# 130B Quantum Physics

## Part 1. Path Integral Quantization

## From Classical to Quantum

### ▪ Historical Review

### ▪ History: What is the Nature of Light?

There has been *two theories* in the history concerning the nature of *light*.

- The **corpuscular (particle) theory**: light is composed of steady stream of *particles* carrying the energy and travelling along rays in the speed of light.
- The **wave theory**: light is *wave-like*, propagating in the space and time.

The long-running dispute about this problem has lasted for centuries.

#### ▫ The Wave-Particle Wars in History

A time-line of "the **wave-particle** wars" in the history of physics. (c.f. Wikipedia: Historical theories about light).

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| Ancient Greece | Pythagorean discipline postulated that every visible object emits a steady **stream of particles**, while Aristotle concluded that light travels in a manner similar to **waves** in the ocean. |
| Early 17th century | R. Descartes proposed light is a kind of **pressure** propagating in the media. |
| 1662 | P. de Fermat stated the **Fermat principle**, the fundamental principle of geometric optics, where light rays are assumed to be trajectories of small particles. |
| 1665 | P. Hooke expressly pointed out the wave theory of light in his book, where light was considered as some kind of **fast pulses**. |
| 1672 | I. Newton conducted the **dispersion** experiment of light. He decomposed white light into seven colors. Thus he explained that light is a mixture of little corpuscles of different colors. His paper was strongly opposed by Hook, and "the first wave-particle war" broke out. |
| 1675 | The phenomenon of **Newton's ring** was discovered by Newton. |

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| 1690 | C. Huygens considered light as longitudinal wave propagating in a media called ether. He introduced the concept of **wave front**, deduced the law of **reflection** and **refraction**, and explained the phenomenon of *Newton's ring* by **wave interference**. The wave theory reached its crest. |
| 1704 | I. Newton published his book *Optiks*, which explained **dispersion**, **double refraction**, and **diffraction** from particle viewpoint. On the other side, Newton integrated the corpuscular theory with his **classical mechanics**, which combined to show enormous strength over the century. |
| Early 18th century | "The first wave-particle war" ends, and corpuscular (particle) theory occupied the mainstream of physics for the following hundred years. |
| 1807 | T. Young conducted the **double-split experiment**, and proposed light to be a **longitudinal wave**, which simply explained the **interference** and **diffraction** of light. Young's experiment triggered "the second wave-particle war". The corpuscular theory could do nothing but to suffer one defeat after another. |
| 1809 | E. Malus discover the **polarization** of light, which could not be explained by *longitudinal* wave theory. This gave the wave theory a heavy strike. |
| 1819 | A. Fresnel submitted a paper, perfectly explained the **diffraction** of light from wave viewpoint based on rigorous mathematical deductions. When Poisson applied this theory to circular disk diffraction, he predicted that a light spot will appear at the center of the shadow of the disk. This unreasonable effect was considered by Poisson as an opposing evidence of the wave theory. However, F. Arago insisted on doing the experiment and proved the existence of the **Poisson spot**. The success of Fresnel's theory won the decisive battle for the wave in "the second wave-particle war". |
| 1821 | Fresnel proposed that light is a **transverse wave**, and successfully explained the *polarization* of light. "The second wave-particle war" ended with the victory of wave theory. |
| 1865 | J. Maxwell formulated the classical theory of **electrodynamics**, which predicted that light is kind of electromagnetic wave. |
| 1887 | H. R. Hertz verified the existence of **electromagnetic wave** in experiments. The speed of the electromagnetic wave is exactly the speed of light. The wave theory of light was firmly established. |
| 1900 | M. Planck obtained the formula of **blackbody radiation**, the **quantum** hypothesis of light was proposed. |
| 1905 | A. Einstein explained the **photoelectric** effect. In Einstein's theory light is consisted of some particles carrying the discrete amount of energy, and can only be absorbed or emitted one by one. The concept of light quantum (**photon**) resurrected the particle theory. "The third wave-particle war" broke out. |

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| 1923 | A. Compton studied the scattering of X-ray by a free electron. The **Compton effect** was discovered, that the frequency of X-ray changes in the scattering. The experiment exactly proved that X-ray is also composed by radiation quantum with certain momentum and energy. |
| 1924 | S. N. Bose considered light as a set of indistinguishable particles and obtained Planck's formula of *blackbody radiation*. **Bose-Einstein statistics** was established, which further supports the idea of particle theory. |
| … | … |

### Concluding Remarks

In fact, "the third wave-particle war" had gone beyond the scope of the nature of *light*. The discussion had been extended to the nature of all *matter* in general.

- Light: originally considered as *wave*, also behaves like *particle*.
- Electrons, $\alpha$ particles ($^4$He nucleus): originally considered as *particles*, also behave like *wave*.

The dispute ends up with the discovery of **wave-particle duality**, which finally leads to the formulation of **quantum mechanics**. Another century has passed, we hope that wave and particle will live in peace under the quantum framework, and there should be no more wars.

# Quantization of Light

## Geometric Optics

**Geometric optics** is the **particle mechanics** of light (light travels *along a path*)

- **Fermat's Principle**: Light always travels along the path of *extremal* optical path length.

$$\boxed{\delta L = 0,} \tag{1}$$

- The **optical path length** is defined by

$$\boxed{L(A \to B) = \int_A^B n\, d s,} \tag{2}$$

where $n$ is the **refractive index** of the medium and $d s$ is an infinitesimal displacement along the ray.

- The *optical path length* is simply related to the *light travelling time* $T$ by $L = c\,T$, where $c$ is the **speed of light** in vacuum. So extremization of either of them will be equivalent.

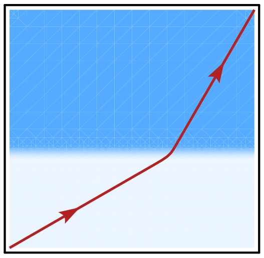
- **Eikonal equation** (*Newton's law* of light)

$$n \frac{d}{d t}\left(n^2 \frac{d \boldsymbol{x}}{d t}\right) = c^2\, \nabla n. \tag{3}$$

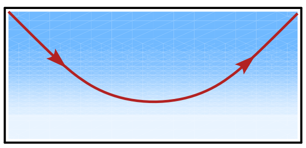
**Exc 1** Derive Eq. (3) from Fermat's principle Eq. (1).

Examples of light rays in the medium by solving Eq. (3):

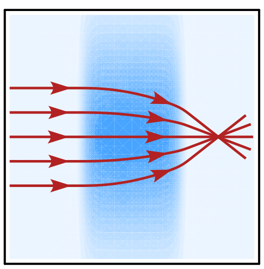
- Refraction (Snell's law)



- Total reflection



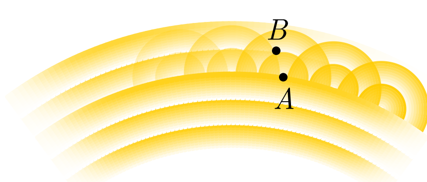
- Gradient-index (GRIN) optics



## Physical Optics

**Physical optics** is the **wave mechanics** of light (light *propagates* in the spacetime as a *wave*).

- **Huygens' Principle**: Every point on the wavefront acts as a *secondary source* emitting *spherical wavelet*. The new wavefront is formed by the *coherent superposition* of these wavelets.




- **Wave propagation**: The **wave amplitude** $\psi_B$ on the *new* wave front is determined by the amplitude $\psi_A$ on the *preceding* wave front, modified by a **phase factor** $e^{i\,\Theta(A\to B)}$ that encodes the accumulated **phase** $\Theta(A \to B)$ during *wave propagation*.

- **Interference effect**: contributions from *different paths* must be collected and summed up (integrated over)

$$\boxed{\psi_B = \int_{A\to B} \psi_A\, e^{i\,\Theta(A\to B)}.} \tag{4}$$

- The accumulated **phase** $\Theta$ is determined by the propagation time $T$ × the frequency $\omega$ of light

$$\boxed{\Theta(A \to B) = \omega\, T(A \to B) = \frac{\omega}{c}\, L(A \to B),} \tag{5}$$

proportional to the *optical path length* $L$ (given that the light propagates with a fixed frequency).

The resulting profile of the wave amplitude throughout the spacetime (or the space) is described by the **wavefunction**

$$\begin{aligned} &\text{spacetime}: \psi(\boldsymbol{x}, t), \\ &\text{space (at fixed-time)}: \psi(\boldsymbol{x}). \end{aligned} \tag{6}$$

- The **magnitude** (or the absolute amplitude) $|\psi|$ of the wave is related to the **intensity** of the light, or the **probability density** to observe a photon at a given position $\boldsymbol{x}$,

$$p(\boldsymbol{x}) = |\psi(\boldsymbol{x})|^2. \tag{7}$$

- **Normalization**: the wavefunction is said to be *normalized*, if

$$\int |\psi(\boldsymbol{x})|^2\, d^D \boldsymbol{x} = \int p(\boldsymbol{x})\, d^D \boldsymbol{x} = 1, \tag{8}$$

a requirement for the total probability to be 1.

## From Fermat to Huygens

Optimizing the *optical path length* $L$ can be viewed as optimizing an **action** $S$

$$S(A \to B) = \frac{\hbar\,\omega}{c}\, L(A \to B), \tag{9}$$

which is defined by properly rescaling $L$ to match the dimension of energy × time.

- Particle mechanics defines the **action** $S$ in the variational principle $\delta S = 0$.
- Wave mechanics defines the **phase** $\Theta$ in the wavelet propagator $e^{i\,\Theta}$.

They are related by

$$\boxed{S(A \to B) = \hbar\, \Theta(A \to B).} \tag{10}$$

The **Planck constant** $\hbar$ provides a natural unit for the action.

Therefore the *particle* and *wave* mechanics are connected by

| The **action** accumulated by particle = the **phase** accumulated by wave. |
|---|

This is also the guiding principle of the **path integral quantization** — a universal approach to promote any classical theory to its quantum version.

# Path Integral Quantization

## ▪ Quantization of Matter

### ▪ Classical Mechanics

**Action**: a function(al) associated to each possible path of a particle,

$$S[x] = \int L(x, \dot{x}, t)\, dt. \tag{11}$$

The **principle of stationary action**: the path taken by the particle $\bar{x}(t)$ is the one for which the action is stationary (to first order), subject to boundary conditions: $\bar{x}(t_0) = x_0$ (*initial*) and $\bar{x}(t_1) = x_1$ (*final*).

$$\delta\, S[x]|_{x=\bar{x}} = \delta \int L(x, \dot{x}, t)\, dt\Big|_{x=\bar{x}} = 0. \tag{12}$$

This leads to the **Euler-Lagrange equation** (the equation of motion),

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}}\right) - \frac{\partial L}{\partial x} = 0, \tag{13}$$

such that the classical path $\bar{x}(t)$ is the solution of Eq. (13). For a *non-relativistic* particle, the Lagrangian takes the form of $L = T - V$, where $T$ is the *kinetic* energy and $V$ is the *potential* energy. For a *relativistic* particle, the action is simply the *proper time* of the path in the spacetime.

HW 1

> For a non-relativistic free particle $L = (m/2)\,\dot{x}^2$.
> (i) Show that the stationary (classical) action $S[\bar{x}]$ corresponding to the classical motion of a free particle travelling from $(x_0, t_0)$ to $(x_1, t_1)$ is $S[\bar{x}] = \frac{m}{2}\,\frac{(x_1 - x_0)^2}{t_1 - t_0}$.
> For this case of the free particle,
> (ii) Show that the spatial derivative of the action $\partial_{x_1} S[\bar{x}]$ is the momentum of the particle.
> (iii) Show that the (negative) temporal derivative of the action $-\partial_{t_1} S[\bar{x}]$ is the energy of the particle.

A **computability problem**: the *principle of stationary action* is formulated as a **deterministic** *global optimization*, which requires exact computations and indefinitely long run time (on any computer).

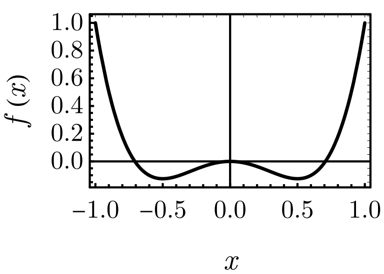
- Nature may not have sufficient *computational resources* to carry out the classical mechanics *precisely*. ⇒ Classical mechanics might actually be realized only *approximately* as a **stochastic** *global optimization*, which is computationally more feasible.
- **Quantum mechanics** takes a *stochastic* approach to optimize the action, which is more natural than the *deterministic* approach of classical mechanics, if we assume only limited computational resource is available to nature.

## Optimization by Interference

Each *path* is associated with an *action*. Quantum mechanics effectively finds the *stationary action* by the **interference** among all possible paths.

Example: find the stationary point(s) of

$$f(x) = -x^2 + 2\,x^4. \tag{14}$$




- Every point $x$ is a legitimate guess of the solution.
- Each point $x$ is associated with an *action* $f(x)$ (the objective function).
- Raise the *action* $f(x)$ to the exponent (as a *phase*): $e^{i f(x)/\hbar}$ ⇒ call it a "probability amplitude" contributed by the point $x$.
  - A "Planck constant" $\hbar = h/(2\pi)$ is introduced as a *hyperparameter* of the algorithm, to control "how quantum" the algorithm will be.
- Contributions from all points must be collected and summed (integrated) up,

$$Z = \int_{-\infty}^{\infty} e^{i f(x)/\hbar}\, dx. \tag{15}$$

The result $Z$ summarizes the probability amplitudes. It is known as the **partition function** of the stationary problem. But it is just a complex number, how do we make use of it? ⇒ Well, we need to analyze how $Z$ is accumulated. Each infinitesimal step in the integral → a infinitesimal **displacement** on the *complex plane*

$$dz = e^{i f(x)/\hbar}\, dx. \tag{16}$$

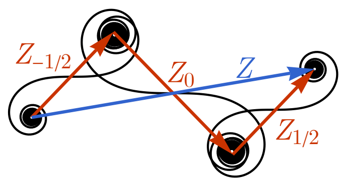
- $dx$ controls the infinitesimal step size,
- $e^{i f(x)/\hbar}$ controls the direction to make the displacement,

- displacement $d z$ is *accumulated* to form the partition function,

$$Z \equiv \int d z. \tag{17}$$

Let us see how the partition function is constructed.

- For small $h$ (classical limit)

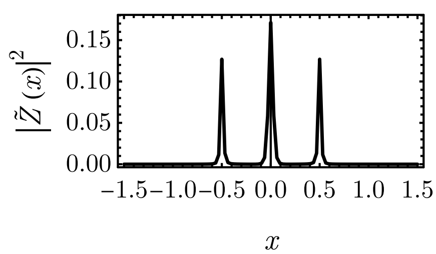



$$Z = Z_{-1/2} + Z_0 + Z_{1/2}, \tag{18}$$

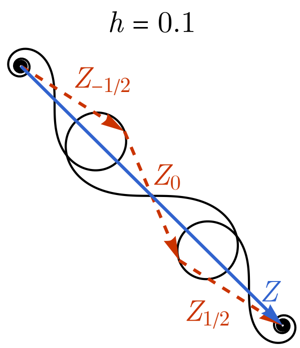
- $Z$ can break up into three smaller contributions, which correspond to the contributions *around* the three **stationary points**: $x = 0, \pm 1/2$.
- Around the *stationary point*, **phase** changes *slowly* $\partial_x f(x) \sim 0 \Rightarrow$ **constructive interference** $\Rightarrow$ *large* contribution to the partition function.
- The solutions of stationary points (*classical* solutions) **emerge** from *interference* due to their *dominant* contribution to the probability amplitude.
- *More precisely, the partition function is actually evaluated with respect to the momentum $k$,

$$Z(k) \equiv \int d z\, e^{i k x} \simeq Z_{-1/2}\, e^{-i k/2} + Z_0 + Z_{1/2}\, e^{i k/2}. \tag{19}$$

Then its Fourier spectrum $\tilde{Z}(x) = \int d k\, Z(k)\, e^{-i k x}$ will reveal the saddle points.

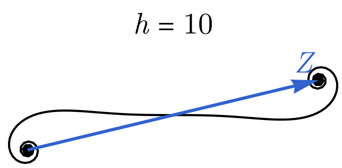



- For intermediate $h$




- The decomposition of $Z$ into three subdominant amplitudes is not very well defined. ⇒ **Quantum fluctuations** start to smear out nearby stationary points.

- For large $h$ (quantum limit)




- Stationary points are indistinguishable if quantum fluctuations are too large. ⇒ As if there is only one (approximate) stationary point around $x = 0$.

- If there is no sufficient resolution power, fine structures in the *action* landscape will be *ignored* by quantum mechanics. In this way, the computational complexity is *controlled*.

Generalize the same problem from stationary *points* to stationary *paths* (in classical mechanics) ⇒ **path integral** formulation of quantum mechanics.

The **Planck constant** characterizes nature's **resolution** (computational precision) of the action.

$$h = 6.62607004 \times 10^{-34}\ \text{J s}. \tag{20}$$

Two nearby paths with an action difference smaller than the Planck constant can not be resolved.

- $h$ is very small (in our everyday unit) ⇒ our nature has a pretty high resolution of action ⇒ no need to worry about the resolution limit in the *macroscopic* world ⇒ classical mechanics works well.

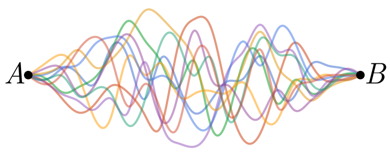
- However, in the *microscopic* world, nature's resolution limit can be approached ⇒ "round-off error" may occur ⇒ one consequence is the *quantization* of atomic orbitals (discrete energy levels etc.).

## ■ Path Integral and Wave Function

- **Feynman's principle**: The **probability** $p_{A\to B}$ for a particle to *propagate* from $A$ to $B$ is given by the square modulus of a complex number $K_{A\to B}$ called the **transition amplitude**

$$p_{A\to B} = |K_{A\to B}|^2. \tag{21}$$

- The **transition amplitude** is given by *adding together* the contributions of *all paths* $x$ from $A$ to $B$.




$$K_{A\to B} \propto \int_{A\to B} \mathcal{D}[x]\, e^{i\, S[x]/\hbar}. \tag{22}$$

- The contribution of each particular path is *proportional* to $e^{i\, S[x]/\hbar}$, where $S[x]$ is the **action** of the path $x$.

In the limit of $\hbar \to 0$, the classical path $\overline{x}$ (that satisfies $\delta S[\overline{x}] = 0$) will dominate the transition amplitude,

$$K_{A\to B} \sim e^{i\, S[\overline{x}]/\hbar}. \tag{23}$$

*Quantum mechanics* reduces to *classical mechanics* in the limit of $\hbar \to 0$.

To make the problem tractable, an important observation is that the *transition amplitude* satisfies a **composition property**

$$K_{A\to B} = \int_C K_{A\to C}\, K_{C\to B}. \tag{24}$$

This allows us the chop up time into slices $t_0 < t_1 < \ldots < t_{N-1} < t_N$,

$$K_{(x_0,t_0)\to(x_N,t_N)} = \int d x_1 \ldots d x_{N-1}\, K_{(x_0,t_0)\to(x_1,t_1)} \ldots K_{(x_{N-1},t_{N-1})\to(x_N,t_N)}. \tag{25}$$

The “front” of transition amplitude propagates in the form of wave ⇒ define the **wavefunction** $\psi(x,\, t)$, which describes the **probability amplitude** to observe the particle at $(x,\, t)$,

$$\psi(x_{k+1},\, t_{k+1}) = \int d x_k\, K_{(x_k,t_k)\to(x_{k+1},t_{k+1})}\, \psi(x_k,\, t_k). \tag{26}$$

If we start with a *initial wavefunction* $\psi(x,\, t_0)$ concentrated at $x_0$, following the time evolution Eq. (26), the *final wavefunction* $\psi(x,\, t_N)$ will give the *transition amplitude* $K_{(x_0,t_0)\to(x_N,t_N)} = \psi(x_N,\, t_N)$. ⇒ It is sufficient to study the evolution of a *generic wavefunction* over one time step, then the dynamical rule can be applied iteratively.

Putting together Eq. (22) and Eq. (26),

$$\psi(x_{k+1},\, t_{k+1}) \propto \int \mathcal{D}[x] \exp\!\left(\frac{i}{\hbar}\, S[x]\right) \psi(x_k,\, t_k), \tag{27}$$

this path integral involves multiple integrals:

- for each given initial point $x_k$, integrate over paths $x(t)$ subject to the boundary conditions $x(t_k) = x_k$ and $x(t_{k+1}) = x_{k+1}$,
- finally integrate over choices of initial point $x_k$.

The **Schrödinger equation** is the equation that governs the **time evolution** of the *wavefunction*, which plays a central role in quantum mechanics. It can be derived from the *path integral* formulation in Eq. (27).

# Deriving the Schrödinger Equation

## Action in a Time Slice

The **action** of a free particle of mass $m$,

$$S[x] = \int_{t_0}^{t_1} dt \, \frac{1}{2} m \dot{x}^2, \tag{28}$$

where the particle starts from $x(t_0) = x_0$, ends up at $x(t_1) = x_1$.

Suppose the time interval $\delta t = t_1 - t_0$ is small, approximate the path of the particle by a *straight line* in the space-time,

$$x(t) = x_0 + v\, t, \tag{29}$$

where the *velocity* $v$ will be a constant

$$v = \frac{x_1 - x_0}{t_1 - t_0} = \frac{x_1 - x_0}{\delta t}. \tag{30}$$

Plug into Eq. (28), we get an estimate of the *action* accumulated as the particle moves from $x_0$ to $x_1$ in time $\delta t$,

$$S[x] = \frac{1}{2} m \left(\frac{x_1 - x_0}{\delta t}\right)^2 \delta t = \frac{m}{2\,\delta t} (x_1 - x_0)^2. \tag{31}$$

## Path Integral in a Time Slice

The wavefunction $\psi(x, t + \delta t)$ in the next time slice is related to the previous one $\psi(x, t)$ by

$$\begin{aligned} \psi(x_1, t + \delta t) &\propto \int d x_0 \exp\left(\frac{i}{\hbar} S[x]\right) \psi(x_0, t) \\ &= \int d x_0 \exp\left(\frac{i\, m}{2\,\hbar\,\delta t} (x_1 - x_0)^2\right) \psi(x_0, t). \end{aligned} \tag{32}$$

- The *proportional sign* "∝" implies that the *normalization factor* is not determined yet. (It will be determined later.)

To proceed we expand $\psi(x_0, t)$ around $x_0 \to x_1$, by defining $x_0 = x_1 + a$, and *Taylor expand* with respect to $a$,

$$\begin{aligned}\psi(x_0,\ t) &= \psi(x_1 + a,\ t)\\ &= \psi(x_1,\ t) + a\,\psi'(x_1,\ t) + \frac{a^2}{2!}\,\psi''(x_1,\ t) + \frac{a^3}{3!}\,\psi^{(3)}(x_1,\ t) + \ldots\\ &= \sum_{n=0}^{\infty} \frac{a^n}{n!}\,\partial_{x_1}^n \psi(x_1,\ t).\end{aligned}$$

Substitute into Eq. (32),

$$\psi(x_1,\ t + \delta t) \propto \sum_{n=0}^{\infty} \int d\,a \exp\left(\frac{i\,m}{2\,\hbar\,\delta t}\ a^2\right) \frac{a^n}{n!}\,\partial_{x_1}^n \psi(x_1,\ t). \tag{34}$$

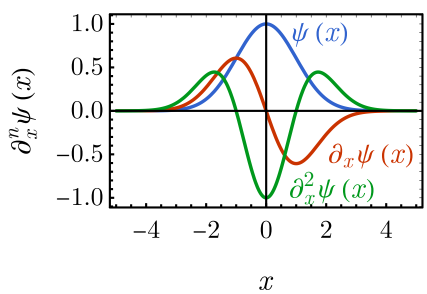
We pack everything related to the integral of $a$ into a coefficient

$$\boxed{\lambda_n \equiv \int d\,a \exp\left(\frac{i\,m}{2\,\hbar\,\delta t}\ a^2\right) \frac{a^n}{n!},} \tag{35}$$

then the time evolution is simply given by (we are free to replace $x_1$ by $x$)

$$\boxed{\psi(x,\ t + \delta t) \propto \sum_{n=0}^{\infty} \lambda_n\,\partial_x^n \psi(x,\ t).} \tag{36}$$

- The idea is that the time-evolved wavefunction can be expressed as the original wavefunction "dressed" by its (different orders of) derivatives.




  - For example, $\psi(x)$ is a wave packet.
  - $\psi(x) + \lambda\,\psi'(x)$: shift the wave packet around.
  - $\psi(x) + \lambda\,\psi''(x)$: expand or shrink the wave packet.
  - **Locality of Physics**: the *time evolution* should only involve *local modifications* of the wavefunction $\psi(x)$ (mostly within the light-cone) in each step.

## Computing the Coefficients $\lambda_n$

The $\lambda_n$ coefficient can be computed by *Mathematica*

$$\lambda_n = \frac{1 + (-1)^n}{2}\ \frac{\sqrt{\pi}}{2^n\,\Gamma\left(1 + \frac{n}{2}\right)} \left(-\frac{i\,m}{2\,\hbar\,\delta t}\right)^{-\frac{1+n}{2}}. \tag{37}$$

**Exc 2**

> Evaluate the integral in Eq. (35) for $\lambda_n$.

- The first term $(1+(-1)^n)/2$ just discriminates *even* and *odd* $n$.

$$\frac{1+(-1)^n}{2} = \begin{cases} 1 & \text{if } n \in \text{even}, \\ 0 & \text{if } n \in \text{odd}. \end{cases} \tag{38}$$

So as long as $n \in$ odd, $\lambda_n = 0$. We only need to consider the case of even $n$.

- For even $n$, the first several $\lambda_n$ are given by

$$\begin{aligned} \lambda_0 &= \sqrt{\pi}\left(-\frac{i\,m}{2\,\hbar\,\delta t}\right)^{-1/2}, \\ \lambda_2 &= \frac{\sqrt{\pi}}{4}\left(-\frac{i\,m}{2\,\hbar\,\delta t}\right)^{-3/2} = \frac{i}{4}\left(\frac{2\,\hbar\,\delta t}{m}\right)\lambda_0, \\ \lambda_4 &= \frac{\sqrt{\pi}}{32}\left(-\frac{i\,m}{2\,\hbar\,\delta t}\right)^{-5/2} = -\frac{1}{32}\left(\frac{2\,\hbar\,\delta t}{m}\right)^2\lambda_0, \\ &\ldots \end{aligned} \tag{39}$$

**Exc 3**

> Compute the first several $\lambda_n$ for even integer $n$ using Eq. (37).

## ▪ Determining the Normalization

Plugging the results of $\lambda_n$ in Eq. (39) into Eq. (36), we get

$$\psi(x,\ t+\delta t) \propto \lambda_0\left(1+\frac{i}{4}\left(\frac{2\,\hbar\,\delta t}{m}\right)\partial_x^2 - \frac{1}{32}\left(\frac{2\,\hbar\,\delta t}{m}\right)^2\partial_x^4 + \ldots\right)\psi(x,\ t). \tag{40}$$

- If we take $\delta t = 0$, all higher order terms vanishes,

$$\psi(x,\ t) \propto \lambda_0\,\psi(x,\ t). \tag{41}$$

So obviously, the *normalization factor* should be such to cancelled out $\lambda_0$.

So we should actually write (in *equal sign*) that

$$\psi(x,\ t+\delta t) = \left(1+\frac{i}{4}\left(\frac{2\,\hbar\,\delta t}{m}\right)\partial_x^2 - \frac{1}{32}\left(\frac{2\,\hbar\,\delta t}{m}\right)^2\partial_x^4 + \ldots\right)\psi(x,\ t). \tag{42}$$

## ▪ Taking the Limit of $\delta t \to 0$

Let us consider the time derivative of the wavefunction

$$\begin{aligned} \partial_t\psi(x,\ t) &= \lim_{\delta t\to 0}\frac{\psi(x,\ t+\delta t)-\psi(x,\ t)}{\delta t} \\ &= \lim_{\delta t\to 0}\frac{1}{\delta t}\left(\frac{i}{4}\left(\frac{2\,\hbar\,\delta t}{m}\right)\partial_x^2 - \frac{1}{32}\left(\frac{2\,\hbar\,\delta t}{m}\right)^2\partial_x^4 + \ldots\right)\psi(x,\ t) \end{aligned} \tag{43}$$

- Only the first term survives under the limit $\delta t \to 0$,

$$\partial_t \psi(x, t) = \frac{i \hbar}{2 m} \partial_x^2 \psi(x, t). \tag{44}$$

- All the higher order terms will have higher powers in $\delta t$, so they should all vanish under the limit $\delta t \to 0$.

By convention, we write Eq. (44) in the following form

$$\boxed{i \hbar \partial_t \psi(x, t) = -\frac{\hbar^2}{2 m} \partial_x^2 \psi(x, t).} \tag{45}$$

This is the **Schrödinger equation** that governs the *time evolution* of the wavefunction of a *free* particle.

## ▪ Adding Potential Energy

Now suppose the particle is not free but moving in a **potential** $V(x)$, the action changes to

$$\boxed{S = \int_{t_0}^{t_1} d t \left(\frac{1}{2} m \dot{x}^2 - V(x)\right),} \tag{46}$$

The *additional* action that will be accumulated over time $\delta t$ will be

$$\Delta S = - V(x) \delta t. \tag{47}$$

Eventually this cause an additional *phase shift* in the wavefunction

$$\begin{aligned}\psi(x, t + \delta t) &= e^{i \Delta S/\hbar} \psi_0(x, t + \delta t) \\ &= e^{-i V(x) \delta t/\hbar} \psi_0(x, t + \delta t) \\ &= \left(1 - \frac{i}{\hbar} V(x) \delta t + \ldots\right) \psi_0(x, t + \delta t),\end{aligned} \tag{48}$$

where $\psi_0$ is the expected wavefunction at $t + \delta t$ without the potential. Combining with the result in Eq. (42), to the first order of $\delta t$ we have

$$\begin{aligned}\psi(x, t + \delta t) &= \left(1 - \frac{i}{\hbar} V(x) \delta t + \ldots\right)\left(1 + \frac{i}{4}\left(\frac{2 \hbar \delta t}{m}\right) \partial_x^2 + \ldots\right) \psi(x, t) \\ &= \left(1 + \frac{i}{4}\left(\frac{2 \hbar \delta t}{m}\right) \partial_x^2 - \frac{i}{\hbar} V(x) \delta t + \ldots\right) \psi(x, t).\end{aligned} \tag{49}$$

Then after taking the $\delta t \to 0$ limit, we arrive at

$$\partial_t \psi(x, t) = \frac{i \hbar}{2 m} \partial_x^2 \psi(x, t) - \frac{i}{\hbar} V(x) \psi(x, t), \tag{50}$$

or equivalently written as

$$i\hbar\,\partial_t\psi(x,t) = -\frac{\hbar^2}{2m}\,\partial_x^2\psi(x,t) + V(x)\,\psi(x,t). \tag{51}$$

This is the **Schrödinger equation** that governs the *time evolution* of the wavefunction $\psi(x, t)$ of a particle moving in a potential $V(x)$.

### Time-Independent Case

If the potential function $V(x)$ is independent of time $t$, the problem can be simplified by a **separation of variables** for $\psi(x, t)$ in the form of

$$\psi(x,t) = \psi(x)\,e^{-i E t/\hbar}. \tag{52}$$

Substitute Eq. (52) into Eq. (51), we arrived as the *stationary* **Schrödinger equation** as an eigen equation,

$$\left(-\frac{\hbar^2}{2m}\,\partial_x^2 + V(x)\right)\psi(x) = E\,\psi(x). \tag{53}$$

**Exc 4** Derive Eq. (53) from Eq. (51).

The solution to the eigen problem provides

- $E_n$: eigen energies,
- $\psi_n(x)$: corresponding eigen wavefunctions,

both labeled by the eigenstate index $n$.

## Semiclassical Approach

### WKB Approximation (General)

**WKB** (Wentzel-Kramers-Brillouin) **approximation**: a method for solving the Schrödinger equation in the *semiclassical* limit where $\hbar \to 0$.

- Goal: find approximate solution of Eq. (51), keeping only the *leading* quantum effects (i.e., the leading terms of $\hbar$).

Postulate a solution for $\psi(x, t)$ of the form

$$\psi(x,t) = A(x,t)\,e^{i S(x,t)/\hbar}. \tag{54}$$

Substitute into the Schrödinger equation,

- To the *leading* (0th) order of $\hbar$, the **action function** $S(x, t)$ is governed by

$$\partial_t S(x,\, t) + \frac{1}{2\, m} (\partial_x S(x,\, t))^2 + V(x) = 0, \tag{55}$$

also known as the **Hamilton-Jacobi equation**.

- In general, given the **Hamiltonian function** $H(\boldsymbol{x},\, \boldsymbol{p},\, t)$ of the system, the *Hamilton-Jacobi equation* reads

  $$\partial_t S(\boldsymbol{x},\, t) + H(\boldsymbol{x},\, \nabla S(\boldsymbol{x},\, t),\, t) = 0. \tag{56}$$

  Eq. (55) is a special case of Eq. (56) for a particle moving in 1D with $H(x,\, p,\, t) = \frac{1}{2\, m}\, p^2 + V(x)$.

- Physical meaning of action derivatives:
  - **Energy**: (negative) rate of action accumulation in **time**

  $$E = -\partial_t S. \tag{57}$$

  - **Momentum**: action accumulation rate in **space** (along every direction), or the spatial *gradient* of action

  $$\boldsymbol{p} = \nabla S. \tag{58}$$

- To the *next leading* (1st) order of $\hbar$,

  $$\partial_t A(x,\, t) + \frac{1}{2\, m} \left(2\, \partial_x A(x,\, t)\, \partial_x S(x,\, t) + A(x,\, t)\, \partial_x^2 S(x,\, t)\right) = 0, \tag{59}$$

  which determines $A(x,\, t)$ from the solution of $S(x,\, t)$.

**Exc 5** Derive Eq. (55) and Eq. (59).

The WKB approach amounts to solving Eq. (55) and Eq. (59), then substitute the solution $S(x,\, t)$ and $A(x,\, t)$ into Eq. (54) to construct the approximate solution for the wavefunction $\psi(x,\, t)$.

## ▪ Solutions of Hamilton-Jacobi Equation

### ▫ Particle in the Free Space

For a particle moving in the free space, the potential will be flat

$$V(x) = 0. \tag{60}$$

Substitute into the Hamilton-Jacobi equation Eq. (55), depending on the initial condition

$$S(x,\, 0) = p\, x = m\, v_0\, x, \tag{61}$$

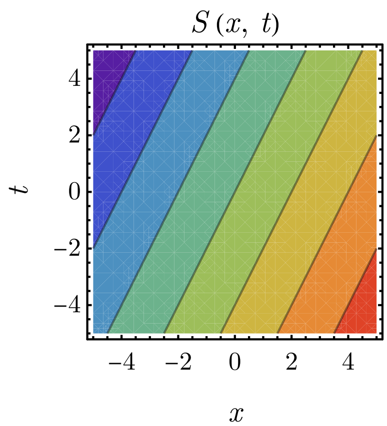
- $v_0$ is the initial **velocity** of the particle at time $t = 0$,
- $p = m\, v_0$ is the **momentum** of the particle, which will remain conserved,

the solution of $S(x, t)$ is

$$\boxed{\begin{aligned} S(x, t) &= p\,x - E\,t \\ &= m\,v_0\,x - \frac{1}{2}\,m\,v_0^2\,t, \end{aligned}} \tag{62}$$

- $E = \frac{1}{2\,m}\,p^2 = \frac{1}{2}\,m\,v_0^2$ is the (kinetic) **energy** of the particle.

  $S(x, t)$ looks like:




- The contours of $S(x, t)$ are wave fronts (equal-phase surface) in the spacetime.
- The solution $S(x, t)$ in Eq. (62) corresponds to a **plane wave** solution of the wavefunction

$$\boxed{\begin{aligned} \psi(x, t) &= e^{i\,S(x,t)/\hbar} \\ &= \exp\left(\frac{i}{\hbar}\,(p\,x - E\,t)\right). \end{aligned}} \tag{63}$$

  This turns out to be the *exact* solution of the Schrödinger equation for a free particle (the WKB approximation becomes exact in this case).

### ▫ Particle under a Constant Force

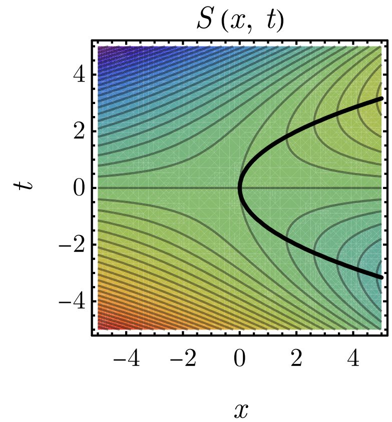
In a linear potential,

$$V(x) = -F\,x, \tag{64}$$

the particle will experience a constant force $F := -\partial_x V(x)$. Plugging $V(x)$ in the Hamilton-Jacobi equation Eq. (55),

$$\partial_t S + \frac{1}{2\,m}\,(\partial_x S)^2 + V(x) = 0, \tag{65}$$

the solution of $S(x, t)$ look like:




- In the $m \to \infty$ limit, $\partial_t S = -V(x)$, such that

$$S(x, t) = -V(x)\, t = F\, x\, t, \tag{66}$$

creating a growing spatial gradient of the action

$$p = \partial_x S = F\, t, \tag{67}$$

corresponding to a momentum that increases in time.

- When $m$ is finite, the kinetic energy $(\partial_x S)^2 / (2\, m)$ grows with the momentum $p = \partial_x S$, which also contributes to the total energy and alters the rate of action accumulation in time. ⇒ This leads to curvature in the constant-action contours, signaling acceleration in the particle's motion.

- The **classical trajectory** (in black) of the particle corresponds to the family of *stationary points* of $S(x, t)$ in the spacetime, which turns out to form a *parabola*

$$x = \frac{1}{2}\, a \left(t + \frac{v_0}{a}\right)^2. \tag{68}$$

  - $v_0 = \dot{x}(t = 0)$ is the initial **velocity** of the particle at time $t = 0$,
  - $a$ is the **acceleration** of the particle. It increases with $F$ and decreases with $m$, and can be verified to follow

$$a = \frac{F}{m}, \tag{69}$$

  which recovers **Newton's 2nd law** ($F = m\, a$).

## WKB Approximation (Time-Independent)

In the *time-independent* case, the **energy** $E$ is a *conserved* quantity, the action can be separated as

$$S(x, t) = W(x) - E\, t, \tag{70}$$

meaning that $\psi(x, t) = \psi(x)\, e^{-i\, E\, t/\hbar}$ with

$$\boxed{\psi(x) = A(x)\, e^{i\, W(x)/\hbar}.} \tag{71}$$

- The spatial part $W(x)$ of the action satisfies the *stationary* **Hamilton-Jacobi equation**, reduced from Eq. (55),

$$\frac{1}{2\, m} (\partial_x W(x))^2 + V(x) = E. \tag{72}$$

**Exc 6** Derive Eq. (72) from Eq. (55).

- Given a time-independent Hamiltonian $H(\boldsymbol{x}, \boldsymbol{p})$, a more general form of Eq. (72) is

$$H(\boldsymbol{x}, \nabla W(\boldsymbol{x})) = E. \tag{73}$$

- Eq. (72) can be solved by introducing the **momentum function** $p(x)$ — the rate that the action is accumulated in space,

$$\boxed{p(x) := \partial_x W(x),} \tag{74}$$

such that Eq. (72) becomes an algebraic equation

$$\frac{p(x)^2}{2\, m} + V(x) = E, \tag{75}$$

with the solution(s) given by

$$\boxed{p(x) = \pm \sqrt{2\, m\, (E - V(x))}\, .} \tag{76}$$

Then the solution of $W(x)$ can be reconstructed by integration

$$W(x) = \int^x p(x')\, d x' = \int^x \sqrt{2\, m\, (E - V(x'))}\; d x'. \tag{77}$$

- Eq. (59) also reduces to its stationary form

$$\partial_x \log A(x) = -\frac{1}{2}\, \partial_x \log p(x), \tag{78}$$

whose solution is

$$A(x) = \frac{C}{\sqrt{p(x)}}\, . \tag{79}$$

**Exc 7** Derive Eq. (78).

Putting Eq. (77) and Eq. (79) together into Eq. (71), the **WKB wavefunction** for a quantum state of energy $E$ is

$$\boxed{\psi(x) \approx \frac{C}{\sqrt{p(x)}} \exp\left(\frac{i}{\hbar} \int^{x} p(x')\, dx'\right),} \tag{80}$$

where $p(x) = \pm\sqrt{2\,m\,(E - V(x))}$ as in Eq. (76), and $C$ serves as the normalization constant for $\psi(x)$ to ensure $\int |\psi(x)|^2 = 1$.

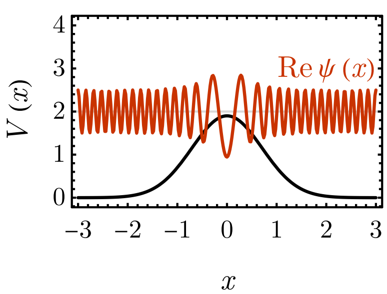
- **Classically allowed regions** ($V(x) < E$):
  - $p(x) \in \mathbb{R}$, the WKB wavefunction $\psi(x)$ exhibits *wavy* behavior.
  - Both $\pm$ solutions of $p(x)$ are valid, corresponding to *right-moving* and *left-moving* waves.
- **Classically forbidden regions** ($V(x) > E$):
  - $p(x) \in \mathbb{I}$, the WKB wavefunction $\psi(x)$ exhibits *exponential decay* (or *grow*) behavior

$$\psi(x) \approx \frac{C}{\sqrt{|p(x)|}} \exp\left(\mp \frac{1}{\hbar} \int^{x} |p(x')|\, dx'\right). \tag{81}$$

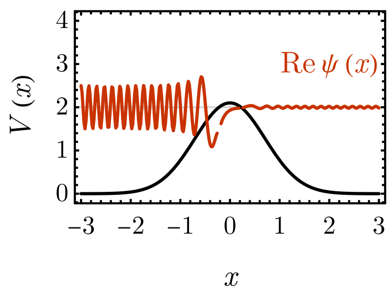
  - Only one of the $\pm$ solutions of $p(x)$ will be valid, which corresponding to the *decaying* wave, as the particle's probability density must diminish as it enters the classical forbidden regions. The invalid solution will correspond to an *growing* wave.
- **Transition region** ($V(x) \to E$): $p(x) \to 0$, the amplitude *diverges* as $p(x)^{-1/2}$, and the WKB wavefunction is *ill-defined*. Joining the WKB wave function across the transition region is a rather complicated task, more can be found in Ref. [1].

Examples of WKB approximations:

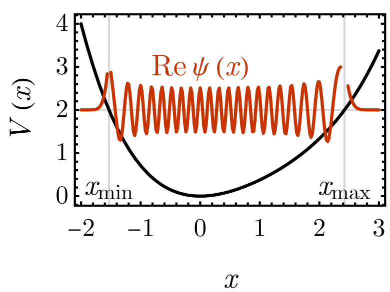
- **Scattering states**
  - **Quantum climbing**: the potential top is *lower* than the energy level $E$.




  - **Quantum tunneling**: the potential top is *higher* than the energy level $E$.




- **Bound state**: the potential grows higher than the energy level $E$ towards both sides.




  - $x_{\min}$, $x_{\max}$: two classical turning points, at which $E = V(x)$ and the particle will be bounced back in the classical limit.
  - Total **phase** acquired by the wavefunction between the classical turning points is given by

$$\Theta(x_{\min} \to x_{\max}) = \frac{1}{\hbar} W(x_{\min} \to x_{\max}), \tag{82}$$

where $W$ is the corresponding **action**,

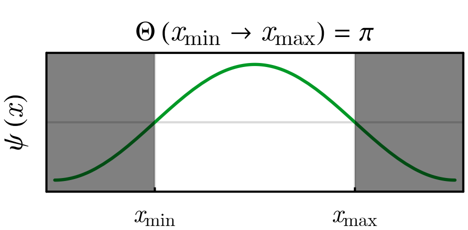
$$W(x_{\min} \to x_{\max}) = \int_{x_{\min}}^{x_{\max}} p(x)\, dx = \int_{x_{\min}}^{x_{\max}} \sqrt{2\, m\, (E - V(x))}\, dx. \tag{83}$$

[1] Wikipedia, WKB approximation.

## ■ Bohr-Sommerfeld Quantization

The WKB approximation can be used to estimate the bound state eigenenergies.

- Intuition: Consider a sine wave, with one node pinned to $x_{\min}$, how to pin another node to $x_{\max}$ by varying $\Theta(x_{\min} \to x_{\max})$?



- **Bohr-Sommerfeld quantization** condition: To confine the wave in the region $[x_{\min}, x_{\max}]$, we must *pin* the *wave nodes* on both turning points, which requires the *phase* acquired between the turning points to be an *integer* of $\pi$, i.e.

$$\boxed{\Theta(x_{\min} \to x_{\max}) = \frac{1}{\hbar} \int_{x_{\min}}^{x_{\max}} \sqrt{2\, m\, (E - V(x))}\, dx = n\, \pi,} \tag{84}$$

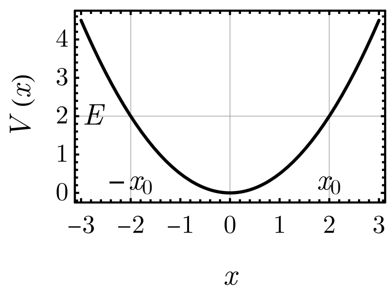
for $n = 1, 2, 3, \ldots$.

Example: Harmonic Oscillator

- Consider the potential

$$V(x) = \frac{1}{2}\, m\, \omega^2\, x^2. \tag{85}$$

  - $\omega$ - angular frequency of the oscillator.




- Let $\pm x_0$ be the turning points, at which $E = V(x)$, such that

$$E = \frac{1}{2}\, m\, \omega^2\, x_0^2. \tag{86}$$

- The Bohr-Sommerfeld quantization condition Eq. (84) requires

$$\frac{m\, \omega}{\hbar} \int_{-x_0}^{x_0} \sqrt{x_0^2 - x^2}\, dx = \frac{\pi\, m\, \omega\, x_0^2}{2\, \hbar} = n\, \pi, \tag{87}$$

  which sets $x_0^2 = 2\, n\, \hbar / (m\, \omega)$. By Eq. (86), the energy that correspond to such turning points is

$$E_n = n\, \hbar\, \omega, \tag{88}$$

  for $n = 1, 2, 3, \ldots$.

This predicts the **energy quantization** with the correct energy level spacing $\hbar\, \omega$. Compare with the exact eigenenergies

$$E_n = \left(n + \frac{1}{2}\right) \hbar\, \omega, \tag{89}$$

the only missing part is the **vacuum energy** $\frac{1}{2}\, \hbar\, \omega$, which requires more rigorous quantum treatment.

**HW 2**

Consider a potential where energy grows linearly with the distance of the particle from the origin:

$V(x) = F\,|x|,$

where $F$ is a constant with the unit of force. Use the Bohr-Sommerfeld quantization condition to estimate the energy levels in this potential. To which power do they scale with the level index $n$?