The Weber equation as a normal form with applications to top of the barrier scattering

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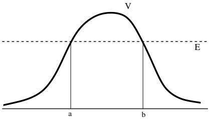
Problem: for Schrödinger equations

$$-\hbar^2\psi''(\xi) + V(\xi)\psi(\xi) = E\psi(\xi)$$



find fine properties of the resolvent and the spectral measure for energies $E \approx \max V$ close to the *top of the potential barrier*, and obtain accurate representations of the resolvent uniformly in small $\hbar$.

The potential satisfies:

- decay: $V \in L^1(\mathbb{R})$
- regularity: $V \in C^v(\mathbb{R})$ with $v \in \{\infty, \omega\}$,
- unique absolute maximum: say at $\xi = 0$, where $V(\xi) = 1 - \xi^2 + O(\xi^3)$.

Problem much studied:

Vast literature devoted to this problem (and its higher-dim) , e.g.: Ramond & al. ('11...'14), Aoki, Kawai & Takei ('09), Bleher ('94), Briet, Combes & Duclos ('87), de Verdiére & Parisse ('94), Gérard & Gigris ('88), Helfer & Sjöstrand ('86), [...] Olver ('59...'75).

Their methods employed vary e.g. analysis of Hamiltonian flow near a hyperbolic fixed point, microlocal analysis, and complex WKB techniques (requiring analytic potentials).

But: they do not produce *multiplicative control of the errors* - needed for using the spectral measure is applications to wave equations (e.g. the wave equation on a Schwarzschild black hole).

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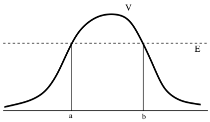
But: they do not produce *multiplicative control of the errors* - needed for using the spectral measure is applications to wave equations (e.g. the wave equation on a Schwarzschild black hole).

Our approach:

we show that for E close enough to max V the Schrödinger eq.

$$-\hbar^2\psi''(\xi) + V(\xi)\psi(\xi) = E\psi(\xi)$$



is $C^\omega[C^\infty]$ equivalent to a Weber equation

$$-\hbar^2\phi''(y) + (\beta - y^2)\phi(y) = E_1\phi(y) \qquad \text{for some } \beta = \beta(E), E_1 \text{ close to } \beta$$

(eq. of the modified parabolic cylinder functions)

Step I. Reduction to a perturbed Weber equation

Theorem 1.
Consider

$$-\hbar^2\psi''(\xi) + V(\xi)\psi(\xi) = E\psi(\xi) \tag{1}$$

where

- $V \in L^1(\mathbb{R})$ and $V \in C^v(\mathbb{R})$ with $v \in \{\infty, \omega\}$,
- $V(\xi)$ has a unique absolute max: $V(\xi) = 1 - \xi^2 + O(\xi^3)$ $(\xi \to 0)$.

Then there exist $\delta > 0$ and

- $\beta = \beta(E)$ of class C^v for $|1 - E| < \delta$
- $y = y(\xi; \beta)$ of class C^v on $\mathbb{R} \times (-\delta, \delta)$

so that (1) becomes

$$\underbrace{\psi_2''(y) = \frac{\beta - y^2}{\hbar^2}\psi_2(y)}_{\text{Weber eq.}} + \underbrace{f(y)\psi_2(y)}_{\text{perturbation}}$$

Note: smoothness regardless of transition between 2 turning points $(\beta > 0)$, one $(\beta = 0)$ or none $(\beta < 0)$.

II. Equivalence to Weber equation with fine control of errors

Theorem 2.
Perturbed Weber eq. $\psi_2'' = \frac{\beta - y^2}{\hbar^2}\psi_2 + f\psi_2$ is equivalent to Weber's eq.

$$\phi''(y) = \frac{\beta - y^2}{\hbar^2}\phi(y)$$

through a transformation

$$\begin{bmatrix} \psi_2 \\ \psi_2' \end{bmatrix} = H(y;\beta,\hbar) \begin{bmatrix} \phi \\ \phi' \end{bmatrix}, \quad H = I + \hbar\, E(y;\beta,\hbar)$$

where the error $E(y;\beta,\hbar)$ is of class C^v and behaves like a symbol, i.e.

$$\|\partial_y^k \partial_\beta^j E\| \leqslant \begin{cases} C_{k,j}\,\langle y\rangle^{-k}\hbar^{-j} & \text{if } \hbar/|\beta| \lesssim 1 \\ \ln(\hbar^{-1}) \quad C_{k,j}\,\langle y\rangle^{-k}\hbar^{-j} & \text{if } \hbar/|\beta| \gg 1 \end{cases}$$

III. Scattering Matrix

The monodromy matrix $\mathcal{M}_W[\phi]$ of the Weber's eq. can be calculated.
Consequence:

$$\mathcal{M}[\psi_2] = (I + \hbar E_1)\,\mathcal{M}_W[\phi]\,(I + \hbar E_2)$$

where

$$(*) \qquad \|\partial_\beta^j E_{1,2}\| \leqslant \begin{cases} C_j\,\hbar^{-j} & \text{if } \hbar/|\beta| \lesssim 1 \\ \ln(\hbar^{-1}) \quad C_j\,\hbar^{-j} & \text{if } \hbar/|\beta| \gg 1 \end{cases}$$

Working back through the equivalence and the changes of variables, the monodromy of $-\hbar^2\psi''(\xi) + V(\xi)\psi(\xi) = E\psi(\xi)$ follows $\rightsquigarrow$ scattering:

Theorem 3. The scattering matrix of the Schrödinger eq.

$$\mathcal{S}(E,\hbar) = \begin{pmatrix} \mathcal{S}_{11} & \mathcal{S}_{12} \\ \mathcal{S}_{21} & \mathcal{S}_{22} \end{pmatrix}, \quad \text{with } \mathcal{S}_{11} = \mathcal{S}_{22}, \quad \mathcal{S}_{12} = -\bar{\mathcal{S}}_{21}\frac{\mathcal{S}_{11}}{\bar{\mathcal{S}}_{11}}$$

is linked to the similar quantities corresponding to the Weber's equation by

$$\mathcal{S}_{ij} = \mathcal{S}_{W,ij}(1 + \hbar e_{ij}) \quad \text{with } e_{ij} \text{ satisfying } (*).$$

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How do $\mathcal{S}_{W,ij}$ look like: for $1-\delta < E \leqslant 1$

$$\mathcal{S}_{W,11} = e^{\frac{i}{\hbar}(I_+(E)+I_-(E))}\, e^{i\theta}\, \frac{1}{\sqrt{1+A^2}}, \qquad \mathcal{S}_{W,21} = e^{\frac{i}{\hbar}2I_-(E)}\, e^{i\theta}\, \frac{-iA}{\sqrt{1+A^2}}$$

where

$$A = e^{\pi\beta/(2\hbar)}, \qquad \theta = \frac{\beta}{2\hbar}\left[1+\ln(2\hbar/|\beta|)\right] + \arg\Gamma\left(\frac{1}{2}+\frac{i\beta}{2\hbar}\right)$$

and

$$I_+(E) := \int_b^{+\infty}\left(\sqrt{E-V(\xi)}-\sqrt{E}\right)d\xi - b\sqrt{E}$$

$$I_-(E) := \int_{-\infty}^{a}\left(\sqrt{E-V(\xi)}-\sqrt{E}\right)d\xi + a\sqrt{E}$$

where $a<0<b$ are the two solutions of $E-V(\xi)=0$.

How do $\mathcal{S}_{W,ij}$ look like: for $1 < E < 1 + \delta$

$$\mathcal{S}_{W,11} = e^{\frac{i}{\hbar}\int_{-\infty}^{+\infty}\left(\sqrt{E-V(\xi)}-\sqrt{E}\right)d\xi}\, e^{i\theta}\, \frac{1}{\sqrt{1+A^2}}$$

$$\mathcal{S}_{W,21} = e^{\frac{2i}{\hbar}\int_{-\infty}^{0}\left(\sqrt{E-V(\xi)}-\sqrt{E}\right)d\xi}\, e^{\frac{i}{\hbar}2\gamma^{-1}\phi_\omega}\, e^{i\theta}\, \frac{-iA}{\sqrt{1+A^2}}$$

with γ depending C^v of $1-E$, $\gamma = 1 + O(1-E)$ and

ϕ_ω has an explicit expression in terms of the Taylor coefficients of V at $\xi = 0$

(heuristic physical interpretation still needs understood).

Proof of Theorem 1: Schrödinger $\rightsquigarrow$ perturbed Weber

Use a Liouville transformation: want a change indep. var. $\xi = \xi(y)$ s.t.

$$[V(\xi) - E]\left(\frac{d\xi}{dy}\right)^2 = \text{quadratic function of } y \qquad (V(\xi) = 1 - \xi^2 + \dots)$$

and we want $\xi(y)$ smooth at both turning points!

Proposition 1.

$(\exists)$ $\tilde{E} = \tilde{E}(E)$ class C^ν for $|1 - E| < 1 + \delta_1$ $(\delta_1 > 0)$

$(\exists)$ $\xi = \xi(y, E)$ 1-to-1, and of class C^ν in (y, E) , $|y| < \delta_2$ so that

$$[V(\xi) - E]\left(\frac{d\xi}{dy}\right)^2 = 1 - y^2 - \tilde{E}$$

Furthermore, $\xi(y, E)$ can be extended 1-to-1, of class C^ν on $\mathbb{R}$.

Recall: $V(\xi) = 1 - \xi^2 + O(\xi^3)$ so for $E < 1$ eq. has two singularities a, b.

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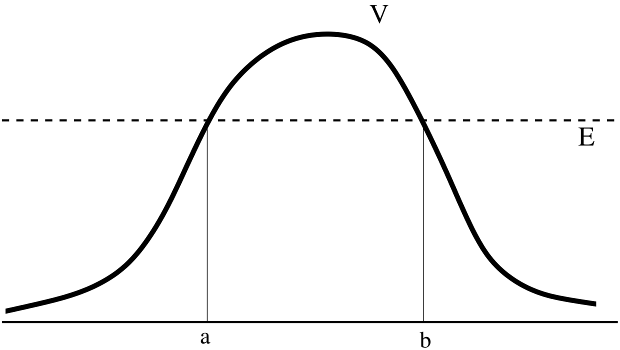

Figure: $E < 1$ with two turning points

Proof of Proposition 1.

In a more convenient notation, and after fidgeting with $V(\xi)$:

Proposition 1 in disguise

There exists $\beta = \beta(\alpha)$ of class C^v so that eq.

$$(\beta - y^2)\left(\frac{dy}{dx}\right)^2 = (\alpha - x^2)\omega(x)^2$$

$(\omega(x) \in C^v,\ \omega(0) = 1)$ has a solution C^v on $(-\delta, \delta) \supset [-\sqrt{\alpha}, \sqrt{\alpha}]$.

Remark A. sol. class C^v at $x = \sqrt{\alpha}$ must satisfy $y(\sqrt{\alpha}) = \pm\sqrt{\beta}$:
and for $x^2 < \alpha$ sol. with $+$ satisfies:

$$\int_{\sqrt{\beta}}^{y} \sqrt{\beta - t^2}\, dt = \int_{\sqrt{\alpha}}^{x} \omega(s)\sqrt{\alpha - s^2}\, ds$$

Proof of Proposition 1. ...p.2

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and for $x^2 < \alpha$ the increasing sol. $y(x)$ must satisfy:

$$\int_{-\sqrt{\beta}}^{y} \sqrt{\beta - t^2}\, dt = \int_{-\sqrt{\alpha}}^{x} \omega(s)\sqrt{\alpha - s^2}\, ds$$

Remark C. But generically it is not the same solution!
It is the same solution iff

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Proof of Proposition 1. ...p.3

...determines uniquely

$$\beta = \frac{2}{\pi} \int_{-\sqrt{\alpha}}^{\sqrt{\alpha}} \omega(s) \sqrt{\alpha - s^2}\, ds = \alpha + O(\alpha^2)$$

- If $V \in C^\omega$ then $\beta(\alpha) \in C^\omega$ for $|\alpha| < \delta_1$
- If $V \in C^\infty$ then $\beta(\alpha) \in C^\infty[0, \delta_1)$. Continue it $C^\infty(-\delta_1, \delta_1)$.

With this β we rewrite the equation

$$(\beta - y^2) \left(\frac{dy}{dx} \right)^2 = (\alpha - x^2) \omega(x)^2$$

in a contractive form as follows.

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In class C^ω: denote $y = \sqrt{\beta/\alpha}[x + (\alpha - x^2)w]$. Eq becomes

$$w = \frac{\alpha}{\beta}\, u(x;\alpha) + w^2 \int_0^1 \frac{(1-\sigma)[x + (\alpha - x^2)w\sigma]}{\sqrt{1 - 2xw\sigma + (x^2-\alpha)w^2\sigma^2}}\, d\sigma := \mathcal{N}(w)$$

where ($u(x,\alpha)$ takes on the burden of proving regularity!, $\int$ super-regular)

$$u(x;\alpha) = (\alpha - x^2)^{-3/2} \int_{-\sqrt{\alpha}}^{x} [\omega(s) - \gamma^{-1}]\sqrt{\alpha - s^2}\, ds \qquad (\gamma = \frac{\alpha}{\beta})$$

Note: $u(x;\alpha) \in C^\omega(\text{polydisk} \setminus (0,0))$ (for our $\beta(\alpha)$!), bc. solves

$$(\alpha - x^2)u' - 3xu = \omega(x) - \gamma^{-1}$$

Hartog's extension thm.: C^ω(polydisk)!
Then show $\mathcal{N}(w)$ is contractive $\rightsquigarrow$ sol. an. in polydisk. Q.E.D.

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Proof of Proposition 1. ...p.5 C^∞ case.

In class C^∞: would like a similar argument, but what is, for $\alpha < 0$,

$$u(x;\alpha) = (\alpha - x^2)^{-3/2} \int_{-\sqrt{\alpha}}^{x} [\omega(s) - \gamma^{-1}]\sqrt{\alpha - s^2}\, ds$$

Inspired by the values on $\mathbb{R}$ in the C^ω case, we should define $u(x;\alpha) =$

$$(\alpha - x^2)^{-\frac{3}{2}} \int_{\pm\sqrt{\alpha}}^{x} ds\, [\omega(s) - \gamma^{-1}]\sqrt{\alpha - s^2}, \qquad -\sqrt{\alpha} < x < \sqrt{\alpha}$$

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$$-(x^2 - \alpha)^{-\frac{3}{2}} \left\{\gamma^{-1}\phi_\omega(\alpha) + \int_0^x ds\, [\omega(s) - \gamma^{-1}]\sqrt{s^2 - \alpha}\right\}, \qquad \alpha \leqslant 0$$

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Proof of Proposition 1. ...p.6 C^∞ case.

In the C^ω case, by analytic cont. in α from $\alpha > 0$ to $\alpha < 0$:

$$u(x;\alpha) = -(x^2-\alpha)^{-\frac{3}{2}} \left\{ \gamma^{-1}\phi_\omega(\alpha) + \int_0^x ds \, [\omega(s) - \gamma^{-1}] \sqrt{s^2-\alpha} \right\}$$

where

$$\phi_\omega(\alpha) = i\alpha\gamma \int_0^1 \omega_{\text{odd}}(it\sqrt{-\alpha}) \sqrt{1-t^2}\, dt$$

Q: How do we define $i\omega_{\text{odd}}(it\sqrt{-\alpha})$ if $\omega \in C^\infty(\mathbb{R})$ only?

I.e., for $\alpha < 0$ define $i\omega_{\text{odd}}(ix)$!

Define $i\omega_{\text{odd}}(ix)$ for $\omega \in C^\infty(-\delta, \delta)$:

- $\omega_{\text{odd}}(x) = x\tilde{\omega}_{\text{even}}(x) = xg_\omega(x^2)$ where $g_\omega \in C^\infty([0, \delta^2])$
- Take g^c_ω any $C^\infty(-\delta^2, \delta^2)$ continuation of g_ω
- Define $\omega_{\text{odd}}(ix) = ixg^c_\omega(-x^2)$ which is in $C^\infty([-\delta, \delta])$.
- Note: $i\omega_{\text{odd}}(ix) \in \mathbb{R}$
- The Taylor coeff. at $x = 0$ of ϕ_ω are explicit and this is all we need (as we will see).

Proof of Proposition 1. ...p.8 C^∞ case.

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- $u(x;\alpha) := \mathcal{J}_\alpha(\omega - \gamma^{-1})$ with $\mathcal{J}_\alpha$=integral op.
- Note: $\mathcal{J}_\alpha$(Chebyshev polyn.)=Gegenbauer polyn.

$$C^{(2)}_{n-1}\left(\frac{x}{\sqrt{\alpha}}\right) = \frac{-n(n+2)}{2}\sqrt{\alpha}\,\mathcal{J}_\alpha\left[U_n\left(\frac{x}{\sqrt{\alpha}}\right)\right]$$

- Approximate $\omega(x) - \gamma^{-1} = \text{Taylor}_N(x,\alpha) + R_N(x)$.
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Proof of Theorem 2.

Theorem 2 is:

$$\underbrace{\psi_2''(y) = \frac{\beta - y^2}{\hbar^2}\psi_2(y)}_{\text{Weber eq.}} + \underbrace{f(y)\psi_2(y)}_{\text{perturbation}}$$

perturbed Weber is equivalent to Weber $\phi''(y) = \frac{\beta - y^2}{\hbar^2}\phi(y)$.

Done by showing that for a fd. system of solutions $\psi_2^{1,2}$:

$$\begin{bmatrix} \psi_2^{1,2} \\ \psi_2^{1,2\,\prime} \end{bmatrix} = \begin{bmatrix} \phi^{1,2} \\ \phi^{1,2\,\prime} \end{bmatrix} (I + \hbar\, E(y;\beta,\hbar))$$

where the error $E(y;\beta,\hbar)$ is of class C^v and satisfies

$$\|\partial_y^k \partial_\beta^j E\| \leqslant \begin{cases} C_{k,j}\,\langle y\rangle^{-k}\hbar^{-j} & \text{if } \hbar/|\beta| \lesssim 1 \\ \ln(\hbar^{-1})\quad C_{k,j}\,\langle y\rangle^{-k}\hbar^{-j} & \text{if } \hbar/|\beta| \gg 1 \end{cases}$$

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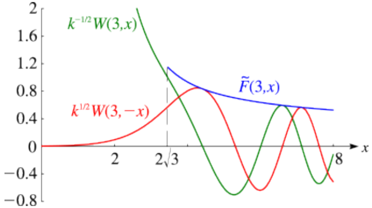
Modified Parabolic Cylinder Functions

Modified Parabolic Cylinder Functions: $\phi''(y) = \frac{\beta - y^2}{\hbar^2}\phi(y)$
Figure *NIST, Digital Libr. of Spec. Func.*

For $\beta > 0$
eq. has two turning points: $\pm\sqrt{\beta}$.



- For $y > \sqrt{\beta}$: oscillatory character
- For $|y| < \sqrt{\beta}$: exponential character
- Study perturbation for $y \geqslant \sqrt{\beta}$, for $y \in (-\epsilon, \sqrt{\beta}]$, matching at $y = \sqrt{\beta}$
- Similar solutions for $y < 0$. Matching at $y = 0 \rightsquigarrow$ monodromy.
- Works only for $\hbar/\beta \lesssim 1$.

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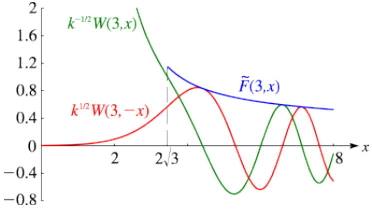

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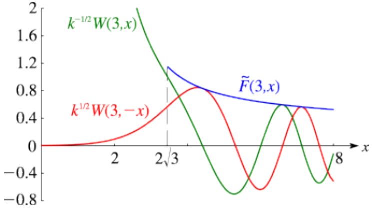

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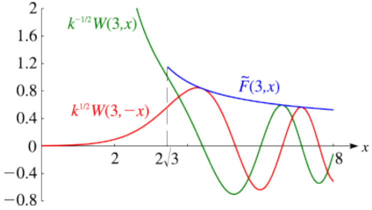

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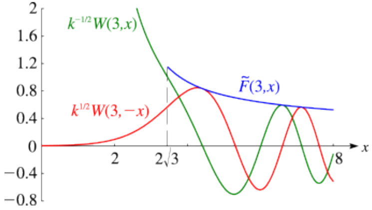

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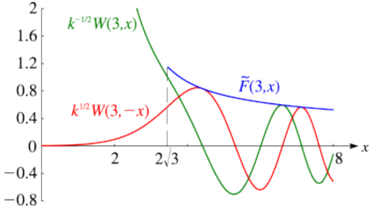

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Proof of Theorem 2: a few technical remarks

For $\hbar/\beta \lesssim 1$:

- Olver ('59) approximation from $+\infty$ and through one turning point, and beyond 0, using Airy functions. (But with additive errors.)
- We turn the perturbed Weber into an integral equation, then use Voltera iterations and lemmas from Costin, O., Donninger, R., Schlag, W., Tanveer, S. *Semiclassical low energy scattering for one-dimensional Schrödinger operators with exponentially decaying potentials*. Ann. Henri Poincaré 13 (2012).

For $\hbar/|\beta| \gg 1$:

The approach above does not apply.

WKB is very involved.

We turn the differential equation into an *integral eq. with a kernel involving modified parabolic cylinder functions* and show it is contractive on $[0, +\infty)$.

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Equivalence for $\hbar/|\beta| \gg 1$:

A few steps below.

Rescale: $y = x\sqrt{\hbar/2}$, $\psi_2(y) = \psi(x\sqrt{\hbar/2}) = u(x)$, $a = \beta/(2\hbar)$ to get

$$\underbrace{u(x)'' = \left(a - \frac{x^2}{4}\right) u(x)}_{\text{Weber eq.}} + \underbrace{\frac{\hbar}{2} f\left(x\sqrt{\hbar/2}\right) u(x)}_{\text{perturbation}} \qquad (2)$$

Approximate solutions by the complex sol. of Weber eq.: $E(a, x)$, $E^*(a, x)$.

Theorem

Let $x \geqslant 0$, $\hbar/|\beta| \gg 1$. *Perturbed Weber eq. has two independent solutions* $u_E(x), u_E^*(x)$

$$u_E(x) = E\,(a,x)\,(1 + e(x;\hbar,\beta)),\;\; u_E^*(x) = E^*\,(a,x)\,(1 + e^*(x;\hbar,\beta)) \quad (3)$$

$$\begin{aligned} |\partial_x^{k+1}\partial_\beta^\ell e(x;\hbar,\beta)| &\lesssim x^{-3-k}\hbar^{-\ell} < x^{-1-k}\hbar^{-\ell+1} && \textit{for } x > \sqrt{2/\hbar} \\ |\partial_x^{k+1}\partial_\beta^\ell e(x;\hbar,\beta)| &\lesssim x^{-1-k}\hbar^{-\ell+1} && \textit{for } x \in [\sqrt{2}, \sqrt{2/\hbar}] \\ |\partial_x^{k+1}\partial_\beta^\ell e(x;\hbar,\beta)| &\lesssim \hbar^{-\ell+1} && \textit{for } x \in [0, \sqrt{2}] \end{aligned} \quad (4)$$

(uniform errors, behaving like a symbol)

Technique of the proof:

Contractive argument:

$$e(x) = \int_\infty^x \frac{1}{E(a,s)^2} \int_\infty^s \frac{\hbar}{2} f(t\sqrt{\hbar/2})\, E(a,t)^2\, (1 + e(t))\, dt\, ds$$

change order of $\int\int$ and use $\left(\frac{E^*}{E}\right)' = \frac{W[E,E^*]}{E^2} = \frac{-2i}{E^2}$ to get

$$e(x) = \frac{i\hbar}{4} \int_\infty^x (1+e(t))\, f(t\sqrt{\hbar/2}) \left(|E(a,t)|^2 - E(a,t)^2 \frac{E^*(a,x)}{E(a,x)}\right) dt =: J[e](x$$

Known estimates for $E(a,x)$ were improved to show symbol behavior, then we proved contraction.
Then inductively, contraction for all derivatives of $e(x)$. Q.E.D.

Conclusions

Scattering for energies near the top of the barrier of the potential is well approximated by the one for a quadratic potential, and the latter can be calculated explicitly.

Having obtained multiplicative errors behaving like a symbol, the quantities can now be used in further calculations.

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Thank You!