Introduction to Semiclassical Asymptotic Analysis: Lecture 1

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Motivating Semiclassical Analysis for Dispersive Waves



3 Nonlinear Problems: The Defocusing Nonlinear Schrödinger Equation as a Case Study

Zabusky and Kruskal's experiment (1965) for the Korteweg-de Vries (KdV) equation

$$u_t + uu_x + \frac{2}{3}u_{xxx} = 0, \quad u(x,0) = 1 + \cos(\pi x/20).$$



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The formation of the "undular bore" becomes much more distinct if the dispersion parameter 2/3 is replaced with a smaller number. Here is a snapshot at t = 0.4 from the solution of the initial-value problem

$$u_t + 6uu_x + 10^{-4}u_{xxx} = 0, \quad u(x,0) = -\operatorname{sech}^2(x).$$



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[Figure taken from a paper of Claeys and Grava.]

Quantifying multiscale phenomena in dispersive wave propagation.

We observe:

- The solutions of typical initial-value problems for KdV have undeniable features including
 - Intervals where the solution is slowly-varying,
 - Intervals where the solution resembles a slowly-varying train of more rapid oscillations, and
 - Moving transitional regions separating the above.
- These features become "sharper" as the dispersion parameter become smaller for fixed initial data. They may be well-defined as suitable mathematical limits as the dispersion parameter tends to zero.

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Similar phenomena occur for other dispersive equations as well...

Another example: the initial-value problem for $u^{\epsilon} = u^{\epsilon}(x, t)$ solving the *sine-Gordon equation*:

$$\epsilon^2 u_{tt}^{\epsilon} - \epsilon^2 u_{xx}^{\epsilon} + \sin(u^{\epsilon}) = 0, \quad x \in \mathbb{R}, \quad t > 0,$$
$$u^{\epsilon}(x, 0) = F(x), \qquad \epsilon u_t^{\epsilon}(x, 0) = G(x).$$

Here $\epsilon > 0$ is a parameter, and *F* and *G* are independent of ϵ . Interesting features of u^{ϵ} become better-resolved as $\epsilon \to 0$ for fixed *F* and *G*...

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Quantifying multiscale phenomena in dispersive wave propagation.

The initial data is $F(x) \equiv 0$ and $G(x) = -3 \operatorname{sech}(x)$ with $\epsilon = 0.1875$.



Quantifying multiscale phenomena in dispersive wave propagation.

The initial data is $F(x) \equiv 0$ and $G(x) = -3 \operatorname{sech}(x)$ with $\epsilon = 0.09375$.



Quantifying multiscale phenomena in dispersive wave propagation.

The initial data is $F(x) \equiv 0$ and $G(x) = -3 \operatorname{sech}(x)$ with $\epsilon = 0.046875$.



Quantifying multiscale phenomena in dispersive wave propagation.

Another example...



The focusing nonlinear Schrödinger equation for $\psi^{\epsilon} = \psi^{\epsilon}(x, t)$:

$$i\epsilon\psi_t^{\epsilon} + \frac{\epsilon^2}{2}\psi_{xx}^{\epsilon} + |\psi^{\epsilon}|^2\psi^{\epsilon} = 0, \quad \psi^{\epsilon}(x,0) = 2\operatorname{sech}(x), \quad \epsilon = 0.4.$$

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Quantifying multiscale phenomena in dispersive wave propagation.

Another example...



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$$i\epsilon\psi_t^{\epsilon} + \frac{\epsilon^2}{2}\psi_{xx}^{\epsilon} + |\psi^{\epsilon}|^2\psi^{\epsilon} = 0, \quad \psi^{\epsilon}(x,0) = 2\operatorname{sech}(x), \quad \epsilon = 0.2.$$

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Quantifying multiscale phenomena in dispersive wave propagation.

Another example...



The focusing nonlinear Schrödinger equation for $\psi^{\epsilon} = \psi^{\epsilon}(x, t)$:

$$i\epsilon\psi_t^{\epsilon} + \frac{\epsilon^2}{2}\psi_{xx}^{\epsilon} + |\psi^{\epsilon}|^2\psi^{\epsilon} = 0, \quad \psi^{\epsilon}(x,0) = 2\operatorname{sech}(x), \quad \epsilon = 0.1.$$

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Quantifying multiscale phenomena in dispersive wave propagation.

Another example...



The focusing nonlinear Schrödinger equation for $\psi^{\epsilon} = \psi^{\epsilon}(x, t)$:

$$i\epsilon\psi_t^\epsilon + rac{\epsilon^2}{2}\psi_{xx}^\epsilon + |\psi^\epsilon|^2\psi^\epsilon = 0, \quad \psi^\epsilon(x,0) = 2\operatorname{sech}(x), \quad \epsilon = 0.05.$$

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This phenomenon is not only present in nonlinear systems. Consider the free-particle (linear) Schrödinger equation

$$i\epsilon\psi_t^\epsilon + \frac{\epsilon^2}{2}\psi_{xx}^\epsilon = 0, \quad \psi^\epsilon(x,0) = \psi_0^\epsilon(x) = \sqrt{\rho_0(x)}e^{iS(x)/\epsilon}, \quad S(x) := \int_0^x u_0(y)\,dy.$$

Here we may consider $\rho_0 : \mathbb{R} \to \mathbb{R}_+$ and $u_0 : \mathbb{R} \to \mathbb{R}$ as fixed and consider what happens as ϵ varies.

This example motivates the terminology "semiclassical limit" for the asymptotic behavior as $\epsilon \to 0$.

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For the linear Schrödinger equation...

Plots of $|\psi^{\epsilon}(x,t)|^2$ for $u_0(x) = -8 \operatorname{sech}^2(x) \tanh(x)$ and $\rho_0(x) = 4 \operatorname{sech}^4(x)$:



 $\epsilon = 0.2$



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What gives rise to semiclassical phenomena? How can we calculate?

The initial-value problem for the linear Schrödinger equation can be solved by the Fourier/Inverse-Fourier transform pair.

• Direct transform:
$$\hat{\psi}_0^{\epsilon}(\lambda) := \frac{1}{2\pi} \int_{\mathbb{R}} \psi_0^{\epsilon}(x) e^{2i\lambda x/\epsilon} dx.$$

2 Time evolution (from taking the direct transform of the Schrödinger equation): $\hat{\psi}^{\epsilon}(\lambda, t) = e^{-2i\lambda^2 t/\epsilon} \hat{\psi}_0^{\epsilon}(\lambda)$.

3 Inverse transform:
$$\psi^{\epsilon}(x,t) = \frac{2}{\epsilon} \int_{\mathbb{R}} \hat{\psi}^{\epsilon}(\lambda,t) e^{-2i\lambda x/\epsilon} d\lambda.$$

Each step involves ϵ in a singular way. Alternately, by carefully exchanging the order of integration in the resulting double integral formula, the problem can also be solved using Green's function:

$$\psi^{\epsilon}(x,t) = \frac{e^{-i\pi/4}}{\sqrt{2\pi\epsilon t}} \int_{\mathbb{R}} e^{iI(\xi;x,t)/\epsilon} \sqrt{\rho_0(\xi)} \, d\xi, \quad t > 0, \quad \text{where}$$
$$I(\xi;x,t) := S(\xi) + \frac{(\xi - x)^2}{2t}$$

What gives rise to semiclassical phenomena? How can we calculate?

Use the *method of stationary phase* to analyze the integral as $\epsilon \downarrow 0$:

$$\psi^{\epsilon}(x,t) = \frac{1}{\sqrt{t}} \sum_{n=0}^{2P} \frac{e^{i\pi((-1)^n - 1)/4}}{\sqrt{|I''(\xi_n; x, t)|}} \sqrt{\rho_0(\xi_n)} e^{iI(\xi_n; x, t)/\epsilon} + \mathcal{O}(\epsilon)$$

where $\xi_n = \xi_n(x, t)$, and $\xi_0 < \xi_1 < \cdots < \xi_{2P}$ are the *stationary phase points*, that is, the roots (assumed simple) of $I'(\xi; x, t) = 0$. Note that

$$I'(\xi; x, t) = u_0(\xi) + \frac{\xi - x}{t} = 0 \quad \Leftrightarrow \quad x = u_0(\xi)t + \xi$$

is the equation for intercepts ξ of characteristics through (x, t) for the formal limit of the Madelung system ($\rho^{\epsilon} := |\psi^{\epsilon}|^2$ and $u^{\epsilon} := \epsilon \operatorname{Im}(\psi_x^{\epsilon}/\psi^{\epsilon})$)

$$\rho_t^{\epsilon} + (\rho^{\epsilon} u^{\epsilon})_x = 0, \quad u_t^{\epsilon} + u^{\epsilon} u_x^{\epsilon} = \frac{\epsilon^2}{2} \left[\frac{\rho_{xx}^{\epsilon}}{2\rho^{\epsilon}} - \left(\frac{\rho_x^{\epsilon}}{2\rho^{\epsilon}} \right)^2 \right].$$

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What gives rise to semiclassical phenomena? How can we calculate?

Here are the characteristic lines in the case $u_0(x) = -8 \operatorname{sech}^2(x) \tanh(x)$:



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What gives rise to semiclassical phenomena? How can we calculate?

The stationary phase formula tells us the following. There is a critical time $t = t_c$ such that:

- If *t* < *t_c* then there is just one characteristic line through each point and hence just one term in the sum. Thus ψ^ϵ(*x*, *t*) looks like a modulated plane wave.
- If $t > t_c$ then there are *caustic curves* $x = x^{\pm}(t)$ with $x^{\pm}(t_c) = x_c$ such that
 - If x < x[−](t) or x > x⁺(t) then there is again just one characteristic through each point and again ψ^ϵ(x, t) looks like a modulated plane wave.
 - If x⁻(t) < x < x⁺(t) then there are *three* lines through each point and hence three terms in the sum. There are three interfering terms in ψ^ε(x, t), and |ψ^ε(x, t)|² becomes highly oscillatory.

The asymptotically abrupt transitions in the (x, t)-plane arise as bifurcation points for characteristics or stationary phase points.

What about nonlinear problems?

Similar precision of analysis is available in principle for nonlinear dispersive wave problems that are integrable by a direct/inverse-scattering transform:

- In place of the Fourier transform of the initial data, we have instead the *direct scattering transform*. Usually requires the analysis of a linear ODE (or PDE) with a *spectral parameter* to obtain scattering data (one or more functions of the spectral parameter).
- Just as in the linear theory, one has explicit exponential evolution of the scattering data in time *t*.
- In place of the inverse-Fourier transform of the time-evolved transform data, one has the *inverse-scattering transform*. Usually requires the solution of a linear Riemann-Hilbert problem (or ∂ problem).

The Defocusing Nonlinear Schrödinger Equation

Let's illustrate these steps in a bit more detail for the defocusing nonlinear Schrödinger equation

$$i\epsilon\psi_t^{\epsilon} + \frac{\epsilon^2}{2}\psi_{xx}^{\epsilon} - |\psi^{\epsilon}|^2\psi^{\epsilon} = 0, \ \psi^{\epsilon}(x,0) = \sqrt{\rho_0(x)}e^{iS(x)/\epsilon}, \ S(x) := \int_0^x u_0(y)\,dy.$$

The PDE is the compatibility condition for the two linear problems ($\lambda \in \mathbb{C}$ is the spectral parameter):

$$\begin{aligned} \boldsymbol{\epsilon} \frac{\partial \mathbf{w}}{\partial x} &= \mathbf{U}\mathbf{w}, \quad \mathbf{U} = \mathbf{U}(x, t, \lambda) := \begin{bmatrix} -i\lambda & \psi^{\epsilon} \\ \psi^{\epsilon *} & i\lambda \end{bmatrix} \\ \boldsymbol{\epsilon} \frac{\partial \mathbf{w}}{\partial t} &= \mathbf{V}\mathbf{w}, \quad \mathbf{V} = \mathbf{V}(x, t, \lambda) := \begin{bmatrix} -i\lambda^2 - i\frac{1}{2}|\psi^{\epsilon}|^2 & \lambda\psi^{\epsilon} + i\frac{1}{2}\epsilon\psi^{\epsilon}_x \\ \lambda\psi^{\epsilon *} - i\frac{1}{2}\epsilon\psi^{\epsilon *}_x & i\lambda^2 + i\frac{1}{2}|\psi^{\epsilon}|^2 \end{bmatrix}. \end{aligned}$$

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The Defocusing Nonlinear Schrödinger Equation

Formal semiclassical limit

Introducing real variables (Madelung, 1926)

$$\rho^{\epsilon} := |\psi^{\epsilon}|^2 \text{ and } u^{\epsilon} := \Im\left\{\frac{\epsilon\psi^{\epsilon}_x}{\psi^{\epsilon}}\right\} \implies \rho^{\epsilon}(x,0) = \rho_0(x) \text{ and } u^{\epsilon}(x,0) = u_0(x),$$

one can check that the defocusing nonlinear Schrödinger equation for ψ^{ϵ} implies the following closed system of equations on ρ^{ϵ} and u^{ϵ} :

$$\frac{\partial \rho^{\epsilon}}{\partial t} + \frac{\partial}{\partial x}(\rho^{\epsilon}u^{\epsilon}) = 0 \quad \text{and} \quad \frac{\partial u^{\epsilon}}{\partial t} + \frac{\partial}{\partial x}\left(\frac{1}{2}u^{\epsilon^2} + \rho^{\epsilon}\right) = \frac{1}{2}\epsilon^2 \frac{\partial F[\rho^{\epsilon}]}{\partial x}$$

where $F[\rho]$ denotes the expression

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ho}{\partial x^2} - \left(rac{1}{2
ho} rac{\partial
ho}{\partial x}
ight)^2.$$

Neglecting $\epsilon^2 F_x$ leads to a closed, ϵ -independent hyperbolic system governing expected limits ρ and u, the *dispersionless defocusing NLS* system.

The Defocusing Nonlinear Schrödinger Equation Direct Scattering Transform: $R_0^{\epsilon} = \mathscr{S}(\psi_0^{\epsilon})$

We need to calculate the Jost solution w of the linear equation

$$\epsilon \frac{d\mathbf{w}}{dx} = \begin{bmatrix} -i\lambda & \sqrt{\rho_0(x)}e^{iS(x)/\epsilon} \\ \sqrt{\rho_0(x)}e^{-iS(x)/\epsilon} & i\lambda \end{bmatrix} \mathbf{w},$$

that is, the solution for $\lambda \in \mathbb{R}$ that is determined (assuming sufficiently rapid decay of ρ_0 for large |x|) by the conditions

$$\mathbf{w}(x) = \begin{bmatrix} e^{-i\lambda x/\epsilon} \\ 0 \end{bmatrix} + R_0^{\epsilon}(\lambda) \begin{bmatrix} 0 \\ e^{i\lambda x/\epsilon} \end{bmatrix} + o(1), \quad x \to +\infty$$

and

$$\mathbf{w}(x) = T_0^{\epsilon}(\lambda) \begin{bmatrix} e^{-i\lambda x/\epsilon} \\ 0 \end{bmatrix} + o(1), \quad x \to -\infty,$$

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for some coefficients $R_0^{\epsilon}(\lambda)$ (the *reflection coefficient*) and $T_0^{\epsilon}(\lambda)$ (the *transmission coefficient*).

The Defocusing Nonlinear Schrödinger Equation Inverse Scattering Transform: $\psi^{\epsilon} = \mathscr{S}^{-1}(e^{2i\lambda^2 t/\epsilon}R_0^{\epsilon})$

For the inverse transform, solve (for each fixed *x* and *t*) the following Riemann-Hilbert problem: seek $\mathbf{M} : \mathbb{C} \setminus \mathbb{R} \to SL(2, \mathbb{C})$ such that:

- Analyticity: M is analytic in each half-plane, and takes boundary values $M_{\pm} : \mathbb{R} \to SL(2, \mathbb{C})$ on the real line from \mathbb{C}_{\pm} .
- Jump Condition: The boundary values are related by

$$\mathbf{M}_{+}(\lambda) = \mathbf{M}_{-}(\lambda) \begin{bmatrix} 1 - |\mathbf{R}_{0}^{\boldsymbol{\epsilon}}(\lambda)|^{2} & -e^{-2i(\lambda x + \lambda^{2}t)/\boldsymbol{\epsilon}} \mathbf{R}_{0}^{\boldsymbol{\epsilon}}(\lambda)^{*} \\ e^{2i(\lambda x + \lambda^{2}t)/\boldsymbol{\epsilon}} \mathbf{R}_{0}^{\boldsymbol{\epsilon}}(\lambda) & 1 \end{bmatrix}, \ \lambda \in \mathbb{R}.$$

• Normalization: As $\lambda \to \infty$, $\mathbf{M}(\lambda) \to \mathbb{I}$.

The solution of the initial-value problem is given by

$$\psi^{\epsilon}(x,t) = 2i \lim_{\lambda \to \infty} \lambda M_{12}(\lambda).$$

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Recall the linear ODE for the Jost vector w:

$$\epsilon \frac{d\mathbf{w}}{dx} = \begin{bmatrix} -i\lambda & \sqrt{\rho_0(x)}e^{iS(x)/\epsilon} \\ \sqrt{\rho_0(x)}e^{-iS(x)/\epsilon} & i\lambda \end{bmatrix} \mathbf{w}.$$

The rapidly oscillatory factors in the coefficient matrix can be removed by a simple substitution:

$$\mathbf{w} = \begin{bmatrix} e^{iS(x)/(2\epsilon)} & 0\\ 0 & e^{-iS(x)/(2\epsilon)} \end{bmatrix} \mathbf{v} = e^{iS(x)\sigma_3/(2\epsilon)} \mathbf{v},$$

leading to

$$\epsilon \frac{d\mathbf{v}}{dx} = \begin{bmatrix} -i(\lambda + \frac{1}{2}u_0(x)) & \sqrt{\rho_0(x)} \\ \sqrt{\rho_0(x)} & i(\lambda + \frac{1}{2}u_0(x)) \end{bmatrix} \mathbf{v}$$

because $S'(x) = u_0(x)$.

Semiclassical Approximation of R_0^{ϵ} The WKB Method

If we try to treat the terms proportional to $\epsilon \ll 1$ as a perturbation, we are led to consider the approximate equation:

$$\begin{bmatrix} -i(\lambda + \frac{1}{2}u_0(x)) & \sqrt{\rho_0(x)} \\ \sqrt{\rho_0(x)} & i(\lambda + \frac{1}{2}u_0(x)) \end{bmatrix} \mathbf{v} \approx \mathbf{0}.$$

Unless the determinant of the coefficient matrix is zero, i.e.,

$$(\lambda + \frac{1}{2}u_0(x))^2 = \rho_0(x),$$

there is no nontrivial solution. This suggests that, away from exceptional points, $d\mathbf{v}/dx$ must be large, proportional to ϵ^{-1} . As the equation is linear, nothing is gained by simply scaling \mathbf{v} by ϵ^{-1} , but $d\mathbf{v}/dx$ can be made large compared to \mathbf{v} by an exponential substitution:

 $\mathbf{v} = e^{f/\epsilon}\mathbf{u}$ for some scalar function $f(x, \lambda)$ to be determined.

Given f, the substitution implies a linear equation for **u**:

$$\epsilon \frac{d\mathbf{u}}{dx} = \begin{bmatrix} -i(\lambda + \frac{1}{2}u_0(x)) - f_x(x,\lambda) & \sqrt{\rho_0(x)} \\ \sqrt{\rho_0(x)} & i(\lambda + \frac{1}{2}u_0(x)) - f_x(x,\lambda) \end{bmatrix} \mathbf{u}.$$

The main idea of the WKB method is to choose *f* so that the modified coefficient matrix is singular, leading to the possibility that **u** may vary slowly, on the scale of *x*. That is, $f_x(x, \lambda)$ should be an eigenvalue of the coefficient matrix

$$\mathbf{H}(x,\lambda) := \begin{bmatrix} -i(\lambda + \frac{1}{2}u_0(x)) & \sqrt{\rho_0(x)} \\ \sqrt{\rho_0(x)} & i(\lambda + \frac{1}{2}u_0(x)) \end{bmatrix}$$

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and, to leading order, u should be a corresponding eigenvector of H.

The exact equation for **u** is

$$\epsilon \frac{d\mathbf{u}}{dx} = (\mathbf{H}(x,\lambda) - f_x(x,\lambda)\mathbb{I})\mathbf{u}$$

and the WKB method is to seek \mathbf{u} in the form of an asymptotic series

$$\mathbf{u} \sim \mathbf{u}_0(x,\lambda) + \epsilon \mathbf{u}_1(x,\lambda) + \epsilon^2 \mathbf{u}_2(x,\lambda) + \cdots, \quad \epsilon \to 0.$$

Substituting this series and equating the terms proportional to the same powers of ϵ leads to the leading-order equation

$$(\mathbf{H}(x,\lambda) - f_x(x,\lambda)\mathbb{I})\mathbf{u}_0(x,\lambda) = \mathbf{0}$$

and the infinite hierarchy of equations for subsequent corrections:

$$(\mathbf{H}(x,\lambda) - f_x(x,\lambda)\mathbb{I})\mathbf{u}_n(x,\lambda) = \frac{d\mathbf{u}_{n-1}}{dx}(x,\lambda), \quad n \ge 1.$$

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Semiclassical Approximation of R_0^{ϵ} The WKB Method

The formalism of the WKB method consists of the following steps:

Fix *f_x(x, λ)* to be an eigenvalue of **H**(*x, λ*) that is smooth as a function of *x* in an interval of interest. The characteristic equation is:

$$f_x(x,\lambda)^2 = \rho_0(x) - (\lambda + \frac{1}{2}u_0(x))^2.$$

This makes $\mathbf{H}(x, \lambda) - f_x(x, \lambda)\mathbb{I}$ a rank one matrix. Its nullspace is spanned by $(M(x, \lambda))$ is an arbitrary nonzero scalar)

$$\mathbf{y}(x,\lambda) := \frac{1}{M(x,\lambda)} \begin{bmatrix} f_x(x,\lambda) - i(\lambda + \frac{1}{2}u_0(x)) \\ \sqrt{\rho_0(x)} \end{bmatrix}$$

and its range is spanned by ($N(x, \lambda)$ is an arbitrary nonzero scalar)

$$\mathbf{z}(x,\lambda) := \frac{1}{N(x,\lambda)} \begin{bmatrix} -f_x(x,\lambda) - i(\lambda + \frac{1}{2}u_0(x)) \\ \sqrt{\rho_0(x)} \end{bmatrix}.$$

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The WKB Method

Pind u₀:

- Solve the leading-order equation by u₀(x, λ) = c₀(x, λ)y(x, λ) for some scalar function c₀ to be determined.
- Ensure the solvability of the next equation in the hierarchy by imposing

$$\det\left(\frac{d\mathbf{u}_0}{dx}(x,\lambda),\mathbf{z}(x,\lambda)\right) = 0$$

This is a linear first-order equation for the scalar $c_0(x, \lambda)$:

$$\frac{dc_0}{dx}(x,\lambda) + \frac{\det\left(\mathbf{y}_x(x,\lambda),\mathbf{z}(x,\lambda)\right)}{\det\left(\mathbf{y}(x,\lambda),\mathbf{z}(x,\lambda)\right)}c_0(x,\lambda) = 0$$

The WKB Method

- Supposing \mathbf{u}_{n-1} is known, find \mathbf{u}_n :
 - The equation $(\mathbf{H}(x,\lambda) f_x(x,\lambda)\mathbb{I})\mathbf{u}_n(x,\lambda) = \mathbf{u}_{n-1,x}(x,\lambda)$ is solvable by construction. Its general solution has the form

$$\mathbf{u}_n(x,\lambda) = \mathbf{u}_n^{(\mathrm{p})}(x,\lambda) + c_n(x,\lambda)\mathbf{y}(x,\lambda)$$

where $\mathbf{u}_n^{(p)}(x, \lambda)$ is any particular solution (chosen to depend smoothly on *x*) and where $c_n(x, \lambda)$ is a scalar to be determined.

Ensure the solvability of the next equation in the hierarchy by imposing the condition

$$\det\left(\frac{d\mathbf{u}_n}{dx}(x,\lambda),\mathbf{z}(x,\lambda)\right) = 0,$$

which is a linear equation for $c_n(x, \lambda)$:

$$\frac{dc_n}{dx}(x,\lambda) + \frac{\det(\mathbf{y}_x(x,\lambda),\mathbf{z}(x,\lambda))}{\det(\mathbf{y}(x,\lambda),\mathbf{z}(x,\lambda))}c_n(x,\lambda) = -\frac{\det(\mathbf{u}_{n,x}^{(p)}(x,\lambda),\mathbf{z}(x,\lambda))}{\det(\mathbf{y}(x,\lambda),\mathbf{z}(x,\lambda))}.$$

Oscillatory and exponential intervals

The nature of the WKB approximation (obtained by truncating the series for **u** at some order) is determined by the sign of $f_x(x, \lambda)^2$. Given $\lambda \in \mathbb{R}$:

- In *x*-intervals where $(\lambda + \frac{1}{2}u_0(x))^2 > \rho_0(x)$, we have $f_x^2 < 0$, so up to a λ -dependent factor, *f* is purely imaginary. This means that the solutions are rapidly oscillatory, and $|e^{\pm f/\epsilon}|$ is independent of *x*.
- In *x*-intervals where $(\lambda + \frac{1}{2}u_0(x))^2 < \rho_0(x)$, we have $f_x^2 > 0$, so up to a λ -dependent factor, *f* is real. This means that the solutions are either exponentially growing or decaying, very rapidly for small ϵ .

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We call the two types of intervals *oscillatory* and *exponential* intervals respectively.

Turning points

Oscillatory intervals abut exponential intervals at *turning points* where $(\lambda + \frac{1}{2}u_0(x))^2 = \rho_0(x)$ and hence $\mathbf{H}(x, \lambda)$ is singular with degenerate eigenvalues. This information can be summarized in a picture:



Here $\alpha(x) := -\frac{1}{2}u_0(x) - \sqrt{\rho_0(x)}$ and $\beta(x) := -\frac{1}{2}u_0(x) + \sqrt{\rho_0(x)}$. For simplicity, we assume that there are at most two turning points $x_-(\lambda) \le x_+(\lambda)$.

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Above barrier reflection

Unless λ lies in the interval $[\lambda_-, \lambda_+] := [\min_x \alpha(x), \max_x \beta(x)]$, there are *no* turning points at all, and all of \mathbb{R} is an oscillatory interval. Suppose that $\lambda > \lambda_+$. Take f_x to be strictly negative imaginary and integrate:

$$f(x,\lambda) = -i \int_0^x \sqrt{(\lambda + \frac{1}{2}u_0(y))^2 - \rho_0(y)} \, dy$$
, (positive root).

Fix the normalizing factors M and N as follows (positive square roots):

$$M(x,\lambda) := i\sqrt{2if_x(x,\lambda)(\lambda + \frac{1}{2}u_0(x)) - 2f_x(x,\lambda)^2}$$
$$N(x,\lambda) := \sqrt{2if_x(x,\lambda)(\lambda + \frac{1}{2}u_0(x)) + 2f_x(x,\lambda)^2}.$$

It follows from the characteristic equation that $\mathbf{y}^{\mathsf{T}}\mathbf{y} = 1$, $\mathbf{z}^{\mathsf{T}}\mathbf{z} = 1$ and $\mathbf{y}^{\mathsf{T}}\mathbf{z} = 0$. Hence if $\mathbf{K} := (\mathbf{y}, \mathbf{z})$, then $\mathbf{K}^{-1} = \mathbf{K}^{\mathsf{T}}$.

Above barrier reflection

Differentiating the identity $\mathbf{K}^{-1}\mathbf{K} = \mathbb{I}$ with respect to *x* gives

$$\frac{d\mathbf{K}^{-1}}{dx}\mathbf{K} + \mathbf{K}^{-1}\frac{d\mathbf{K}}{dx} = \mathbf{0}.$$

Since $\mathbf{K}^{-1} = \mathbf{K}^{\mathsf{T}}$, $\mathbf{K}^{-1}\mathbf{K}_{x}$ is skew-symmetric, and therefore

$$0 = (\mathbf{K}^{-1}\mathbf{K}_x)_{11} = \frac{\det(\mathbf{y}_x, \mathbf{z})}{\det(\mathbf{y}, \mathbf{z})}.$$

The differential equation for $c_0(x, \lambda)$ therefore dramatically simplifies, having general solution $c_0 = c_0(\lambda)$.

In the absence of turning points, the uniform accuracy of the WKB approximation for $x \in \mathbb{R}$ can be justified rigorously, and the Jost solution has the form

$$\mathbf{w}(x,\lambda) = c_0(\lambda)e^{iS(x)\sigma_3/(2\epsilon)}e^{f(x,\lambda)/\epsilon}\mathbf{y}(x,\lambda) + O(\epsilon).$$

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Above barrier reflection

A direct calculation gives:

$$\lim_{x \to \pm \infty} e^{i\lambda x/\epsilon} \cdot e^{iS(x)\sigma_3/(2\epsilon)} e^{f(x,\lambda)/\epsilon} \mathbf{y}(x,\lambda) = \exp\left(\frac{i}{\epsilon} \int_0^{\pm \infty} \left[\lambda + \frac{1}{2}u_0(y) - \sqrt{(\lambda + \frac{1}{2}u_0(y))^2 - \rho_0(y)}\right] dy\right) \begin{bmatrix} -1\\0 \end{bmatrix}$$

Therefore, taking

$$c_0(\lambda) := -\exp\left(-\frac{i}{\epsilon}\int_0^{+\infty} \left[\lambda + \frac{1}{2}u_0(y) - \sqrt{(\lambda + \frac{1}{2}u_0(y))^2 - \rho_0(y)}\right] dy\right),$$

the Jost solution satisfies

$$\mathbf{w}(x,\lambda) = T_0^{\boldsymbol{\epsilon}}(\lambda) \begin{bmatrix} e^{-i\lambda x/\boldsymbol{\epsilon}} \\ 0 \end{bmatrix} + o(1), \quad x \to -\infty,$$

and

$$\mathbf{w}(x,\lambda) = \begin{bmatrix} e^{-i\lambda x/\epsilon} \\ 0 \end{bmatrix} + R_0^{\epsilon}(\lambda) \begin{bmatrix} 0 \\ e^{i\lambda x/\epsilon} \end{bmatrix} + o(1), \quad x \to +\infty, \quad \text{where}$$

Above barrier reflection

$$T_0^{\epsilon}(\lambda) = \exp\left(-\frac{i}{\epsilon} \int_{-\infty}^{+\infty} \left[\lambda + \frac{1}{2}u_0(y) - \sqrt{(\lambda + \frac{1}{2}u_0(y))^2 - \rho_0(y)}\right] dy\right) + O(\epsilon)$$

and

$$R_0^{\epsilon}(\lambda) = O(\epsilon).$$

Therefore, the reflection coefficient is small (of order ϵ) for $\lambda > \lambda_+$. Completely analogous calculations show that the same holds for $\lambda < \lambda_-$.

Going to higher order shows that (assuming ρ_0 and u_0 are smooth) $R_0^{\epsilon}(\lambda) = O(\epsilon^N)$ for arbitrary *N*. The reflection coefficient is small beyond all orders in absence of turning points.

Below barrier reflection and tunneling

Now let us assume that $\lambda_{-} < \lambda < \lambda_{+}$ so that there are precisely two turning points $x_{-}(\lambda) < x_{+}(\lambda)$, dividing \mathbb{R} into three intervals:

- *I*_− := (−∞, *x*_−(λ)), in which the WKB method predicts oscillatory solutions.
- *I*₀ := (*x*₋(λ), *x*₊(λ)), in which the WKB method predicts exponentially growing and decaying solutions.
- *I*₊ := (*x*₊(λ), +∞), in which the WKB method again predicts oscillatory solutions.



Below barrier reflection and tunneling

There are two essential issues to be addressed:

- For $x \in I_0$, the rigorous analysis of the WKB method is complicated by exponential amplification of errors. Small errors introduced at a point $x_0 \in I_0$ can only be controlled if the initial-value problem for the ODE is solved in the direction of exponential growth of the WKB approximation.
- 2 The WKB method fails entirely in neighborhoods of the two turning points, where f_x vanishes like a square root.

We will construct the scaled Jost solution $\mathbf{w}(x, \lambda)/T_0^{\epsilon}(\lambda)$ which is defined by the condition that

$$\frac{1}{T_0^{\boldsymbol{\epsilon}}(\lambda)}\mathbf{w}(x,\lambda) = \begin{bmatrix} e^{-i\lambda x/\boldsymbol{\epsilon}} \\ 0 \end{bmatrix} + o(1), \quad x \to -\infty.$$

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Below barrier reflection and tunneling

By our previous analysis we can show that the following is valid for $-\frac{1}{2}u_0(-\infty) < \lambda < \lambda_+$:

$$\frac{1}{T_0^{\epsilon}(\lambda)}\mathbf{w}(x,\lambda) = C^{\epsilon}(\lambda)e^{iS(x)\sigma_3/(2\epsilon)}e^{f_-(x,\lambda)/\epsilon}\mathbf{y}_-(x,\lambda) + O(\epsilon), \quad x \in I_-,$$

where:

•
$$|C^{\epsilon}(\lambda)| = 1$$
,
• $f_{-}(x,\lambda) = -i \int_{x_{-}(\lambda)}^{x} \sqrt{(\lambda + \frac{1}{2}u_{0}(y))^{2} - \rho_{0}(y)} \, dy$, (positive root),
• $\mathbf{y}_{-}(x,\lambda) = \frac{1}{M_{-}(x,\lambda)} \left[\frac{f_{-x}(x,\lambda) - i(\lambda + \frac{1}{2}u_{0}(x))}{\sqrt{\rho_{0}(x)}} \right]$, and
• $M_{-}(x,\lambda) = i\sqrt{2if_{-x}(x,\lambda)(\lambda + \frac{1}{2}u_{0}(x)) - 2f_{-x}(x,\lambda)^{2}}$, (positive root).
the error estimate of $O(\epsilon)$ holds pointwise in *x* and also uniformly on
py subinterval of *L*, bounded away from *x*_{-}(\lambda).

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Connection problems

For *x* in the other two intervals, I_0 and I_+ , we may expect that the same solution $\mathbf{w}(x, \lambda)/T_0^{\epsilon}(\lambda)$ is approximated by linear combinations of WKB solutions (exponential character in I_0 and oscillatory character in I_+). But to obtain the coefficients in these linear combinations, we must somehow pass over the turning points $x_{\pm}(\lambda)$ where WKB fails.

Some insight is gained by making the substitution

$$\mathbf{v} = \begin{bmatrix} 1 & 1 \\ i & -i \end{bmatrix} \tilde{\mathbf{v}}$$

into the equation $\epsilon \mathbf{v}_x = \mathbf{H}(x, \lambda)\mathbf{v}$, with the result:

$$\epsilon \frac{d\tilde{\mathbf{v}}}{dx} = i \begin{bmatrix} 0 & \alpha(x) - \lambda \\ \beta(x) - \lambda & 0 \end{bmatrix} \tilde{\mathbf{v}},$$

recalling $\alpha(x) := -\frac{1}{2}u_0(x) - \sqrt{\rho_0(x)}$ and $\beta(x) := -\frac{1}{2}u_0(x) + \sqrt{\rho_0(x)}$.

Connection problems

Taylor expanding the coefficient matrix about $x = x_{-}(\lambda)$ where $\beta(x) - \lambda$ has a simple root, and keeping only the first nonzero term from each matrix element yields

$$\epsilon \frac{d\tilde{\mathbf{v}}}{dx} \approx i \begin{bmatrix} 0 & \alpha(x_{-}(\lambda)) - \lambda \\ \beta'(x_{-}(\lambda))(x - x_{-}(\lambda)) & 0 \end{bmatrix} \tilde{\mathbf{v}}$$

Note that $\alpha(x_{-}(\lambda)) - \lambda < 0$ while $\beta'(x_{-}(\lambda)) > 0$. Replacing \approx with = we obtain the first-order system form of *Airy's equation*:

$$\frac{d^2\tilde{v}_1}{dy^2} = y\tilde{v}_1, \quad \tilde{v}_2 = i\frac{(\epsilon\beta'(x_-(\lambda)))^{1/3}}{(\lambda - \alpha(x_-(\lambda)))^{2/3}}\frac{d\tilde{v}_1}{dy},$$

where

$$y = \beta'(x_{-}(\lambda))^{1/3}(\lambda - \alpha(x_{-}(\lambda)))^{1/3}\frac{x - x_{-}(\lambda)}{\epsilon^{2/3}}.$$

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Connection problems

Linearly independent solutions to Airy's equation $\tilde{v}_1'(y) = y \tilde{v}_1(y)$ are the functions $\tilde{v}_1(y) = \operatorname{Ai}(y)$ and $\tilde{v}_1(y) = \operatorname{Bi}(y)$:



and as $y \to -\infty$,

$$\begin{aligned} \operatorname{Ai}(y) &= \frac{1}{\sqrt{\pi}|y|^{1/4}} \left[\sin\left(\frac{2}{3}|y|^{3/2} + \frac{\pi}{4}\right) + O(|y|^{-3/2}) \right] \\ \operatorname{Bi}(y) &= \frac{1}{\sqrt{\pi}|y|^{1/4}} \left[\cos\left(\frac{2}{3}|y|^{3/2} + \frac{\pi}{4}\right) + O(|y|^{-3/2}) \right]. \end{aligned}$$

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Connection problems

The formal procedure for going through the turning point $x_{-}(\lambda)$ is:

- Expand the WKB formula from region I_- , $\mathbf{v} \approx e^{f_-(x,\lambda)/\epsilon} \mathbf{y}_-(x,\lambda)$, assuming that $x_-(\lambda) x$ is small and positive. Keep only the dominant terms, and eliminate $x_-(\lambda) x$ in favor of the Airy independent variable *y*.
- Identify the result with linear combinations of the asymptotic forms of Ai(y), Bi(y) and their derivatives for large negative y.
- Seplace these asymptotic forms by the corresponding asymptotic forms now valid for large positive *y*, keeping only dominant terms (in the limit *y* → +∞), and eliminate *y* in favor of *x* − *x*_−(*λ*).
- Compare with expansions of WKB formulae for v valid in region I_0 (exponential interval) assuming $x x_-(\lambda)$ is small (as in step 1).

It is not a pretty calculation, but it is straightforward. It identifies the proper combination of WKB formulae in region I_0 corresponding to the WKB approximation $\mathbf{v} \approx e^{f_-(x,\lambda)/\epsilon} \mathbf{y}_-(x,\epsilon)$ valid in region I_- .

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Connection problems

The result of this calculation is the following WKB formula valid for $x \in I_0$. It contains only the WKB exponential growing to the right.

$$\frac{1}{T_0^{\epsilon}(\lambda)}\mathbf{w}(x,\lambda) = -C^{\epsilon}(\lambda)e^{iS(x)\sigma_3/(2\epsilon)}e^{f_0(x,\lambda)/\epsilon}\mathbf{y}_0(x,\lambda)(1+O(\epsilon)), \quad x \in I_0,$$

where

•
$$f_0(x,\lambda) = \int_{x_-(\lambda)}^x \sqrt{\rho_0(y) - (\lambda + \frac{1}{2}u_0(y))^2} \, dy$$
 (positive root),
• $\mathbf{y}_0(x,\lambda) = \frac{1}{M_0(x,\lambda)} \begin{bmatrix} f_{0x}(x,\lambda) - i(\lambda + \frac{1}{2}u_0(x)) \\ \sqrt{\rho_0(x)} \end{bmatrix}$, and
• $M_0(x,\lambda) = \left(2f_{0x}(x,\lambda)^2 - 2if_{0x}(x,\lambda)(\lambda + \frac{1}{2}u_0(x))\right)^{1/2}$ (principal branch of the square root).

Carrying out similar steps to connect through the next turning point $x_+(\lambda)$, assuming that $\beta(x_+(\lambda)) - \lambda$ and $\beta'(x_+(\lambda)) < 0$ while $\lambda - \alpha(x_+(\lambda)) > 0$, yields:

Connection problems

$$\frac{1}{T_0^{\boldsymbol{\epsilon}}(\lambda)} \mathbf{w}(x,\lambda) = C^{\boldsymbol{\epsilon}}(\lambda) e^{\tau(\lambda)/\boldsymbol{\epsilon}} e^{iS(x)\sigma_3/(2\boldsymbol{\epsilon})} \left[e^{f_+(x,\lambda)/\boldsymbol{\epsilon}} \mathbf{y}_+(x,\lambda) - e^{-f_+(x,\lambda)/\boldsymbol{\epsilon}} \mathbf{z}_+(x,\lambda) + O(\boldsymbol{\epsilon}) \right], \quad x \in I_+, \quad \text{where}$$
• $\tau(\lambda) := \int_{x_-(\lambda)}^{x_+(\lambda)} \sqrt{\rho_0(y) - (\lambda + \frac{1}{2}u_0(y))^2} \, dy \text{ (positive root)},$
• $f_+(x,\lambda) := -i \int_{x_+(\lambda)}^x \sqrt{(\lambda + \frac{1}{2}u_0(y))^2 - \rho_0(y)} \, dy \text{ (positive root)},$
• $\mathbf{y}_+(x,\lambda) = \frac{1}{M_+(x,\lambda)} \left[f_{+x}(x,\lambda) - i(\lambda + \frac{1}{2}u_0(x)) \\ \sqrt{\rho_0(x)} \right],$
• $\mathbf{z}_+(x,\lambda) = \frac{1}{N_+(x,\lambda)} \left[-f_{+x}(x,\lambda) - i(\lambda + \frac{1}{2}u_0(x)) \\ \sqrt{\rho_0(x)} \right],$
• $M_+(x,\lambda) = i\sqrt{2if_{+x}(x,\lambda)(\lambda + \frac{1}{2}u_0(x)) - 2f_{+x}(x,\lambda)^2} \text{ and}$
 $N_+(x,\lambda) = \sqrt{2if_{+x}(x,\lambda)(\lambda + \frac{1}{2}u_0(x)) + 2f_{+x}(x,\lambda)} \text{ (positive roots)}.$

Extraction of the reflection and transmission coefficients

Now we recall that the coefficients $R_0^{\epsilon}(\lambda)$ and $T_0^{\epsilon}(\lambda)$ are defined by the way that the Jost solution $\mathbf{w}(x, \lambda)$ behaves in the limit $x \to +\infty$:

$$\mathbf{w}(x,\lambda) = \begin{bmatrix} e^{-i\lambda x/\epsilon} \\ 0 \end{bmatrix} + R_0^{\epsilon}(\lambda) \begin{bmatrix} 0 \\ e^{i\lambda x/\epsilon} \end{bmatrix} + o(1), \quad x \to +\infty.$$

Dividing by $T_0^{\epsilon}(\lambda)$ and using the WKB formula for $\mathbf{w}(x,\lambda)/T_0^{\epsilon}(\lambda)$ valid for $x \in I_+$ to let $x \to +\infty$ allows us to obtain approximations for $R_0^{\epsilon}(\lambda)$ and $T_0^{\epsilon}(\lambda)$. We only need the following formulae:

$$\lim_{x \to +\infty} \mathbf{y}_+(x,\lambda) = \begin{bmatrix} -1 \\ 0 \end{bmatrix}, \quad \lim_{x \to +\infty} \mathbf{z}_+(x,\lambda) = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \text{ and as } x \to +\infty,$$

$$f_{+}(x,\lambda) = -i(\lambda + \frac{1}{2}u_{0}(+\infty))(x - x_{+}(\lambda))$$
$$-i\int_{x_{+}(\lambda)}^{+\infty} \left[\sqrt{(\lambda + \frac{1}{2}u_{0}(y))^{2} - \rho_{0}(y)} - (\lambda + \frac{1}{2}u_{0}(+\infty))\right] dy + o(1),$$

$$S(x) = u_0(+\infty)x + \int_0^{+\infty} \left[u_0(y) - u_0(+\infty) \right] dy + o(1).$$

Summary: asymptotic formula for R_0^{ϵ}

WKB analysis, plus connection analysis based on Airy functions near turning points, therefore yields the following results:

• If
$$\lambda < \lambda_{-} := \inf_{x \in \mathbb{R}} \alpha(x)$$
 or $\lambda > \lambda_{+} := \sup_{x \in \mathbb{R}} \beta(x)$, then $R_{0}^{\epsilon}(\lambda) = O(\epsilon)$ (smaller if u_{0} and ρ_{0} are smoother).

• If $\lambda \in (\lambda_{-}, \lambda_{+})$, then:

$$R_0^{\epsilon}(\lambda) = e^{-2i\Phi(\lambda)/\epsilon} (1+O(\epsilon)) \quad \text{and} \quad |T_0^{\epsilon}(\lambda)|^2 = e^{-2\tau(\lambda)/\epsilon} (1+O(\epsilon))$$

where

$$\begin{aligned} \tau(\lambda) &:= \int_{x_-(\lambda)}^{x_+(\lambda)} \sqrt{\rho_0(y) - (\lambda + \frac{1}{2}u_0(y))^2} \, dy \\ \Phi(\lambda) &:= \frac{1}{2}S(x_+(\lambda)) + \lambda x_+(\lambda) \\ &\quad - \int_{x_+(\lambda)}^{+\infty} \left[\sigma \sqrt{(\lambda + \frac{1}{2}u_0(y))^2 - \rho_0(y)} - (\lambda + \frac{1}{2}u_0(y)) \right] \, dy \\ \sigma &:= \operatorname{sgn}(\lambda + \frac{1}{2}u_0(+\infty)). \end{aligned}$$

Notes about accuracy and rigor

The formal calculations described above can be justified rigorously in some situations.

- The best method for dealing rigorously with turning points is due to Langer. He avoids Taylor expansion of the coefficient matrix to arrive at Airy's equation by introducing simultaneously
 - A nonlinear change of independent variable *x* → *y* that is more than a simple rescaling, and
 - A gauge transformations (pointwise linear map of the vector $\tilde{\mathbf{v}}$) and he arrives at a rewriting of the original system as a formally small perturbation of Airy's equation that holds in neighborhoods of each turning point that don't need to shrink with ϵ .
- The error terms in Langer's transformation are controlled by working with the Volterra integral equations equivalent to the perturbed initial-value problem (Duhamel's formula).
- These methods are all quite sensitive to geometric details of the graphs of α and β. The connection problem is solved for simple or double turning points.

Since $|R_0^{\epsilon}(\lambda)|^2 + |T_0^{\epsilon}(\lambda)|^2 = 1$ holds, we will approximate $R_0^{\epsilon}(\lambda)$ for all $\lambda \in \mathbb{R}$ by:

$$\tilde{R}_0^{\epsilon}(\lambda) := \chi_{[\lambda_-,\lambda_+]}(\lambda) \sqrt{1 - e^{-2\tau(\lambda)/\epsilon}} e^{-2i\Phi(\lambda)/\epsilon}$$

In the next lecture, we will formulate the Riemann-Hilbert problem of inverse scattering with \tilde{R}_0^{ϵ} in place of R_0^{ϵ} . Then we will show how to analyze its solution in the same asymptotic limit, $\epsilon \to 0$.

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