 - i\tilde{a}) + \ln\left(\frac{1 + i\tilde{a} - \tilde{\varkappa}_N^{(s)}}{\sqrt{2\tilde{E}_N}}\right)\left(\tilde{E}_N - \tilde{a}^2 - \frac{\tilde{a}^2}{\sqrt{1-2\tilde{E}_N}}\right) + \right.$$

$$\left. + \frac{\tilde{a}^2}{\sqrt{1-2\tilde{E}_N}}\ln\frac{\sqrt{1-2\tilde{E}_N} + i\tilde{a} - \tilde{\varkappa}_N^{(s)}}{\sqrt{1-2\tilde{E}_N} + i\tilde{a} + \tilde{\varkappa}_N^{(s)}} - \tilde{a}^2\ln\tilde{a} + \tilde{a}^2\frac{i\pi}{2}\right], \qquad \tilde{\varkappa}_N^{(s)} \equiv \varkappa_N^{(s)}/\omega x_0$$

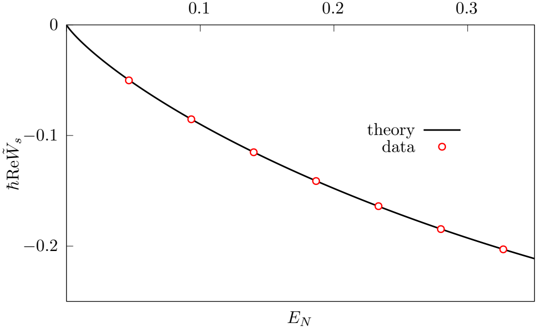
Numerical Test

$$\hbar \ln |\mathcal{A}| = \hbar \mathrm{Re}\ \tilde{W}_s + \frac{9}{4}\hbar \ln \hbar + \hbar \ln |P(E_N)| + \hbar \ln |\cos(\arg P(E_N) + \mathrm{Im}\ \tilde{W}_s)|$$

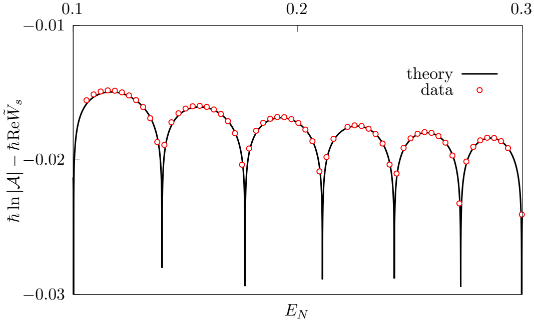
1. $\lim_{\hbar \to 0} \hbar \ln |\mathcal{A}| = \hbar \mathrm{Re}\ \tilde{W}_s$ – suppression exponent
2. $\hbar \ln |\mathcal{A}| - \hbar \mathrm{Re}\ \tilde{W}_s$ – prefactor (for finite $\hbar$)

$\omega = x_0 = 1, \ a = 0.1$

Suppression Exponent:



Prefactor ($\hbar = 1.6 \cdot 10^{-3}$):



Results:

1. Original Landau method is not applicable for potentials with soft singularities. We generalized Landau method to such potentials.
2. We obtained analytical formula for matrix elements in a particular model and confirmed it with high-precise numerical calculations.
3. There are the first steps of generalizing Exact WKB method to potentials with branching points.

Future: Exact quantization conditions for potentials with branch point singularities?

Thank you for attention!

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