Quantum Mechanics

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, theories of light in history).

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	Dutch physicist 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. The wave theory reached its crest.
1704	I. Newton published his book *Optiks*, which explained dispersion, double refraction, Newton's ring 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 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.

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 (^{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*)
- Its basic principle is **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

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

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

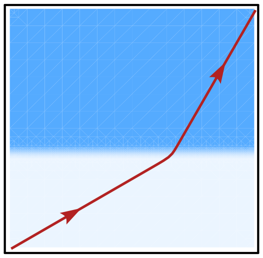
  - The *optical path length* is simply related to the *light travelling time* T by $L = c\, T$, where c is the **speed of light** in vacuum. So extremization of either of them will be equivalent.

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

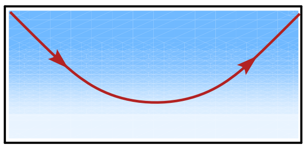
$$n \frac{d}{d t}\left(n^2 \frac{d \boldsymbol{x}}{d t}\right) = \boldsymbol{\nabla} n. \tag{3}$$

  It can be derived from *Fermat's principle*.

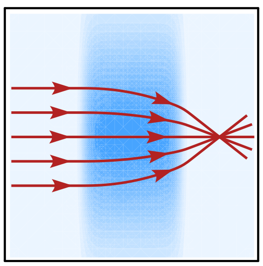
- Refraction (Snell's law)



- Total reflection



- Gradient-index (GRIN) optics



Physical Optics

- **Physical optics** is the **wave mechanics** of light (light *propagates* in the spacetime as a *wave*)
- Its basic principle is **Huygens' Principle**

Every point on the wavefront is a source of spherical wavelet. Wavelets from the past wavefront interferes to determine the new wavefront.

$$\boxed{\psi = \psi_0\, e^{i\,\Theta}.} \tag{4}$$

The new wave amplitude ψ receives contribution from the previous one ψ_0 with additional phase factor $e^{i\,\Theta}$.

- **Interference effect**: contributions from *different paths* must be collected and summed up

$$\psi_B = \int_{A\to B} \psi_A\, e^{i\,\Theta(A\to B)}. \tag{5}$$

- The accumulated phase Θ is determined by the propagation time × the frequency of light

$$\Theta = \omega\, T = \frac{\omega}{c}\, L. \tag{6}$$

The **phase** is proportional to the *optical path length* (given that the light propagates with a fixed frequency).

What about the **amplitude** of the wave? It is related to the *intensity* of the light, or the *probability density* to observe a photon,

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

From Fermat to Huygens

Optimizing the *optical path length* L can be viewed as optimizing an **action** $S = (\hbar\,\omega\,/\,c)\,L$ (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** Θ in the wavelet propagator $e^{i\,\Theta}$.

They are related by

$$\boxed{S = \hbar\,\Theta.} \tag{8}$$

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 procedure to promote 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,

$$S[x] = \int L(x,\, \dot{x},\, t)\, d\,t. \tag{9}$$

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*).

$$\delta\, S[x]|_{x=\overline{x}} = \delta \int L(x,\, \dot{x},\, t)\, d\,t\Big|_{x=\overline{x}} = 0. \tag{10}$$

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

$$\frac{d}{d\,t}\left(\frac{\partial L}{\partial \dot{x}}\right) - \frac{\partial L}{\partial x} = 0, \tag{11}$$

such that the classical path $\bar{x}(t)$ is the solution of Eq. (11). 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).

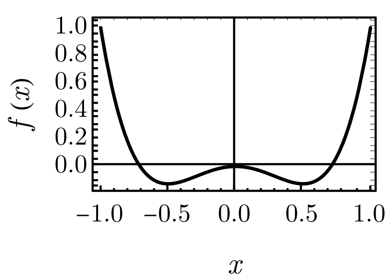
- Nature may not have sufficient *computational resources* to carry out the classical mechanics *precisely*. ⇒ Classical mechanics might actually be realized only *approximately* as a **stochastic** *global optimization*, which is computationally more feasible.
- **Quantum mechanics** takes a *stochastic*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

$$f(x) = -x^2 + 2\,x^4. \tag{12}$$



- 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,

$$Z = \int_{-\infty}^{\infty} e^{i f(x)/\hbar}\, d x. \tag{13}$$

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*

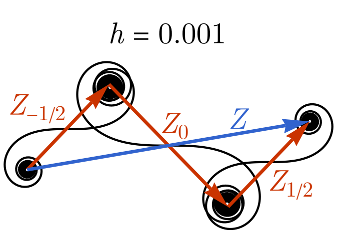
$$d z = e^{i f(x)/\hbar}\, d x. \tag{14}$$

- $d x$ 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,

$$Z \equiv \int d z. \tag{15}$$

Let us see how the partition function is constructed.

- For small h (classical limit)

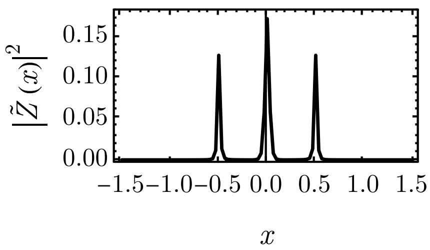


$$Z = Z_{-1/2} + Z_0 + Z_{1/2}, \tag{16}$$

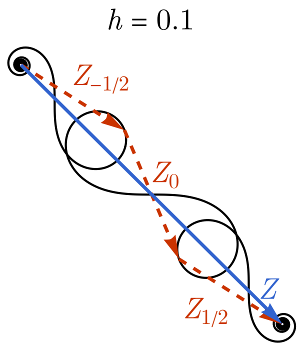
  - Z can break up into three smaller contributions, which correspond to the contributions *around* the three **stationary points**: $x = 0, \pm 1/2$.
  - Around the *stationary point*, **phase** changes *slowly* $\partial_x f(x) \sim 0$ ⇒ **constructive interference** ⇒ *large* contribution to the partition 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,

$$Z(k) \equiv \int d z\, e^{i k x} \simeq Z_{-1/2}\, e^{-i k/2} + Z_0 + Z_{1/2}\, e^{i k/2}. \tag{17}$$

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

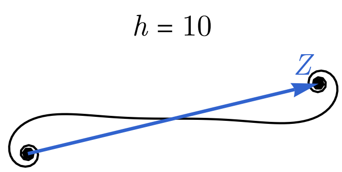


- For intermediate h



  - 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.

$$h = 6.62607004 \times 10^{-34}\,\text{J s}. \tag{18}$$

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.).

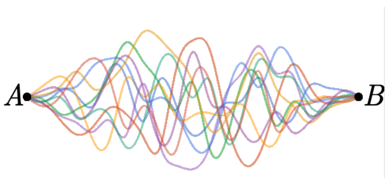
Path Integral and Wave Function

Feynman's 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**

$$\boxed{p_{A\to B} = |K_{A\to B}|^2.} \tag{19}$$

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



$$\boxed{K_{A\to B} \propto \int_{A\to B} \mathcal{D}[x]\, e^{i\,S[x]/\hbar}.} \tag{20}$$

- 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 $\bar{x}$ (that satisfies $\delta S[\bar{x}] = 0$) will dominate the transition amplitude,

$$K_{A\to B} \sim e^{i\,S[\bar{x}]/\hbar}. \tag{21}$$

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**

$$K_{A\to B} = \int_C K_{A\to C}\, K_{C\to B}. \tag{22}$$

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

$$K_{(x_0,t_0)\to(x_N,t_N)} = \int d\,x_1 \ldots d\,x_{N-1}\, K_{(x_0,t_0)\to(x_1,t_1)} \ldots K_{(x_{N-1},t_{N-1})\to(x_N,t_N)}. \tag{23}$$

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

$$\psi(x_{k+1}, t_{k+1}) = \int d\,x_k\, K_{(x_k,t_k)\to(x_{k+1},t_{k+1})}\, \psi(x_k, t_k). \tag{24}$$

If we start with a *initial wave function* $\psi(x, t_0)$ concentrated at x_0, following the time evolution Eq. (24), the *final wave function* $\psi(x, t_N)$ 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 wave function* over one time step, then the dynamical rule can be applied iteratively.

Putting together Eq. (20) and Eq. (24),

$$\psi(x_{k+1},\, t_{k+1}) \propto \int \mathcal{D}[x] \exp\left(\frac{i}{\hbar} S[x]\right) \psi(x_k,\, t_k), \tag{25}$$

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 *wave function*, which plays a central role in quantum mechanics. It can be derived from the *path integral* formulation in Eq. (25).

■ Deriving the Schrödinger Equation

■ Action in a Time Slice

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

$$\boxed{S[x] = \int_{t_0}^{t_1} d\,t\, \frac{1}{2}\, m\, \dot{x}^2,} \tag{26}$$

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,

$$x(t) = x_0 + v\, t, \tag{27}$$

where the *velocity* v will be a constant

$$v = \frac{x_1 - x_0}{t_1 - t_0} = \frac{x_1 - x_0}{\delta t}. \tag{28}$$

Plug into Eq. (26), we get an estimate of the *action* accumulated as the particle moves from x_0 to x_1 in time δt,

$$S[x] = \frac{1}{2}\, m \left(\frac{x_1 - x_0}{\delta t}\right)^2 \delta t = \frac{m}{2\,\delta t}\,(x_1 - x_0)^2. \tag{29}$$

■ Path Integral in a Time Slice

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

$$\begin{aligned}\psi(x_1, t+\delta t) &\propto \int d x_0 \exp\left(\frac{i}{\hbar} S[x]\right) \psi(x_0, t) \\ &= \int d x_0 \exp\left(\frac{i m}{2 \hbar \delta t} (x_1 - x_0)^2\right) \psi(x_0, t).\end{aligned} \tag{30}$$

- 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,

$$\begin{aligned}\psi(x_0, t) &= \psi(x_1 + a, t) \\ &= \psi(x_1, t) + a \psi'(x_1, t) + \frac{a^2}{2!} \psi''(x_1, t) + \frac{a^3}{3!} \psi^{(3)}(x_1, t) + \ldots \\ &= \sum_{n=0}^{\infty} \frac{a^n}{n!} \partial_{x_1}^n \psi(x_1, t).\end{aligned} \tag{31}$$

Substitute into Eq. (30),

$$\psi(x_1, t+\delta t) \propto \sum_{n=0}^{\infty} \int d a \exp\left(\frac{i m}{2 \hbar \delta t} a^2\right) \frac{a^n}{n!} \partial_{x_1}^n \psi(x_1, t). \tag{32}$$

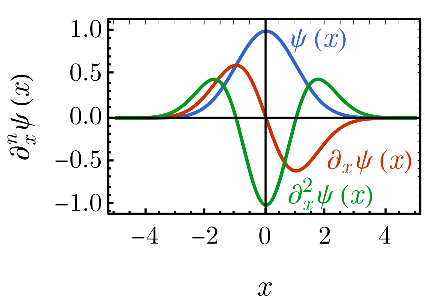
We pack everything related to the integral of a into a coefficient

$$\boxed{\lambda_n \equiv \int d a \exp\left(\frac{i m}{2 \hbar \delta t} a^2\right) \frac{a^n}{n!},} \tag{33}$$

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

$$\boxed{\psi(x, t+\delta t) \propto \sum_{n=0}^{\infty} \lambda_n \partial_x^n \psi(x, t).} \tag{34}$$

- The idea is that the time-evolved wave function can be expressed as the original wave function "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 wave function $\psi(x)$ (within the light-cone) in each step.

Computing the Coefficients λ_n

The λ_n coefficient can be computed by *Mathematica*

$$\lambda_n = \frac{1+(-1)^n}{2}\,\frac{\sqrt{\pi}}{2^n\,\Gamma\left(1+\frac{n}{2}\right)}\left(-\frac{i\,m}{2\,\hbar\,\delta t}\right)^{-\frac{1+n}{2}}. \tag{35}$$

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

$$\frac{1+(-1)^n}{2} = \begin{cases} 1 & \text{if } n\in\text{even}, \\ 0 & \text{if } n\in\text{odd}. \end{cases} \tag{36}$$

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 λ_n are given by

$$\begin{aligned} \lambda_0 &= \sqrt{\pi}\left(-\frac{i\,m}{2\,\hbar\,\delta t}\right)^{-1/2}, \\ \lambda_2 &= \frac{\sqrt{\pi}}{4}\left(-\frac{i\,m}{2\,\hbar\,\delta t}\right)^{-3/2} = \frac{i}{4}\left(\frac{2\,\hbar\,\delta t}{m}\right)\lambda_0, \\ \lambda_4 &= \frac{\sqrt{\pi}}{32}\left(-\frac{i\,m}{2\,\hbar\,\delta t}\right)^{-5/2} = -\frac{1}{32}\left(\frac{2\,\hbar\,\delta t}{m}\right)^2\lambda_0, \\ &\ldots \end{aligned} \tag{37}$$

Determining the Normalization

Plugging the results of λ_n in Eq. (37) into Eq. (34), we get

$$\psi(x,\,t+\delta t)\propto\lambda_0\left(1+\frac{i}{4}\left(\frac{2\,\hbar\,\delta t}{m}\right)\partial_x^2-\frac{1}{32}\left(\frac{2\,\hbar\,\delta t}{m}\right)^2\partial_x^4+\ldots\right)\psi(x,\,t). \tag{38}$$

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

$$\psi(x,\,t)\propto\lambda_0\,\psi(x,\,t). \tag{39}$$

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

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

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

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

Let us consider the time derivative of the wave function

$$\begin{aligned}\partial_t \psi(x,\ t) &= \lim_{\delta t \to 0} \frac{\psi(x,\ t+\delta t) - \psi(x,\ t)}{\delta t} \\ &= \lim_{\delta t \to 0} \frac{1}{\delta t} \left(\frac{i}{4} \left(\frac{2\,\hbar\,\delta t}{m} \right) \partial_x^2 - \frac{1}{32} \left(\frac{2\,\hbar\,\delta t}{m} \right)^2 \partial_x^4 + \ldots \right) \psi(x,\ t)\end{aligned} \tag{41}$$

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

$$\partial_t \psi(x,\ t) = \frac{i\,\hbar}{2\,m}\,\partial_x^2 \psi(x,\ t). \tag{42}$$

- 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. (42) in the following form

$$\boxed{i\,\hbar\,\partial_t \psi(x,\ t) = -\frac{\hbar^2}{2\,m}\,\partial_x^2 \psi(x,\ t).} \tag{43}$$

This is the **Schrödinger equation** that governs the *time evolution* of the wave function 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

$$\boxed{S = \int_{t_0}^{t_1} d t \left(\frac{1}{2}\,m\,\dot{x}^2 - V(x) \right),} \tag{44}$$

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

$$\Delta S = -\,V(x)\,\delta t. \tag{45}$$

Eventually this cause an additional *phase shift* in the wave function

$$\begin{aligned}\psi(x,\ t+\delta t) &= e^{i\,\Delta S/\hbar}\,\psi_0(x,\ t+\delta t) \\ &= e^{-i\,V(x)\,\delta t/\hbar}\,\psi_0(x,\ t+\delta t) \\ &= \left(1 - \frac{i}{\hbar}\,V(x)\,\delta t + \ldots\right) \psi_0(x,\ t+\delta t),\end{aligned} \tag{46}$$

where ψ_0 is the expected wave function at $t+\delta t$ without the potential. Combining with the result in Eq. (40), to the first order of δt we have

$$\psi(x,\ t+\delta t) = \left(1 - \frac{i}{\hbar}\ V(x)\,\delta t + \ldots\right)\left(1 + \frac{i}{4}\left(\frac{2\,\hbar\,\delta t}{m}\right)\partial_x^2 + \ldots\right)\psi(x,\ t)$$
$$= \left(1 + \frac{i}{4}\left(\frac{2\,\hbar\,\delta t}{m}\right)\partial_x^2 - \frac{i}{\hbar}\ V(x)\,\delta t + \ldots\right)\psi(x,\ t). \tag{47}$$

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

$$\partial_t \psi(x,\ t) = \frac{i\,\hbar}{2\,m}\,\partial_x^2 \psi(x,\ t) - \frac{i}{\hbar}\ V(x)\,\psi(x,\ t), \tag{48}$$

or equivalently written as

$$\boxed{i\,\hbar\,\partial_t \psi(x,\ t) = -\frac{\hbar^2}{2\,m}\,\partial_x^2 \psi(x,\ t) + V(x)\,\psi(x,\ t).} \tag{49}$$

This is the **Schrödinger equation** that governs the *time evolution* of the wave function of a particle moving in a potential $V(x)$.

Single-Particle Quantum Mechanics

▪ Wave Mechanics v.s. Matrix Mechanics

▪ Functions as Vectors

To specify a **function** ψ is to specify the values $\psi(x)$ of the function at each point $x \Rightarrow$ these values can be arranged into an infinite-dimensional **vector**

$$\psi(x) \sim (\ \cdots\ \ \psi(0)\ \ \cdots\ \ \psi(0.01)\ \ \cdots\ \ \psi(0.5)\ \ \cdots\ )^{\mathsf{T}}. \tag{50}$$

- Elements of the vector are labeled by real numbers $x \in \mathbb{R}$ (instead of integers). The vector is like a *look-up table* representation of the function.

Quantum states of particles are represented by ~~state vectors~~ **wave functions**.

- The **ket state**:

$$|\psi\rangle \doteq \psi(x). \tag{51}$$

$\psi : \mathbb{R} \to \mathbb{C}$ is a complex function in general.

- The **bra state**:

$$\langle\psi| \doteq \psi^*(x). \tag{52}$$

- **Inner product** of *bra* and *ket*

$$\boxed{\langle\phi \mid \psi\rangle = \int d\,x\,\phi^*(x)\,\psi(x),} \tag{53}$$

as a functional generalization of $\langle \phi \mid \psi \rangle = \sum_i \phi_i^* \psi_i$.

- **Normalized state**: $|\psi\rangle$ is normalized iff

$$\langle \psi \mid \psi \rangle = \int d x \, \psi^*(x) \, \psi(x) = \int d x \, |\psi(x)|^2 = 1. \tag{54}$$

- **Orthogonal states**: two states $|\phi\rangle$ and $|\psi\rangle$ are orthogonal iff

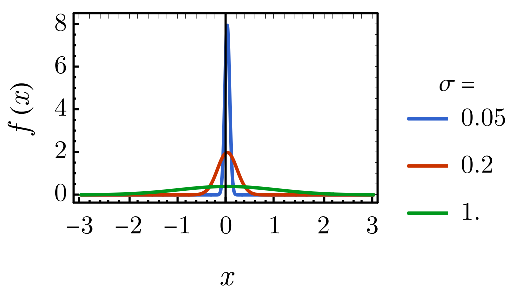
$$\langle \phi \mid \psi \rangle = \int d x \, \phi^*(x) \, \psi(x) = 0. \tag{55}$$

Can we find a complete set of **orthonormal basis**?

Dirac δ-function: a infinitely sharp peak of unit area.

- It can be considered as the limit of Gaussians with $\sigma \to 0$

$$\delta(x) = \lim_{\sigma \to 0} \frac{1}{\sqrt{2\pi} \, \sigma} \, e^{-\frac{x^2}{2\sigma^2}}. \tag{56}$$



Loosely speaking

$$\delta(x) = \begin{cases} 0 & \text{if } x \neq 0, \\ \infty & \text{if } x = 0 \text{ (ill–defined)}. \end{cases} \tag{57}$$

- The area under the curve remains unity as the limit is taken, i.e. $\int \delta(x) \, d x = 1$, as a functional generalization of $\sum_i \delta_{ij} = 1$.
- Multiplying $\delta(x - a)$ with an ordinary function $\psi(x)$ is the same as multiplying $\psi(a)$, i.e. $\delta(x - a) \, \psi(x) = \psi(a) \, \delta(x - a)$, because the product is *zero anyway* except at point a. In particular,

$$\int \delta(x - a) \, \psi(x) \, d x = \psi(a). \tag{58}$$

This can be thought as the *defining property* of the Dirac δ-function: *convolution* of $\delta(x - a)$ with any function $\psi(x)$ *picks out* the value of the function $\psi(a)$ at point a. It is a functional generalization of $\sum_j \delta_{ij} \, \psi_j = \psi_i$.

The *Dirac δ-function* can be used to construct a set of *orthonormal basis*: called the **position basis**, labeled by $x_1 \in \mathbb{R}$

$$|x_1\rangle \doteq \delta(x - x_1). \tag{59}$$

- x_1 labels the basis state,

- x is a dummy variable of the corresponding wave function.
- The wave function $\delta(x - x_1)$ describes the state that the particle is at a *definite position* x_1. It can be prepared by measuring the position and then post-select based on the measurement outcome.

We can check the orthogonality,

$$\langle x_1 \mid x_2 \rangle = \int \delta(x - x_1)\, \delta(x - x_2)\, d x = \delta(x_1 - x_2), \tag{60}$$

which is a functional generalization of $\langle i \mid j \rangle = \delta_{ij}$.

- Thus $|x\rangle$ ($x \in \mathbb{R}$) for a set of **orthonormal basis** of the Hilbert space of a particle (the Hilbert space dimension is infinite) $\Rightarrow$ the **single-particle Hilbert space**.
- Any state in the *single-particle Hilbert space* is a linear superposition of these basis states

$$\boxed{|\psi\rangle = \int d x\, \psi(x)\, |x\rangle,} \tag{61}$$

  as a functional generalization of $|\psi\rangle = \sum_i \psi_i\, |i\rangle$.
- The wave function of a state $|\psi\rangle$ can be extracted by the inner product with position basis

$$\langle x \mid \psi \rangle = \int \delta(x' - x)\, \psi(x')\, d x' = \psi(x), \tag{62}$$

  as a functional generalization of $\psi_i = \langle i \mid \psi \rangle$.

Statistical interpretation: given a particle described by the state $|\psi\rangle$, as we measure the *position* of a particle, the **probability density** to find the particle at position x is given by

$$\boxed{p(x) = |\langle x \mid \psi \rangle|^2 = |\psi(x)|^2.} \tag{63}$$

After the measurement, the state of the particle *collapses* to the position basis state $|x\rangle$ that corresponds to the measurement outcome x.

Operators as Matrices

Operator takes one function to another function, e.g. $\partial_x \sin(x) = \cos(x)$. **Linear operators** in the *single-particle Hilbert space* are linear superpositions of basis operators $|x_1\rangle\langle x_2|$:

$$\boxed{\hat{M} = \int d x_1\, d x_2\, |x_1\rangle\, M(x_1, x_2)\, \langle x_2|.} \tag{64}$$

- Operator acting on a state $|\psi\rangle$,

$$\begin{aligned}\hat{M}\, |\psi\rangle &= \int d x_1\, d x_2\, d x_3\, |x_1\rangle\, M(x_1, x_2)\, \langle x_2 \mid x_3 \rangle\, \psi(x_3)\\ &= \int d x_1\, d x_2\, d x_3\, |x_1\rangle\, M(x_1, x_2)\, \delta(x_2 - x_3)\, \psi(x_3)\end{aligned} \tag{65}$$

$$= \int d x_1\, d x_2\, |x_1\rangle\, M(x_1, x_2)\, \psi(x_2).$$

If we define a new wave function ϕ via the following **convolution**

$$\phi(x_1) = \int d x_2\, M(x_1, x_2)\, \psi(x_2), \tag{66}$$

where $M(x_1, x_2)$ is the **convolution kernel**, we can write

$$\hat{M}\, |\psi\rangle = |\phi\rangle = \int d x_1\, |x_1\rangle\, \phi(x_1). \tag{67}$$

Applying an *operator* to *a state* $\doteq$
convolute the *kernel* of the operator with the *wave function* of the state.

So an operator does change the state in general (unless it is the identity operator).

- The **identity operator** is represented by the *δ-function convolution kernel* $M(x_1, x_2) = \delta(x_1 - x_2)$, because $\int d x_2\, \delta(x_1 - x_2)\, \psi(x_2) = \psi(x_1)$ does not really change the wave function. So the identity operator can be written as

$$\mathbb{1} = \int d x_1\, d x_2\, |x_1\rangle\, \delta(x_1 - x_2)\, \langle x_2| = \int d x\, |x\rangle\, \langle x|, \tag{68}$$

a functional generalization of $\sum_i |i\rangle\, \langle i| = \mathbb{1}$.

- Since the **operator** is specified by a two-variable function $M(x_1, x_2)$, it can be viewed as an *infinite-dimensional* **matrix**

$$\hat{M} \doteq M(x_1, x_2) \;\text{ or }\; \begin{pmatrix} \ddots & \vdots & \iddots \\ \cdots & M(x_1, x_2) & \cdots \\ \iddots & \vdots & \ddots \end{pmatrix}. \tag{69}$$

x_1, x_2 are row and column indices (indexed by real numbers).

Hermitian conjugate of operator,

$$\hat{M}^\dagger = \int d x_1\, d x_2\, |x_1\rangle\, M^*(x_2, x_1)\, \langle x_2|. \tag{70}$$

- **Hermitian** operator: $\hat{L}^\dagger = \hat{L}$. Hermitian operators correspond to **physical observables**.
  - The **expectation value** of $\hat{L}$ on the state $|\psi\rangle$ is given by

$$\boxed{\langle \hat{L}\rangle \equiv \langle\psi|\, \hat{L}\, |\psi\rangle = \int d x_1\, d x_2\, \psi^*(x_1)\, L(x_1, x_2)\, \psi(x_2).} \tag{71}$$

- **Unitary** operator: $\hat{U}^\dagger\, \hat{U} = \hat{U}\, \hat{U}^\dagger = \mathbb{1}$.

■ Momentum Operator

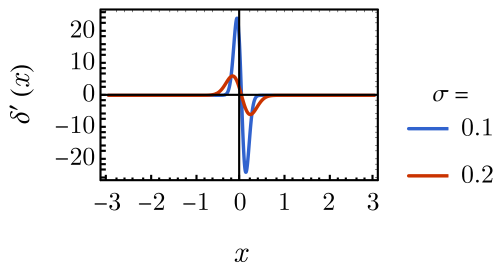
How do we think of the differential operator as a matrix?

The **differential operator** ∂_x is represented by the *convolution kernel* $\delta'(x_1 - x_2)$.

$$\partial_x = \int \mathbb{d} x_1 \, \mathbb{d} x_2 \, |x_1\rangle \, \delta'(x_1 - x_2) \, \langle x_2|. \tag{72}$$

- $\delta'(x) = \partial_x \delta(x)$ is the first derivative of the Dirac δ-function. Think in terms of the limit

$$\delta'(x) = \lim_{\sigma \to 0} \frac{-x}{\sqrt{2\pi} \, \sigma^3} \, e^{-\frac{x^2}{2\sigma^2}}. \tag{73}$$



- $\delta'(x_1 - x_2)$ can be either understood as $\partial_{x_1} \delta(x_1 - x_2)$ or as $-\partial_{x_2} \delta(x_1 - x_2)$. Under convolution,

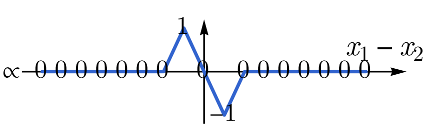
$$\begin{aligned}
&\int \mathbb{d} x_2 \, \delta'(x_1 - x_2) \, \psi(x_2) \\
&= \int \mathbb{d} x_2 (-\partial_{x_2} \delta(x_1 - x_2)) \, \psi(x_2) \\
&= \int \mathbb{d} x_2 \, \delta(x_1 - x_2) \, (\partial_{x_2} \psi(x_2)) \\
&= \partial_{x_1} \psi(x_1),
\end{aligned} \tag{74}$$

  so the kernel $\delta'(x_1 - x_2)$ indeed implements differentiation under convolution.

- In the matrix form,

$$\begin{aligned}
\partial_x |\psi\rangle &\doteq \lim_{\delta x \to 0} \frac{1}{2\,\delta x} \begin{pmatrix} \ddots & \ddots & & & \\ \ddots & 0 & 1 & & \\ & -1 & 0 & 1 & \\ & & -1 & 0 & \ddots \\ & & & \ddots & \ddots \end{pmatrix} \begin{pmatrix} \vdots \\ \psi(x - \delta x) \\ \psi(x) \\ \psi(x + \delta x) \\ \vdots \end{pmatrix} \\
&= \lim_{\delta x \to 0} \frac{\psi(x + \delta x) - \psi(x - \delta x)}{2\,\delta x} \doteq |\partial_x \psi\rangle.
\end{aligned} \tag{75}$$

  Note: to discretize $\delta'(x_1 - x_2)$ without losing its essential meaning, we can consider

  $\delta'(x_1 - x_2) \propto$ 

- Higher order derivatives: just multiply the matrix n times.

$$\partial_x^n \doteq \delta^{(n)}(x_1 - x_2) \text{ or } \lim_{\delta x \to 0} \frac{1}{(2\,\delta x)^n} \begin{pmatrix} \ddots & \ddots & & & \\ \ddots & 0 & 1 & & \\ & -1 & 0 & 1 & \\ & & -1 & 0 & \ddots \\ & & & \ddots & \ddots \end{pmatrix}^n .$$

The matrix representation of ∂_x is **not Hermitian**! $\Rightarrow$ ∂_x is not a Hermitian operator, as

$$\begin{aligned} (\partial_x)^\dagger &= \int d\,x_1\, d\,x_2\, |x_1\rangle\, \delta'^*(x_2 - x_1)\, \langle x_2| \\ &= -\int d\,x_1\, d\,x_2\, |x_1\rangle\, \delta'(x_1 - x_2)\, \langle x_2| \\ &= -\partial_x . \end{aligned} \tag{77}$$

We can make it Hermitian by giving it an imaginary factor $-i\,\hbar$, and define:

$$\boxed{\hat{p} = -i\,\hbar\,\partial_x = -i\,\hbar \int d\,x_1\, d\,x_2\, |x_1\rangle\, \delta'(x_1 - x_2)\, \langle x_2|.} \tag{78}$$

Now $\hat{p}$ is *Hermitian*, what *physical observable* does it correspond to? - It is the **momentum operator**. Why?

A hand-waving argument: the idea of path integral is that the phase Θ of the wave function ~ the action S of the particle (by $\Theta = S/\hbar$), i.e.

$$\psi \sim e^{i\,\Theta} \sim e^{i\,S/\hbar}, \tag{79}$$

therefore

$$\hat{p}\,\psi = -i\,\hbar\,\partial_x\, e^{i\,S/\hbar} \sim -i\,\hbar \left(\frac{i\,\partial_x S}{\hbar}\right) e^{i\,S/\hbar} \sim (\partial_x S)\,\psi. \tag{80}$$

So the eigenvalues of $\hat{p}$ would better correspond to $\partial_x S$, or more precisely, the *variation* of the *action* with respect to the final *position*, which is the **momentum** in classical mechanics (recall the result of HW 1).

■ Position Operator

Position of the particle is also an *physical observable*. What *Hermitian operator* does it correspond to?

The **position operator**:

$$\boxed{\hat{x} = \int d\,x\, |x\rangle\, x\, \langle x|.} \tag{81}$$

It is a *diagonal* operator (like a diagonal matrix) in the *position basis* $\Rightarrow$ it just *marks* each **position eigenstate** $|x\rangle$ by the **position eigenvalue** x (which is the coordinate of the particle). It is a generalized example of the *spectral decomposition* of Hermitian operators $L = \sum_i |\lambda_i\rangle\, \lambda_i\, \langle\lambda_i|$.

- The *position operator* $\hat{x}$ acting on a state $|\psi\rangle = \int d\,x\, |x\rangle\, \psi(x)$

$$\hat{x}\,|\psi\rangle = \int d\,x\,d\,x'\,|x\rangle\,x\,\langle x \mid x'\rangle\,\psi(x')$$
$$= \int d\,x\,d\,x'\,|x\rangle\,x\,\delta(x-x')\,\psi(x')$$
$$= \int d\,x\,(x\,\psi(x))\,|x\rangle.$$

In terms of the wave function $\psi(x)$, the position operator basically multiplies the wave function by the position x:

$$\psi(x) \overset{\hat{x}}{\to} x\,\psi(x). \tag{83}$$

A sloppy notation:

$$\hat{x}\,\psi(x) = x\,\psi(x). \tag{84}$$

- The *momentum operator* $\hat{p}$ acting on a state $|\psi\rangle = \int d\,x\,|x\rangle\,\psi(x)$

$$\hat{p}\,|\psi\rangle = \int d\,x\,|x\rangle\,(-i\,\hbar\,\partial_x\psi(x)). \tag{85}$$

Another sloppy notation:

$$\hat{p}\,\psi(x) = -i\,\hbar\,\partial_x\psi(x). \tag{86}$$

Uncertainty Relation

So the *position* operator *marks* the wave function by x, the *momentum* operator *mixes* (changes) the wave function by derivatives. Markers and mixers do *not commute*!

$$\boxed{[\hat{x}, \hat{p}] = i\,\hbar.} \tag{87}$$

To see this, study how they act on a state

$$\begin{aligned}\hat{x}\,\hat{p}\,\psi(x) &= -i\,\hbar\,x\,\partial_x\psi(x),\\ \hat{p}\,\hat{x}\,\psi(x) &= -i\,\hbar\,\partial_x(x\,\psi(x)) = -i\,\hbar\,\psi(x) - i\,\hbar\,x\,\partial_x\psi(x),\end{aligned} \tag{88}$$

so the commutator

$$\begin{aligned}[\hat{x}, \hat{p}]\,\psi(x) &= (\hat{x}\,\hat{p} - \hat{p}\,\hat{x})\,\psi(x)\\ &= -i\,\hbar\,x\,\partial_x\psi(x) + i\,\hbar\,\psi(x) + i\,\hbar\,x\,\partial_x\psi(x)\\ &= i\,\hbar\,\psi(x),\end{aligned} \tag{89}$$

"eliminate" $\psi(x)$ from both sides $\Rightarrow [\hat{x}, \hat{p}] = i\,\hbar\,\mathbb{1}$.

Uncertainty Relation (between position and momentum): on any given state $|\psi\rangle$ of a particle, measure the position x and the momentum p (in separate experiments) repeatedly, the statistics of the measurement outcomes must obey

$$\boxed{(\text{std}\,x)\,(\text{std}\,p) \geq \frac{1}{2}\,|\langle[\hat{x}, \hat{p}]\rangle| = \frac{\hbar}{2}.} \tag{90}$$

- If the particle has a *precise position*, i.e. (std x) → 0, its *momentum* must *fluctuate* infinitely strong, i.e. (std p) → ∞.
- If we want to probe smaller and smaller structures of our space, we must use particles (say photons) with larger and larger momentum, until the energy $E = c\,p$ of the photon becomes so large that the photon itself collapses into a black hole under its own gravity. ⇒ Quantum mechanics imposes a fundamental resolution limit of the space: the **Planck length**

$$\ell_P = \sqrt{\frac{\hbar\, G}{c^3}} \approx 1.616229\,(38) \times 10^{-35}\ \text{m}. \tag{91}$$

HW 2

> Consider a state $|\psi\rangle = \int d x\, \psi(x)\, |x\rangle$ described by the following wave function with a tunable parameter σ:
> $\psi(x) = \frac{1}{\pi^{1/4}\,\sigma^{1/2}} \exp\left(-\frac{x^2}{2\,\sigma^2}\right)$
> (i) Check that the state is normalized $\langle \psi \mid \psi \rangle = 1$, regardless of the value of σ.
> (ii) Evaluate the expectation values: $\langle \hat{x} \rangle$, $\langle \hat{p} \rangle$, $\langle \hat{x}^2 \rangle$, $\langle \hat{p}^2 \rangle$ in terms of σ.
> (iii) Based on the result of (ii), calculate (std x) and (std p) in terms of σ. Do they satisfy the uncertainty relation?

Dynamics and Symmetry

Hamiltonian and Time Evolution

Hamiltonian of a non-relativistic particle in classical mechanics

$$H = \frac{p^2}{2\,m} + V(x). \tag{92}$$

In quantum mechanics, just promote every physical observable to its operator,

$$\begin{aligned} \hat{H} &= \frac{\hat{p}^2}{2\,m} + V(\hat{x}) \\ &= -\frac{\hbar^2}{2\,m}\,\partial_x^2 + V(\hat{x}). \end{aligned} \tag{93}$$

- By $V(\hat{x})$ we mean

$$V(\hat{x}) = \int d x\, |x\rangle\, V(x)\, \langle x|. \tag{94}$$

This is always how we define a function of an operator. Its action on a wave function $\psi(x)$ (in the position basis) is simply to multiply it by $V(x)$, sloppy notation:

$$V(\hat{x})\,\psi(x) = V(x)\,\psi(x). \tag{95}$$

The **Schrödinger equation** we derived previously in Eq. (49) matches its general form of

$$\boxed{i\,\hbar\,\partial_t|\psi\rangle = \hat{H}\,|\psi\rangle.} \tag{96}$$

The **Hamiltonian operator** $\hat{H}$ is *Hermitian*. What *physical observable* does it correspond to? - Answer: the **energy**. Why?

A hand-waving argument: the idea of path integral is that the phase Θ of the wave function ~ the action S of the particle (by $\Theta = S/\hbar$), i.e.

$$\psi \sim e^{i\,\Theta} \sim e^{i\,S/\hbar}, \tag{97}$$

therefore

$$\hat{H}\,\psi = i\,\hbar\,\partial_t\,e^{i\,S/\hbar} \sim i\,\hbar\left(\frac{i\,\partial_t S}{\hbar}\right)e^{i\,S/\hbar} \sim (-\partial_t S)\,\psi. \tag{98}$$

So the eigenvalues of $\hat{H}$ would better correspond to $-\partial_t S$, or more precisely, the (negative) *variation* of the *action* with respect to the final *time*, which is the **energy** in classical mechanics (recall the result of HW 1).

Time evolution is **unitary**

$$\boxed{|\psi(t)\rangle = \hat{U}(t)\,|\psi(0)\rangle,} \tag{99}$$

and it is *generated* by the **Hamiltonian**,

$$\boxed{\hat{U}(t) = e^{-i\,\hat{H}\,t/\hbar}.} \tag{100}$$

Then $|\psi(t)\rangle$ can be further used to calculate the evolution of operator expectation values ...

In the **Heisenberg picture**, the state remains fixed while the operator evolves in time

$$\boxed{\hat{L}(t) = \hat{U}(t)^\dagger\,\hat{L}\,\hat{U}(t),} \tag{101}$$

described by the **Heisenberg equation**

$$\boxed{i\,\hbar\,\partial_t\,\hat{L}(t) = \left[\hat{L}(t),\,\hat{H}\right].} \tag{102}$$

This will provide an equivalent description for the evolution of the operator expectation values.

HW 3 Consider $\hat{H} = \frac{1}{2}\,\hat{p}^2 + \frac{1}{2}\,\hat{x}^2$, derive the Heisenberg equation for operator $\hat{a} = \frac{1}{\sqrt{2}}\,(\hat{x} + i\,\hat{p})$.

■ Momentum and Space Translation

The *momentum operator* $\hat{p}$, as a *Hermitian* operator, must also be able to generate a *unitary* operator. So what is the unitary operator generated by momentum? - Answer: it is the **space translation** operator

$$\boxed{\hat{T}(a) = e^{i\,\hat{p}\,a/\hbar}.} \tag{103}$$

- Acting on a wave function $\psi(x)$

$$\begin{aligned}
&\hat{T}(a)\,\psi(x) = e^{i\,\hat{p}\,a/\hbar}\,\psi(x)\\
&= \exp(a\,\partial_x)\,\psi(x)\\
&= \left(\mathbb{1} + a\,\partial_x + \frac{a^2}{2!}\,\partial_x^2 + \frac{a^3}{3!}\,\partial_x^3 + \ldots\right)\psi(x)\\
&= \psi(x) + a\,\psi'(x) + \frac{a^2}{2!}\,\psi''(x) + \frac{a^3}{3!}\,\psi^{(3)}(x) + \ldots\\
&= \psi(x+a).
\end{aligned} \tag{104}$$

So the unitary operator $\hat{T}(a)$ implements the space translation $x \to x + a$, it is called the **space translation operator**.

- Another equivalent definition of $\hat{T}(a)$ is

$$\boxed{\hat{T}(a) = \int d\!\!\!\!\;d\,x\,|x - a\rangle\,\langle x|.} \tag{105}$$

Such that given the state $|\psi\rangle = \int d\,x\,\psi(x)\,|x\rangle$

$$\begin{aligned}
&\hat{T}(a)\,|\psi\rangle = \int d\,x\,d\,x'\,|x - a\rangle\,\langle x \mid x'\rangle\,\psi(x')\\
&= \int d\,x\,d\,x'\,|x - a\rangle\,\delta(x - x')\,\psi(x')\\
&= \int d\,x\,\psi(x)\,|x - a\rangle\\
&= \int d\,x\,\psi(x + a)\,|x\rangle.
\end{aligned} \tag{106}$$

- The inverse translation should be given by the *Hermitian conjugate*,

$$\hat{T}^{-1}(a) = \hat{T}^{\dagger}(a) = \int d\,x\,|x\rangle\,\langle x - a| = \int d\,x\,|x + a\rangle\,\langle x| = T(-a). \tag{107}$$

HW 4

> Staring from the commutation relation $[\hat{x}, \hat{p}] = i\,\hbar$ introduced in Eq. (87).
> (i) Show that $\left[\hat{x}, \hat{p}^n\right] = i\,\hbar\,n\,\hat{p}^{n-1}$ for all $n \in \mathbb{N}$ by induction.
> (ii) Use the above result to show that $[\hat{x}, F(\hat{p})] = i\,\hbar\,\partial_{\hat{p}} F(\hat{p})$ for generic function F.
> (ii) Apply the above result to the translation operator $\hat{T}(a)$ defined in Eq. (103) to show that $\left[\hat{x}, \hat{T}(a)\right] = -a\,\hat{T}(a)$.
> The final result implies that the position operator is indeed translated by the translation operator $\hat{T}(a)\,\hat{x}\,\hat{T}^{\dagger}(a) = \hat{x} + a\,\mathbb{1}$.

■ Symmetry and Conservation Laws

Applying the translation operator to:

- the position operator $\hat{x}$ → will shift the position

$$\begin{aligned}
&\hat{T}(a)\,\hat{x}\,\hat{T}^{\dagger}(a)\\
&= \int d x_1\,|x_1 - a\rangle\,\langle x_1| \int d x_2\,|x_2\rangle\,x_2\,\langle x_2| \int d x_3\,|x_3\rangle\,\langle x_3 - a|\\
&= \int d x_1\,d x_2\,d x_3\,|x_1 - a\rangle\,\langle x_1 \mid x_2\rangle\,x_2\,\langle x_2 \mid x_3\rangle\,\langle x_3 - a|\\
&= \int d x_1\,|x_1 - a\rangle\,x_1\,\langle x_1 - a|\\
&= \int d x\,|x\rangle\,(x + a)\,\langle x|\\
&= \int d x\,|x\rangle\,x\,\langle x| + a \int d x\,|x\rangle\,\langle x|\\
&= \hat{x} + a\,\mathbb{1}.
\end{aligned} \tag{108}$$

- the momentum operator $\hat{p}$ → will do nothing

$$\begin{aligned}
&\hat{T}(a)\,\hat{p}\,\hat{T}^{\dagger}(a)\\
&= e^{i\,\hat{p}\,a/\hbar}\,\hat{p}\,e^{-i\,\hat{p}\,a/\hbar}\\
&= e^{i\,\hat{p}\,a/\hbar}\,e^{-i\,\hat{p}\,a/\hbar}\,\hat{p}\\
&= \hat{p}.
\end{aligned} \tag{109}$$

- the Hamiltonian $\hat{H}$ → will only translate the potential profile

$$\begin{aligned}
&\hat{T}(a)\,\hat{H}\,\hat{T}^{\dagger}(a)\\
&= \hat{T}(a)\left(\frac{\hat{p}^2}{2\,m} + V(\hat{x})\right)\hat{T}^{\dagger}(a)\\
&= \frac{\hat{p}^2}{2\,m} + V(\hat{x} + a).
\end{aligned} \tag{110}$$

The *Hamiltonian* will be *invariant* under *space translation*, iff the potential is flat (position independent)

$$V(x + a) = V(x), \tag{111}$$

i.e. $V(x) = \text{const}$. In this case, we say the particle respects the **space translation symmetry**.

What is the significance of the **space translation symmetry**?

If $\hat{T}(a)\,\hat{H}\,\hat{T}^{\dagger}(a) = \hat{H}$ for any a, we can consider the limit $a \to 0$, then we must at least have

$$\hat{T}(a)\,\hat{H}\,\hat{T}^{\dagger}(a) = e^{i\,\hat{p}\,a/\hbar}\,\hat{H}\,e^{-i\,\hat{p}\,a/\hbar}$$

$$= \left(\mathbb{1} + \frac{i\,\hat{p}\,a}{\hbar} + \ldots\right) \hat{H} \left(\mathbb{1} - \frac{i\,\hat{p}\,a}{\hbar} + \ldots\right)$$
$$= \hat{H} + \frac{i\,a}{\hbar}\left[\hat{p}, \hat{H}\right] + O\left(a^2\right) = \hat{H},$$

meaning that to the first order in a, the commutator must vanish

$$\left[\hat{p}, \hat{H}\right] = 0. \tag{113}$$

According to the **Heisenberg equation** of operator dynamics

$$i\,\hbar\,\partial_t\,\hat{p}(t) = \left[\hat{p}(t), \hat{H}\right] = 0, \tag{114}$$

the **momentum** of the particle is **conserved**.

Noether's theorem: every **continuous (differentiable) symmetry** of a physical system implies a corresponding **conservation law**.

- **Space translation** symmetry ⇔ **Momentum** conservation
- **Time translation** symmetry ⇔ **Energy** conservation

In quantum mechanics, *symmetries* are implemented by **unitary** operators, the corresponding **Hermitian generators** will describe the corresponding *conserved physical observables*.

What if the Hamiltonian is *momentum independent*? Does the **momentum translation** symmetry implies the **position conservation**? Yes!

$$\hat{H} = \frac{\hat{p}^2}{2\,m} + V(\hat{x}) \xrightarrow{m\to\infty} \hat{H} = V(\hat{x}). \tag{115}$$

The Hamiltonian becomes momentum independent in the limit of large particle mass. ⇒ In this limit, the position of the particle remains unchanged in time ⇒ Heavy particles are hard to move.

Wave-Particle Duality

Momentum Basis

The **momentum operator** $\hat{p}$ is a **Hermitian** operator in the *single-particle Hilbert space*. *Eigenstates* of the momentum operator should form a complete set of *orthonormal basis* as well ⇒ the **momentum basis**.

$$\hat{p}\,|p\rangle = p\,|p\rangle. \tag{116}$$

- Eigenstates $|p\rangle$ are labeled by momentum eigenvalues $p \in \mathbb{R}$.
- Any state in the *single-particle Hilbert space* can is a linear superposition of the momentum basis states,

$$\boxed{|\tilde{\psi}\rangle = \int đ p\,\tilde{\psi}(p)\,|p\rangle.} \tag{117}$$

- Given the state $|\tilde{\psi}\rangle$, the probability density to observe the particle with momentum p is

$$\boxed{p(p) = \left|\langle p \mid \tilde{\psi}\rangle\right|^2 = \left|\tilde{\psi}(p)\right|^2.} \tag{118}$$

We are free to choose basis: the *position* and *momentum* basis states can be written in terms of each other

$$\boxed{\begin{aligned} |p\rangle &= \frac{1}{\sqrt{2\pi\hbar}} \int dx\, e^{i p x/\hbar} |x\rangle, \\ |x\rangle &= \frac{1}{\sqrt{2\pi\hbar}} \int dp\, e^{-i p x/\hbar} |p\rangle. \end{aligned}} \tag{119}$$

- The normalization factor $1/\sqrt{2\pi\hbar}$ is just a matter of convention.

To verify the first equation in Eq. (119)

$$\begin{aligned} \hat{p}\,|p\rangle &= \frac{1}{\sqrt{2\pi\hbar}} \int dx \left(-i\hbar\,\partial_x e^{i p x/\hbar}\right) |x\rangle \\ &= \frac{1}{\sqrt{2\pi\hbar}} \int dx \left(p\, e^{i p x/\hbar}\right) |x\rangle \\ &= p\,|p\rangle. \end{aligned} \tag{120}$$

This implies

$$\boxed{\begin{aligned} \langle x \mid p\rangle &= \frac{1}{\sqrt{2\pi\hbar}}\, e^{i p x/\hbar}, \\ \langle p \mid x\rangle &= \frac{1}{\sqrt{2\pi\hbar}}\, e^{-i p x/\hbar}, \end{aligned}} \tag{121}$$

which leads to the second equation in Eq. (119). The second equation further implies that

$$\boxed{\begin{aligned} \hat{x} &= i\hbar\,\partial_p, \\ \hat{p} &= -i\hbar\,\partial_x. \end{aligned}} \tag{122}$$

For a *free* particle, the Hamiltonian is a function of momentum only

$$\hat{H} = \frac{\hat{p}^2}{2m}, \tag{123}$$

so the momentum eigenstates $|p\rangle$ are also energy eigenstates,

$$\hat{H}\,|p\rangle = \frac{p^2}{2m}\,|p\rangle. \tag{124}$$

The *position space* wave function of *momentum eigenstate* is given by

$$\langle x \mid p \rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{i\,p\,x/\hbar}, \tag{125}$$

also known as the **plane wave** solution of a free particle. However this wave function is not normalizable, indicating that the idea of free particle in a infinite space is not quite physical (in reality, particles are usually subject to some confining potential).

▪ Fourier Transform

The fact that both position and momentum basis are *complete* ⇒ implies the following resolutions of identity, see Eq. (68),

$$\boxed{\mathbb{1} = \int d\,x\,|x\rangle\,\langle x| = \int d\,p\,|p\rangle\,\langle p|.} \tag{126}$$

Combining two identity operator ⇒ still an identity operator

$$\begin{aligned} \mathbb{1} &= \int d\,x\,d\,p\,|x\rangle\,\langle x \mid p\rangle\,\langle p| = \frac{1}{\sqrt{2\pi\hbar}} \int d\,x\,d\,p\,|x\rangle\,e^{i\,p\,x/\hbar}\,\langle p|, \\ \mathbb{1} &= \int d\,x\,d\,p\,|p\rangle\,\langle p \mid x\rangle\,\langle x| = \frac{1}{\sqrt{2\pi\hbar}} \int d\,x\,d\,p\,|p\rangle\,e^{-i\,p\,x/\hbar}\,\langle x|. \end{aligned} \tag{127}$$

They can be use to transform wave functions between position and momentum basis, e.g.

$$\begin{aligned} &\int d\,x\,\psi(x)\,|x\rangle \\ &= \frac{1}{\sqrt{2\pi\hbar}} \int d\,x\,d\,p\,|p\rangle\,e^{-i\,p\,x/\hbar}\,\langle x| \int d\,x'\,\psi(x')\,|x'\rangle \\ &= \frac{1}{\sqrt{2\pi\hbar}} \int d\,x\,d\,p\,d\,x'\,|p\rangle\,e^{-i\,p\,x/\hbar}\,\psi(x')\,\delta(x-x') \\ &= \frac{1}{\sqrt{2\pi\hbar}} \int d\,x\,d\,p\,|p\rangle\,e^{-i\,p\,x/\hbar}\,\psi(x) \\ &= \int d\,p\,\tilde{\psi}(p)\,|p\rangle, \end{aligned} \tag{128}$$

where $\tilde{\psi}(p)$ is related to $\psi(x)$ by **Fourier transforms**,

$$\boxed{\begin{aligned} \tilde{\psi}(p) &= \frac{1}{\sqrt{2\pi\hbar}} \int d\,x\,e^{-i\,p\,x/\hbar}\,\psi(x), \\ \psi(x) &= \frac{1}{\sqrt{2\pi\hbar}} \int d\,p\,e^{i\,p\,x/\hbar}\,\tilde{\psi}(p). \end{aligned}} \tag{129}$$

- In Eq. (128), the *same* state is written in two *different* ways:
  - as a superposition of *position* basis $\int d\,x\,\psi(x)\,|x\rangle$,

- as a superposition of *momentum* basis $\int d p\, \tilde{\psi}(p)\, |p\rangle$,

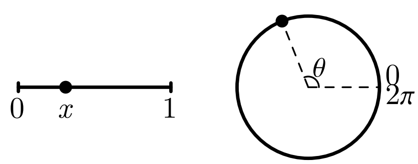
  The superposition coefficients $\psi(x)$ and $\tilde{\psi}(p)$ will be related by *Fourier transforms*, for the two descriptions to be equivalent.

- Sometimes we call $\psi(x)$ the *position (real) space* wave function and $\tilde{\psi}(p)$ the *momentum space* wave function.
- This is an example of **duality** in physics: two seemly *different descriptions* actually correspond to the *same physics*.
- The *Fourier transform* is also a special case of the more general **representation transformation**, which transforms between two arbitrary sets of basis.

Quantum Planar Rotor

Rotor Basis

A **planar rotor** is a particle living on a ring:



- $x \in [0, 1)$ with periodic boundary condition, i.e. $x = 1$ is equivalent to $x = 0$.
- Or in terms of angular variable $\theta = 2\pi x$, s.t. $\theta \in [0, 2\pi)$ with $\theta = 2\pi$ equivalent to $\theta = 0$.

The planar rotor *Hilbert space* can be spanned by a set of basis states $|\theta\rangle$ labeled by the angle $\theta \in [0, 2\pi)$, called the **angular (position) basis** or the **rotor basis**.

- $|\theta\rangle$ describes the state that the rotor is at a definite angular position θ.
- All states $|\theta\rangle$ form a *orthonormal* basis

$$\boxed{\langle\theta_1 \mid \theta_2\rangle = \delta(\theta_1 - \theta_2 \bmod 2\pi).} \tag{130}$$

- Any state of the planar rotor can be expanded as a linear superposition of the rotor basis states

$$\boxed{|\psi\rangle = \int_0^{2\pi} d\theta\, \psi(\theta)\, |\theta\rangle.} \tag{131}$$

  Hereinafter, the integration of any angular variable θ is always assumed to be from 0 to 2π, as $\int_0^{2\pi} d\theta$.

- The *periodicity* of $\theta \Rightarrow |\theta\rangle$ and $|\theta \pm 2\pi\rangle$ are the *same* state (just different names). Any *physical* state/operator should be *invariant* under $\theta \to \theta \pm 2\pi$.

To avoid this naming redundancy, it is better to think that each θ actually labels an element $e^{i\theta}$ in the **U(1) group**, with the *group multiplication* rule

$$e^{i\theta_1} e^{i\theta_2} = e^{i(\theta_1+\theta_2)}. \tag{132}$$

■ Rotation and Angular Momentum

Rotation operator: a *unitary* operator in the rotor Hilbert space that implements the *rotation* $\theta \to \theta+\alpha$.

$$\boxed{\hat{R}(\alpha) = \int d\theta\, |\theta-\alpha\rangle\langle\theta|.} \tag{133}$$

As a unitary operator, the *rotation operator* $\hat{R}(\alpha)$ also has a **Hermitian generator** $\hat{N}$,

$$\boxed{\hat{R}(\alpha) = e^{i\hat{N}\alpha}.} \tag{134}$$

- The operator $\hat{N}$ can be found via

$$\begin{aligned}\hat{N} &= \lim_{\alpha\to 0}\left(-i\,\partial_\alpha \hat{R}(\alpha)\right)\\ &= \lim_{\alpha\to 0}\left(-i\,\partial_\alpha \int d\theta\, |\theta-\alpha\rangle\langle\theta|\right)\\ &= \lim_{\alpha\to 0}\left(-i\,\partial_\alpha \int d\theta_1\, d\theta_2\, |\theta_1\rangle\,\delta(\theta_1-\theta_2+\alpha)\,\langle\theta_2|\right)\\ &= \lim_{\alpha\to 0}\int d\theta_1\, d\theta_2\, |\theta_1\rangle\,(-i\,\delta'(\theta_1-\theta_2+\alpha))\,\langle\theta_2|\\ &= \int d\theta_1\, d\theta_2\, |\theta_1\rangle\,(-i\,\delta'(\theta_1-\theta_2))\,\langle\theta_2|\end{aligned} \tag{135}$$

- Acting $\hat{N}$ on a state $|\psi\rangle = \int d\theta\,\psi(\theta)\,|\theta\rangle$,

$$\begin{aligned}\hat{N}\,|\psi\rangle &= \int d\theta\, d\theta'\, |\theta\rangle\,(-i\,\delta'(\theta-\theta'))\,\psi(\theta')\\ &= \int d\theta\, d\theta'\, |\theta\rangle\,(-i\,\delta(\theta-\theta')\,\partial_{\theta'}\psi(\theta'))\\ &= \int d\theta\,(-i\,\partial_\theta\psi(\theta))\,|\theta\rangle,\end{aligned} \tag{136}$$

  the effect is like (in sloppy notation)

$$\hat{N}\,\psi(\theta) = -i\,\partial_\theta\psi(\theta). \tag{137}$$

Thus we identify the rotation generator $\hat{N}$ to be

$$\boxed{\hat{N} = -i\,\partial_\theta = -i\int d\theta_1\, d\theta_2\, |\theta_1\rangle\,\delta'(\theta_1-\theta_2)\,\langle\theta_2|.} \tag{138}$$

The **rotation generator** should be related to the **angular momentum** operator $\hat{L}$. The precise relation is

$$\hat{L} = \hat{N}\,\hbar, \tag{139}$$

as $\hbar$ provides a natural unit for angular momentum (since they have the same dimension). If we set $\hbar = 1$, we may also call $\hat{N}$ as the (dimensionless) *angular momentum* operator of a planar rotor.

▪ Angular Momentum Quantization

What are the *eigenvalues* and *eigenstates* of the angular momentum operator $\hat{N}$? To figure out, we need to solve the eigen equation:

$$\hat{N}\,|N\rangle = N\,|N\rangle, \tag{140}$$

where the **eigenstate** $|N\rangle$ is label by the **eigenvalue** N, and can be written as a *linear superposition* of the *rotor basis* $|\theta\rangle$

$$|N\rangle = \int d\theta\,|\theta\rangle\,\langle\theta \mid N\rangle, \tag{141}$$

with the wave function (the superposition coefficient) $\langle\theta \mid N\rangle$. Plugging Eq. (138) and Eq. (141) into Eq. (140), we obtain

$$-i\,\partial_\theta\langle\theta \mid N\rangle = N\,\langle\theta \mid N\rangle \Rightarrow \langle\theta \mid N\rangle \propto e^{i\,N\,\theta}. \tag{142}$$

After normalization

$$\boxed{|N\rangle = \frac{1}{\sqrt{2\,\pi}}\int d\theta\;e^{i\,N\,\theta}\,|\theta\rangle.} \tag{143}$$

HW 5 Verify that the state $|N\rangle$ in Eq. (143) has been properly normalized, s.t. $\langle N \mid N\rangle = 1$.

But recall the **periodic boundary condition** (or called the **compactification condition**): $|\theta\rangle$ is equivalent to $|\theta \pm 2\,\pi\rangle$ ⇒ **physical states** must be *invariant* under $\theta \to \theta \pm 2\,\pi$ ⇒ the eigenstate $|N\rangle$ is physical iff

$$\begin{aligned}|N\rangle &= \hat{R}(2\,\pi)\,|N\rangle\\ &= e^{2\,\pi\,i\,\hat{N}}\,|N\rangle\\ &= e^{2\,\pi\,i\,N}\,|N\rangle,\end{aligned} \tag{144}$$

which requires $e^{2\,\pi\,i\,N} = 1$, i.e. the eigenvalue N must be an **integer**

$$\boxed{N = 0, \pm 1, \pm 2, \ldots \text{ or } N \in \mathbb{Z}.} \tag{145}$$

- If the *coordinate* is **compact** (like θ), the *momentum* will be **quantized** (like N).
- The integer N is also called the angular momentum **quantum number**. As we restore the dimension, the angular momentum is quantized to $N\,\hbar$ (in unit of $\hbar$).

The state $|N\rangle$ describes a quantum planar rotor with definite angular momentum N (or more precisely $N\hbar$).

- $|N=0\rangle$ state: a *equal weight* and *equal phase* superposition of all rotor basis

$$|N\rangle = \frac{1}{\sqrt{2\pi}} \int d\theta \, |\theta\rangle. \tag{146}$$

  - Zero angular momentum ⇒ the rotor is "static" (but not in the classical sense).
  - The probability to find the rotor at angle θ: $p(\theta) = 1/(2\pi)$ ⇒ the rotor rests everywhere with equal probability ⇒ manifesting the *uncertainty relation* and *quantum fluctuations*.
- $N > 0$ states ⇒ *positive* angular momentum ⇒ *counterclockwise* rotating rotors.
- $N < 0$ states ⇒ *negative* angular momentum ⇒ *clockwise* rotating rotors.

Representation Transformation

As *eigenstates* of a *Hermitian* operator $\hat{N}$, the states $|N\rangle$ also form a complete set of orthonormal basis for the rotor Hilbert space, called the **angular momentum basis**.

- Unlike the *rotor basis*, the *angular momentum basis* is **discrete**. Its orthonormality implies

$$\langle N_1 \mid N_2\rangle = \delta_{N_1 N_2}. \tag{147}$$

  Its completeness implies

$$\mathbb{1} = \sum_{N\in\mathbb{Z}} |N\rangle\langle N|. \tag{148}$$

- The two sets of basis are related by

$$\boxed{\begin{aligned} |N\rangle &= \frac{1}{\sqrt{2\pi}} \int_{U(1)} d\theta \, e^{i N\theta} |\theta\rangle, \\ |\theta\rangle &= \frac{1}{\sqrt{2\pi}} \sum_{N\in\mathbb{Z}} e^{-i N\theta} |N\rangle. \end{aligned}} \tag{149}$$

- The basis transformations are implemented by **Fourier transforms**

$$\begin{aligned} \mathbb{1} &= \frac{1}{\sqrt{2\pi}} \sum_{N\in\mathbb{Z}} \int_{U(1)} d\theta \, |\theta\rangle \, e^{i N\theta} \langle N|, \\ \mathbb{1} &= \frac{1}{\sqrt{2\pi}} \sum_{N\in\mathbb{Z}} \int_{U(1)} d\theta \, |N\rangle \, e^{-i N\theta} \langle \theta|. \end{aligned} \tag{150}$$

Free Planar Rotor

A *free* planar rotor is described by the following Hamiltonian

$$\hat{H} = \frac{1}{2I} \hat{L}^2 = \frac{\hbar^2}{2I} \hat{N}^2 = -\frac{\hbar^2}{2I} \partial_\theta^2, \tag{151}$$

where $I = m R^2$ is the **moment of inertia**. $\hat{H}$ = the kinetic energy (operator) of the rotor. To make life easier, let us set $\hbar^2 I^{-1} = 1$ (as our energy unit) and consider

$$\boxed{\hat{H} = \frac{1}{2}\hat{N}^2.} \tag{152}$$

The *angular momentum* eigenstates $|N\rangle$ are automatically *energy* eigenstates

$$\boxed{\begin{aligned}&\hat{H}\,|N\rangle = E_N\,|N\rangle,\\ &E_N = \frac{1}{2}N^2.\end{aligned}} \tag{153}$$

- The eigenenergies are **discrete** ⇒ **energy levels**.
- The *lowest* energy eigenstate $|0\rangle$ is called the **ground state**. All the other *higher* energy eigenstates $|N\rangle$ (for $N = \pm 1, \pm 2, \ldots$) are **excited states**.
- The *ground* state of the free planar rotor is *unique* (*non-degenerated*). All the *excited* states are *two-fold degenerated*, i.e. **level degeneracy** = 2.

For $N \neq 0$, the two states $|N\rangle$ and $|-N\rangle$ are related by the **reflection symmetry**, under which $\theta \to -\theta$ and $N \to -N$.

- The symmetry can be implemented by the *unitary* operator $\hat{P}$

$$\boxed{\hat{P} = \int d\theta\,|-\theta\rangle\,\langle\theta| = \sum_N |-N\rangle\,\langle N|.} \tag{154}$$

- It is a $\mathbb{Z}_2$ symmetry, i.e. $\hat{P}^2 = \mathbb{1}$, so $\hat{P}^{-1} = \hat{P}^\dagger = \hat{P}$.
- The Hamiltonian $\hat{H}$ is *invariant* under the symmetry transformation $\hat{P}$

$$\hat{P}\,\hat{H}\,\hat{P} = \hat{H}, \tag{155}$$

because $\hat{H}$ and $\hat{P}$ commute.

HW 6

(i) Use Eq. (149) to show that $\int d\theta\,|-\theta\rangle\,\langle\theta|$ and $\sum_N |-N\rangle\,\langle N|$ are the same operator.
(ii) Show that $\hat{H}$ and $\hat{P}$ commute, i.e. $\hat{H}\,\hat{P} = \hat{P}\,\hat{H}$.

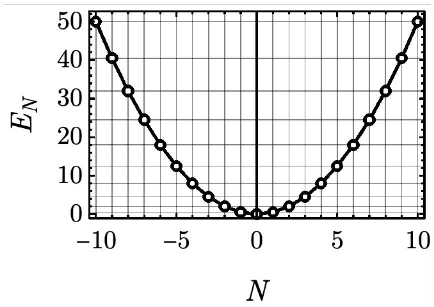
Using Eq. (155), can show that

$$E_N\,|N\rangle = \hat{H}\,|N\rangle = \hat{P}\,\hat{H}\,\hat{P}\,|N\rangle = \hat{P}\,\hat{H}\,|-N\rangle = E_{-N}\,\hat{P}\,|-N\rangle = E_{-N}\,|N\rangle, \tag{156}$$

meaning that $E_N = E_{-N}$. So $|N\rangle$ and $|-N\rangle$ state must have the same energy (as long as $N \neq 0$) ⇒ hence the *two-fold* degeneracy of excited levels is *enforced* by **symmetry**.

The energy has a quadratic dependence on the quantum number N,

$$E_N = \frac{1}{2} N^2. \tag{157}$$



- **Density of state**: number of states per energy interval (usually defined in the thermodynamic limit to smooth out the discreteness).

$$D(E) = \frac{d N}{d E} \propto \frac{1}{\sqrt{E}}. \tag{158}$$

If the rotor is *electrically charged*, it can be driven by electromagnetic field. It can absorb an incident photon of frequency ω and transits from the ground state $|0\rangle$ to an excited state $|N\rangle$, if $\hbar\,\omega = E_N - E_0$. The absorption rate (at low temperature) will be proportional to $D(E_0 + \hbar\,\omega)$.

Raising and Lowering Operators

We have defined the *angular momentum* operator $\hat{N}$ of the planar rotor. What about the *angular position* operator $\hat{\theta}$? - We may attempt to define:

$$\hat{\theta} = \int d\theta\,|\theta\rangle\,\theta\,\langle\theta|. \tag{159}$$

However, it is ill-defined, because it is *not invariant* under the 2π-rotation.

$$\hat{R}(2\pi)\,\hat{\theta}\,\hat{R}^\dagger(2\pi) = \hat{\theta} + 2\pi\,\mathbb{1} \neq \hat{\theta}. \tag{160}$$

So the operator $\hat{\theta}$ is *unphysical*.

Then what operator(s) should we measure to determine the "position" of the rotor? - The **raising** and **lowering** operators,

$$\boxed{e^{\pm i\,\hat{\theta}} = \int d\theta\,|\theta\rangle\,e^{\pm i\,\theta}\,\langle\theta|.} \tag{161}$$

- $e^{+i\,\hat{\theta}}$: **raising operator**, $e^{-i\,\hat{\theta}}$ **lowering operator**.

- Or to be *Hermitian*, what we really measure should be the real and imaginary parts of $e^{\pm i\,\hat{\theta}}$

$$\begin{aligned} \cos\hat{\theta} &= \int d\theta\,|\theta\rangle\cos\theta\,\langle\theta|, \\ \sin\hat{\theta} &= \int d\theta\,|\theta\rangle\sin\theta\,\langle\theta|. \end{aligned} \tag{162}$$

Why are $e^{\pm i\hat{\theta}}$ called *raising* and *lowering*?

$$
\begin{aligned}
e^{\pm i\hat{\theta}}|N\rangle &= e^{\pm i\hat{\theta}} \frac{1}{\sqrt{2\pi}} \int d\theta\, e^{i N\theta} |\theta\rangle \\
&= \frac{1}{\sqrt{2\pi}} \int d\theta\, e^{i N\theta}\, e^{\pm i\hat{\theta}} |\theta\rangle \\
&= \frac{1}{\sqrt{2\pi}} \int d\theta\, e^{i N\theta}\, e^{\pm i\theta} |\theta\rangle \\
&= \frac{1}{\sqrt{2\pi}} \int d\theta\, e^{i (N\pm 1)\theta} |\theta\rangle \\
&= |N \pm 1\rangle.
\end{aligned}
\tag{163}
$$

Because $e^{\pm i\hat{\theta}}$ indeed raise or lower the *angular momentum* of the planar rotor.

$$\boxed{e^{\pm i\hat{\theta}} = \sum_N |N \pm 1\rangle \langle N|.} \tag{164}$$

To compare:

- $\hat{\theta}$ generates the shift of angular momentum $e^{\pm i\hat{\theta}} = \sum_N |N \pm 1\rangle \langle N|$.
- $\hat{N}$ generates the rotation $e^{i\hat{N}\alpha} = \int d\theta\, |\theta - \alpha\rangle \langle\theta|$.

HW 7

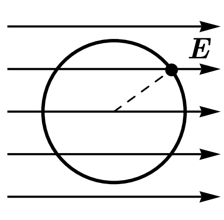
> A free planar rotor, described by the Hamiltonian $\hat{H} = \frac{1}{2}\hat{N}^2$, was initial prepared in the state $|\psi(0)\rangle = (4\pi)^{-1/2} \int d\theta \left(1 + e^{i\theta}\right) |\theta\rangle$. Find the expectation value of the raising operator $e^{i\hat{\theta}}$ as a function of time t. (May set $\hbar = 1$ for simplicity.)

■ Charged Rotor in Electric Field

The electric field provides a **potential energy** for the charged particle

$$V(\theta) = g\,(1 - \cos\theta), \tag{165}$$

where $g = q\,R\,|\boldsymbol{E}|$ characterizes the strength of the electric field.



The Hamiltonian operator

$$\boxed{\hat{H} = \frac{1}{2}\hat{N}^2 + g\left(\mathbb{1} - \cos\hat{\theta}\right).} \tag{166}$$

The potential term g can be written as raising/lowering operators

$$\begin{aligned}\hat{H} &= \frac{1}{2}\hat{N}^2 + g\,\mathbb{1} - \frac{g}{2}\left(e^{+i\hat{\theta}} + e^{-i\hat{\theta}}\right)\\ &= \sum_N\left(\left(\frac{N^2}{2} + g\right)|N\rangle\langle N| - \frac{g}{2}|N+1\rangle\langle N| - \frac{g}{2}|N-1\rangle\langle N|\right).\end{aligned} \tag{167}$$

This provides a matrix representation of the Hamiltonian

$$\hat{H} \doteq \begin{pmatrix} \ddots & \ddots & & & & & \\ \ddots & 2+g & -g/2 & & & & \\ & -g/2 & 1/2+g & -g/2 & & & \\ & & -g/2 & g & -g/2 & & \\ & & & -g/2 & 1/2+g & -g/2 & \\ & & & & -g/2 & 2+g & \ddots \\ & & & & & \ddots & \ddots \end{pmatrix}. \tag{168}$$

Eigenvalues and eigenstates of $\hat{H}$ can be obtained by diagonalizing the Hamiltonian (using the matrix form).

$$\hat{H}|n\rangle = E_n|n\rangle. \tag{169}$$

Let us do it numerically:

- In numerics, we need to *truncate* the angular momentum basis to $N \in [-M, M]$, altogether $2M+1$ basis states. If we only care about the **low-energy physics**, large angular momentum states are not important.

```
M = 32;
```

- We will consider a relatively *large* g, such that the rotor is almost pinned around $\theta = 0$ to do *small* oscillations ⇒ approximated by a **harmonic oscillator**.

```
g = 256;
```

$$\hat{H} \xrightarrow{\theta\to 0} \frac{1}{2}\hat{N}^2 + \frac{g}{2}\hat{\theta}^2 + \ldots. \tag{170}$$

- Construct and diagonalize the Hamiltonian (a $(2M+1)\times(2M+1)$ matrix)

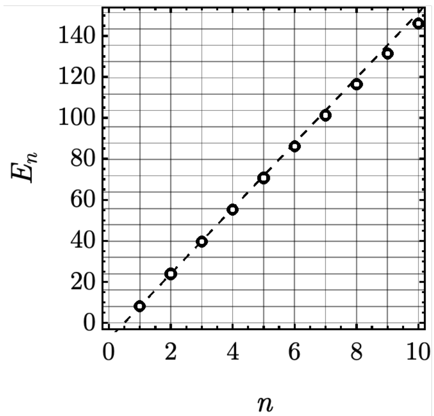
```
H = SparseArray[{Band[{1, 1}] → Range[-M, M]^2 / 2 + g,
    Band[{1, 2}] → -g / 2, Band[{2, 1}] → -g / 2}, {2 M + 1, 2 M + 1}];
eigs = SortBy[First]@Thread@Eigensystem@N@H;
```

- Now `eigs` contains the full list of $(E_n, |n\rangle)$ pairs (that solves the eigen equation Eq. (169)), with $|n\rangle$ represented by a state vector $\tilde{\psi}_n$ in the angular momentum basis (each with $2M+1$ components)

$$|n\rangle = \sum_N \tilde{\psi}_{n,N} \, |N\rangle. \tag{171}$$

- The low-lying energy levels ($n \ll M$) follow a *linear* relation with the level index $n \Rightarrow$ the neighboring level spacings are equal (denoted as $\hbar\,\omega$)

$$E_n \simeq \hbar\,\omega\left(n + \frac{1}{2}\right). \tag{172}$$



In fact ω is related to g by $\omega = g^{1/2}$ (to be discussed later).

- The *density of state* is uniform (E independent) at low-energy

$$D(E) = \frac{d\,n}{d\,E} \simeq \frac{1}{\hbar\,\omega} = \text{const.} \tag{173}$$

Applying the electric field changes the low-energy density of state drastically. This is a measurable effect in the absorption spectrum $D(E_0 + \hbar\,\omega)$.

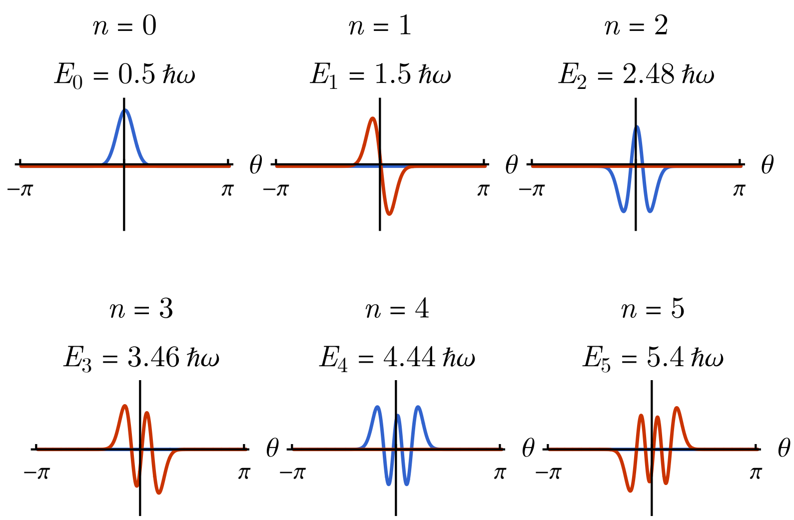
- What does the wave function of each eigenstate look like in the rotor basis?

$$\begin{aligned}|n\rangle &= \sum_N \tilde{\psi}_{n,N} \, |N\rangle \\ &= \frac{1}{\sqrt{2\,\pi}} \int d\theta \sum_N \tilde{\psi}_{n,N} \, e^{i\,N\,\theta} \, |\theta\rangle \\ &= \int d\theta \, \psi_n(\theta) \, |\theta\rangle,\end{aligned} \tag{174}$$

where $\psi_n(\theta)$ is given by

$$\psi_n(\theta) = \frac{1}{\sqrt{2\,\pi}} \sum_N \tilde{\psi}_{n,N} \, e^{i\,N\,\theta}. \tag{175}$$

Some examples of the wave function $\psi_n(\theta)$ (blue - $\operatorname{Re}\psi_n(\theta)$, red - $\operatorname{Im}\psi_n(\theta)$):



■ Potential Momentum

We have been talking about a quantum particle moving in a (energy) potential $V(x)$,

$$\hat{H} = \frac{\hat{p}^2}{2\,m} + V(\hat{x}). \tag{176}$$

- **Potential energy**: as the particle moves from one *position* x_1 to another x_2, if $V(x_1) \neq V(x_2)$, the difference $V(x_2) - V(x_1)$ will be released in the form of *energy* (and can be converted to the kinetic energy).

  For a particle with charge q in an electrostatic potential $\varphi(x)$, we have $V(x) = q\,\varphi(x)$.

Is there also something like a potential **momentum**?

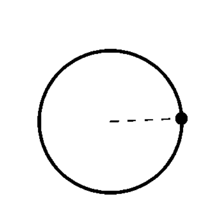
- **Potential momentum**: as the particle travels from one *time* t_1 to another t_2, if $q\,A(t_1) \neq q\,A(t_2)$, the difference $q\,A(t_2) - q\,A(t_1)$ will be released in the form of *momentum* (and can be converted to the kinetic momentum).

Is there any example of potential momentum?

Yes. A *charged* particle q on a ring with *magnetic flux* threading through the ring. Suppose we gradually turn on/off the **magnetic field** $\boldsymbol{B}$, according to **Faraday's law** of induction,

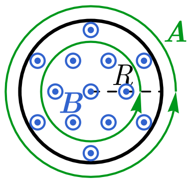
$$\int_\Sigma \frac{\partial \boldsymbol{B}}{\partial t} \cdot d\,\boldsymbol{S} = -\oint_{\partial\Sigma} \boldsymbol{E} \cdot d\,\boldsymbol{l}, \tag{177}$$

an induced **electric field** $\boldsymbol{E}$ will be generated to accelerate/decelerate the charge.



The particle starts from rest. Just by threading the magnetic flux through the ring, the particle acquires (**angular**) **momentum**. ⇒ *Magnetic* field $\boldsymbol{B}$ generates a "potential momentum" $q\,\boldsymbol{A}$ for the surrounding charged particle

$$\int_\Sigma \boldsymbol{B}\cdot d\,\boldsymbol{S} = \oint_{\partial\Sigma} \boldsymbol{A}\cdot d\,\boldsymbol{l} \xRightarrow{\text{on the ring}} A = \frac{B\,R}{2}. \tag{178}$$



Eq. (177) and Eq. (178) implies $\boldsymbol{E} = -\partial_t\,\boldsymbol{A}$ in this case
⇒ $\partial_t(m\,\boldsymbol{v}) = \boldsymbol{F} = q\,\boldsymbol{E} = -\partial_t(q\,\boldsymbol{A})$
⇒ $\partial_t(m\,\boldsymbol{v} + q\,\boldsymbol{A}) = 0$,

such that (the *kinetic* momentum $m\,\boldsymbol{v}$ + the *potential* momentum $q\,\boldsymbol{A}$ =) the total momentum is *conserved.*

How does the potential momentum enter the Hamiltonian?

The *conserved* energy/momentum are time/space translation *generators.* ⇒ They are directly related to the differential operators ∂_t or ∂_x, including the contributions from both the **kinetic** and the **potential** parts.

$$\begin{cases} i\,\hbar\,\partial_t = H = \frac{1}{2}\,m\,v^2 + q\,\varphi, \\ -i\,\hbar\,\partial_x = p = m\,v + q\,A, \end{cases} \Rightarrow H = \frac{1}{2\,m}\,(p - q\,A)^2 + q\,\varphi. \tag{179}$$

The **Schrödinger equation** of charged particle in electromagnetic field (in one-dimensional space)

$$i\,\hbar\,\partial_t\psi = \hat{H}\,\psi = \left[\frac{1}{2\,m}\,(-i\,\hbar\,\partial_x - q\,A)^2 + q\,\varphi\right]\psi. \tag{180}$$

(A, φ) are also called the **gauge** potential. What do we mean by "gauge"? For simplicity, let us set $\hbar = 1$ and $q = 1$,

$$(i\,\partial_t - \varphi)\,\psi = \frac{1}{2\,m}\,(-i\,\partial_x - A)^2\,\psi. \tag{181}$$

- Wave function $\psi(x, t)$ is not physical, only the probability distribution $p(x, t) = |\psi(x, t)|^2$ is physical.
- Attaching an arbitrary phase $\chi(x, t)$ to the wave function at each space time point

  $$\psi(x, t) \to e^{i\,\chi(x,t)}\,\psi(x, t) \tag{182}$$

  does not affect $p(x, t)$ ⇒ Eq. (182) is a **gauge transformation** (= do-nothing/renaming)
- However, gauge transformation *does* affect how ∂_t and ∂_x act on the wave function!

$$i\,\partial_t\psi \to i\,\partial_t\left(e^{i\,\chi}\,\psi\right) = e^{i\,\chi}(i\,\partial_t - \partial_t\,\chi)\,\psi,$$
$$-i\,\partial_x\psi \to -i\,\partial_x\left(e^{i\,\chi}\,\psi\right) = e^{i\,\chi}(-i\,\partial_x + \partial_x\,\chi)\,\psi. \tag{183}$$

φ and A must *transform accordingly* to keep the Schrödinger equation invariant

$$\boxed{\begin{aligned}&\varphi \to \varphi - \partial_t\,\chi,\\ &A \to A + \partial_x\,\chi,\\ &\psi \to e^{i\,\chi}\,\psi.\end{aligned}} \tag{184}$$

The equations in Eq. (184) is the full set of gauge transformations for both the gauge potentials (**gauge field**) and the wave function of charged particles (**matter field**).

*In higher dimensional space-time, using the relativistic notation $A^\mu = (\varphi, \boldsymbol{A})$

$$\psi \to e^{i\,\chi}\,\psi,\;\; A_\mu \to A_\mu + \partial_\mu\,\chi. \tag{185}$$

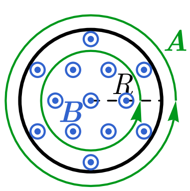
The local phase redundancy of quantum wave function $\Leftrightarrow$ the gauge redundancy of A_μ (under gauge transformation the electromagnetic field strength $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ remains unchanged).

Charged Rotor in Magnetic Field

If the charged particle is confined on a ring (as a planar rotor), with **magnetic flux** Φ through the ring, the Hamiltonian will be

$$\hat{H} = \frac{\hbar^2}{2\,I}\left(\hat{N} - N_\Phi\right)^2, \tag{186}$$

where $N_\Phi = \Phi/\Phi_0$ and $\Phi_0 = h/q$ is the **magnetic flux quantum**.



- Magnetic flux $\Phi = \int_\Sigma \boldsymbol{B}\cdot d\boldsymbol{S} = \oint_{\partial\Sigma}\boldsymbol{A}\cdot d\boldsymbol{l}$,

$$\Phi = \pi\,R^2\,B = 2\,\pi\,R\,A. \tag{187}$$

- Linear potential momentum $q\,\boldsymbol{A}$

$$q\,A = \frac{q\,\Phi}{2\,\pi\,R}. \tag{188}$$

- Angular potential momentum $\boldsymbol{L}_\Phi = \boldsymbol{R}\times(q\,\boldsymbol{A})$

$$L_\Phi = R\,(q\,A) = \frac{q\,\Phi}{2\,\pi}. \tag{189}$$

in unit of $\hbar$ (recall that $L = \hbar\,N$)

$$N_\Phi = \frac{L_\Phi}{\hbar} = \frac{q\,\Phi}{2\,\pi\,\hbar} = \frac{\Phi}{(h/q)} = \frac{\Phi}{\Phi_0}. \tag{190}$$

Physical meaning of N_Φ: *number* of magnetic flux in unit of the flux quantum. Note: the flux quantum depends on the charge carrier q: electrons in a metallic nano-ring $q = e$, Cooper pairs in a superconducting ring (SQUID) $q = 2\,e$.

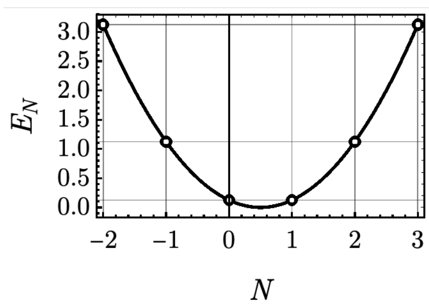
Again, let us set $\hbar^2\, I^{-1} = 1$, and consider

$$\boxed{\hat{H} = \frac{1}{2}\left(\hat{N} - N_\Phi\,\mathbb{1}\right)^2.} \tag{191}$$

Obviously, angular momentum eigenstates $|N\rangle$ are still energy eigenstates, but the energy spectrum is shifted by N_Φ (tunable by magnetic flux Φ)

$$\boxed{\begin{aligned} &\hat{H}\,|N\rangle = E_N\,|N\rangle, \\ &E_N = \frac{1}{2}\,(N - N_\Phi)^2. \end{aligned}} \tag{192}$$

If Φ is fine tuned to $\Phi = \Phi_0/2$, i.e. $N_\Phi = 1/2$,



The *two-fold* degenerated ground states $|N = 0\rangle$ and $|N = 1\rangle$ can be treated as a **qubit**, if the excitation gap is sufficiently large.

*In fact, similar Hamiltonian is used to realize the **superconducting qubit** for quantum computation,

$$H = \frac{1}{2}\,E_C\left(\hat{N} - N_g\,\mathbb{1}\right)^2 - E_J \cos\hat{\theta}, \tag{193}$$

although the physical meaning of $\hat{N}$ and $\cos\hat{\theta}$ are interpreted differently:

- $\hat{N}$: the number of Cooper pairs in the capacitor,
- $\cos\hat{\theta}$: the operator describing Cooper pair tunneling through a Josephson junction.

It is so far the most popular qubit architecture, under active development by Google, Microsoft, IBM, Rigetti, and Intel.

Reference

[1] R. Shankar, Principles of Quantum Mechanics. Plenum Press, New York. (1994)