Exercise 4: Theorem of Coleman

Theorem: Let f_W be a solution of

$$(-\partial_\tau^2 - W(\tau))\, f(\tau) = 0$$

with initial conditions $f_W(0) = 0$, $\dot{f}_W(0) = 1$,

then

$$\frac{\det(-\partial_\tau^2 - U(\tau))}{\det(-\partial_\tau^2 - V(\tau))} = \frac{f_U(t)}{f_V(t)} .$$

with $\tau \in [0,t]$ on $\mathcal{H} := \{ \varphi \in L^2([0,t]) \mid \varphi(0) = 0 = \varphi(t) \}$

Proof: Let $\{\lambda_n^W\}_{n=0,1,2,\dots}$ be the discrete spectrum of $(-\partial_\tau^2 - W(\tau))$ on $\mathcal{H}$, real and bounded from below

no degeneracy

- $$g(\lambda) := \frac{\det(-\partial_\tau^2 - U(\tau) - \lambda)}{\det(-\partial_\tau^2 - V(\tau) - \lambda)} = \frac{\prod_{n=0}^{\infty} (\lambda_n^U - \lambda)}{\prod_{n=0}^{\infty} (\lambda_n^V - \lambda)}, \quad \lambda \in \mathbb{C}$$

$$\left.\begin{array}{l} \text{has simple zeros at } \lambda = \lambda_n^U \\ \text{has simple poles at } \lambda = \lambda_n^V \end{array}\right\} \Rightarrow g \text{ meromorphic } \mathbb{C}$$

- $h(\lambda) := \dfrac{f_{U+\lambda}(t)}{f_{V+\lambda}(t)}$

obviously $(-\partial_\tau^2 - W(\tau)) f_{W+\lambda}(\tau) = \lambda f_{W+\lambda}$

$\rightsquigarrow$ λ is eigenvalue iff $f_{W+\lambda}(t) = 0$

$\rightsquigarrow$ $h(\lambda)$ has zeros at $\lambda = \lambda_n^U$
and poles at $\lambda = \lambda_n^V$ (simple?)

- g/h = analytic function without poles and zeros on $\mathbb{C}$

For $\lambda \to \infty$ $\quad g(\lambda) \to 1$, $\quad h(\lambda) \to 1$ $\quad$ as details of U and V become irrelevant

$\rightsquigarrow$ g/h is bounded on $\mathbb{C}$ with $\lim\limits_{\lambda\to\infty} \dfrac{g(\lambda)}{h(\lambda)} = 1$

Liouville $\Rightarrow$ $\dfrac{g(\lambda)}{h(\lambda)} \equiv 1$

for $\lambda = 0$ follows Theorem of Coleman

(see Felsager p. 197 ff)

Exercise 5: Quasi-classical approx. for Green's function

- Starting point is propagator

$$K(\vec{x}'',\vec{x}',t) \approx \sum_{x_\alpha}^{t\text{ fixed}} \left(\frac{i}{2\pi\hbar}\right)^{d/2} \sqrt{\det\left(\frac{\partial^2 S_\alpha}{\partial \vec{x}''\partial \vec{x}'}\right)}\, e^{\frac{i}{\hbar}S_\alpha}$$

$$S_\alpha \equiv S_\alpha(\vec{x}'',\vec{x}';t) = \int_0^t d\tau \left[\frac{m}{2}\dot{\vec{x}}_\alpha^2(\tau) - V(x_\alpha(\tau))\right]$$

with $m\ddot{\vec{x}}_\alpha = -\vec{\nabla}V(\vec{x})$, $\vec{x}_\alpha(0)=\vec{x}'$, $\vec{x}_\alpha(t)=\vec{x}''$

- Green's function:

$$G(\vec{x}'',\vec{x}',E) := \langle\vec{x}''|\frac{1}{E-H}|\vec{x}'\rangle = \frac{1}{i\hbar}\int_0^\infty dt\, e^{\frac{i}{\hbar}Et}\langle\vec{x}''|e^{-\frac{i}{\hbar}Ht}|\vec{x}'\rangle$$

$\operatorname{Im} E > 0$

$$\approx \frac{1}{i\hbar}\left(\frac{i}{2\pi\hbar}\right)^{d/2}\int_0^\infty dt \sum_{x_\alpha}^{t\text{ fixed}} \sqrt{\det\frac{\partial^2 S_\alpha}{\partial\vec{x}''\partial\vec{x}'}}\, e^{\frac{i}{\hbar}(S_\alpha+Et)}$$

for small $\hbar$ only quadratic fluctuation around stationary phase contribute (at $t=t_\beta$)

$$\left.\frac{\partial S_\alpha}{\partial t}\right|_{t_\beta} + E = 0 \quad \text{at } t=t_\beta$$

$\leadsto$ $E = -\left.\frac{\partial S}{\partial t}\right|_{t_\beta}$ = conserved energy

$\leadsto$ only paths w. energy E contribute
↑ classical

Hence $$\int_0^\infty dt \sum_{x_\alpha}^{t \text{ fixed}} (\dots) = \sum_{x_\alpha}^{E \text{ fixed}} \int_0^\infty dt\, (\dots)$$

with $$S_\alpha + Et \approx S_\alpha(x'', x', t_\beta) + E t_\beta + \frac{1}{2} \left.\frac{\partial^2 S_\alpha}{\partial t^2}\right|_{t_\beta} (t - t_\beta)^2 + \dots$$

Recall: Hamilton's characteristic function

$$W_\alpha(x'', x', E) := S_\alpha(x'', x', t) + Et \quad \text{with } E = -\frac{\partial S_\alpha}{\partial t}$$

and $t = t(E)$

Fresnel integral: $$\int_0^\infty dt \exp\left\{\frac{i}{2\hbar} \left.\frac{\partial^2 S_\alpha}{\partial t^2}\right|_{t_\beta} (t - t_\beta)^2\right\} \approx \sqrt{\frac{2\pi i\hbar}{\partial^2 S_\alpha / \partial t^2|_{t_\beta}}}$$

Green's function result:

$$\boxed{G(\vec{x}'', \vec{x}'; E) = \frac{1}{i\hbar} \sum_{x_\alpha}^{E \text{ fixed}} \left(\frac{i}{2\pi\hbar}\right)^{\frac{d-1}{2}} \sqrt{D_\alpha}\, e^{\frac{i}{\hbar} W_\alpha}}$$

with $$D_\alpha := -\frac{\det \frac{\partial^2 S_\alpha}{\partial \vec{x}'' \partial \vec{x}'}}{\partial^2 S / \partial t^2} \overset{*}{=} \det \begin{pmatrix} \frac{\partial^2 W_\alpha}{\partial \vec{x}'' \partial \vec{x}'} & \frac{\partial^2 W_\alpha}{\partial \vec{x}' \partial E} \\ \frac{\partial^2 W_\alpha}{\partial \vec{x}'' \partial E} & \frac{\partial^2 W_\alpha}{\partial E^2} \end{pmatrix}$$

Original work: M. Gutzwiller, JMP 8 (1967) 1971–2000

see also book by Schulman

Proof of ⊛:

$$W(x'',x',E) = S(x'',x',t) + Et$$

$$\frac{\partial S}{\partial t} = -E \quad , \quad t = \frac{\partial W}{\partial E}$$

Legendre transf.

- $$\frac{\partial^2 S}{\partial t^2} = -\frac{\partial E}{\partial t} = -\left(\frac{\partial^2 W}{\partial E^2}\right)^{-1}$$

- $$\frac{\partial S}{\partial x''}\bigg|_{t \text{ fixed}} = \frac{\partial W}{\partial x''}\bigg|_t - \frac{\partial E}{\partial x''}\bigg|_t t = \frac{\partial W}{\partial x''} + \frac{\partial W}{\partial E}\frac{\partial E}{\partial x''}\bigg|_t - \frac{\partial E}{\partial x''}\bigg|_t \frac{\partial W}{\partial E} = \frac{\partial W}{\partial x''}$$

- $$\frac{\partial^2 S}{\partial x''\partial x'}\bigg|_t = \frac{\partial^2 W}{\partial x'\partial x''} + \frac{\partial^2 W}{\partial x''\partial E}\frac{\partial E}{\partial x'}\bigg|_t$$

with $0 = \frac{\partial t}{\partial x'}\Big|_t = \frac{\partial^2 W}{\partial x'\partial E}\Big|_t = \frac{\partial^2 W}{\partial x'\partial E} + \frac{\partial^2 W}{\partial E^2}\frac{\partial E}{\partial x'}\Big|_t$

$$\rightsquigarrow \quad \frac{\partial E}{\partial x'}\bigg|_t = -\frac{\partial^2 W}{\partial x'\partial E}\left(\frac{\partial^2 W}{\partial E^2}\right)^{-1}$$

$$\rightsquigarrow \quad \frac{\partial^2 S}{\partial x''\partial x'}\bigg|_t = \frac{\partial^2 W}{\partial x''\partial x'} - \frac{\partial^2 W}{\partial x''\partial E}\frac{\partial^2 W}{\partial x'\partial E} \bigg/ \frac{\partial^2 W}{\partial E^2}$$

Result:

$$-\frac{\partial^2 S}{\partial x''\partial x'}\bigg|_t \bigg/ \frac{\partial^2 S}{\partial t^2} = \frac{\partial^2 W}{\partial x''\partial x'}\frac{\partial^2 W}{\partial E^2} - \frac{\partial^2 W}{\partial x''\partial E}\frac{\partial^2 W}{\partial x'\partial E}$$

$$= \det\begin{pmatrix} \frac{\partial^2 W}{\partial x''\partial x'} & \frac{\partial^2 W}{\partial x'\partial E} \\ \frac{\partial^2 W}{\partial x''\partial E} & \frac{\partial^2 W}{\partial E^2} \end{pmatrix} = D_\alpha$$

#

Summary:

$$G(x'',x',E) \approx \frac{1}{i\hbar}\left(\frac{i}{2\pi\hbar}\right)^{\frac{d-1}{2}} \sum_{x_\alpha}^{E} \sqrt{|D_\alpha|}\, e^{\frac{i}{\hbar}W_\alpha}\, e^{-i\frac{\pi}{2}\mu_\alpha}$$

μ_α: Maslov Index = No. of negative eigenvalues of D_α

= Morse Index (+1) in case $\frac{\partial^2 S}{\partial t^2} < 0$

Example: 1-dim. free particle (has only 1 path ⤳ no α)

$$S = \frac{m}{2t}(x''-x')^2 \quad , \quad E = \frac{m}{2}\left(\frac{x''-x'}{t}\right)^2 \quad , \quad S = Et$$

$$\leadsto t = \sqrt{\frac{m}{2E}}\,|x''-x'| \quad , \quad \frac{\partial^2 S}{\partial x''\partial x'} = -\frac{m}{t} \quad , \quad \frac{\partial^2 S}{\partial t^2} = \frac{m}{t^3}(x''-x')^2 > 0$$

$$\Rightarrow D = -\frac{\partial^2 S}{\partial x''\partial x'} \Big/ \frac{\partial^2 S}{\partial t^2} = \frac{m}{t}\,\frac{t^3}{m}\,\frac{1}{(x''-x')^2} = \frac{t^2}{(x''-x')^2} = \frac{m}{2E} > 0$$

$$W = S + Et = 2Et = \sqrt{2mE}\,|x''-x'|$$

$$\leadsto \frac{\partial^2 W}{\partial x''\partial x'} = 0 \, , \quad \frac{\partial^2 W}{\partial x''\partial E} = \pm\sqrt{\frac{m}{2E}} = -\frac{\partial^2 W}{\partial x'\partial E} \quad \text{for} \quad \begin{array}{l} x''>x' \\ x''<x' \end{array}$$

$$\leadsto D = \frac{m}{2E} \quad ✓ \quad \text{consistent}$$

$$\Rightarrow \quad \underline{\underline{G(x'',x',E) = \frac{1}{i\hbar}\sqrt{\frac{m}{2E}}\; e^{\frac{i}{\hbar}\sqrt{2mE}\,|x''-x'|}}}$$

is exact in 1-d and 3-d

Free particle in d-dimension

$$G(\vec{x}'', \vec{x}', E) = \langle \vec{x}'' | \frac{1}{E - \vec{p}^2/2m} | \vec{x}' \rangle$$

$$= \frac{2}{i\hbar} \left(\frac{m}{2\pi i\hbar} \right)^{d/2} \left(\frac{2E}{m r^2} \right)^{\frac{d-2}{4}} K_{\frac{d-2}{2}} \left(\frac{r}{i\hbar} \sqrt{2mE} \right)$$

$$= \underbrace{\frac{m}{i\hbar} \frac{1}{(2\pi i\hbar)^{\frac{d-1}{2}}} (2mE)^{\frac{d-3}{4}} \frac{1}{r^{\frac{d-1}{2}}} e^{\frac{i}{\hbar}\sqrt{2mE}\, r}}_{\text{quasi-cl. result}} \; \underbrace{{}_2F_0\left(\frac{d-1}{2}, \frac{3-d}{2}, \frac{\hbar}{2 i r \sqrt{2mE}} \right)}_{\text{Power series in } \hbar}$$

Here $r := |\vec{x}'' - \vec{x}'|$, $K_\nu(z)$ mod. Bessel-function

$${}_2F_0(a, b, z) := \sum_{n=0}^{\infty} \frac{(a)_n (b)_n}{n!} z^n, \quad (a)_n := \frac{\Gamma(a+n)}{\Gamma(a)} \text{ Pochhammer symbol}$$

power series in z

terminates when a or b is negativ integer

$${}_2F_0(0, b, z) = 1 = {}_2F_0(a, 0, z)$$

Exercise 6: The WKB formula via path integration

Here only $d = 1$

$$W_\alpha(x'', x', E) = \int_0^t d\tau \left(\frac{m}{2} \dot{x}_\alpha^2 - V(x_\alpha) \right) + Et = \int_0^t d\tau \, m \dot{x}_\alpha^2$$

$$= \int_{x'}^{x''} dx \, P_E(x) \quad \text{with} \quad P_E(x) := \pm \sqrt{2m(E - V(x))}$$

$$\Rightarrow \frac{\partial P_E(x)}{\partial E} = \frac{m}{P_E(x)}$$

Hence $\dfrac{\partial W_\alpha}{\partial x'} = -P_E(x')$ and $\dfrac{\partial W_\alpha}{\partial x''} = +P_E(x'')$ $\Rightarrow$ $\dfrac{\partial^2 W_\alpha}{\partial x'' \partial x'} = 0$

as x', x'' and E are independent

$$\Rightarrow D_\alpha = -\frac{\partial^2 W_\alpha}{\partial x'' \partial E} \frac{\partial^2 W_\alpha}{\partial x' \partial E} = \frac{\partial P_E(x')}{\partial E} \frac{\partial P_E(x'')}{\partial E} = \frac{m^2}{P_E(x') P_E(x'')}$$

Note: D_α changes sign along x_α whenever momentum changes sign!

$\Rightarrow$ μ_α = number of turning points along x_α

Classification of classical paths:

			x'	x''
1.	$P(x') > 0$	$P(x'') > 0$	$\bullet\!\rightarrow$	$\rightarrow\!\bullet$
2.	$P(x') < 0$	$P(x'') > 0$	$\leftarrow\!\bullet$	$\rightarrow\!\bullet$
3.	$P(x') > 0$	$P(x'') < 0$	$\bullet\!\rightarrow$	$\bullet\!\leftarrow$
4.	$P(x') < 0$	$P(x'') < 0$	$\leftarrow\!\bullet$	$\bullet\!\leftarrow$

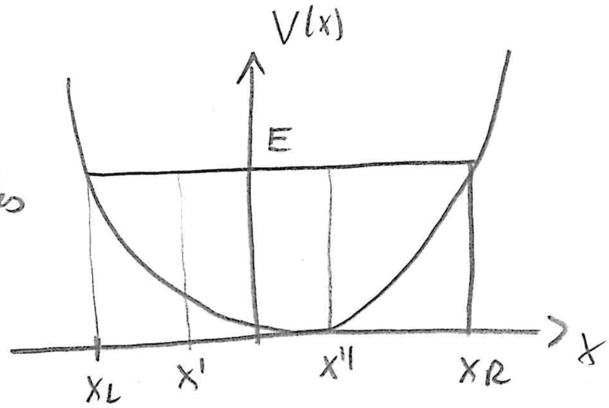
Let: $w(z) := \int_{x_L}^{z} dx \sqrt{2m(E - V(x))}$ with $V(x_{L/R}) = E$ left/right turning points

$$W_\alpha[x] \equiv W_K^{(i)} = W_0^{(i)} + 2K\, w(x_R)$$

Path belongs to class i with K full cycles

$$\mu_\alpha[x] \equiv \mu_K^{(i)} = \mu_0^{(i)} + 2K$$

2 turning point for full cycle

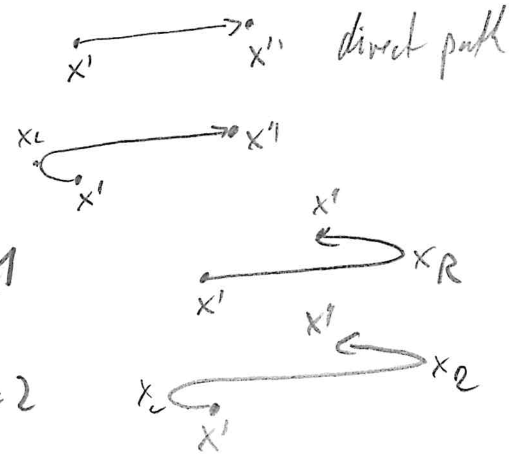


$$W_0^{(1)} = w(x'') - w(x') \,, \quad \mu_0^{(1)} = 0$$

$$W_0^{(2)} = w(x'') + w(x') \,, \quad \mu_0^{(2)} = 1$$

$$W_0^{3} = 2w(x_R) - w(x') - w(x'') \,, \quad \mu_0^{(3)} = 1$$

$$W_0^{4} = 2w(x_R) + w(x') - w(x'') \,, \quad \mu_0^{(4)} = 2$$



$$\Rightarrow \sum_{x_L}^{E} (\dots) = \sum_{k=0}^{\infty} \sum_{i=1}^{4} (\dots)$$

Result:

$$G(x'', x', E) \approx \frac{1}{i\hbar} \frac{m}{\sqrt{|p(x'')p(x')|}} \sum_{i=1}^{4} e^{\frac{i}{\hbar} W_0^{(i)} - \frac{i\pi}{2}\mu_0^{(i)}} \underbrace{\sum_{k=0}^{\infty} \underbrace{e^{\frac{i}{\hbar} 2k w(x_R)} \, e^{-\frac{i}{2}\pi 2k}}_{\exp\{ik(\frac{2}{\hbar} w(x_R) - \pi)\}}}_{= \frac{1}{1 - \exp\{i(\frac{2}{\hbar} w(x_R) - \pi)\}}}$$

$$\approx \frac{m}{i\hbar} \left[2m(E - V(x'))(E - V(x''))\right]^{-\frac{1}{4}} \frac{\sum_{i=1}^{4} \exp\{i(\frac{W_0^{(i)}}{\hbar} - \frac{\pi}{2}\mu_0^{(i)})\}}{1 - \exp\{i(\frac{2}{\hbar} w(x_R) - \pi)\}}$$

- Poles: $\frac{2}{\hbar} w(x_R) - \pi = 2\pi n$, $n \in \mathbb{N}_0$ as $w(x_R) \geq 0$

$$\Rightarrow w(x_R) = \pi\hbar(n + \tfrac{1}{2}) \Rightarrow \boxed{\int_{x_L}^{x_R} dx \sqrt{2m(E - V(x))} = \pi\hbar(n + \tfrac{1}{2})}$$

WKB Formula good for large n or E

exact for HO and Morse-Oscillator!

• Residues: $\operatorname*{Res}_{E=E_n} \langle x''| \frac{1}{E-H} |x'\rangle = \varphi_n^*(x')\, \varphi_n(x'')$

$$\Longrightarrow \boxed{\varphi_n(x) \approx \sqrt{\frac{4\pi}{T_n}}\, \frac{\sin\left(\frac{W(x)}{\hbar} + \frac{\pi}{4}\right)}{\sqrt{2m(E-V(x))}}}$$ see Landau/Lifshitz

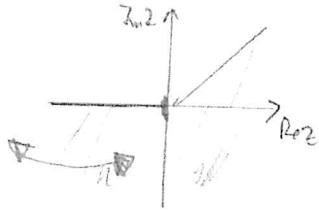
with $T_n := 2\int_{x_L}^{x_R} dx \sqrt{\frac{m}{2(E_n - V(x))}}$ = cl. period for $E=E_n$

Exercise 7: Proof of modified Weber formula

We start with Gradsteyn / Ryshik #6.633 (2)   Weber's formula

$$\int_0^\infty dx\, x\, e^{-\rho^2 x^2} J_\nu(ax)\, J_\nu(bx) = \frac{1}{2\rho^2}\, e^{-\frac{a^2+b^2}{4\rho^2}}\, I_\nu\left(\frac{ab}{2\rho^2}\right)$$

$$\mathrm{Re}\,\rho^2 > 0, \quad \mathrm{Re}\,\nu > -1, \quad a,b > 0$$



Note: $I_\nu(z) = e^{-i\frac{\pi}{2}\nu} J_\nu(iz)$ for $-\pi < \arg z \le \frac{\pi}{2}$

Let $z = -iar$ $a,r>0$ ⇝ $\arg z = -\frac{\pi}{2}$

⇝ $I_\nu(-iar) = e^{-i\frac{\pi}{2}\nu} J_\nu(ar)$

Let $\alpha := i\rho^2$ ⇝ $\mathrm{Im}\,\alpha > 0$

$$\int_0^\infty dr\, r\, e^{i\alpha r^2} I_\nu(-iar)\, I_\nu(-ibr)\, e^{i\pi\nu} = \frac{i}{2\alpha}\, e^{-\frac{i}{4\alpha}(a^2+b^2)}\, I_\nu\left(\frac{ab}{-2i\alpha}\right)$$

$$I_\nu(z\, e^{m\pi i}) = e^{m\nu\pi i} I_\nu(z), \quad z = \frac{ab}{2i\alpha}, \quad m = 1$$

$$\int_0^\infty dr\, r\, e^{i\alpha r^2} I_\nu(-iar)\, I_\nu(-ibr) = \frac{i}{2\alpha}\, e^{-\frac{i}{4\alpha}(a^2+b^2)}\, I_\nu\left(-i\frac{ab}{2\alpha}\right)$$

modified Weber formula