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).

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 .

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 <i>Optiks</i> , 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 <i>polarization</i> 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.	

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, α particles (⁴He 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.

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

• The optical path length is defined by

$$L(A \to B) = \int_{A}^{B} n \, ds, \tag{2}$$

where n is the **refractive index** of the medium and ds 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)

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

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

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

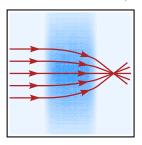
• Refraction (Snell's law)



• Total reflection



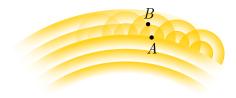
• Gradient-index (GRIN) optics



■ 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 ψ_B on the new wave front is determined by the amplitude ψ_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)

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

• The accumulated **phase** Θ is determined by the propagation time $T \times$ the frequency ω of

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

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

spacetime:
$$\psi(\mathbf{x}, t)$$
,
space (at fixed-time): $\psi(\mathbf{x})$. (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 x,

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

• Normalization: the wavefunction is said to be normalized, if

$$\int |\psi(\boldsymbol{x})|^2 d^D \boldsymbol{x} = \int p(\boldsymbol{x}) d^D \boldsymbol{x} = 1,$$
(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 \times time.

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

They are related by

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

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 $\overline{x}(t)$ is the one for which the action is stationary (to first order), subject to boundary conditions: $\overline{x}(t_0) = x_0$ (initial) and $\overline{x}(t_1) = x_1$ (final).

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

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 $\overline{x}(t)$ 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.

For a non-relativistic free particle $L = (m/2) \dot{x}^2$.

(i) Show that the stationary (classical) action $S[\overline{x}]$ corresponding to the classical motion of a free particle travelling from (x_0, t_0) to (x_1, t_1) is $S[\overline{x}] = \frac{m}{2} \frac{(x_1 - x_0)^2}{t_1 - t_0}$.

For this case of the free particle,

- (ii) Show that the spatial derivative of the action $\partial_{x_1} S[\overline{x}]$ is the momentum of the particle.
- (iii) Show that the (negative) temporal derivative of the action $-\partial_{t_1} S[\overline{x}]$ is the energy of the particle.

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

HW 1 any computer).

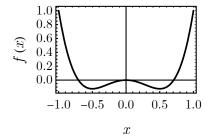
- Nature may not have sufficient computational resources to carry out the classical mechanics precisely. \Rightarrow Classical mechanics might actually be realized only approximately as a **stochastic** global optimization, which is computationally more feasible.
- Quantum mechanics takes a *stochastic* 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

$$f(x) = -x^2 + 2x^4. (14)$$



- 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): $e^{i f(x)/\hbar} \Rightarrow$ 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? \Rightarrow Well, we need to analyze how Z is accumulated. Each infinitesimal step in the integral \rightarrow 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,

 \bullet displacement dz is accumulated to form the partition function,

$$Z = \int dz. \tag{17}$$

Let us see how the partition function is constructed.

• For small h (classical limit)

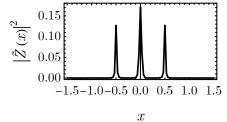
$$h = 0.001$$
 $Z_{-1/2}$
 Z_{0}
 $Z_{1/2}$

$$Z = Z_{-1/2} + Z_0 + Z_{1/2}, (18)$$

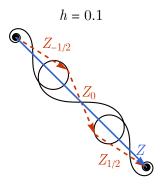
- Z can break up into three smaller contributions, which correspond to the contributions around the three stationary points: $x = 0, \pm 1/2$.
- Around the stationary point, phase changes slowly $\partial_x f(x) \sim 0 \Rightarrow$ constructive interference $\Rightarrow large$ contribution to the partition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

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

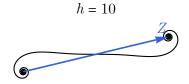
Then its Fourier spectrum $\tilde{Z}(x)=\int\!\!d\,k\,Z(k)\,e^{-i\,k\,x}$ will reveal the saddle points.



 \bullet For intermediate h



- The decomposition of Z into three subdominant amplitudes is not very well defined. \Rightarrow 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.

$$h = 6.62607004 \times 10^{-34} \,\mathrm{J}\,\mathrm{s}.$$
 (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) \Rightarrow our nature has a pretty high resolution of action \Rightarrow no need to worry about the resolution limit in the macroscopic world \Rightarrow classical mechanics works well.
- However, in the microscopic world, nature's resolution limit can be approached \Rightarrow "round-off error" may occur \Rightarrow one consequence is the quantization of atomic orbitals (discrete energy levels etc.).

■ Path Integral and Wave Function

Feynman's principles:

• 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**

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

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



$$K_{A\to B} \propto \int_{A\to B} \mathcal{D}[x] e^{iS[x]/\hbar}.$$
 (22)

• The contribution of each particular path is *proportional* to $e^{iS[x]/\hbar}$, 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,

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

$$K_{A\to B} = \int_C K_{A\to C} K_{C\to B}.$$
 (24)

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

$$K_{(x_0,t_0)\to(x_N,t_N)} = \int dx_1 \dots dx_{N-1} K_{(x_0,t_0)\to(x_1,t_1)} \dots K_{(x_{N-1},t_{N-1})\to(x_N,t_N)}.$$
(25)

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

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

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

 $K_{(x_0,t_0)\to(x_N,t_N)} = \psi(x_N, t_N)$. \Rightarrow 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),

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

this path integral involves multiple integrals:

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

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

$$\psi(x_1, t + \delta t) \propto \int dx_0 \exp\left(\frac{i}{\hbar} S[x]\right) \psi(x_0, t)$$

$$= \int dx_0 \exp\left(\frac{i m}{2 \hbar \delta t} (x_1 - x_0)^2\right) \psi(x_0, t).$$
(32)

• The proportional sign "\infty" 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,

$$\psi(x_0, t) = \psi(x_1 + a, t)
= \psi(x_1, t) + a \psi'(x_1, t) + \frac{a^2}{2!} \psi''(x_1, t) + \frac{a^3}{3!} \psi^{(3)}(x_1, t) + \dots
= \sum_{n=0}^{\infty} \frac{a^n}{n!} \partial_{x_1}^n \psi(x_1, t).$$
(33)

Substitute into Eq. (32),

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

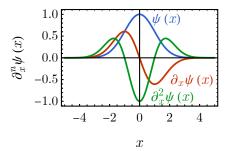
We pack everything related to the integral of a into a coefficient

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

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

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

• 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 λ_n

The λ_n coefficient can be computed by *Mathematica*

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

Evaluate the integral in Eq. (35) for λ_n .

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

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

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

• For even n, the first several λ_n are given by

$$\lambda_{0} = \sqrt{\pi} \left(-\frac{i m}{2 \hbar \delta t} \right)^{-1/2},$$

$$\lambda_{2} = \frac{\sqrt{\pi}}{4} \left(-\frac{i m}{2 \hbar \delta t} \right)^{-3/2} = \frac{i}{4} \left(\frac{2 \hbar \delta t}{m} \right) \lambda_{0},$$

$$\lambda_{4} = \frac{\sqrt{\pi}}{32} \left(-\frac{i m}{2 \hbar \delta t} \right)^{-5/2} = -\frac{1}{32} \left(\frac{2 \hbar \delta t}{m} \right)^{2} \lambda_{0},$$
(39)

Compute the first several λ_n for even integer n using Eq. (37).

■ Determining the Normalization

Plugging the results of λ_n in Eq. (39) into Eq. (36), we get

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

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

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

So obviously, the normalization factor should be such to cancelled out λ_0 .

So we should actually write (in equal sign) that

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

■ Taking the Limit of $\delta t \rightarrow 0$

Let us consider the time derivative of the wavefunction

$$\partial_{t}\psi(x, t) = \lim_{\delta t \to 0} \frac{\psi(x, t + \delta t) - \psi(x, t)}{\delta t}$$

$$= \lim_{\delta t \to 0} \frac{1}{\delta t} \left(\frac{i}{4} \left(\frac{2 \hbar \delta t}{m} \right) \partial_{x}^{2} - \frac{1}{32} \left(\frac{2 \hbar \delta t}{m} \right)^{2} \partial_{x}^{4} + \dots \right) \psi(x, t)$$
(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 δt , so they should all vanish under the limit $\delta t \to 0$.

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

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

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

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

The additional action that will be accumulated over time δt will be

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

Eventually this cause an additional phase shift in the wavefunction

$$\psi(x, t + \delta t) = e^{i \Delta S/\hbar} \psi_0(x, t + \delta t)$$

$$= e^{-i V(x) \delta t/\hbar} \psi_0(x, t + \delta t)$$

$$= \left(1 - \frac{i}{\hbar} V(x) \delta t + \dots\right) \psi_0(x, t + \delta t),$$
(48)

where ψ_0 is the expected wavefunction at $t + \delta t$ without the potential. Combining with the result in Eq. (42), to the first order of δt we have

$$\psi(x, t + \delta t) = \left(1 - \frac{i}{\hbar} V(x) \delta t + \dots\right) \left(1 + \frac{i}{4} \left(\frac{2 \hbar \delta t}{m}\right) \partial_x^2 + \dots\right) \psi(x, t)$$

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

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

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

Exc d 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

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

Substitute into the Schrödinger equation,

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

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

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

• In general, given the **Hamiltonian function** H(x, p, t) of the system, the *Hamilton-Jacobi* equation reads

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

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

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

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

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

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

• To the next leading (1st) order of \hbar ,

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

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

Exc

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

$$V(x) = 0. ag{60}$$

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

$$S(x, 0) = p x = m v_0 x, (61)$$

- 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,

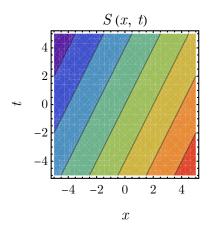
the solution of S(x, t) is

$$S(x, t) = p x - E t$$

$$= m v_0 x - \frac{1}{2} m v_0^2 t,$$
(62)

• $E = \frac{1}{2m} p^2 = \frac{1}{2} m v_0^2$ 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

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

$$= \exp\left(\frac{i}{\hbar} (p x - E t)\right).$$
(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

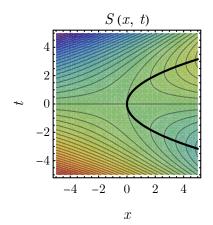
In a linear potential,

$$V(x) = -F x, (64)$$

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

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

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



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

$$S(x, t) = -V(x) t = F x t,$$
 (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 $(\partial_x S)^2/(2m)$ grows with the momentum $p = \partial_x S$, which also contributes to the total energy and alters the rate of action accumulation in time. \Rightarrow 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

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

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

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

Derive Eq. (72) from Eq. (55).

• Given a time-independent Hamiltonian H(x, p), a more general form of Eq. (72) is $H(\boldsymbol{x}, \nabla W(\boldsymbol{x})) = E.$ (73)

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

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

such that Eq. (72) becomes an algebraic equation

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

with the solution(s) given by

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

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

$$W(x) = \int_{-\infty}^{x} p(x') dx' = \int_{-\infty}^{x} \sqrt{2 m (E - V(x'))} dx'.$$
 (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

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

Derive Eq. (78).

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

$$\psi(x) \approx \frac{C}{\sqrt{p(x)}} \exp\left(\frac{i}{\hbar} \int_{-\pi}^{x} p(x') dx'\right),$$
(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 $\int |\psi(x)|^2 = 1$.

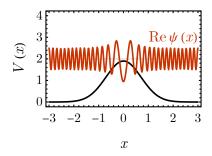
- Classically allowed regions (V(x) < E):
 - $p(x) \in \mathbb{R}$, the WKB wavefunction $\psi(x)$ exhibits wavy behavior.
 - Both \pm solutions of p(x) are valid, corresponding to right-moving and left-moving waves.
- Classically forbidden regions (V(x) > E):
 - $p(x) \in \mathbb{I}$, the WKB wavefunction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

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

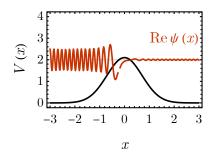
- Only one of the \pm solutions of p(x) will be valid, which corresponding to the *decaying* wave, as the particle's probability density must diminish as it enters the classical forbidden regions. The invalid solution will correspond to an *growing* wave.
- Transition region $(V(x) \to E)$: $p(x) \to 0$, 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:

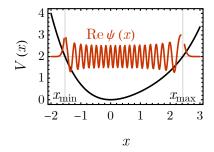
- Scattering states
 - Quantum climbing: the potential top is *lower* than the energy level E.



• 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**,

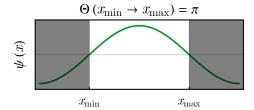
$$W(x_{\min} \to x_{\max}) = \int_{x_{\min}}^{x_{\max}} p(x) \, dx = \int_{x_{\min}}^{x_{\max}} \sqrt{2 \, m \, (E - V(x))} \, dx. \tag{83}$$

[1] Wikipedia, WKB approximation.

■ Bohr-Sommerfeld Quantization

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

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



• 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 π , i.e.

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

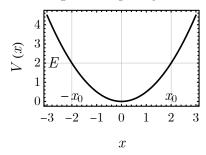
for n = 1, 2, 3, ...

Example: Harmonic Oscillator

• Consider the potential

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

• ω - 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, ...

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.

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?

Path Integral with Gauge Background

■ Gauge Structure and Berry Phase

■ Phase Ambiguities

At its core, quantum mechanics is a **probability theory**. It postulate to model the probability density p(x) by a squared norm

$$p(\mathbf{x}) = |\psi(\mathbf{x})|^2,\tag{90}$$

just to ensure the positive semi-definite property $p(x) \ge 0$.

The wavefunction $\psi(x)$ itself serves as a mathematical parameter of the probability model, not a physical observable, and is therefore subject to some degree of ambiguity or redundancy.

• Global phase ambiguity. A global phase rotation of the wavefunction (where "global" means α does not depend on x)

$$\psi(x) \to e^{i\alpha} \, \psi(x) \tag{91}$$

has no consequence on the expectation value $\langle O \rangle$ of any physical observable O in any case

$$\langle O \rangle = \int \psi^*(\mathbf{x}) \ O(\mathbf{x}, \mathbf{x}') \, \psi(\mathbf{x}') \, d^D \mathbf{x} \, d^D \mathbf{x}'. \tag{92}$$

Conclusion: quantum states \in projective Hilbert space, where global phase is always unphysical.

• Local phase ambiguity (Gauge redundancy). We can push this idea further: if we restrict ourself to diagonal observables in the position basis, i.e., functions f(x) that depends only on \boldsymbol{x} (but not \boldsymbol{p}), then any local phase rotation

$$\psi(x) \to e^{i\chi(x)} \psi(x) \tag{93}$$

will leave all expectation values $\langle f(x) \rangle$ invariant,

$$\langle f(\boldsymbol{x}) \rangle := \int f(\boldsymbol{x}) |\psi(\boldsymbol{x})|^2 d^D \boldsymbol{x} = \int f(\boldsymbol{x}) p(\boldsymbol{x}) d^D \boldsymbol{x}$$
 (94)

since the probability density $p(\mathbf{x})$ is unchanged.

- If $p(\mathbf{x}) = |\psi(\mathbf{x})|^2$ was the only *physical* probability distribution to be modeled, any $\psi(\mathbf{x})$ related by *local* phase rotation Eq. (93) should be treated as *equivalent*.
- This represents a **gauge redundancy**: multiple mathematical descriptions (e.g. wavefunctions) describing the same physical reality (e.g. position distribution).

Quantum decoherence gives the deeper reason of why only *diagonal* observables are measurable.

- Environmental monitoring: The environment has a natural tendency to monitor the local density p(x) of particles in the space.
 - Effectively performing weak continuous measurement of x.
 - Inducing **decoherence** in the position basis: rapid decay of *off-diagonal* coherence $\rho(x, x')$ of the density matrix for $x \neq x'$.
- Consequence 1: **Dephasing noise**.
 - The measurement randomizes the **phase** of $\psi(x)$ at every position independently.
 - Relative phase between $\psi(x)$ and $\psi(x')$ no longer comparable, allowing *local* phase rotation as Eq. (93) to become a *redundancy*.
- Consequence 2: Gauge projection.
 - The measurement *collapse* the system towards the **particle number** eigenstates, suppressing the *number fluctuations*.
 - Effectively imposing a gauge constraint (like Gauss law), that couples the particle to an emergent gauge field, allowing particles to interact with each other through emergent gauge forces.

■ Gauge Transformation

If the gauge freedom is an (emergent) redundancy, it should have no physical consequence. For example, it should not affect the **quantum dynamics** governed by the **Schrödinger equation**.

However, the standard Schrödinger equation is *not* invariant under the **gauge** transformation

$$\psi(x, t) \to e^{i\chi(x,t)} \psi(x, t), \tag{95}$$

unless we modify it appropriately.

• Start from the free Schrödinger equation

$$i \,\hbar \,\partial_t \psi(\boldsymbol{x}, \, t) = -\frac{\hbar^2}{2 \, m} \,\nabla^2 \psi(\boldsymbol{x}, \, t), \tag{96}$$

under gauge transformation $\psi \to e^{i\chi} \psi$ in Eq. (95), the derivative operators picks up extra terms involving $\partial_t \chi$ and $\nabla \chi$,

$$i \hbar (\partial_t + i \partial_t \chi(\mathbf{x}, t)) \psi(\mathbf{x}, t) = -\frac{\hbar^2}{2 m} (\nabla + i \nabla \chi(\mathbf{x}, t))^2 \psi(\mathbf{x}, t), \tag{97}$$

and the equation does *not* remain invariant.

Show that Eq. (96) becomes to Eq. (97) under gauge transformation.

- To restore the **gauge invariance**, we introduce **gauge fields**:
 - Scalar potential: $\Phi(x, t)$ a scalar field in the spacetime
 - Vector potential: A(x, t) a vector field in the spacetime and replace derivatives by **covariant derivatives**:

$$\partial_{t} \to D_{t} := \partial_{t} + \frac{i}{\hbar} \Phi(\boldsymbol{x}, t),$$

$$\nabla \to \boldsymbol{D} := \nabla - \frac{i}{\hbar} \boldsymbol{A}(\boldsymbol{x}, t),$$
(99)

Then Eq. (96) can be recast into the gauge-invariant Schrödinger equation

$$i\hbar D_t \psi(\boldsymbol{x}, t) = \frac{1}{2m} (-i\hbar \boldsymbol{D})^2 \psi(\boldsymbol{x}, t), \tag{100}$$

or more explicitly,

$$i \hbar \partial_t \psi(\boldsymbol{x}, t) = \left(\frac{1}{2 m} \left(-i \hbar \nabla - \boldsymbol{A}(\boldsymbol{x}, t)\right)^2 + \Phi(\boldsymbol{x}, t)\right) \psi(\boldsymbol{x}, t). \tag{101}$$

Under gauge transformation, the wavefunction ψ and the gauge fields (Φ, A) must transform together as

$$\psi(\boldsymbol{x}, t) \to e^{i\chi(\boldsymbol{x}, t)} \psi(\boldsymbol{x}, t),$$

$$\Phi(\boldsymbol{x}, t) \to \Phi(\boldsymbol{x}, t) - \partial_t \chi(\boldsymbol{x}, t),$$

$$\boldsymbol{A}(\boldsymbol{x}, t) \to \boldsymbol{A}(\boldsymbol{x}, t) + \nabla \chi(\boldsymbol{x}, t),$$
(102)

to ensure the covariance of the quantum dynamics.

■ Semiclassical Interpretation

In the WKB approximation Eq. (54), we write the wavefunction as $\psi = A e^{i S/\hbar}$. (103)

Plugging the WKB ansatz into the gauge-invariant Schrödinger equation Eq. (100) yields:

$$(-\partial_t S - \Phi) = \frac{1}{2m} (\nabla S - \mathbf{A})^2. \tag{104}$$

Given that the spacetime derivatives of the action S is associated to **energy** $E = -\partial_t S$ and **momentum** $p = \nabla S$, Eq. (104) can be written as

$$(E - \Phi) = \frac{1}{2m} (\mathbf{p} - \mathbf{A})^2. \tag{105}$$

This reveals the physical meaning of gauge fields:

- Scalar potential Φ: **potential energy**,
- Vector potential A: potential momentum.

Note: Energy and Momentum each have three distinct forms

$$\frac{|\text{Total} = \text{Kinetic} + \text{Potential}|}{|\text{Energy}|} E = \frac{1}{2} m \dot{x}^2 + \Phi \qquad (106)$$
Momentum $|p| = m \dot{x} + A$

Exc g Show that both equations in Eq. (106) are consistent with Eq. (105).

- **Total** (or **Canonical**): appear directly in *conservation laws* and determine the *action* accumulated in spacetime.
- **Kinetic**: directly linked to the particle's motion (velocity \dot{x}).
- Potential: exist independently of particle motion, contributing even when the particle is at rest $(\dot{x} = 0)$, representing the interaction with the background field in the spacetime.

Question: What are their dynamical consequences?

Newton's 2nd law — the force F causes the kinetic momentum $(m \dot{x})$ to change in time:

$$\mathbf{F} = \frac{d}{dt}(m\,\dot{\mathbf{x}}) = \frac{d\,\mathbf{p}}{dt} - \frac{d\,\mathbf{A}}{dt}\,,\tag{107}$$

in two distinct ways:

- $d \mathbf{p} / d t = \partial_t \mathbf{p} + \dot{\mathbf{x}} \cdot \nabla \mathbf{p}$, in which
 - $\nabla p = 0$, as x and p are independent variables,
 - Maxwell relation: $\partial_t \nabla S = \nabla \partial_t S$ implies

$$\partial_t \mathbf{p} = -\nabla E = (\nabla \mathbf{A}) \cdot \dot{\mathbf{x}} - \nabla \Phi. \tag{108}$$

• $d\mathbf{A}/dt = \partial_t \mathbf{A} + \dot{\mathbf{x}} \cdot \nabla \mathbf{A}$.

Put together, F takes the form as an electromagnetic force

$$F = -\nabla \Phi - \partial_t \mathbf{A} + (\nabla \mathbf{A}) \cdot \dot{\mathbf{x}} - \dot{\mathbf{x}} \cdot \nabla \mathbf{A}$$

$$= \mathbf{E} + \dot{\mathbf{x}} \times \mathbf{B},$$
(109)

as long as we define

$$E = -\nabla \Phi - \partial_t \mathbf{A},$$

$$B = \nabla \times \mathbf{A}.$$
(110)

Justify Eq. (108) and Eq. (109).

Obviously, E and B should be interpreted as **electric** and **magnetic** fields, allowing F to be consistently identified as the force exerted by the electromagnetic field on a charged particle.

Conclusion: Gauge fields (Φ, A) are not merely mathematical constructs to maintain gauge invariance; they give rise to the physical electromagnetic interactions among quantum particles. Remarkably, the **electromagnetic forces** familiar from our everyday classical experience emerge profoundly from the **local phase ambiguity** of matter at the *quantum* level.

■ Math Interlude: Lorentz Vectors

It is more convenient to unify time and space, as well as energy and momentum.

- Spacetime: Introduce $x = (x^0, x^1, x^2, x^3)$ to denote the coordinate of a spacetime point,
 - $t = x^0$: time,
 - $x = (x^1, x^2, x^3)$: space,

and denote these components as $x^{\mu}(\mu = 0, 1, 2, 3)$ jointly. x is said to be a **Lorentz vector**.

• Spacetime derivatives: Partial derivatives in the spacetime are defined as

$$\partial_{\mu} f(x) = \lim_{\delta x \to 0} \frac{f(x + \delta x) - f(x)}{\delta x^{\mu}},\tag{111}$$

- $\partial_t = \partial_0$: temporal derivative,
- $\nabla = (\partial_1, \partial_2, \partial_3)$: spatial derivatives.
- Energy-momentum: Introduce $p = (p^0, p^1, p^2, p^3)$ to denote the energy and momentum,
 - $E = p^0 = -p_0$: energy,
 - $p = (p^1, p^2, p^3) = (p_1, p_2, p_3)$: momentum.
- Gauge field: Introduce $A = (A^0, A^1, A^2, A^3)$ to denote the gauge field,
 - $\Phi = A^0 = -A_0$: scalar potential,
 - $A = (A^1, A^2, A^3) = (A_1, A_2, A_3)$: vector potential.

• Covariant derivatives: Operators in Eq. (99) can now be unified as a single Lorentz vector operator

$$D_{\mu} = \partial_{\mu} - \frac{i}{\hbar} A_{\mu},\tag{112}$$

- $D_t = D_0$: covariant temporal derivative,
- $D = (D_1, D_2, D_3)$: covariant spatial derivative.

Raising and **lowering** the index of a Lorentz vector is done by the **Lorentz metric** $g_{\mu\nu}$ or $g^{\mu\nu}$,

$$a_{\mu} = g_{\mu\nu} \ a^{\nu}, \ a^{\mu} = g^{\mu\nu} \ a_{\nu},$$
 (113)

where *repeated* indices are automatically summed over (**contracted**) following the **Einstein** sum rule. The Lorentz metric is given by

$$g_{\mu\nu} = g^{\mu\nu} = \text{diag}(-1, +1, +1, +1). \tag{114}$$

Rule of thumb: In index contraction, the *upper* index can only contract with the *lower* index and vice versa.

$$a^{\mu} b_{\mu} \checkmark \text{ ok}$$
 $a^{\mu} b^{\mu} \times \text{no!}$
 $a_{\mu} b_{\mu} \times \text{no!}$

More explicitly, the following expressions are all valid and equal

$$a^{\mu} b_{\mu} = a^{0} b_{0} + a^{1} b_{1} + a^{2} b_{2} + a^{3} b_{3}$$

$$= a^{\mu} g_{\mu\nu} b^{\nu} = -a^{0} b^{0} + a^{1} b^{1} + a^{2} b^{2} + a^{3} b^{3}$$

$$= a_{\mu} g^{\mu\nu} b_{\nu} = -a_{0} b_{0} + a_{1} b_{1} + a_{2} b_{2} + a_{3} b_{3}.$$
(115)

■ Berry Phase

Berry phase is the *phase* accumulated by the wavefunction as a particle travels through the spacetime *adiabatically*.

• A processes is said to be **adiabatic**, if it happens *slowly* over a long time, i.e. the rates of change in physical observables tend to zero. In terms of the motion of a particle, it means the *velocity* of the particle is *almost zero* throughout the process:

$$\dot{x} \to 0.$$
 (116)

Eq. (116) is also called the adiabatic limit.

• In the adiabatic limit, the **action** of the particle is accumulated by the **potential** energy and momentum

$$-\partial_t S = E = \Phi,$$

$$\nabla S = \mathbf{p} = \mathbf{A}.$$
(117)

as the kinetic energy and momentum vanishes when $\dot{x} \to 0$.

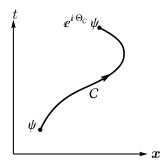
• Given that phase is related to action, the **Berry phase** that a particle accumulates along a spacetime trajectory C is given by the **path integral** that computes the accumulated action

$$\Theta_C = \frac{S_C}{\hbar} = \frac{1}{\hbar} \int_C -\Phi \, dt + \mathbf{A} \cdot d\mathbf{x} = \frac{1}{\hbar} \int_C A_\mu \, dx^\mu. \tag{118}$$

Justify Eq. (118).

Such that adiabatically propagating the wave amplitude ψ along trajectory $\mathcal C$ will acquire the Berry phase shift:

$$\psi \stackrel{C}{\to} e^{i\Theta_C} \psi = \exp\left(\frac{i}{\hbar} \int_C A_\mu \, dx^\mu\right) \psi. \tag{119}$$



• For infinitesimal transportation $C: x \to x + \delta x$,

$$\psi \to e^{\frac{i}{\hbar} A_{\mu} \delta x^{\mu}} \psi. \tag{120}$$

• Under gauge transformation

$$A_{\mu}(x) \to A_{\mu}(x) + \partial_{\mu} \chi(x),$$
 (121)

• the Berry phase along an **open trajectory** C is not gauge invariant (hence not a physical observable):

$$\Theta_C \to \Theta_C + \chi(x_{\text{end}}) - \chi(x_{\text{start}}),$$
 (122)

where x_{start} , $x_{\text{end}} = \partial C$ are the starting and ending point of C.

• the Berry phase around a **closed loop** (Wilson loop) is gauge invariant, and is a physical observable.

■ Gauge Field and Electrodynamics

■ Gauge Connection

Previously, we have introduced the covariant derivative D_{μ} to make the Schrödinger equa-

tion gauge invariant, but is there a deeper motivation behind this? In calculus, the **derivative** of a function tells us how much the function changes between nearby points

$$\partial_x f(x) = \lim_{\delta x \to 0} \frac{f(x + \delta x) - f(x)}{\delta x}.$$
 (123)

But this assumes we can *compare* the values of the function at different points directly.

• Problem: If the wavefunction $\psi(x)$ has local phase ambiguity,

$$\psi(x) \to e^{i\chi(x)} \psi(x), \tag{124}$$

meaning that $\psi(x)$ at each point x is defined up to a phase rotation, there will be no basis to compare wavefunctions between distinct points.

There is a similar issue in **finance**: you cannot directly compare currencies from different countries by their face values!

• Are the following amounts of money the same?



• You should first move (parallel transport) the money to the same place before comparing.

During the conversion, the money will be multiplied by the *exchange rate* (exponential gauge connection), e.g.

$$e^{0.076961} \in 100 = \$108, \ e^{-2.01741} \, \$100 = \$13.3.$$
 (125)

• Solution: Similarly, to define a meaningful derivative for the wavefunction, we have to introduce a **gauge connection** $A_{\mu}(x)$ to keep track of the *phase rotation* needed to transport $\psi(x+\delta x)$ back to the point x for comparison, for every point x along any direction μ .

This allows us to (re)define the **covariant derivative**:

$$D_{\mu} \psi(x) = \lim_{\delta x \to 0} \frac{e^{-\frac{i}{\hbar} A_{\nu}(x) \, \delta x^{\nu}} \, \psi(x + \delta x) - \psi(x)}{\delta \, x^{\mu}}. \tag{126}$$

- Interpretation: $\psi(x + \delta x)$ has accumulated a Berry phase of $\exp(\frac{i}{\hbar} A_{\nu}(x) \delta x^{\nu})$ compare to $\psi(x)$ as the particle travels adiabatically. So when pulling $\psi(x + \delta x)$ back to the point x, this phase should be compensated by the opposite phase factor $\exp(-\frac{i}{\hbar} A_{\nu}(x) \delta x^{\nu})$ before comparing.
- Expressed in terms of the usual partial derivative modified by the gauge connection,

$$D_{\mu} = \partial_{\mu} - \frac{i}{\hbar} A_{\mu}(x), \tag{127}$$

which exactly reproduces Eq. (112).

Show Eq. (127) follows from Eq. (126) by taking the limit.

• The covariant derivative commute with the gauge transformation

$$\psi(x) \to e^{i\chi(x)} \psi(x),$$

$$A_{\mu}(x) \to A_{\mu}(x) + \partial_{\mu}\chi(x),$$
(128)

as adapted from Eq. (102).

• The apparent deformation of the wavefunction ψ from x to $x + \delta x$ can be expressed as

$$\psi(x+\delta x) = e^{\frac{i}{\hbar}A_{\mu}(x)\delta x^{\mu}} e^{\delta x^{\mu}D_{\mu}} \psi(x), \tag{129}$$

which contains two contributions

- the intrinsic deformation under parallel transport $\psi \to e^{\delta x^{\mu} D_{\mu}} \psi$, which is generated by the covariant derivative D_{μ} ,
- the **background** deformation in terms of the Berry phase $\psi \to e^{(i/\hbar) A_{\mu}(x) \delta x^{\mu}} \psi$ accumulated along the gauge connection A_{μ} .

■ Gauge Curvature

Exchanging currencies in cycles typically results in a loss. Why?



Because the global foreign exchange market is not flat—the mismatch around a closed loop is a measure of curvature.

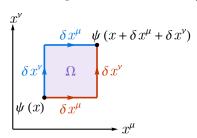
In gauge theory, the gauge curvature $F_{\mu\nu}$ measures the adiabatic action accumulated per area when transporting the wavefunction around the area boundary in spacetime.

$$S = \oint_{\partial \Omega} A_{\mu} \, dx^{\mu} = \int_{\Omega} F_{\mu\nu} \, dx^{\mu} \, dx^{\nu}. \tag{130}$$

• Operational definition: Mathematically, the gauge curvature $F_{\mu\nu}$ is defined by the commutator of covariant derivatives

$$[D_{\mu}, D_{\nu}] \psi = -\frac{i}{\hbar} F_{\mu\nu} \psi, \tag{131}$$

which measures the amount of non-commutativity to transport the wavefunction along two distinct spacetime directions μ and ν .



Exc

Using Eq. (129), prove Eq. (131) by comparing the above two paths to transport $\psi(x)$ to $\psi(x + \delta x^{\mu} + \delta x^{\nu})$.

• Physical meaning: In electromagnetism, $F_{\mu\nu}$ corresponds to the electromagnetic field strength tensor,

$$F_{\mu\nu} = \partial_{\mu} A_{\nu} - \partial_{\nu} A_{\mu}. \tag{132}$$

Exc

Derive Eq. (132) from Eq. (131).

• Electric field: $\boldsymbol{E} = (E^1, E^2, E^3)$, with $E^i := -F_{0i}$.

$$\boldsymbol{E} = -\nabla \Phi - \partial_t \boldsymbol{A}. \tag{133}$$

• Magnetic field: $\mathbf{B} = (B^1, B^2, B^3)$, with $B^i := \frac{1}{2} \epsilon^{ijk} F_{jk}$.

$$B = \nabla \times A. \tag{134}$$

Exc

Check that \boldsymbol{E} and \boldsymbol{B} are gauge invariant. Therefore, they are physical observables.

■ Particle in Gauge Field

In quantum mechanics, the time-evolution is generated by the Hamiltonian operator \hat{H} .

• Schrödinger picture: state evolves in time, operator remains fixed.

$$i \,\hbar \,\partial_t \psi = \hat{H} \,\psi. \tag{135}$$

• **Heisenberg picture**: operator evolves in time, state remains fixed.

$$i \,\hbar \,\partial_t \,\hat{O} = \left[\,\hat{O}, \,\hat{H} \,\right]. \tag{136}$$

Note: Eq. (136) assumes \hat{O} has no explicit time dependence, if not, its explicit time derivative will also contribute to the rate of change of \hat{O} .

Compare Eq. (135) with Eq. (101), we conclude that the Hamiltonian of the gauge-invariant Schrödinger equation is

$$\hat{H}(\hat{\boldsymbol{x}},\,\hat{\boldsymbol{p}},\,t) = \frac{1}{2\,m} \left(\hat{\boldsymbol{p}} - \hat{\boldsymbol{A}}(\hat{\boldsymbol{x}},\,t)\right)^2 + \hat{\Phi}(\hat{\boldsymbol{x}},\,t),\tag{137}$$

where

- \hat{x} is the coordinate operator.
- $\hat{p} = -i \hbar \nabla$ is the momentum operator.
- They satisfy the canonical commutation relation

$$\begin{bmatrix} \hat{x}_i, \, \hat{p}_j \end{bmatrix} = i \, \hbar \, \delta_{ij} \, \mathbb{I}.$$
Exc 16 Verify Eq. (138).

• $\hat{\Phi}$ and \hat{A} are operator functions (of \hat{x}) that also has explicit time dependence.

Using the Heisenberg equation Eq. (136), we can compute time derivatives of the particle position operator \hat{x}

• 1st order (velocity operator)

$$\partial_t \hat{\boldsymbol{x}} = \frac{1}{i \, \hbar} [\hat{\boldsymbol{x}}, \, \hat{H}] = \frac{\hat{\boldsymbol{p}} - \hat{\boldsymbol{A}}}{m} \,. \tag{139}$$

• 2nd order (acceleration operator)

$$\partial_t^2 \hat{\boldsymbol{x}} = -\frac{1}{m} \, \partial_t \hat{\boldsymbol{A}} + \frac{1}{i \, \hbar} \left[\partial_t \hat{\boldsymbol{x}}, \, \hat{H} \right]$$

$$= \frac{1}{m} \left(\hat{\boldsymbol{E}} + \frac{1}{2} \left(\partial_t \hat{\boldsymbol{x}} \times \hat{\boldsymbol{B}} - \hat{\boldsymbol{B}} \times \partial_t \hat{\boldsymbol{x}} \right) \right),$$
(140)

where $\hat{\boldsymbol{E}}$ and $\hat{\boldsymbol{B}}$ operators are defined by

$$\hat{\boldsymbol{E}} = -\nabla \hat{\boldsymbol{\Phi}} - \partial_t \hat{\boldsymbol{A}},$$

$$\hat{\boldsymbol{B}} = \nabla \times \hat{\boldsymbol{A}}.$$
(141)

Derive Eq. (139) and Eq. (140).

Eq. (140) describes the quantum dynamics of a charged particle in an electromagnetic field in the Heisenberg picture:

$$m \,\partial_t^2 \,\hat{\boldsymbol{x}} = \hat{\boldsymbol{E}} + \frac{1}{2} \left(\partial_t \,\hat{\boldsymbol{x}} \times \hat{\boldsymbol{B}} - \hat{\boldsymbol{B}} \times \partial_t \,\hat{\boldsymbol{x}} \right). \tag{142}$$

In contrast, the **classical dynamics** is described by

$$m \ddot{x} = F = E + \dot{x} \times B, \tag{143}$$

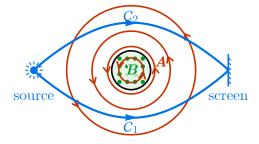
where all quantities commute. In the quantum case, however, $\partial_t \hat{x}$ and \hat{B} generally do not commute, so their cross product must be symmetrized as in Eq. (142).

■ Aharonov-Bohm Effect

In quantum mechanics, the *motion* of a charged particle can be *influenced* by the **gauge fields** Φ and A through **quantum interference**, even in the *absence* of electromagnetic fields (i.e. E = B = 0) when there is no Lorentz force acting on the particle at all!

- Setup: Aharonov-Bohm Experiment
 - Physical Arrangement: Consider a long, thin solenoid carrying a magnetic flux ϕ_B . Outside the solenoid, the magnetic field \boldsymbol{B} is zero, but the vector potential \boldsymbol{A} is nonzero. For any surface $\boldsymbol{\mathcal{S}}$ that fully covers the solenoid, we have

$$\phi_B = \int_{\mathcal{S}} \mathbf{B} \cdot d\mathbf{\sigma} = \oint_{\partial \mathcal{S}} \mathbf{A} \cdot d\mathbf{l}. \tag{144}$$



- **Interferometry**: A beam of electrons is split into two paths that *encircle* the solenoid in opposite directions and then recombine to produce an *interference* pattern.
- Key idea: Even when B = 0 outside the solenoid, the **vector potential** A influences the *phase* of the wavefunction.
 - When an electron travels along a path C, the wavefunction acquires a **Berry phase**:

$$\psi \stackrel{C}{\to} \psi e^{i\Theta_C} = \psi \exp\left(\frac{i \ q}{\hbar} \int_C \mathbf{A} \cdot d\mathbf{x}\right),\tag{145}$$

where q = -e is recovered to represent the electron charge.

• The **phase difference** between the two paths is

$$\Delta\Theta = \Theta_{C_1} - \Theta_{C_2} = \frac{q}{\hbar} \left(\int_{C_1} \mathbf{A} \cdot d\mathbf{x} - \int_{C_2} \mathbf{A} \cdot d\mathbf{x} \right). \tag{146}$$

• By applying Stokes' theorem over the surface S enclosed by the loop $C=C_1-C_2=\partial S$,

$$\Delta\Theta = -\frac{q}{\hbar} \int_{\mathcal{S}} (\nabla \times \mathbf{A}) \cdot d\mathbf{\sigma} = \frac{q \, \phi_B}{\hbar},\tag{147}$$

where ϕ_B is the magnetic flux through S (which equals to the flux inside the solenoid as long as S covers the solenoid fully).

This phase shift manifests as a shift in the interference fringes when the two parts of the beam are recombined.

- Application: Superconducting Quantum Interference Device (SQUID)
 - A SQUID consists of a superconducting loop containing a Josephson junction (serving as the screen) and exploit quantum interference to detect extremely subtle changes in maqnetic flux inside the loop.
 - By harnessing the quantum-level sensitivity of the Aharonov-Bohm (AB) effect, SQUIDs can measure magnetic fields as faint as 5×10^{-18} T at microscopic scales.
 - SQUIDs also play a pivotal role in quantum computing, as an approach towards superconducting qubits.
- Question: What Is Physical about Gauge Fields?
 - Gauge Potentials vs. Field Strengths: Traditionally, one might think only the fields E and **B** are physical since they are gauge invariant and can be measured directly by forces. However, the AB effect shows that the potentials Φ and A also have direct physical consequences—they affect the phase of a quantum wavefunction.
 - Holonomy and Berry Phase: The Berry phase around any closed loop is gauge invariant, and should be *physical*. All such **closed-loop Berry phases** (aka. the **holonomies**) form the *complete* set of physical observables of a gauge theory. The AB phase is an example of a holonomy: the phase accumulated around a closed loop depends on the *curvature* (here, the magnetic flux ϕ_B) enclosed by the loop.

Path Integral of Spin

■ Dynamics of Classical Spinning Top

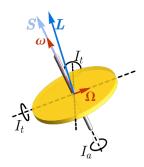
The classical motion of a **spinning top** is governed by

$$\tau = \frac{dL}{dt},\tag{148}$$

where

- τ torque exerted on the top,
- L angular momentum of the top, decomposed into components parallel $I_a \omega$ and perpendicular $I_t \Omega$ to the spinning axis





- I_a axial moment of inertia (about the spinning axis),
- I_t transverse moment of inertia (about either of the two equivalent transverse axes)
- ω axial angular velocity (along the spinning axis)
- Ω transverse angular velocity, describing the instantaneous rotation rate of the spinning axis itself.

Substitute Eq. (149) into Eq. (148),

$$\tau = I_a \frac{d\omega}{dt} + I_t \frac{d\Omega}{dt}.$$
 (150)

• Transverse Torque Assumption: Assume τ has no component along the spinning axis, so the magnitude of ω remains constant. Only its direction changes due to the rotation of the spinning axis:

$$\frac{d\omega}{dt} = \mathbf{\Omega} \times \omega,\tag{151}$$

Eq. (150) becomes

$$\tau = I_a \,\mathbf{\Omega} \times \omega + I_t \,\frac{d\,\mathbf{\Omega}}{d\,t}.\tag{152}$$

We are mainly interested in the motion of the spinning axis, represented by the unit vector

$$n = -\frac{\omega}{\omega}.$$
 (153)

Similar to Eq. (151), n also gets rotated by Ω as

$$\frac{d\,\mathbf{n}}{d\,t} = \mathbf{\Omega} \times \mathbf{n},\tag{154}$$

from which Ω can be "solved" and expressed as

$$\Omega = n \times \frac{d \, n}{d \, t} \,. \tag{155}$$

Derive Eq. (155) from Eq. (154).

Substitute Eq. (155) into Eq. (152), and cross product with n from right on both sides, we obtain

$$I_t \left(\frac{d^2 \mathbf{n}}{d t^2} \right)_{\perp} = \mathbf{\tau} \times \mathbf{n} - \frac{d \mathbf{n}}{d t} \times \mathbf{S}, \tag{156}$$

where

- $S := I_a \omega = S n$ spin angular momentum (parallel to the spinning axis),
- $(\ddot{n})_{\perp} = \ddot{n} (\ddot{n} \cdot n) \ n$ component of acceleration \ddot{n} in the tangent plane.

Derive Eq. (156).

■ Electromagnetic Analogy

The motion of the spinning axis n (spin dynamics) can be interpreted as the motion of a charged particle on a unit sphere in an electromagnetic field (charge dynamics on a sphere).

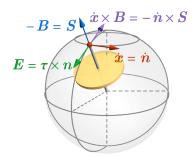
• Analogy: Compare the spin dynamics in Eq. (156) and the charge dynamics in Eq. (143)

spin:
$$I_t(\ddot{\boldsymbol{n}})_{\perp} = \boldsymbol{\tau} \times \boldsymbol{n} - \dot{\boldsymbol{n}} \times \boldsymbol{S}$$

charge: $m \, \ddot{\boldsymbol{x}} = \boldsymbol{E} + \dot{\boldsymbol{x}} \times \boldsymbol{B}$ (157)

Spin dynamics	Charge dynamics
Spin orientation : \boldsymbol{n}	Charge position : \boldsymbol{x}
Moment of inertia : I_t	Mass (interia): m
Torque-induced force : $\tau \times n$	Electric field : \boldsymbol{E}
Spin angular momentum : – $oldsymbol{S}$	Magnetic field : \boldsymbol{B}

• Similarity: Just as in electromagnetism, where the Lorentz force deflects a charge moving in a magnetic field, the spin-induced term $-\dot{n} \times S$ generates precession of the spinning axis.



• Difference: The constraint to the sphere makes the spin dynamics non-Euclidean, confined to a 2D *curved* surface.

- Effective Gauge Field: Introduce the effective gauge field (Φ, A) on the sphere, such that
 - Effective **electric field**:

$$E(n) = -\nabla_{\perp} \Phi(n), \tag{158}$$

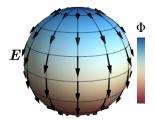
where

- the unit vector $\mathbf{n} = (\cos \phi \sin \theta, \sin \phi \sin \theta, \cos \theta)$ can be parametrized by the **polar angle** $\theta \in [0, \pi]$ and the **azimuthal angle** $\phi \in [0, 2\pi)$,
- then the gradient operator in the tangent space reads

$$\nabla_{\perp} := \mathbf{e}_{\theta} \,\partial_{\theta} + \mathbf{e}_{\phi} \, \frac{1}{\sin \theta} \, \partial_{\phi}, \tag{159}$$

with e_{θ} and e_{ϕ} being basis vectors along θ and ϕ directions.

In this way, E is guaranteed to lie in the tangent plane, the same as the torque-induced force $\tau \times n$.



Example: a spinning top in a uniform gravity field $\Phi(\mathbf{n}) \propto n_z = \cos \theta$,

$$\mathbf{E} = -\nabla_{\perp} \Phi = \mathbf{e}_{\theta} \sin \theta. \tag{160}$$

• Effective magnetic field:

$$B(n) = -S(n) = -S(n) = \nabla \times A(n). \tag{161}$$

where $S = I_a \omega$ is the spin angular momentum (magnitude). The magnetic field points towards the origin, where there is effective an **magnetic monopole**.