The WKB Method

MAT633 Mathematical Field Theory Exam

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Motivation

Goal: Obtaining approximate solutions of the Schrödinger equation, WKB method. Developed by Gregor Wentzel, Hendrik Anthony Kramers, and Léon Brillouin in 1926.

Earlier appearances of essentially equivalent methods are from: Francesco Carlini in 1817, Joseph Liouville and George Green in 1837, Lord Rayleigh in 1912, Richard Gans in 1915, and Harold Jeffreys in 1923.

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$$\mathrm{WKB} \xrightarrow{?} \mathrm{CLGRGJWKB}$$

Overview

Overview

Physical WKB Approximation

Recall the Schrödinger Equation (SE)

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi \, .$$

with the Schrödinger operator

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + m_{V(x)}$$

which has solutions $\psi = \psi(x,t) : \mathbb{R}^n \times \mathbb{R} \to \mathbb{C}$. We look for stationary states, i.e. solutions to the SE of the form

$$\psi(x,t) = \varphi(x) e^{-i\omega t}$$

Free particle

Stationary states follow the time-independent SE

$$(\hat{H} - E)\varphi(x) = 0 \quad \text{with} \quad E = \hbar\omega$$

Hence φ an eigenstate of the linear differential operator $\hat{H}$ with eigenvalue E, which represents the energy of the system.
Simplest case: Free particle ($V = \mathrm{const.}$ and $V' = 0$). Ansatz:

$$\varphi(x) = e^{ix\xi} \iff \hbar^2\|\xi\|^2 = 2m(E - V)$$

for some $\xi \in \mathbb{R}^n$.

Free particle

Example

Free particle for $n = 1$:

$$\varphi(x) = e^{ix\xi} \iff \hbar^2\xi^2 = 2m(E - V)$$

- *Case 1: $E > V$. Then*

$$\xi = \pm\frac{\sqrt{2m(E - V)}}{\hbar} \in \mathbb{R}$$

solutions are oscillatory and bounded, but not square-integrable.

- *Case 2: $V > E$. Then $\xi \sim \sqrt{E - V}$ imaginary, hence $\varphi(x)$ unbounded.*

Phase function ansatz

For more interesting examples, we must assume $V' \neq 0$.

Basic idea of WKB

If V varies (slowly) with x, so should ξ vary with $x \longrightarrow$ de Broglie wavelength $\lambda \ll V/V'$

Replace $\xi \in \mathbb{R}^n$ with the real-valued phase function $S(x)$, ansatz $\varphi(x) = e^{iS(x)/\hbar}$.
Plugging the ansatz into the time-independent SE, we get

$$(\hat{H} - E)\varphi(x) = \left[\frac{\|\nabla S(x)\|^2}{2m} + \big(V(x) - E\big) - \frac{i\hbar}{2m}\Delta S(x)\right]\varphi(x) \overset{!}{=} \mathcal{O}(\hbar^1)$$

Note that $\varphi(x) = \mathcal{O}(\hbar^0)$.

Phase function ansatz

This implies

Hamilton-Jacobi equation

$$H\left(x_1, \ldots, x_n, \frac{\partial S}{\partial x_1}, \ldots, \frac{\partial S}{\partial x_n}\right) \equiv \frac{\|\nabla S(x)\|^2}{2m} + V(x) \stackrel{!}{=} E$$

Definition

We call a phase function $S : \mathbb{R}^n \to \mathbb{R}$ **admissible** if it satisfies the Hamilton-Jacobi equation.

We then also write

$$(\hat{H} - E)\varphi = \mathcal{O}(\hbar)\,,$$

because the error is of order $\hbar$, i.e. φ an eigenstate of $\hat{H}$ with eigenvalue E modulo order $\hbar$.

Semi-classical approximation

How to improve accuracy in terms of $\hbar$? Cannot choose better S, as physically $|\varphi(x)|^2 = |e^{iS(x)/\hbar}| = 1$ (probability density) is too restrictive $\longrightarrow$ multiply ansatz by an amplitude function,

$$\varphi(x) = e^{iS(x)/\hbar} a(x)$$

Let S be admissible. Plugging ansatz in:

$$\begin{aligned}(\hat{H} - E)\varphi(x) &= -\frac{1}{2m}\left[i\hbar a \Delta S + 2i\hbar(\nabla S)\cdot(\nabla a) + \hbar^2 \Delta a - a\underbrace{\left(\|\nabla S\|^2 + 2m(V - E)\right)}_{\to 0}\right] e^{iS/\hbar} \\ &= -\frac{1}{2m}\left[i\hbar\left(a\Delta S + 2(\nabla S \cdot \nabla a)\right) + \hbar^2 \Delta a\right] e^{iS/\hbar} \stackrel{!}{=} \mathcal{O}(\hbar^2)\,,\end{aligned}$$

hence $a(x)$ needs to satisfy the

Homogeneous transport equation

$$a\Delta S + 2\nabla S \cdot \nabla a = 0\,.$$

Semi-classical approximation

Definition

We call $\varphi = e^{iS/\hbar}a$ with $S(x)$ admissible and $a(x)$ satisfying the homogeneous transport equation the **semi-classical approximation**.

Example

For $n = 1$, we can solve directly the Hamilton-Jacobi equation

$$S'(x) = \pm\sqrt{2m\big(E - V(x)\big)}\,,$$

as well as the homogeneous transport equation

$$aS'' + 2a'S' \stackrel{!}{=} 0 \implies (a^2S')' = 0$$
$$\implies a = \frac{c}{\sqrt{S'}} = \frac{c}{\big(2m(E-V)\big)^{1/4}}\,.$$

Generalisation

Extend the preceding procedure to arbitrary degree of precision:

$$\varphi(x) = e^{iS(x)/\hbar}\big(a_0(x) + \hbar a_1(x)\big)$$

Let $e^{iS/\hbar}a_0$ be a semi-classical approximation. Then

$$(\hat{H} - E)\varphi(x) = -\frac{1}{2m}\left[i\hbar^2\Big(a_1\Delta S + 2(\nabla S \cdot \nabla a_1) - i\Delta a_0\Big) + \hbar^3\Delta a_1\right]e^{iS/\hbar} \stackrel{!}{=} \mathcal{O}(\hbar^3)\,,$$

hence a_1 needs to satisfy the

Inhomogeneous transport equation

$$a_1\Delta S + 2\nabla S \cdot \nabla a_1 = i\Delta a_0\,.$$

Generalisation

In general, a solution to the eigenstate problem modulo terms of order $\mathcal{O}(\hbar^n)$ is given by a WKB ansatz of the form

$$\varphi = e^{iS/\hbar} \sum_{k=0}^{n} a_k \hbar^k$$

$\rightarrow$ asymptotic series, where S is admissible (satisfies the Hamilton-Jacobi equation), a_0 satisfies the homogeneous transport equation, and a_k satisfies the inhomogeneous transport equation

$$a_k \Delta S + 2\nabla S \cdot \nabla a_k = i\Delta a_{k-1}\,.$$

for all $k = 1, \ldots, n$

With this method from QM, we now turn to geometric considerations from CM.

Overview

Geometry of the WKB method

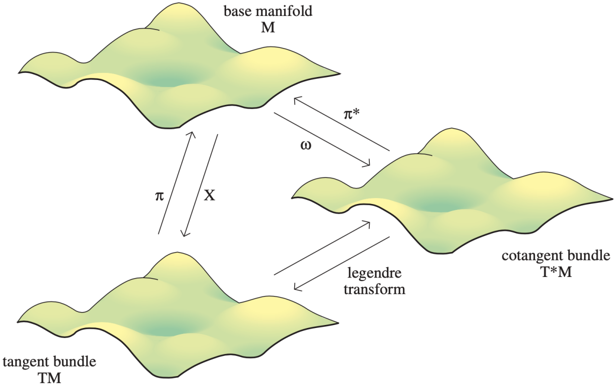

Figure: Source: Peter Mann - Lagrangian and Hamiltonian dynamics

Geometry of admissible phase functions

Geometrical consideration of the phase function S for $n = 1$:

- Classical phase space/plane $T^*\mathbb{R} \cong \mathbb{R}$ with coordinates (q, p)
- View $dS = S'dx : \mathbb{R} \to T^*\mathbb{R}$ as 1-form, $p = S' = \sqrt{2m\big(E - V(x)\big)}$
- Generally: S admissible $\iff$ $L \equiv \mathrm{im}(dS) \subseteq H^{-1}(E)$

Fundamental link between CM and QM

When the image of dS lies in a level manifold of the classical hamiltonian, S may be viewed as the phase function of a first-order approximate solution of the SE.

Geometry of admissible phase functions

The image $L = \mathrm{im}(dS)$ fulfils the following:

1. L is an n-dimensional submanifold of $H^{-1}(E)$
2. The pullback of Poincaré-Cartan form $\theta = p_i dq^i$ on $T^*\mathbb{R}^n$ to L is exact
3. The restriction of the canonical projection $\pi^* : T^*\mathbb{R}^n \to \mathbb{R}^n$ to L induces a diffeomorphism $L \cong \mathbb{R}^n$

Corollary

L is a lagrangian submanifold of $H^{-1}(E)$.

This is too restrictive! General L are not projectable, and θ is only closed.

Geometry of admissible phase functions

Example

For **1D oscillator***, level sets of hamiltonian are lagrangian submanifolds in the phase plane, specifically ellipses. Pull-back of pdq is closed but not exact. Recall that* $S^1 \ncong \mathbb{R}$*. Oscillator still described by trajectory* $\to$ *classically, state of system represented by* L *(projectable or not) rather than by the phase function* S*.*

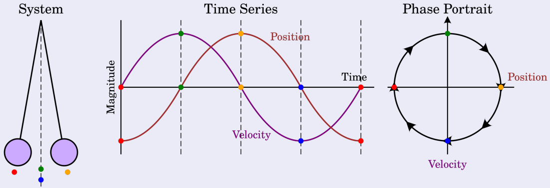

Figure: *Source: Wikipedia*

Starting point of geometrical approach to **microlocal analysis**.

Symplectic formulation of Hamilton-Jacobi

Recall: for hamiltonian function $H : T^*\mathbb{R}^n \cong \mathbb{R}^{2n} \to \mathbb{R}$, hamiltonian vector field is

$$X_H = \dot{q}\frac{\partial}{\partial q} + \dot{p}\frac{\partial}{\partial p} = \frac{\partial H}{\partial p}\frac{\partial}{\partial q} - \frac{\partial H}{\partial q}\frac{\partial}{\partial p}$$

Let ω be the canonical symplectic form on the phase space. Then:

Geometric Hamilton-Jacobi equation

$\iota_{X_H}(\omega) = dH$

$\rightarrow$ Blackboard

Coordinate-free representation of Hamilton's equation, which we retrieve locally.

Symplectic formulation of Hamilton-Jacobi

- $L \subseteq H^{-1}(E) \implies TL \subseteq \ker(dH) \iff \omega = dq^i \wedge dp_i$ vanishes on subspace of $T_p(T^*\mathbb{R}^n)$ gen. by T_pL and $X_H(p)$ for all $p \in L$
- Restriction of ω to $T_p(T^*\mathbb{R}^n)$ at any p is a symplectic form
- Subspaces of $T_p(T^*\mathbb{R}^n)$ on which ω vanishes are at most of dimension n
- X_H is tangent to L

Hamilton-Jacobi theorem

A function $H : \mathbb{R}^{2n} \to \mathbb{R}$ is locally constant on a lagrangian submanifold $L \subset \mathbb{R}^{2n}$ if and only if the hamiltonian vector field X_H is tangent to L.

Corollary

L locally closed $\implies$ L is invariant under the flow of X_H

The End

Thank you for your attention!

Appendix

3. Geometry of transport equation

4. Application example in quantum mechanics

Overview

3. Geometry of transport equation

4. Application example in quantum mechanics

Geometry of transport equation

We have seen the geometric formulation of the first-order WKB approximation $\varphi = e^{iS/\hbar}$ in form of the Geometric HJ equation and the HJ theorem.

We can extend this to the semi-classical approximation $\varphi = e^{iS/\hbar}a(x)$. Recall:

Homogeneous transport equation

$$a\Delta S + 2\nabla S \cdot \nabla a = 0$$

Multiplying by a yields

$$\nabla\left(a^2 \nabla S\right) = 0$$

as a condition of that vector field $\rightarrow$ lift to $L = \mathrm{im}(dS)$.

Geometry of transport equation

For $H(q,p) = \sum p^i/2 + V(q)$, we have the restriction

$$X_H|_L = \sum_j \left(\frac{\partial S}{\partial x_j} \frac{\partial}{\partial q_j} - \frac{\partial V}{\partial q_j} \frac{\partial}{\partial p_j} \right).$$

The projection $X_H|_L$ onto $\mathbb{R}^n$ (with coordinates x), denoted $X_H^{(x)}$ yields ∇S, hence the homogeneous transport equation

$$a\Delta S + 2\sum_j \frac{\partial a}{\partial x_j} \frac{\partial S}{\partial x_j} = 0$$

tells us that $\nabla(a^2 X_H^{(x)}) = 0$

Geometry of transport equation

We can reformulation $a^2 X_H^{(x)}$ being divergence-free as

$$\mathcal{L}(X_H^{(x)}(a^2|dx|)) = 0\,,$$

with $|dx| = |dx_1 \wedge \cdots \wedge dx_n|$ the canonical density on $\mathbb{R}^n$.

Equation equivalent to the fact that the pull-back of $a^2|dx|$ to L via π is invariant under flow of X_H (since X_H tangent to L, Lie derivative invariant under diffeomorphism).

Geometric interpretation. . .

. . . of a as a half-density on L invariant by X_H.

Hence, a geometric semi-classical state is a lagrangian submanifold L of $\mathbb{R}^{2n}$ equipped with a half-density a.

Example

For **1D oscillator***, stationary classical states are $L = H^{-1}(E) \subset \mathbb{R}^{2n}$. Up to constant, there is a unique invariant volume element for the hamiltonian flow of H on every level curve of H. Hence an L with the square root of the volume element constitutes a semi-classical stationary state for the harmonic oscillator.*

Overview

3. Geometry of transport equation

4. Application example in quantum mechanics

Application example in quantum mechanics

Recall:

Definition

We call $\varphi = e^{iS/\hbar}a$ with $S(x)$ admissible and $a(x)$ satisfying the homogeneous transport equation the **semi-classical approximation**.

Example

For $n = 1$, we can solve directly for the phase

$$S'(x) = \pm\sqrt{2m\big(E - V(x)\big)} = p\,,$$

and the amplitude

$$a = \frac{c}{\sqrt{S'}} = \frac{c}{\big(2m(E-V)\big)^{1/4}}\,.$$

Application example in quantum mechanics

The first-order WKB approximation only works for p sufficiently large, and breaks down at turning points. Here, we need the semi-classical approximation.

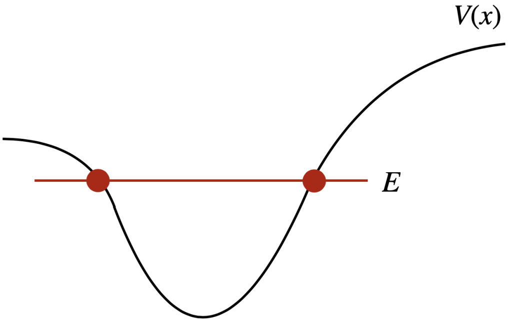

Figure: Source: Massimiliano Grazzini, Quantum Mechanics I

Application example in quantum mechanics

We approximate the general semi-classical state

$$\psi(x) \sim \frac{1}{\sqrt{p}} e^{\pm \frac{i}{\hbar} \int p dx}$$

by approximating the potential close to the turning point

$$E - V(x) \sim -V'(x_0)(x - x_0)\,.$$

Via analytic continuation, this leads us to:

Quantisation condition

$$\frac{1}{2\pi\hbar} \oint p dx = n + \frac{1}{2}$$

Application example in quantum mechanics

Example

The quantisation condition can be used to derive the (discrete!) spectrum of the harmonic oscillator, $V(x) = \frac{1}{2}m\omega^2 x^2$. *Solving*

$$\frac{1}{2\pi\hbar}\oint \sqrt{2m(E - V(x))}\,dx = \frac{\sqrt{2m}}{\pi\hbar}\int_{-x_0}^{x_0}\sqrt{\left(E - \frac{1}{2}m\omega^2 x^2\right)}\,dx \overset{!}{=} n + \frac{1}{2}$$

(with $x_0 + \sqrt{\frac{2E}{m\omega^2}}$*) for the energy yields*

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right).$$