- Consider quantisation of a system of N point particles with spin propagating in a 3-dimensional Euclidean space.
- In CM each particle is described by a pair of canonically conjugate vectors of coordinates and momenta, and by a spin vector of constant length.
- The phase space of such a system is $\Pi_{a=1}^{N}(\mathbb{R}^6\times S_a^2)=\mathbb{R}^{6N}\times\Pi_{a=1}^{N}\ S_a^2$
- The spin spheres S_a^2 may have different radii for different particles.
- The Poisson structure of this phase space is given by

$$\begin{aligned}&\{p_a^\alpha\,,\,x_b^\beta\}=\delta_{ab}\delta^{\alpha\beta}\,,\quad \{x_a^\alpha\,,\,x_b^\beta\}=0\,,\quad \{p_a^\alpha\,,\,p_b^\beta\}=0\,,\quad \alpha,\beta=1,2,3\,,\quad a,b=1,\dots,N\,,\\ &\{s_a^\alpha\,,\,s_b^\beta\}=-\delta_{ab}\epsilon^{\alpha\beta\gamma}s_b^\gamma\,,\quad \sum_\alpha(s_a^\alpha)^2=\rho_a^2=\text{const}\,,\quad \{s_a^\alpha\,,\,x_b^\beta\}=0\,,\quad \{s_a^\alpha\,,\,p_b^\beta\}=0\end{aligned}\tag{1}$$

(i) $\vec{x}_a=(x_a^1\,,\,x_a^2\,,\,x_a^3)$, $\vec{p}_a=(p_a^1\,,\,p_a^2\,,\,p_a^3)$, and $\vec{s}_a=(s_a^1,s_a^2,s_a^3)$ are vectors of coordinates, momenta, and spins of the a-th particle.

(ii) We often denote the full set of coordinates, momenta and spins by $\{z^i\}$, and write the Poisson bracket of z^i as $\{z^i\,,\,z^j\}=\omega^{ij}(z)$.

THE POSTULATES OF QUANTUM MECHANICS

I. State of a system

- Classical Mechanics

  The state of a mechanical system at any given time t_0 is specified by the full set of coordinates $\{z^i\}$, i.e. by a point in the phase space of the system.

- Quantum Mechanics

  The quantum state of the mechanical system at any given time t_0 is represented by a vector $|\psi\rangle$ in a Hilbert space.

  Since the sum of two vectors is a vector, if $|\psi\rangle$ and $|\xi\rangle$ represent possible states of a system so does their arbitrary linear combination $a|\psi\rangle + b|\xi\rangle$.

  This is called **the principle of superposition**.

II. Coordinates

- Classical Mechanics

  The real coordinates $\{z^i\}$ of the phase space at any given time t_0 have the Poisson brackets

$$\{z^i\,,\, z^j\} = \omega^{ij}(z) \tag{2}$$

  given explicitly for a system of N point particles with spin by (1).

- Quantum Mechanics

  (a) The real coordinates z^i are represented at any given time t_0 by Hermitian operators $\hat{Z}^i$ which satisfy the following commutation relations

$$\begin{aligned}
&\frac{\mathrm{i}}{\hbar}[\hat{P}^\alpha_a\,,\,\hat{X}^\beta_b] = \delta_{ab}\delta^{\alpha\beta}\hat{I}\,, \quad [\hat{X}^\alpha_a\,,\,\hat{X}^\beta_b] = 0\,, \quad [\hat{P}^\alpha_a\,,\,\hat{P}^\beta_b] = 0\,, \quad \alpha,\beta = 1,2,3\,, \quad a,b = 1,\ldots,N\,,\\
&\frac{\mathrm{i}}{\hbar}[\hat{S}^\alpha_a\,,\,\hat{S}^\beta_b] = -\delta_{ab}\epsilon^{\alpha\beta\gamma}\hat{S}^\gamma_b\,, \quad \sum_\alpha(\hat{S}^\alpha_a)^2 = s_a(s_a+1)\hbar^2\hat{I}\,, \quad [\hat{S}^\alpha_a\,,\,\hat{X}^\beta_b] = 0\,, \quad [\hat{S}^\alpha_a\,,\,\hat{P}^\beta_b] = 0
\end{aligned} \tag{3}$$

  where s_a is the spin of the a-th particle.

  (b) The Hilbert space $\mathscr{H}$ is the tensor product of Hilbert spaces of individual particles of the system

$$\mathscr{H} = \mathscr{H}_1 \otimes \mathscr{H}_2 \otimes \cdots \otimes \mathscr{H}_N = \prod_{a=1}^N \otimes \mathscr{H}_a \tag{4}$$

  (c) The operators $\hat{X}^\alpha_a$, $\hat{P}^\alpha_a$ and $\hat{S}^\alpha_a$ of the a-th particle only act in the Hilbert space $\mathscr{H}_a$ of this particle.

(d) The Hilbert space $\mathscr{H}_a$ of the a-th particle is the tensor product of a Hilbert space of dimension $2s_a+1$ which we denote by $\mathscr{H}_a^{\hat{s}}$, and an infinite dimensional Hilbert space which we denote by $\mathscr{H}_a^{\hat{x}\hat{p}}$

$$\mathscr{H}_a = \mathscr{H}_a^{\hat{s}} \otimes \mathscr{H}_a^{\hat{x}\hat{p}} \tag{5}$$

(e) The Hermitian spin operators $\hat{S}_a^\alpha$ only act in $\mathscr{H}_a^{\hat{s}}$. The pair $(\hat{S}_a^\alpha/\mathrm{i}\hbar\,,\,\mathcal{H}_a^{\hat{s}})$ is a spin s_a, $2s_a+1$-dimensional irreducible representation of the Lie algebra $\mathfrak{su}(2)$.

(f) The Hilbert space $\mathscr{H}_a^{\hat{x}\hat{p}}$ is the tensor product of three infinite dimensional Hilbert spaces which we denote by $\mathscr{H}_a^\alpha$, $\alpha=1,2,3$

$$\mathscr{H}_a^{\hat{x}\hat{p}} = \mathscr{H}_a^1 \otimes \mathscr{H}_a^2 \otimes \mathscr{H}_a^3 \tag{6}$$

(g) For each $a=1,\ldots,N$ and $\alpha=1,2,3$ the Hermitian operators of coordinates $\hat{X}_a^\alpha$ and momenta $\hat{P}_a^\alpha$ satisfy the canonical commutation relations of the Heisenberg algebra. They only act in $\mathscr{H}_a^\alpha$ and provide a unitary irreducible representation of the Heisenberg algebra in $\mathscr{H}_a^\alpha$.

If some particles of a system are indistinguishable, that is they have the same spin, mass, electric charge and so on, then the postulate requires refinement which will be discussed later.

III. Observables

- Classical Mechanics

  Every observable (or dynamical variable) at any given time t_0 is a real-valued function $a(z)$ such as z^i themselves, the Hamiltonian, angular momentum and so on.

  The coordinates $\{z^i\}$ of the phase space specify a state of the system and simultaneously are observables.

- Quantum Mechanics

  Observables are Hermitian operators acting in $\mathscr{H}$. The operator $\hat{A}(\hat{Z})$ corresponding at any given time t_0 to a classical observable $a(z)$ is given by

$$\hat{A}(\hat{Z}) = \frac{1}{2}\Big(a(\hat{Z}) + a(\hat{Z})^\dagger\Big) \tag{7}$$

  The eigenvectors of an observable operator are **complete**. Any vector in the Hilbert space of the system can be expressed as a linear combination of them.

IV. Measurements

- Classical Mechanics

  If the system at any given time t_0 is in a state specified by $\{z^i\}$, measurement of the observable a at t_0 will yield a value $a(z)$.

  The state will remain unaffected by the measurement.

- Quantum Mechanics

  If the system at any given time t_0 is in a state $|\psi\rangle$, measurement of the observable $\hat{A}$ at this time will yield one of the eigenvalues a with probability

$$P(a) = \frac{\langle\psi|\alpha\rangle\langle\alpha|\psi\rangle}{\langle\psi|\psi\rangle\langle\alpha|\alpha\rangle} \tag{8}$$

  where $|\alpha\rangle$ is an eigenstate of $\hat{A}$ with the eigenvalue a: $\hat{A}|\alpha\rangle = a|\alpha\rangle$.

  The state of the system will change from $|\psi\rangle$ to $|\alpha\rangle$ as a result of the measurement.

  Therefore, the measurement is represented by the projection operator applied to the state $|\psi\rangle$

$$\hat{\Pi}_\alpha = \frac{1}{\langle\alpha|\alpha\rangle}|\alpha\rangle\langle\alpha| \tag{9}$$

  The postulate as stated only applies to observables with discrete and non-degenerate spectrum, and requires modifications for other observables which will be discussed later.

V. Dynamics

- Classical Mechanics

  An observable $a(z,t)$ changes with time according to Hamilton's equation

$$\frac{da}{dt} = \frac{\partial a}{\partial t} + \{H \, , \, a\} = \frac{\partial a}{\partial t} + \frac{\partial H}{\partial z^j}\,\omega^{ji}(z)\frac{\partial a}{\partial z^i} \tag{10}$$

  where $H = H(z,t)$ is the Hamiltonian of the system.

- Quantum Mechanics

  (i) The Heisenberg Picture

  An observable $\hat{A}(\hat{Z},t)$ changes with time according to the Heisenberg equation

$$\frac{d\hat{A}}{dt} = \frac{\partial \hat{A}}{\partial t} + \frac{\mathrm{i}}{\hbar}\big[\hat{H} \, , \, \hat{A}\big] \tag{11}$$

  where $\hat{H}(\hat{Z},t) = (H(\hat{Z},t) + H(\hat{Z},t)^\dagger)/2$ is the quantum Hamiltonian operator corresponding to the classical Hamiltonian of the system.

  The state $|\psi\rangle$ of the system remains stationary: $|\psi(t)\rangle = |\psi(t_0)\rangle = |\psi\rangle$.

  (ii) The Schrödinger Picture

  The state vector $|\psi\rangle$ obeys the Schrödinger equation

$$\mathrm{i}\,\hbar\frac{d}{dt}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle \, , \quad |\psi(t_0)\rangle = |\psi\rangle \tag{12}$$

  The operators $\hat{Z}^i$, and therefore any observable which only depends on $\hat{Z}^i$ (no explicit time dependence), remain stationary: $\hat{Z}^i(t) = \hat{Z}^i(t_0) = \hat{Z}^i$

Comments on Postulates I-III

There is no logical or intuitive explanation of these postulates. They were formulated in an attempt to explain experimental results, and completely contradict our every day intuition.

I. The quantum state of the mechanical system at any given time t_0 is represented by a vector $|\psi\rangle$ in a Hilbert space.

   (a) It states that a system is described by a ket $|\psi\rangle$ in an infinite dimensional Hilbert space.

   (b) A vector in general has an infinite number of components in a given basis.

   (c) Even for a single particle we need infinitely many numbers to describe its state at a given time.

II. The second postulate explains how individual particles are described in the Hilbert space $\mathscr{H}$ of states of a system of N particles.

   (a) Introduce special operators $\hat{Z}^i$ acting in $\mathscr{H}$, and satisfying the commutation relations (3)

$$\frac{\mathrm{i}}{\hbar}[\hat{P}_a^\alpha\,,\,\hat{X}_b^\beta] = \delta_{ab}\delta^{\alpha\beta}\hat{I}\,,\quad [\hat{X}_a^\alpha\,,\,\hat{X}_b^\beta] = 0\,,\quad [\hat{P}_a^\alpha\,,\,\hat{P}_b^\beta] = 0\,,\quad \alpha,\beta = 1,2,3\,,\quad a,b = 1,\dots,N\,,$$
$$\frac{\mathrm{i}}{\hbar}[\hat{S}_a^\alpha\,,\,\hat{S}_b^\beta] = -\delta_{ab}\epsilon^{\alpha\beta\gamma}\hat{S}_b^\gamma\,,\quad \sum_\alpha(\hat{S}_a^\alpha)^2 = s_a(s_a+1)\hbar^2\hat{I}\,,\quad [\hat{S}_a^\alpha\,,\,\hat{X}_b^\beta] = 0\,,\quad [\hat{S}_a^\alpha\,,\,\hat{P}_b^\beta] = 0$$

   - Coincide with the Poisson algebra of the coordinates z^i of the phase space if one replaces the commutators by the Poisson brackets according to the rule

$$\frac{\mathrm{i}}{\hbar}[\,\bullet\,,\,\bullet\,]\;\mapsto\;\{\bullet\,,\,\bullet\} \tag{13}$$

     This rule allows one to recover CM from QM in the limit $\hbar \to 0$.

- They do not change under an arbitrary unitary similarity transformation of the operators $\hat{Z}^i$

$$\hat{Z}^i \mapsto \hat{U}^\dagger \hat{Z}^i \hat{U}\,, \quad \hat{U}^\dagger \hat{U} = \hat{I} \tag{14}$$

These transformations play the role of canonical transformations.

(b) Use the structure of the commutation relations to explain how individual particles, and degrees of freedom of a particle are embedded in $\mathscr{H}$.

Mathematically, the operators $\hat{Z}^i$ satisfying (3) act in the Hilbert space $\mathscr{H}$ irreducibly.

(c) Due to the tensor product structure of $\mathscr{H}$ we can consider approximate QM systems which describe particles with spin in $d = 0, 1, 2$ space dimensions.

Just remove unnecessary Hilbert spaces from the Hilbert space $\mathscr{H}_a$.

(i) If particles are heavy enough their motion in space can be approximately described by CM. To describe quantum motion we keep only the spin space $\mathscr{H}_a^{\hat{s}}$ in each $\mathscr{H}_a$. In particular, if all particles do not move then they interact with each other only through their spins, and their dynamics is described by H which is a matrix acting in a finite dimensional Hilbert space.

(ii) If all particles are placed in an almost impenetrable tube, then their dynamics can be described by one-dim QM where each $\mathscr{H}_a$ is the tensor product of the spin space $\mathscr{H}_a^{\hat{s}}$ and the coordinate-momentum space $\mathscr{H}_a^1$.

(iii) Similarly, if we place all particles between almost impenetrable parallel plates then we get two-dim QM with $\mathscr{H}_a = \mathscr{H}_a^{\hat{s}} \otimes \mathscr{H}_a^1 \otimes \mathscr{H}_a^2$

(d) We can consider QM in space of any dimension d. However, spin degrees of freedom would be described by irreps of the Lie algebra $\mathfrak{so}(d)$ of the group of rotations $SO(d, \mathbb{R})$ in $\mathbb{R}^d$.

III. Observables are Hermitian operators acting in $\mathscr{H}$. The operator $\hat{A}(\hat{Z})$ corresponding at any given time t_0 to a classical observable $a(z)$ is given by

$$\hat{A}(\hat{Z}) = \frac{1}{2}\Big(a(\hat{Z}) + a(\hat{Z})^\dagger\Big) \tag{15}$$

(a) Explains how quantum observables are constructed from their classical counterparts.

(b) Observables are Hermitian operators because according to the fourth postulate we can measure eigenvalues of observable operators.

(c) The eigenvectors of an observable operator must span the whole Hilbert space because in infinite dimensional Hilbert space there are Hermitian operators whose eigenvectors do not span it. The inclusion of these "bad" operators in the set of observables would violate the probabilistic interpretation of QM encoded in postulate IV.

(d) The prescription (15) explaining how to construct quantum observable $\hat{A}$ from classical observable a guarantees that $\hat{A}$ is a Hermitian operator.

- For example, consider the following Hamiltonian of a one-dimensional particle

$$H(x,p) = \frac{p^2}{2m} + \frac{kx^2}{2} + p\,A(x) \tag{16}$$

where $A(x)$ is any function of x. Then, the quantum Hamiltonian is

$$\hat{H}(\hat{X},\hat{P}) = \frac{\hat{P}^2}{2m} + \frac{k\hat{X}^2}{2} + \frac{1}{2}\,\hat{P}\,A(\hat{X}) + \frac{1}{2}\,A(\hat{X})\,\hat{P} \;\neq\; H(\hat{X},\hat{P}) \tag{17}$$

Note that $H(\hat{X},\hat{P})$ is not a Hermitian operator.

- The prescription (15) is ambiguous. Consider

$$a(x,p) = x^2p^2 \tag{18}$$

By using (15) we get

$$\hat{A}_1(\hat{X},\hat{P}) = \frac{1}{2}\hat{X}^2\hat{P}^2 + \frac{1}{2}\hat{P}^2\hat{X}^2 \tag{19}$$

Let's now write $a(x,p)$ in a different form

$$a(x,p) = x\,p\,x\,p \tag{20}$$

Classically, it is the same function but now (15) gives

$$\begin{aligned}\hat{A}_2(\hat{X},\hat{P}) &= \frac{1}{2}\hat{X}\hat{P}\hat{X}\hat{P} + \frac{1}{2}\hat{P}\hat{X}\hat{P}\hat{X} = \frac{1}{2}\hat{X}(\hat{X}\hat{P} - \mathrm{i}\hbar)\hat{P} + \frac{1}{2}\hat{P}(\hat{P}\hat{X} + \mathrm{i}\hbar)\hat{X} \\ &= \hat{A}_1(\hat{X},\hat{P}) - \frac{\mathrm{i}\hbar}{2}\hat{X}\hat{P} + \frac{\mathrm{i}\hbar}{2}\hat{P}\hat{X} = \hat{A}_1(\hat{X},\hat{P}) + \frac{\hbar^2}{2}\end{aligned} \tag{21}$$

Thus, we got two Hermitian operators corresponding to one and the same function. In fact, there are two more forms of $a(x,p)$, and if we take any linear combination of them reproducing $a(x,p)$ then we can have any coefficient in front of $\hbar^2$ in the formula above.

- This is called operator ordering ambiguity, and only an experiment can determine which ordering is the right one.

Discussion of Postulate IV

- QM makes only probabilistic predictions for the result of a measurement of an observable.
- Iit assigns probabilities only for obtaining some eigenvalue of the observable.
- The only possible values of any observable are its eigenvalues, that is we measure the spectrum of an observable operator.

The spectrum of a Hermitian operator can be discrete, continuous or even mixed.

I. **Discrete and non-degenerate spectrum**

The system is in a state $|\psi\rangle$, and $|\alpha_i\rangle$ is an eigenvector of an observable $\hat{A}$ with an eigenvalue a_i

$$\hat{A}|\alpha_i\rangle = a_i|\alpha_i\rangle \,, \quad a_i \neq a_j \text{ if } i \neq j \,, \quad i, j = 1, 2, \dots \tag{22}$$

The eigenvectors are normalisable and orthogonal to each other.

(a) The probability to find the system in the eigenstate α_i, and to measure its eigenvalue a_i, is

$$P(a_i) = P_i \equiv \frac{\langle\psi|\alpha_i\rangle\langle\alpha_i|\psi\rangle}{\langle\psi|\psi\rangle\langle\alpha_i|\alpha_i\rangle} \tag{23}$$

- The probability does not change if $|\psi\rangle$ and $|\alpha_i\rangle$ are multiplied by any numbers c and d.
- Any two vectors differing by a complex factor describe one and the same physical state. A physical state is described by a **ray** of vectors

$$|\psi\rangle \sim c\,|\psi\rangle \,, \quad c \in \mathbb{C} \tag{24}$$

(b) Given any vector from a ray we can normalise it, and, unless said oppositely, all vectors will be assumed to be normalised: $\langle\psi|\psi\rangle = \langle\alpha_i|\alpha_i\rangle = 1$.

- Even with this normalisation we still have the freedom of multiplying any $|\psi\rangle$ by an arbitrary complex number $e^{\mathrm{i}\varphi}$ of modulus 1.
- The set of all normalised vectors does not form a vector space, and we need to normalise a linear combination of normalised vectors.

(c) The probability formula (23) then simplifies

$$P_i = \langle\psi|\alpha_i\rangle\langle\alpha_i|\psi\rangle = |\langle\alpha_i|\psi\rangle|^2 \,, \quad \langle\psi|\psi\rangle = \langle\alpha_i|\alpha_i\rangle = 1 \tag{25}$$

- α_i form an orthonormal basis, and expanding $|\psi\rangle$ in this basis we get

$$|\psi\rangle = \sum_i |\alpha_i\rangle\langle\alpha_i|\psi\rangle \tag{26}$$

- The probability to find the system in the eigenstate α_i is equal to the absolute value squared of the i-th component of the state vector $|\psi\rangle$ in the basis of $|\alpha\rangle$'s.
- Since the projection operator along the eigenstate $|\alpha_i\rangle$ is given by

$$\hat{\Pi}_i = |\alpha_i\rangle\langle\alpha_i| \,, \tag{27}$$

P_i is equal to the length squared of the projection of the vector $|\psi\rangle$ along $|\alpha_i\rangle$

$$\langle\hat{\Pi}_i\psi|\hat{\Pi}_i\psi\rangle = \langle\psi|\hat{\Pi}_i^2|\psi\rangle = \langle\psi|\hat{\Pi}_i|\psi\rangle = \langle\psi|\alpha_i\rangle\langle\alpha_i|\psi\rangle = P_i \tag{28}$$

- The total probability of finding the system in any eigenstate is equal to 1

$$\sum_i P_i = \sum_i\langle\psi|\alpha_i\rangle\langle\alpha_i|\psi\rangle = \langle\psi|\sum_i |\alpha_i\rangle\langle\alpha_i|\psi\rangle = \langle\psi|\psi\rangle = 1 \tag{29}$$

(d) If $|\psi\rangle$ is an eigenstate $|\alpha_i\rangle$, every measurement of $\hat{A}$ is certain to return the same value a_i. We say that $|\alpha_i\rangle$ is a **determinate state** for the observable $\hat{A}$.

- When two determinate states $|\alpha_1\rangle$ and $|\alpha_2\rangle$ are superposed to form another state

$$|\psi\rangle = \frac{c\,|\alpha_1\rangle + d\,|\alpha_2\rangle}{\sqrt{|c|^2 + |d|^2}} \tag{30}$$

one gets the indeterminate state.

- Measurement of $\hat{A}$ can yield either a_1 or a_2 with probabilities $|c|^2/(|c|^2 + |d|^2)$ and $|d|^2/(|c|^2 + |d|^2)$, respectively.

II. **Discrete and degenerate spectrum**

Some orthonormal eigenvectors $|\alpha_1\rangle$ and $|\alpha_2\rangle$ have the same eigenvalue a.

The vectors $|\alpha_1\rangle$ and $|\alpha_2\rangle$ span the eigenspace $\mathscr{V}_a$ of $\hat{A}$ with eigenvalue a.

(a) The probability to find the system in the eigenstate $|\alpha_i\rangle$ is still equal to $P_i = |\langle\alpha_i|\psi\rangle|^2$, $i = 1, 2$

(b) In an experiment we find the probability $P(a)$ to measure the eigenvalue a, and it is equal to

$$P(a) = P_1 + P_2 = |\langle\alpha_1|\psi\rangle|^2 + |\langle\alpha_2|\psi\rangle|^2 \tag{31}$$

- Since the projection operator onto the eigenspace $\mathscr{V}_a$ is given by

$$\hat{\Pi}_{\mathscr{V}_a} = |\alpha_1\rangle\langle\alpha_1| + |\alpha_2\rangle\langle\alpha_2|\,, \tag{32}$$

$P(a)$ is equal to the length squared of the projection of $|\psi\rangle$ onto the eigenspace $\mathscr{V}_a$

$$\langle\hat{\Pi}_{\mathscr{V}_a}\psi|\hat{\Pi}_{\mathscr{V}_a}\psi\rangle = \langle\psi|\hat{\Pi}^2_{\mathscr{V}_a}|\psi\rangle = \langle\psi|\hat{\Pi}_{\mathscr{V}_a}|\psi\rangle = \langle\psi|\alpha_1\rangle\langle\alpha_1|\psi\rangle + \langle\psi|\alpha_2\rangle\langle\alpha_2|\psi\rangle = P(a) \tag{33}$$

- This formula is valid for any degeneracy of the spectrum, and we can replace the formula (8) in postulate IV by

$$P(a) = \langle\psi|\hat{\Pi}_{\mathscr{V}_a}|\psi\rangle \tag{34}$$

  where $\hat{\Pi}_{\mathscr{V}_a}$ is the projection operator for the eigenspace $\mathscr{V}_a$ with eigenvalue a.

(c) **Example.** The XXX periodic Heisenberg spin 1/2 chain of length 2 is described by

$$\hat{H} = 4\sum_{\alpha=1}^{3} S_1^\alpha S_2^\alpha \tag{35}$$

The Hamiltonian acts in the tensor product of 2 copies of two-dim spaces (spin up-down)

$$\mathscr{H} = \mathbb{C}^2 \otimes \mathbb{C}^2 \tag{36}$$

and the spin 1/2 operator $S_i^\alpha = \hbar\sigma_i^\alpha/2$ acts only on the particle at the i-th site

$$S_1^\alpha = S^\alpha \otimes I\,, \quad S_2^\alpha = I \otimes S^\alpha \tag{37}$$

The orthonormal vectors

$$|e_1\rangle \equiv \;|\uparrow\uparrow\rangle\,, \quad |e_0\rangle \equiv \;\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)\,, \quad |e_{-1}\rangle \equiv \;|\downarrow\downarrow\rangle\,, \tag{38}$$

are eigenvectors of $\hat{H}$ with the eigenvalue $E_1 = \hbar^2$ while the vector

$$|f\rangle \equiv \;\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \tag{39}$$

is an eigenvector of $\hat{H}$ with the eigenvalue $E_0 = -3\hbar^2$.

Consider the state

$$]\psi\rangle = \frac{1}{2}(|\uparrow\uparrow\rangle + |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle + |\downarrow\downarrow\rangle) \tag{40}$$

Find the probabilities to measure E_0 and E_1.

We compute

$$\begin{aligned}
\langle e_1|\psi\rangle &= \langle\uparrow\uparrow|\frac{1}{2}(|\uparrow\uparrow\rangle + |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle + |\downarrow\downarrow\rangle) = \frac{1}{2} \\
\langle e_0|\psi\rangle &= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)\frac{1}{2}(|\uparrow\uparrow\rangle + |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle + |\downarrow\downarrow\rangle) = 0 \\
\langle e_{-1}|\psi\rangle &= \langle\downarrow\downarrow|\frac{1}{2}(|\uparrow\uparrow\rangle + |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle + |\downarrow\downarrow\rangle) = \frac{1}{2} \\
\langle f|\psi\rangle &= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)\frac{1}{2}(|\uparrow\uparrow\rangle + |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle + |\downarrow\downarrow\rangle) = \frac{1}{\sqrt{2}}
\end{aligned} \tag{41}$$

Thus,

$$P(E_1) = \frac{1}{4} + 0 + \frac{1}{4} = \frac{1}{2}, \quad P(E_0) = \frac{1}{2} \tag{42}$$

III. **Continuous spectrum**

(a) The spectrum of some important Hermitian operators, e.g. $\hat{X}$ and $\hat{P}$, is continuous.

- Their eigenvectors are not normalisable, they are not in Hilbert space and they do not represent possible physical states.
- They are δ-function normalised and complete, and any vector can be expanded over them.
- Formula (8) in postulate IV cannot be used because $\langle\alpha|\alpha\rangle = \infty$.

(b) Consider an observable $\hat{W}$ with a continuous non-degenerate spectrum w, and δ-function normalised eigenvectors $|w\rangle$: $\hat{W}|w\rangle = w|w\rangle$.

- An arbitrary normalised vector $|\psi\rangle$ can be expanded as

$$|\psi\rangle = \int dw\, |w\rangle\langle w|\psi\rangle\,, \quad \langle w|w'\rangle = \delta(w - w') \tag{43}$$

- Introduce an auxiliary one-dim set, called the w space, the points in which are labeled by w.
- Think about the coefficients $\langle w|\psi\rangle$ as values of a complex-valued function of w.

(c) This function is denoted by $\psi(w)$ and is called **the wave function in the w space**.

- Examples are the wave functions in the x and p spaces.
- The operator $\hat{W}$ acts on $\psi(w)$ just by multiplication: $\hat{W}\psi(w) = w\psi(w)$.
- There is just one space, the Hilbert space, to which the state vector $|\psi\rangle$ belongs.
- The w space, the x space, etc. are auxiliary manifolds introduced to visualise the components of the infinite-dimensional vector $|\psi\rangle$ in the $\hat{W}$ basis, the $\hat{X}$ basis, and so on.

(d) The wave function $\psi(w)$ is also called the **probability amplitude** for finding the system at the position w in the w space.

(e) Is $|\langle w|\psi\rangle|^2 = |\psi(w)|^2$ the probability for finding the system with a value w for $\hat{W}$?

- The number of possible values for w is infinite
- The system total probability is unity
- Each single value of w can be assigned only an infinitesimal probability.

(f) One interprets $P(w) = |\langle w|\psi\rangle|^2$ to be the **probability density** at w

- $P(w)dw$ is the probability of obtaining a result between w and $w + dw$.
- This definition meets the requirement that the total probability be unity

$$\int dw\, P(w) = \int dw\, |\langle w|\psi\rangle|^2 = \int dw\, \langle\psi|w\rangle\langle w|\psi\rangle = \langle\psi| \int dw\, |w\rangle\langle w|\psi\rangle = \langle\psi|\hat{I}|\psi\rangle = 1 \tag{44}$$

- The completeness relation is crucial for the probabilistic interpretation of QM.

(g) The position operator $\hat{X}$, and the momentum operator $\hat{P}$ have continuous spectra.

- The wave function in the $\hat{X}$ basis (or the x space), $\psi(x)$, is usually referred to as either the wave function in the coordinate space (representation) or as just the wave function
- $|\psi(x)|^2 dx$ is the probability for finding the particle in the space interval $[x, x + dx]$.
- The wave function in the $\hat{P}$ basis (or the p space), $\psi(p)$, is usually referred to as the wave function in the momentum space (representation)
- $|\psi(p)|^2 dp$ is the probability for finding the particle with momentum between p and $p + dp$.

(h) Let us recall and adjust our previous discussion of the operators $\hat{X}$ and $\hat{K}$.

- The eigenvectors of $\hat{X}$ and $\hat{P}$ are denoted as usual by $|x\rangle$ and $|p\rangle$.
- In the coordinate basis the action of $\hat{X}$ and $\hat{P}$ on a wave function $\psi(x)$ is

$$\hat{X}\psi(x) = x\psi(x)\,, \quad \hat{P}\psi(x) = -\mathrm{i}\,\hbar\,\frac{d}{dx}\psi(x) \tag{45}$$

- Their δ-function normalised eigenstates in the coordinate space are

$$\begin{aligned} \hat{X}\psi_a(x) = a\,\psi_a(x) \quad &\Rightarrow \quad \psi_a(x) = \delta(x-a) \\ \hat{P}\psi_p(x) = p\,\psi_p(x) \quad &\Rightarrow \quad \psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}}e^{\mathrm{i}\,p\,x/\hbar} \end{aligned} \tag{46}$$

- The eigenkets of $\hat{P}$ have the following expansion over the coordinate basis

$$|p\rangle = \int dx\,\frac{1}{\sqrt{2\pi\hbar}}e^{\mathrm{i}\,p\,x/\hbar}\,|x\rangle \quad \Rightarrow \quad \langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{\mathrm{i}\,p\,x/\hbar} \tag{47}$$

- $\hat{X}$ and $\hat{P}$ act on a momentum space wave function $\psi(p)$ by

$$\hat{X}\psi(p) = \mathrm{i}\,\hbar\,\frac{d}{dp}\psi(p)\,, \quad \hat{P}\psi(p) = p\,\psi(p) \tag{48}$$

- Their δ-function normalised eigenstates in the momentum space are

$$\begin{aligned} \hat{X}\psi_x(p) = x\,\psi_x(p) \quad &\Rightarrow \quad \psi_x(p) = \frac{1}{\sqrt{2\pi\hbar}}e^{-\mathrm{i}\,p\,x/\hbar} \\ \hat{P}\psi_k(p) = k\,\psi_k(p) \quad &\Rightarrow \quad \psi_k(p) = \delta(p-k) \end{aligned} \tag{49}$$

- The eigenkets of $\hat{X}$ have the following expansion over the momentum basis

$$|x\rangle = \int dp \, \frac{1}{\sqrt{2\pi\hbar}} e^{-\mathrm{i}\, p\, x/\hbar} \, |p\rangle \quad \Rightarrow \quad \langle p|x\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{-\mathrm{i}\, p\, x/\hbar} \tag{50}$$

- The wave functions in the coordinate and momentum representations are related by

$$\begin{aligned} \psi(x) &= \langle x|\psi\rangle = \langle x| \int dp \, \psi(p) \, |p\rangle = \frac{1}{\sqrt{2\pi\hbar}} \int dp \, e^{\mathrm{i}\, p\, x/\hbar} \, \psi(p) \\ \psi(p) &= \langle p|\psi\rangle = \langle p| \int dx \, \psi(x) \, |x\rangle = \frac{1}{\sqrt{2\pi\hbar}} \int dx \, e^{-\mathrm{i}\, p\, x/\hbar} \, \psi(x) \end{aligned} \tag{51}$$

- $\psi(x)$ and $\psi(p)$ are two different functions related to each other by the Fourier transform.

(i) Consider a system of N spinless particles

- Since all $(\hat{X}_a^\alpha) = (\hat{X}_a, \hat{Y}_a, \hat{Z}_a)$ commute with each other there is the simultaneous eigenbasis

$$\big|x_1, y_1, z_1; x_2, y_2, z_2; \ldots; x_N, y_N, z_N\big\rangle$$

of these operators.

- It is called the coordinate basis and normalised as

$$\langle x_1, y_1, \ldots, z_N|x_1', y_1', \ldots, z_N'\rangle = \delta(x_1 - x_1')\delta(y_1 - y_1') \cdots \delta(z_N - z_N') \tag{52}$$

- A state vector $|\psi\rangle$ can be expanded as

$$|\psi\rangle = \int dx_1 dy_1 \cdots dz_N \, |x_1, y_1, \ldots, z_N\rangle\langle x_1, y_1, \ldots, z_N|\psi\rangle \tag{53}$$

- The wave function becomes a square-integrable function of all $3N$ coordinates

$$\psi(x_1, y_1, \dots, z_N) = \langle x_1, y_1, \dots, z_N | \psi \rangle \tag{54}$$

- The coordinate and momenta operators act on the wave function as

$$\begin{aligned} \hat{X}_a^\alpha \psi(x_1^1, x_1^2, \dots, x_N^3) &= x_a^\alpha \psi(x_1^1, x_1^2, \dots, x_N^3) \\ \hat{P}_a^\alpha \psi(x_1^1, x_1^2, \dots, x_N^3) &= -\mathrm{i}\hbar \frac{\partial}{\partial x_a^\alpha} \psi(x_1^1, x_1^2, \dots, x_N^3) \end{aligned} \tag{55}$$

- $|\psi(x_1, y_1, \dots, z_N)|^2 dx_1 dy_1 \cdots dz_N$ is the probability for finding each of the particles in its own box, i.e. the a-th particle in its space box $[x_a, x_a + dx_a] \times [y_a, y_a + dy_a] \times [z_a, z_a + dz_a]$.
- One can also consider the simultaneous eigenbasis $|p_1^x, p_1^y, p_1^z; \dots; p_N^x, p_N^y, p_N^z\rangle$ of the momentum operators, called the momentum basis.

(j) If particles have spin then for each particle we would need an additional discrete index.

- The wave function becomes a collection of wave functions

$$\psi_{k_1 k_2 \cdots k_N}(x_1, y_1, z_1; x_2, y_2, z_2; \dots; x_N, y_N, z_N) \tag{56}$$

  where k_a is a spin index of the a-th particle and takes $2s_a + 1$ values.
- The spin operators acting on the wave functions can change their indices.
- The wave functions are normalised as follows

$$\int dx_1 dy_1 \cdots dz_N \sum_{k_1, k_2, \dots, k_N} \psi^*_{k_1 k_2 \cdots k_N}(x_1, y_1, \dots, z_N) \psi_{k_1 k_2 \cdots k_N}(x_1, y_1, \dots, z_N) = 1 \tag{57}$$

  which is required by the probabilistic interpretation.

IV. **Collapse of the state vector**

Another important aspect of postulate IV is that as P. A. M. Dirac said

"A measurement always causes the system to jump into an eigenstate of the dynamical variable that is being measured."

This phenomenon is called the **collapse of the state vector**.

(a) Before the measurement $|\psi\rangle$ is

$$|\psi\rangle = \sum_i |\alpha_i\rangle\langle\alpha_i|\psi\rangle \,, \quad \hat{A}\,|\alpha_i\rangle = a_i\,|\alpha_i\rangle \tag{58}$$

- When the measurement is performed, the system is "thrown into" one of $|\alpha_i\rangle$'s, say $|\alpha_1\rangle$

$$|\psi\rangle \xrightarrow{\text{measurement}} |\alpha_1\rangle \tag{59}$$

- If we repeat the experiment with this or an equivalent system being in $|\psi\rangle$ then we may find it in any other eigenstate, say $|\alpha_2\rangle$.
- To determine the probability $|\langle\alpha_1|\psi\rangle|^2$ for the system to end up in $|\alpha_1\rangle$ we perform many measurements on an ensemble of identically prepared physical systems, all in $|\psi\rangle$.
- Such an ensemble is known as a **pure ensemble**.
- To verify that after each measurement on the ensemble the system jumps into an eigenstate of $\hat{A}$ we perform a second measurement immediately after the first, and get the same result

$$|\psi\rangle \xrightarrow{\hat{A}\text{ measured, } a_1 \text{ obtained}} |\alpha_1\rangle \xrightarrow{\hat{A}\text{ measured, } a_1 \text{ always obtained}} |\alpha_1\rangle \tag{60}$$

(b) This discussion applies to observables with non-degenerate spectrum.

- If the spectrum is degenerate, say $a_2 = a_1$, then

$$|\psi\rangle \xrightarrow{\hat{A} \text{ measured, } a_1 \text{ obtained}} |\alpha_1'\rangle \equiv \frac{|\alpha_1\rangle\langle\alpha_1|\psi\rangle + |\alpha_2\rangle\langle\alpha_2|\psi\rangle}{\sqrt{|\langle\alpha_1|\psi\rangle|^2 + |\langle\alpha_2|\psi\rangle|^2}} = \frac{|\alpha_1\rangle\langle\alpha_1|\psi\rangle + |\alpha_2\rangle\langle\alpha_2|\psi\rangle}{\sqrt{P(a_1)}} \tag{61}$$

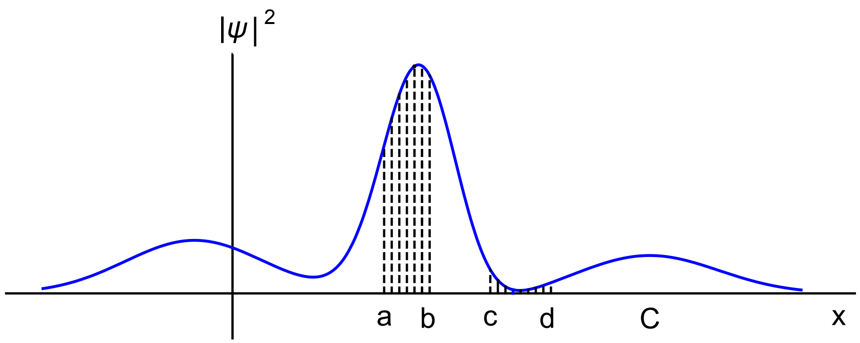
- This is generalised to any degeneracy

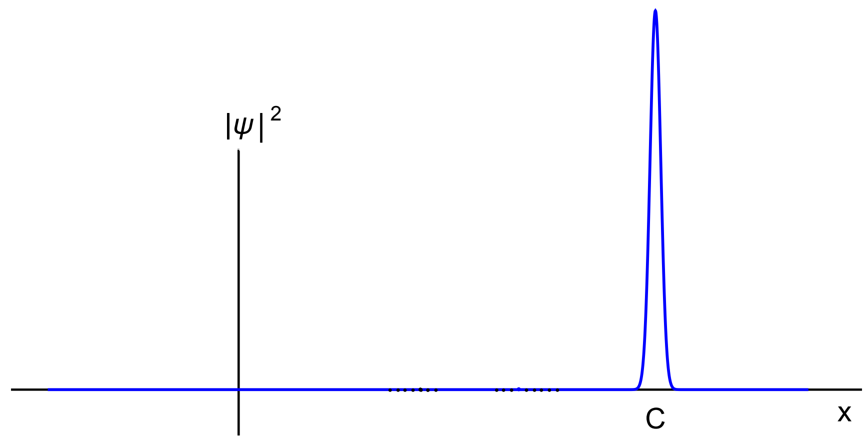
$$|\psi\rangle \xrightarrow{\hat{A} \text{ measured, } a \text{ obtained}} |\alpha\rangle \equiv \frac{\hat{\Pi}_{\mathscr{V}_a}|\psi\rangle}{\sqrt{\langle\hat{\Pi}_{\mathscr{V}_a}\psi|\hat{\Pi}_{\mathscr{V}_a}\psi\rangle}} = \frac{\hat{\Pi}_{\mathscr{V}_a}|\psi\rangle}{\sqrt{P_{\mathscr{V}_a}}} \tag{62}$$

  where $\hat{\Pi}_{\mathscr{V}_a}$ is the projection operator for the eigenspace $\mathscr{V}_a$ with eigenvalue a.
- If the initial state was known then after the measurement the system is the eigenstate of $\hat{A}$ given by the formula.
- If $|\psi\rangle$ was not known then all we find is that the system is in some state in the eigenspace $\mathscr{V}_a$.

(c) If an observable has continuous spectrum then its eigenstates are not normalisable, and after a measurement of the observable a physical state cannot collapse to one of them.

- Consider for example a typical wave function of a particle in one-dimensional coordinate space shown on the left picture below.





- The probability of finding the particle in the interval $[a, b]$ is much higher than, say, in $[c, d]$.
- The particle can be found anywhere in the space.
- If a measurement shows that the particle is at C then as a result of the measurement the wave function collapses to a spike at C whose width depends on the precision of the measurement.
- The second measurement performed immediately after the frst one and with the same precision will find the particle again at C.
- As time passes, the spike will spread out, and we would find the particle anywhere in the space with some probability.

The Stern-Gerlach experiment

The Stern-Gerlach experiment with silver atoms was conducted in 1922 and demonstrated the necessity for a change of the concepts of CM.

(a) Consider a silver atom as a spin 1/2 point particle.

We want to subject a beam of silver atoms to an inhomogeneous magnetic field,

and need to know how a magnetic field interacts with the spin degrees of freedom of the particle.

(b) The spin and a magnetic field are axial vectors $\Rightarrow$ the simplest interaction term is

$$H_{\text{int}} = -\gamma\, \vec{B}(\vec{x}) \cdot \vec{s} = -\gamma \sum_{\alpha=1}^{3} B^{\alpha} s^{\alpha} \tag{63}$$

- $\vec{x}$ is the radius-vector and $\vec{s}$ is the spin vector of the particle
- $\vec{B}$ is the inhomogeneous magnetic field
- the constant γ is called the **gyromagnetic ratio**
- the product $\vec{\mu} \equiv \gamma\, \vec{s}$ is called the **magnetic moment** of the particle.

(c) Since the electric charge of a silver atom is zero, there is no other interaction of the atom with the magnetic field.

(d) The total Hamiltonian is

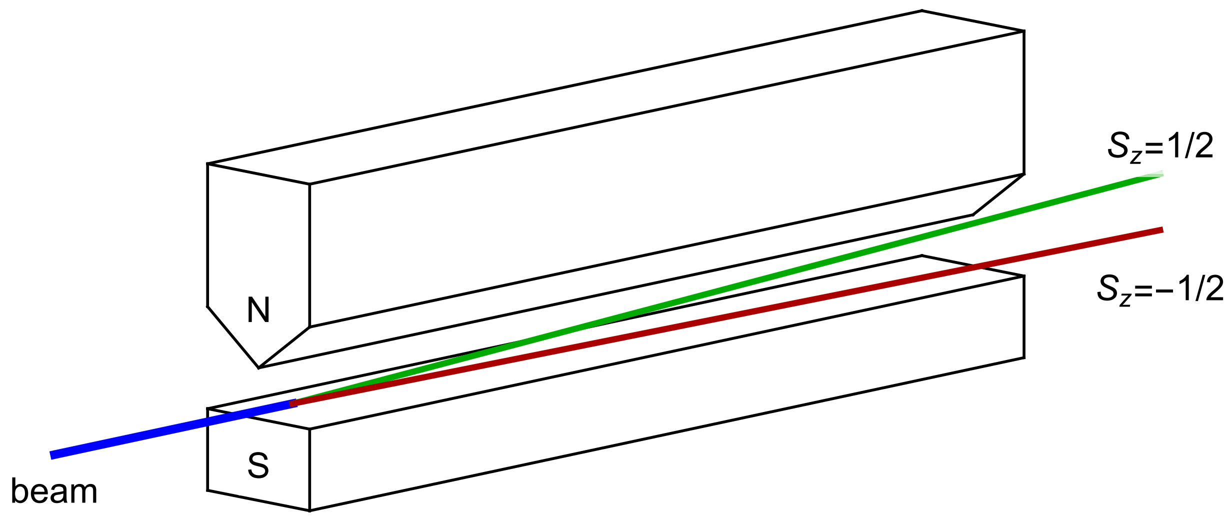
$$H = \frac{p^2}{2m} + H_{\text{int}} = \frac{p^2}{2m} - \gamma \sum_{\alpha=1}^{3} B^\alpha s^\alpha$$

(e) The classical eom of a spinning particle are

$$\begin{aligned} \dot{p}^\alpha &= \{H\,,\,p^\alpha\} = \gamma\,\frac{\partial \vec{B}}{\partial x^\alpha}\cdot\vec{s}\,, \quad m\dot{x}^\alpha = p^\alpha \\ \dot{s}^\alpha &= \{H\,,\,s^\alpha\} = -\gamma\sum_{\rho=1}^{3} B^\rho\{s^\rho\,,\,s^\alpha\} = \gamma\sum_{\beta,\rho=1}^{3} B^\rho\epsilon^{\rho\alpha\beta}s^\beta = \gamma\sum_{\beta,\rho=1}^{3}\epsilon^{\alpha\beta\rho}s^\beta B^\rho = (\vec{\mu}\times\vec{B})^\alpha \end{aligned} \tag{64}$$

- The force the particle experiences depends on the spin orientation.
- The magnetic field can be used to separate atoms with different spin orientations.

(f) In Stern-Gerlach experiment a beam of silver atoms is sent between two powerful magnets



- One magnet has one pole sharpened to a knife edge while the other is approximately flat.
- With this geometry the magnetic field increases in intensity upwards, so atoms that have their spins up are deflected upwards and the other atoms are deflected downwards.
- The atoms in the beam are randomly oriented $\Rightarrow$ expect a continuous bundle of beams coming out of the SG device because all values of s^z could be realised between $-|\vec{s}|$ and $|\vec{s}|$.
- Experiments show that the original beam splits into two distinct components, and therefore only two values of the z-component of $\vec{s}$ are observed.
- Measurements show that $s^z = \pm\hbar/2$.
- If we would oriented the SG device differently we would conclude that the projection of the spin vector on any axis can only take two values $\pm\hbar/2$.

(g) Quantum mechanically the result of the SG experiment can be easily explained.

- The coordinates, momenta, spins and the Hamiltonian become operators

$$\hat{H} = \frac{1}{2m}\sum_{\alpha=1}^{3}\hat{P}^\alpha\hat{P}^\alpha - \gamma\sum_{\alpha=1}^{3}B^\alpha(\hat{X})\hat{S}^\alpha \tag{65}$$

- $\hat{X}^\alpha$ commute with $\hat{S}^\alpha \;\Rightarrow\;$ there is no ordering ambiguity.
- The operators act in $\mathscr{H} = \mathscr{H}^{\hat{s}} \otimes \mathscr{H}^{\hat{x}\hat{p}}$.
  The state vector of an atom in the beam in the coordinate representation is

$$|\psi\rangle = \int d^3x \left(\psi_\uparrow(\vec{x})\,|\vec{x},\uparrow\rangle + \psi_\downarrow(\vec{x})\,|\vec{x},\downarrow\rangle \right), \quad \vec{x} = (x,y,z) = (x^1,x^2,x^3) \tag{66}$$

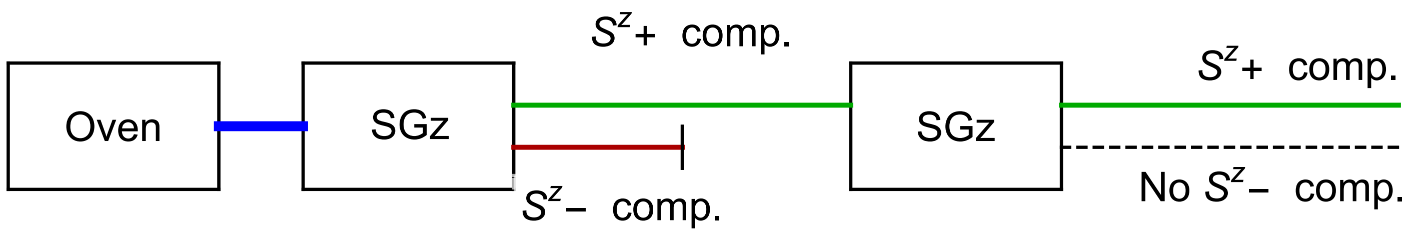
  where the basis kets are eigenstates of $\hat{X}^\alpha$ and $\hat{S}^z = \hat{S}^3$

$$\hat{X}^\alpha\,|\vec{x},\uparrow\rangle = x^\alpha\,|\vec{x},\uparrow\rangle\,, \quad \hat{S}^z\,|\vec{x},\uparrow\rangle = \frac{\hbar}{2}\,|\vec{x},\uparrow\rangle\,, \quad \hat{X}^\alpha\,|\vec{x},\downarrow\rangle = x^\alpha\,|\vec{x},\downarrow\rangle\,, \quad \hat{S}^z\,|\vec{x},\downarrow\rangle = -\frac{\hbar}{2}\,|\vec{x},\downarrow\rangle$$

- The SG device measures $\hat{S}^z \;\Rightarrow\;$ the state vector of each atom collapses into an eigenvector of $\hat{S}^z$.
- Spins are randomly oriented in the beam $\;\Rightarrow\;$ half of the atoms collapses into spin-up state and the other half into spin-down.

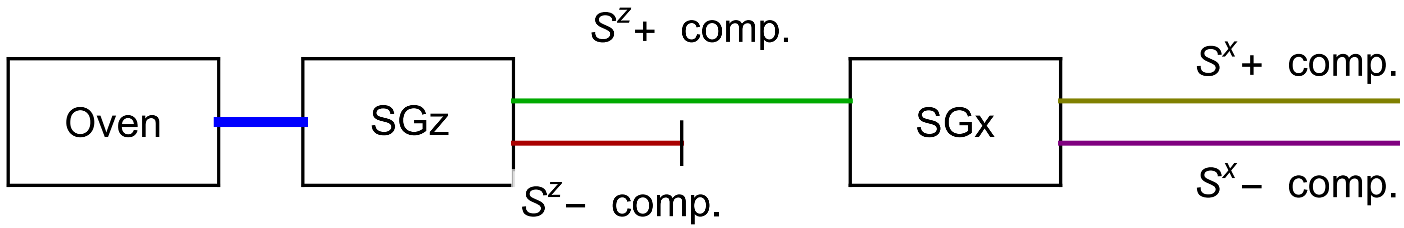
(h) One can verify experimentally whether after the SG measurement the atoms continue to stay in their spin eigenstates.

i. Consider the atomic beam going through several SG devices in sequence.



- A beam is split by the first SG device into an $\hat{S}^z$ up and an $\hat{S}^z$ down beams, and the $\hat{S}^z$ down beam is blocked.
- The remaining $\hat{S}^z$ up beam is subjected by another SG device with the same magnetic field.
- Atoms are in the eigenstate of $\hat{S}^z \;\Rightarrow\;$ all atoms coming from the device have spins up.

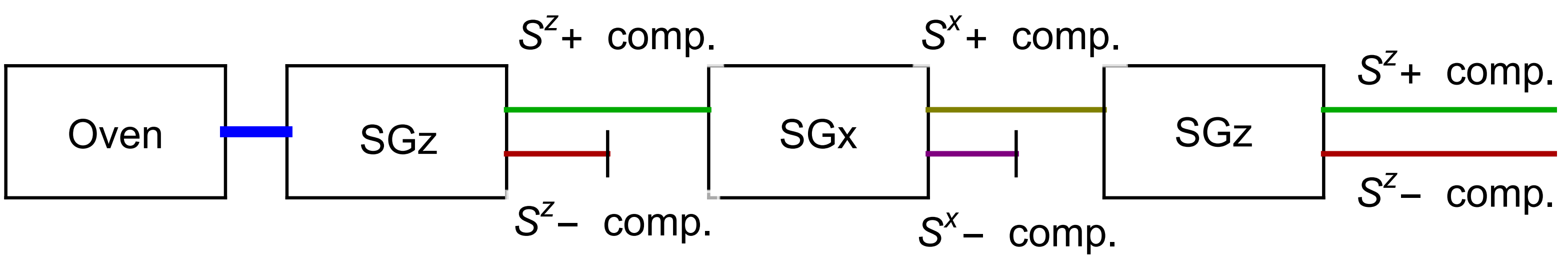
ii. If the second SG device is rotated so that it measured the S^x component



then with equal probability the state vectors of atoms in the remaining beam will collapse into the two eigenstates of $\hat{S}^x$, because the state $|S^z+\rangle \equiv |\uparrow\rangle$ can be decomposed as

$$|S^z+\rangle = \frac{1}{\sqrt{2}}\frac{|S^z+\rangle + |S^z-\rangle}{\sqrt{2}} + \frac{1}{\sqrt{2}}\frac{|S^z+\rangle - |S^z-\rangle}{\sqrt{2}} = \frac{1}{\sqrt{2}}|S^x+\rangle + \frac{1}{\sqrt{2}}|S^x-\rangle \tag{67}$$

iii. If we now block the S^x- component and let the remaining beam to go through a third SG device measuring again the S^z component



then the beam will split again into an $\hat{S}^z$ up and an $\hat{S}^z$ down beams of the same intensity.

More on measurements

I. **Expectation value and the uncertainty**

Given a pure ensemble in a state $|\psi\rangle$, to predict the probability the measurement of an observable $\hat{A}$ will yield an eigenvalue a one has to solve the eigenvalue problem of the operator $\hat{A}$.

It is very detailed information, and often we just need

(a) An average over the ensemble, called the **expectation value**, $\langle \hat{A} \rangle$

- It is just the mean value defined in statistics

$$\begin{aligned} \langle \hat{A} \rangle &= \sum_i P(a_i) a_i = \sum_i |\langle \alpha_i | \psi \rangle|^2 a_i = \sum_i \langle \psi | \alpha_i \rangle \langle \alpha_i | \psi \rangle a_i = \sum_i \langle \psi | a_i | \alpha_i \rangle \langle \alpha_i | \psi \rangle \\ &= \sum_i \langle \psi | \hat{A} | \alpha_i \rangle \langle \alpha_i | \psi \rangle = \langle \psi | \hat{A} \sum_i |\alpha_i \rangle \langle \alpha_i | \psi \rangle = \langle \psi | \hat{A} \hat{I} | \psi \rangle = \langle \psi | \hat{A} | \psi \rangle \end{aligned} \tag{68}$$

- Thus, the expectation value of $\hat{A}$ taken with respect to state $|\psi\rangle$ is

$$\langle \hat{A} \rangle = \langle \psi | \hat{A} | \psi \rangle \equiv \langle \hat{A} \rangle_\psi \tag{69}$$

- If the system is in an eigenstate of $\hat{A}$ then $\langle \hat{A} \rangle = \langle \psi | \hat{A} | \psi \rangle = a \langle \psi | \psi \rangle = a$.

(b) The **standard deviation**

$$\Delta\hat{A} = \sqrt{\langle(\hat{A} - \langle\hat{A}\rangle)^2\rangle} \tag{70}$$

- It measures the average fluctuation around the mean.
- In QM it is referred to as the **uncertainty in** $\hat{A}$.
- $\Delta\hat{A}$ can be calculated if just the state and the operator are given

$$\Delta\hat{A} = \sqrt{\langle\psi|(\hat{A} - \langle\hat{A}\rangle)^2|\psi\rangle} \tag{71}$$

- If the spectrum of $\hat{A}$ and probabilities are known then

$$(\Delta\hat{A})^2 = \sum_i P(a_i)(a_i - \langle\hat{A}\rangle)^2 \tag{72}$$

for discrete spectrum, and

$$(\Delta\hat{A})^2 = \int da\, P(a)(a - \langle\hat{A}\rangle)^2 \tag{73}$$

for continuous.

- $(\Delta\hat{A})^2$ is known as the **dispersion** of $\hat{A}$

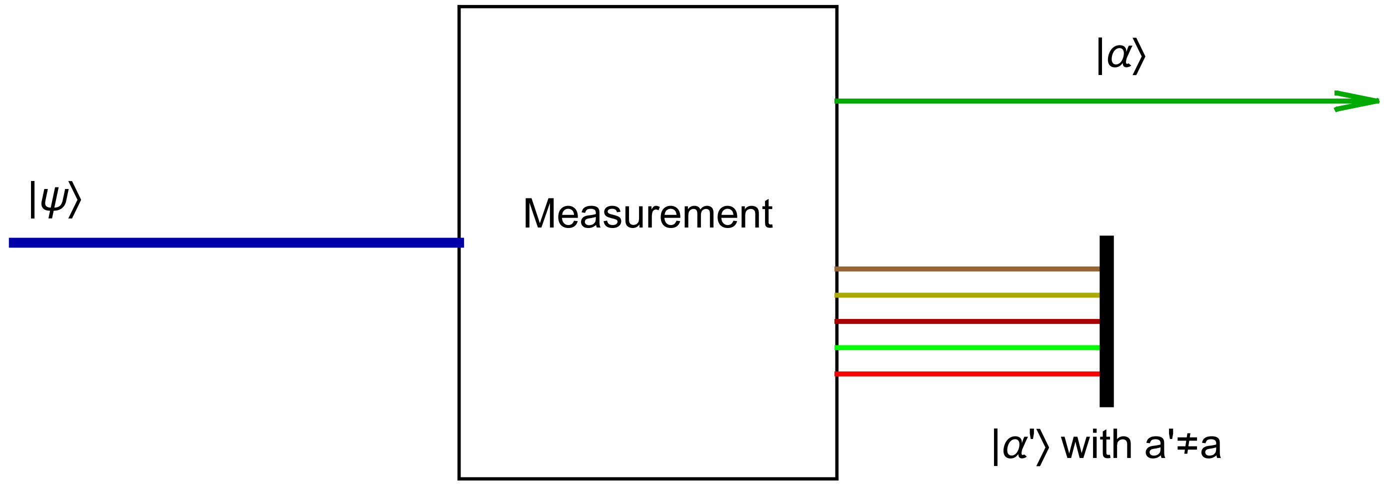
$$(\Delta\hat{A})^2 = \langle(\hat{A} - \langle\hat{A}\rangle)^2\rangle = \langle\left(\hat{A}^2 - 2\hat{A}\langle\hat{A}\rangle + \langle\hat{A}\rangle^2\right)\rangle = \langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2 \geq 0 \tag{74}$$

because for a Hermitian operator $\langle\hat{A}^2\rangle = \langle\psi|\hat{A}\hat{A}|\psi\rangle = |\hat{A}|\psi\rangle|^2 \geq 0$

- Usually, $\langle\hat{A}\rangle$ and $\Delta\hat{A}$ provide us with a fairly good description of the state.
For example, if a particle has $\langle\hat{X}\rangle = a$ and $\Delta\hat{X} = \Delta$ we know that the particle is likely to be spotted near $x = a$, with deviations of order Δ.

II. **Compatible observables**

(a) The SG device combined with blocking one of the spin components works as a filter and leads to the notion of **selective measurement** or **filtration**.



- It is a measurement process by a device which selects only one of the eigenstates of $\hat{A}$, say $|\alpha\rangle$, and rejects all others
- Mathematically filtration amounts to applying the projection operator $\hat{\Pi}_\alpha$ to $|\psi\rangle$

$$\hat{\Pi}_\alpha|\psi\rangle = |\alpha\rangle|\langle\alpha|\psi\rangle \tag{75}$$

- The probability of obtaining the eigenstate $|\alpha\rangle$ is $P(a) = |\langle\alpha|\psi\rangle|^2$.

(b) If having prepared an eigenstate $|\alpha\rangle$ of $\hat{A}$ we immediately measure an observable $\hat{B}$ the system will collapse into an eigenstate $|\beta\rangle$ of $\hat{B}$

- $|\beta\rangle$ in general is not an eigenstate of $\hat{A}$.
- If $|\beta\rangle$ is also an eigenstate of $\hat{A}$ then we denote it by $|\alpha\beta\rangle$, and it satisfies

$$\hat{A}|\alpha\beta\rangle = a|\alpha\beta\rangle \,, \quad \hat{B}|\alpha\beta\rangle = b|\alpha\beta\rangle \tag{76}$$

- If the spectrum of $\hat{A}$ is degenerate the state $|\alpha\beta\rangle$ may be different from $|\alpha\rangle$ but the eigenvalue remains the same.
- The necessary condition for $|\alpha\beta\rangle$ to be a simultaneous eigenvector of $\hat{A}$ and $\hat{B}$ is

$$(\hat{A}\hat{B} - \hat{B}\hat{A})|\alpha\beta\rangle = 0 \tag{77}$$

(c) Observables $\hat{A}$ and $\hat{B}$ are called **compatible** if they commute $[\hat{A}\,,\,\hat{B}] = 0$, and **incompatible** if they do not commute $[\hat{A}\,,\,\hat{B}] \neq 0$.
$\hat{S}^z$ and $\hat{\vec{S}}^2$ are compatible, but $\hat{S}^z$ and $\hat{S}^x$ are incompatible observables.

(d) If two Hermitian operators $\hat{A}$ and $\hat{B}$ commute then a complete basis of simultaneous eigenstates can be found. Consider operators with discrete spectra and construct such a basis.

- We first find any basis of one of the operators, say $\hat{A}$

$$\hat{A}|\alpha_i\rangle = a_i|\alpha_i\rangle \tag{78}$$

- Since $\hat{A}$ and $\hat{B}$ commute the state $\hat{B}|\alpha_i\rangle$ is an eigenstate of $\hat{A}$ with the same eigenvalue a_i

$$\hat{A}(\hat{B}|\alpha_i\rangle) = \hat{B}\hat{A}|\alpha_i\rangle = a_i(\hat{B}|\alpha_i\rangle) \tag{79}$$

- Thus, if $|\alpha_i\rangle$ is the only eigenvector with the eigenvalue a_i then $\hat{B}|\alpha_i\rangle$ must be proportional to $|\alpha_i\rangle$: $\hat{B}|\alpha_i\rangle = b_i|\alpha_i\rangle$, and therefore it is an eigenvector of $\hat{B}$ with the eigenvalue b_i.
- If the eigenvalue a_i is degenerate we consider the eigenvalue problem for $\hat{B}$ restricted to the subspace $\mathscr{V}_{a_i}$ spanned by all eigenvectors of $\hat{A}$ with the eigenvalue a_i.
- The eigenvectors of $\hat{B}$ on this subspace are also eigenvectors of $\hat{A}$ with the eigenvalue a_i.

(e) This consideration can be extended to a set of mutually commuting observables,
and the eigenvalues of these observables can be used to label their simultaneous eigenstates.

(f) Eventually we find a **maximal** set of commuting observables so that we cannot add any more independent observables to our list without violating mutual commutativity.

(g) An example is a system of N spinless particles in the coordinate basis of all position operators.

(h) Consider the following measurements of compatible $\hat{A}$ and $\hat{B}$

$$|\psi\rangle \xrightarrow{\hat{A}\text{ measured, } a \text{ obtained}} |\alpha\rangle \xrightarrow{\hat{B}\text{ measured, } b \text{ obtained}} |\alpha\beta\rangle \xrightarrow{\hat{A}\text{ measured, } a \text{ obtained}} |\alpha\beta\rangle \tag{80}$$

- We first measure $\hat{A}$, and $|\psi\rangle$ collapses to an eigenstate $|\alpha\rangle$ of $\hat{A}$ with the eigenvalue a.
- Then, we measure $\hat{B}$, and $|\alpha\rangle$ may collapse to an eigenstate $|\alpha\beta\rangle$ of $\hat{B}$ different from $|\alpha\rangle$.
- $|\alpha\beta\rangle$ is an eigenstate of $\hat{A}$ with the same eigenvalue a, and the last measurement of $\hat{A}$ will leave the state $|\alpha\beta\rangle$ untouched.
- $\hat{A}$ measurements and $\hat{B}$ measurements do not interfere which explains the term compatible.
- As a result of filtrations we have prepared a simultaneous eigenstate of $\hat{A}$ and $\hat{B}$.

III. **The uncertainty relation**

(a) If two observables are incompatible then they do not have a complete basis of simultaneous eigenstates but they still may have some common eigenstates.

(b) The position and momentum operators $\hat{X}$ and $\hat{P}$ are incompatible

$$[\hat{X}\,,\ \hat{P}] = \mathrm{i}\hbar \tag{81}$$

and have no simultaneous eigenkets.

(c) **The uncertainty relation.** Let $\hat{A}$ and $\hat{B}$ be observables. Then for any state the following inequality holds

$$\Delta\hat{A}\,\Delta\hat{B} \geq \frac{1}{2}|\langle[\hat{A}\,,\ \hat{B}]\rangle| \tag{82}$$

Proof.

- We use the Schwarz inequality

$$\langle\alpha|\alpha\rangle\langle\beta|\beta\rangle \geq |\langle\alpha|\beta\rangle|^2 \qquad \forall\ |\alpha\rangle\,,\ |\beta\rangle \tag{83}$$

- To prove it consider $(\langle\alpha| + \lambda^*\langle\beta|)(|\alpha\rangle + \lambda|\beta\rangle) \geq 0$, and sett $\lambda = -\langle\beta|\alpha\rangle/\langle\beta|\beta\rangle$.
- The Schwarz inequality is saturated only if $|\beta\rangle = c|\alpha\rangle$
- Let $|\psi\rangle$ be any state, $\langle\hat{A}\rangle = \langle\psi|\hat{A}|\psi\rangle\ \ \forall\ \hat{A}$, and

$$|\alpha\rangle = (\hat{A} - \langle\hat{A}\rangle)|\psi\rangle\,, \quad \langle\alpha|\alpha\rangle = \Delta\hat{A}^2\,, \quad |\beta\rangle = (\hat{B} - \langle\hat{B}\rangle)|\psi\rangle\,, \quad \langle\beta|\beta\rangle = \Delta\hat{B}^2 \tag{84}$$

- The Schwarz inequality gives

$$\Delta\hat{A}^2\Delta\hat{B}^2 \geq \langle\alpha|\beta\rangle\langle\beta|\alpha\rangle \tag{85}$$

- We find

$$
\begin{aligned}
\langle\alpha|\beta\rangle &= \langle\psi|(\hat{A}-\langle\hat{A}\rangle)(\hat{B}-\langle\hat{B}\rangle)|\psi\rangle = \langle\hat{A}\hat{B}\rangle - \langle\hat{A}\rangle\langle\hat{B}\rangle \\
&= \langle\Big(\frac{1}{2}(\hat{A}\hat{B}+\hat{B}\hat{A}) + \frac{1}{2}(\hat{A}\hat{B}-\hat{B}\hat{A})\Big)\rangle - \langle\hat{A}\rangle\langle\hat{B}\rangle = \frac{1}{2}\langle[\hat{A}\,,\,\hat{B}]_+\rangle + \frac{1}{2}\langle[\hat{A}\,,\,\hat{B}]\rangle - \langle\hat{A}\rangle\langle\hat{B}\rangle
\end{aligned} \tag{86}
$$

  where $[\hat{A}\,,\,\hat{B}]_+ \equiv \hat{A}\hat{B}+\hat{B}\hat{A} = [\hat{B}\,,\,\hat{A}]_+$ is the **anti-commutator** of $\hat{A}$ and $\hat{B}$.
- Thus,

$$
\begin{aligned}
\langle\alpha|\beta\rangle\langle\beta|\alpha\rangle &= \Big(\frac{1}{2}\langle[\hat{A}\,,\,\hat{B}]_+\rangle + \frac{1}{2}\langle[\hat{A}\,,\,\hat{B}]\rangle - \langle\hat{A}\rangle\langle\hat{B}\rangle\Big)\Big(\frac{1}{2}\langle[\hat{B}\,,\,\hat{A}]_+\rangle + \frac{1}{2}\langle[\hat{B}\,,\,\hat{A}]\rangle - \langle\hat{B}\rangle\langle\hat{A}\rangle\Big) \\
&= \Big(\frac{1}{2}\langle[\hat{A}\,,\,\hat{B}]_+\rangle - \langle\hat{A}\rangle\langle\hat{B}\rangle\Big)^2 - \frac{1}{4}\langle[\hat{A}\,,\,\hat{B}]\rangle^2
\end{aligned} \tag{87}
$$

- Since

$$
\frac{1}{2}\langle[\hat{A}\,,\,\hat{B}]_+\rangle - \langle\hat{A}\rangle\langle\hat{B}\rangle = \frac{1}{2}\langle[\hat{A}-\langle\hat{A}\rangle\,,\,\hat{B}-\langle\hat{B}\rangle]_+\rangle \tag{88}
$$

  we get

$$
\Delta\hat{A}^2\Delta\hat{B}^2 \geq \frac{1}{4}\langle[\hat{A}-\langle\hat{A}\rangle\,,\,\hat{B}-\langle\hat{B}\rangle]_+\rangle^2 - \frac{1}{4}\langle[\hat{A}\,,\,\hat{B}]\rangle^2 \tag{89}
$$

- Since $\hat{A}$ and $\hat{B}$ are Hermitian, their anti-commutator is Hermitian too and their expectation values are real.
- Thus, the first term in (89) is the square of a real number and therefore nonnegative.
- The commutator of Hermitian operators is anti-Hermitian and therefore its expectation value is purely imaginary. Thus, the second term in (89) is nonnegative too.
- Finally, dropping the first term and taking the square root we get the uncertainty relation

(d) If $\hat{A}$ and $\hat{B}$ are compatible

- The uncertainty relation (82) does not lead to any restriction on $\Delta\hat{A}\,,\,\Delta\hat{B}$.
- The general uncertainty relation (89) takes the form

$$\Delta\hat{A}^2\Delta\hat{B}^2 \geq \Big(\frac{1}{2}\langle[\hat{A}\,,\,\hat{B}]_+\rangle - \langle\hat{A}\rangle\langle\hat{B}\rangle\Big)^2 = \Big(\langle\hat{A}\hat{B}\rangle - \langle\hat{A}\rangle\langle\hat{B}\rangle\Big)^2 \tag{90}$$

  because only the first term in (89) contributes.
- Thus, even in case of compatible observables we can get restriction on $\Delta\hat{A}\,,\,\Delta\hat{B}$ from (89).

IV. **The minimum uncertainty packet**

(a) If $\hat{A} = \hat{X}$ anf $\hat{B} = \hat{P}$ we get the famous Heisenberg uncertainty relation

$$\Delta\hat{X}\Delta\hat{P} \geq \frac{\hbar}{2} \tag{91}$$

(b) If we have determined the position of a particle with high precision then we cannot really say anything definite about the momenta, and vice versa.

(c) Let us find the wave function $\psi(x)$ which saturates the lower bound of (91).

- Since the Schwarz inequality saturates if $|\beta\rangle = c|\alpha\rangle$, we must have

$$(\hat{P} - \langle\hat{P}\rangle)|\psi\rangle = c(\hat{X} - \langle\hat{X}\rangle)|\psi\rangle \tag{92}$$

- The general uncertainty relation (89) requires

$$\langle[\hat{X} - \langle\hat{X}\rangle\,,\,\hat{P} - \langle\hat{P}\rangle]_+\rangle = 0 \tag{93}$$

- To simplify the notations let us denote

$$a \equiv \langle \hat{X} \rangle \,, \quad p \equiv \langle \hat{P} \rangle \tag{94}$$

- We first show that c is imaginary.

i. Multiply (92) by $\langle \psi | (\hat{X} - a)$

$$\langle (\hat{X} - a \rangle)(\hat{P} - p \rangle)\rangle = c \langle (\hat{X} - a)^2 \rangle \tag{95}$$

ii. Take Hermitian conjugate of (95), and add the result to (95)

$$\langle [\hat{X} - a \,,\, \hat{P} - p]_+ \rangle = (c^* + c) \langle (\hat{X} - a)^2 \rangle \tag{96}$$

iii. The l.h.s. of this equation must be zero due to (93), and therefore

$$c = \mathrm{i}\,\kappa \,, \quad \kappa \in \mathbb{R} \tag{97}$$

- In the coordinate space eq.(92) takes the form

$$(-\mathrm{i}\hbar \frac{d}{dx} - p)\psi(x) = \mathrm{i}\,\kappa\,(x - a)\psi(x) \tag{98}$$

- Divide both side of this equation by $\psi(x)$

$$-\mathrm{i}\hbar \frac{d \ln \psi}{dx} = p + \mathrm{i}\,\kappa\,(x - a) \tag{99}$$

- Solve the equation

$$\psi(x) = A \,\exp(\frac{\mathrm{i}}{\hbar} px - \frac{\kappa}{2\hbar}(x - a)^2) \tag{100}$$

where A is a constant.

- The wave function must be normalisable $\Rightarrow \ \kappa > 0$.
- Introduce

$$\Delta^2 \equiv \frac{\hbar}{\kappa}, \quad \Delta > 0 \tag{101}$$

The solution takes the form

$$\psi(x) = A \, \exp\big(\frac{\mathrm{i}}{\hbar} p x - \frac{(x-a)^2}{2\Delta^2}\big) \tag{102}$$

- Up to a phase A can be found from the normalisation condition

$$\int dx \, |\psi(x)|^2 = |A|^2 \int dx e^{-\frac{(x-a)^2}{\Delta^2}} = |A|^2 \Delta \int dx e^{-x^2} = |A|^2 \Delta \sqrt{\pi} = 1 \tag{103}$$

- Choosing $A = e^{-\mathrm{i}\, p\, a/\hbar} / \sqrt{\sqrt{\pi}\Delta}$, we get the final form of the solution

$$\psi(x) = \frac{1}{\sqrt{\sqrt{\pi}\Delta}} \exp\big(\frac{\mathrm{i}}{\hbar} p(x-a) - \frac{(x-a)^2}{2\Delta^2}\big) \tag{104}$$

- Thus the minimum uncertainty wave function is a **Gaussian wave packet** of arbitrary width and centre.

Quantum dynamics

I. The Heisenberg picture

A. It is the most natural one from the point of view of the quantisation procedure and postulates

- The coordinates, momenta and any real function on the phase space of a classical system become Hermitian operators
- The Poisson bracket is replaced by the commutator
- Under the replacement rules Hamilton's equation becomes the Heisenberg equation
- The quantum state of the mechanical system at any given time t_0 can be thought of as a quantum analog of initial coordinates and momenta which obviously do not change in time.

B. Given a state vector $|\psi\rangle$ and an observable $\hat{A}$, we are interested in the probability to measure one of the eigenvalues of $\hat{A}$.

- The probability is given by $P(a) = |\langle\alpha|\psi\rangle|^2$ where $\hat{A}\,|\alpha\rangle = a\,|\alpha\rangle\,,\ \langle\alpha|\alpha\rangle = 1$
- In the Heisenberg picture the state vector is time-independent
- $\hat{A}$ in general depends on time
- The eigenstates of $\hat{A}$, and the corresponding probabilities, are also time-dependent.

C. Consider observables $\hat{A}$ which have no explicit time dependence that is their time dependence only comes from the Heisenberg equation

$$\frac{d\hat{A}(t)}{dt} = \frac{\mathrm{i}}{\hbar}\big[\hat{H}\,,\;\hat{A}(t)\big]\,, \quad \hat{A}(t_0) \equiv \hat{A}_0 \tag{105}$$

where $\hat{H} = \hat{H}(\hat{Z}(t), t)$ is the Hamiltonian of the system which may explicitly depend on time.

D. Introduce a unitary operator $\hat{U}(t, t_0)$ which is called the **evolution operator**, and satisfies

$$\mathrm{i}\,\hbar\,\frac{d\hat{U}(t,t_0)}{dt} = \hat{U}(t,t_0)\,\hat{H}(\hat{Z}(t),t)\,, \quad \hat{U}(t_0\,,\;t_0) = \hat{I} \tag{106}$$

E. The Heisenberg equation (105) is solved by

$$\hat{A}(t) = \hat{U}^\dagger(t,t_0)\,\hat{A}_0\,\hat{U}(t,t_0) \tag{107}$$

$$\begin{aligned}\frac{d\hat{A}(t)}{dt} &= \frac{d\hat{U}^\dagger(t,t_0)}{dt}\hat{A}_0\hat{U}(t,t_0) + \hat{U}^\dagger(t,t_0)\,\hat{A}_0\,\frac{d\hat{U}(t,t_0)}{dt} \\ &= \frac{\mathrm{i}}{\hbar}\hat{H}(\hat{Z}(t),t)\,\hat{U}^\dagger(t,t_0)\hat{A}_0\hat{U}(t,t_0) - \frac{\mathrm{i}}{\hbar}\hat{U}^\dagger(t,t_0)\,\hat{A}_0\,\hat{U}(t,t_0)\,\hat{H}(\hat{Z}(t),t) = \frac{\mathrm{i}}{\hbar}\big[\hat{H}\,,\;\hat{A}(t)\big]\end{aligned} \tag{108}$$

F. The formula

$$\hat{A}(t) = \hat{U}^\dagger(t, t_0)\, \hat{A}_0\, \hat{U}(t, t_0)$$

is very important. It tells us that

(i) The observables $\hat{A}(t_0)$ and $\hat{A}(t)$ are unitarily equivalent.
Thus, the quantum dynamics is a unitary similarity transformation.

(ii) The fundamental commutation relations (3) do not change with time.

(iii) The eigenvalues of an observable $\hat{A}$ do not depend on time.

- Indeed, if $\hat{A}(t_0)|\alpha(t_0)\rangle = a|\alpha(t_0)\rangle$ then

$$\hat{U}(t, t_0)\hat{A}(t)\hat{U}^\dagger(t, t_0)|\alpha(t_0)\rangle = a|\alpha(t_0)\rangle \quad \Rightarrow \quad \hat{A}(t)\hat{U}^\dagger(t, t_0)|\alpha(t_0)\rangle = a\, \hat{U}^\dagger(t, t_0)|\alpha(t_0)\rangle \tag{109}$$

- Thus, $|\alpha(t)\rangle = \hat{U}^\dagger(t, t_0)|\alpha(t_0)\rangle$ is an eigenvector of $\hat{A}(t)$ with the same eigenvalue a.

(iv) The eigenvectors of any observable form a complete basis

- The quantum evolution is a time-dependent unitary transformation of the basis.
- It is a passive transformation because it does not change the Hilbert space vectors.

G. The quantum dynamics is encoded in the evolution operator.

(i) It satisfies (eq.(106))

$$\mathrm{i}\,\hbar\, \frac{d\hat{U}(t, t_0)}{dt} = \hat{U}(t, t_0)\, \hat{H}(\hat{Z}(t), t)\,, \quad \hat{U}(t_0\,,\, t_0) = \hat{I}$$

(ii) The Hamiltonian $\hat{H}(\hat{Z}(t), t)$ can be manipulated as

$$\hat{H}(\hat{Z}(t), t) = \hat{H}\Big(\hat{U}^\dagger(t, t_0)\, \hat{Z}_0\, \hat{U}(t, t_0)\,,\, t\Big) = \hat{U}^\dagger(t, t_0)\, \hat{H}(\hat{Z}_0\,,\, t)\, \hat{U}(t, t_0) \tag{110}$$

(iii) Thus,

$$\hat{U}(t,t_0)\,\hat{H}(\hat{Z}(t),t) = \hat{H}(\hat{Z}_0\,,\,t)\,\hat{U}(t,t_0) \tag{111}$$

Clearly, the same formula applies to any operator which is a function of $\hat{Z}(t)$ and t.

(iv) Thus, equation

$$\mathrm{i}\,\hbar\,\frac{d\hat{U}(t,t_0)}{dt} = \hat{U}(t,t_0)\,\hat{H}(\hat{Z}(t),t)\,, \quad \hat{U}(t_0\,,\,t_0) = \hat{I}$$

can be written in the equivalent form

$$\mathrm{i}\,\hbar\,\frac{d\hat{U}(t,t_0)}{dt} = \hat{H}(\hat{Z}_0,t)\,\hat{U}(t,t_0)\,, \quad \hat{U}(t_0\,,\,t_0) = \hat{I} \tag{112}$$

H. This form is known as the **Schrödinger equation for the evolution operator**

(i) It is used to find the evolution operator as a function of $\hat{H}(t) \equiv \hat{H}(\hat{Z}_0,t)$ for any $\hat{H}(t)$ with a given time dependence.

(ii) The Hamiltonian has no time dependence

$$\hat{U}(t,t_0) = \exp\Big(-\frac{\mathrm{i}}{\hbar}(t-t_0)\hat{H}\Big) \tag{113}$$

(iii) The Hamiltonian depends on time but $\hat{H}(t_1)$ commutes with $\hat{H}(t_2)$ for all t_1, t_2

$$\hat{U}(t,t_0) = \exp\Big(-\frac{\mathrm{i}}{\hbar}\int_{t_0}^{t} d\tau\,\hat{H}(\tau)\Big) \tag{114}$$

(iv) In the general case the solution to (112) is given by the time-ordered exponential

$$\hat{U}(t,t_0) = \mathcal{T}\exp\Big(-\frac{\mathrm{i}}{\hbar}\int_{t_0}^{t} d\tau\, \hat{H}(\tau)\Big) \tag{115}$$

- For any operator $\hat{A}$, we define $\mathcal{T}\exp\Big(\int_{t_0}^{t} d\tau\, \hat{A}(\tau)\Big)$ by the series expansion

$$\begin{aligned}\mathcal{T}\exp\Big(\int_{t_0}^{t} d\tau\, \hat{A}(\tau)\Big) &\equiv \sum_{n=0}^{\infty}\frac{1}{n!}\int_{t_0}^{t} d\tau_1 \cdots \int_{t_0}^{t} d\tau_n\, \mathcal{T}\Big\{\hat{A}(\tau_1)\cdots\hat{A}(\tau_n)\Big\} \\ &= \sum_{n=0}^{\infty}\int_{t_0}^{t} d\tau_1 \cdots \int_{t_0}^{t} d\tau_n\, \theta(\tau_1-\tau_2)\theta(\tau_2-\tau_3)\cdots\theta(\tau_{n-1}-\tau_n)\,\hat{A}(\tau_1)\hat{A}(\tau_2)\cdots\hat{A}(\tau_n) \\ &= \sum_{n=0}^{\infty}\int_{t_0}^{t} d\tau_1 \int_{t_0}^{t_1} d\tau_2 \cdots \int_{t_0}^{t_{n-1}} d\tau_n\, \hat{A}(\tau_1)\hat{A}(\tau_2)\cdots\hat{A}(\tau_n)\end{aligned} \tag{116}$$

- To prove the formula, differentiate it with respect to t.
- The symbol $\mathcal{T}$ denotes the time-ordering operator which orders time-dependent operators in a monomial in the decreasing order.
- For example,

$$\mathcal{T}\Big\{\hat{A}(\tau_1)\hat{B}(\tau_2)\Big\} = \theta(\tau_1-\tau_2)\hat{A}(\tau_1)\hat{B}(\tau_2) + \theta(\tau_2-\tau_1)\hat{B}(\tau_2)\hat{A}(\tau_1) \tag{117}$$

- For a product of n operators one gets $n!$ terms which explains the disappearance of $n!$ from the second line in (116).

II. **The Schrödinger picture**

A. Let us explain how one can go from the Heisenberg picture to the Schrödinger picture.

(i) Ccalculate the probability to measure one of the eigenvalues of $\hat{A}(t)$

$$P(a,t) = |\langle\alpha(t)|\psi\rangle|^2 = |\langle\hat{U}^\dagger(t,t_0)\alpha(t_0)|\psi\rangle|^2 = |\langle\alpha(t_0)|\hat{U}(t,t_0)|\psi\rangle|^2 = |\langle\alpha(t_0)|\psi(t)\rangle|^2 \tag{118}$$

- We introduced the time-dependent state vector

$$|\psi(t)\rangle \equiv \hat{U}(t,t_0)|\psi\rangle\,, \quad |\psi(t_0)\rangle = |\psi\rangle \tag{119}$$

- Formula (118) can be interpreted as the probability to measure one of the eigenvalues of $\hat{A}_0 = \hat{A}(t_0)$ at time t for the system described by the time-dependent state vector $|\psi(t)\rangle$.

(ii) This is the Schrödinger picture where observables without explicit time dependence (only depend on $\hat{Z}^i$) remain stationary while the state vector $|\psi\rangle$ evolves.

(iii) Derive the Schrödinger equation

$$\mathrm{i}\,\hbar\frac{d}{dt}|\psi(t)\rangle = \mathrm{i}\,\hbar\frac{d}{dt}\hat{U}(t,t_0)|\psi\rangle = \hat{H}(\hat{Z}_0,t)\,\hat{U}(t,t_0)|\psi\rangle = \hat{H}(\hat{Z}_0,t)|\psi(t)\rangle \tag{120}$$

(iv) In the Schrödinger picture the quantum evolution can be thought of as an active time-dependent unitary transformation of the Hilbert space vectors.

(v) Probabilities and expectation values of operators are independent of the picture used.

B. Let the Hamiltonian be time-independent and let its spectrum and eigenstates be known.

(i) The evolution operator can be written in an explicit form

(ii) It can then be used to find $|\psi(t)\rangle$

(iii) Let us have another time-independent observable $\hat{A}$ compatible with $\hat{H}$.

- There is a complete basis of simultaneous eigenvectors

$$\hat{A}|\alpha_i\rangle = a_i|\alpha_i\rangle\,, \quad \hat{H}|\alpha_i\rangle = E_i|\alpha_i\rangle \tag{121}$$

- The evolution operator can be expanded as

$$\hat{U}(t,0) = \exp\Big(-\frac{\mathrm{i}}{\hbar}\hat{H}t\Big) = \sum_i\sum_j |\alpha_i\rangle\langle\alpha_i|\exp\Big(-\frac{\mathrm{i}}{\hbar}\hat{H}t\Big)|\alpha_j\rangle\langle\alpha_j| = \sum_i |\alpha_i\rangle\exp\Big(-\frac{\mathrm{i}}{\hbar}E_it\Big)\langle\alpha_i| \tag{122}$$

  where we set $t_0 = 0$ to simplify the notations.

- Given an initial ket

$$|\psi\rangle = \sum_i |\alpha_i\rangle\langle\alpha_i|\psi\rangle \tag{123}$$

  it evolves to

$$|\psi(t)\rangle = \sum_i |\alpha_i\rangle\exp\Big(-\frac{\mathrm{i}}{\hbar}E_it\Big)\langle\alpha_i|\sum_j|\alpha_j\rangle\langle\alpha_j|\psi\rangle = \sum_i |\alpha_i\rangle\exp\Big(-\frac{\mathrm{i}}{\hbar}E_it\Big)\langle\alpha_i|\psi\rangle \tag{124}$$

- The expansion coefficients change as

$$\langle\alpha_i|\psi\rangle \mapsto \langle\alpha_i|\psi(t)\rangle = \exp\Big(-\frac{\mathrm{i}}{\hbar}E_it\Big)\langle\alpha_i|\psi\rangle \tag{125}$$

  and their modulus do not change.

(iv) The probability of finding the system in an eigenstate of $\hat{H}$ does not depend on time.

(v) For this reason an energy eigenstate is often referred to as a **stationary state**.

(vi) A particular case of interest is where the initial state is one of the eigenstate $|\alpha_i\rangle$

$$|\alpha_i\rangle \mapsto |\alpha_i(t)\rangle = |\alpha_i\rangle \exp\Big(-\frac{\mathrm{i}}{\hbar}E_i t\Big) \tag{126}$$

- A simultaneous eigenstate of $\hat{H}$ and $\hat{A}$ remains one at all times; its phase can modulate.
- It is an expected because in the Heisenberg picture both $\hat{A}$ and $\hat{H}$ remain time-independent.
- That's why an observable compatible with $\hat{H}$ is called an integral of the motion.

(vii) The expectation value of any observable wrt an energy eigenstate does not change in time

$$\langle\alpha_i(t)|\hat{B}|\alpha_i(t)\rangle = \langle\alpha_i| \exp\Big(\frac{\mathrm{i}}{\hbar}E_i t\Big)\hat{B} \exp\Big(-\frac{\mathrm{i}}{\hbar}E_i t\Big)|\alpha_i\rangle = \langle\alpha_i|\hat{B}|\alpha_i\rangle \tag{127}$$

(viii) Consider a superposition of energy eigenstates which is a **nonstationary state**

$$|\psi\rangle = \sum_i c_i|\alpha_i\rangle\,, \quad |\psi(t)\rangle = \sum_i c_i \exp\Big(-\frac{\mathrm{i}}{\hbar}E_i t\Big)|\alpha_i\rangle \tag{128}$$

- Then

$$\begin{aligned}\langle\psi(t)|\hat{B}|\psi(t)\rangle &= \sum_i c_i^* \exp\Big(\frac{\mathrm{i}}{\hbar}E_i t\Big)\langle\alpha_i|\hat{B}\sum_j c_j \exp\Big(-\frac{\mathrm{i}}{\hbar}E_j t\Big)|\alpha_j\rangle \\ &= \sum_{i,j} c_i^* c_j \langle\alpha_i|\hat{B}|\alpha_j\rangle \exp\Big(-\frac{\mathrm{i}}{\hbar}(E_j - E_i)t\Big)\end{aligned} \tag{129}$$

- The expectation value consists of oscillating terms whose frequencies are determined by Bohr's frequency condition

$$\omega_{ij} = \frac{E_i - E_j}{\hbar} \tag{130}$$

III. **The Schrödinger wave equation**

A. It is often convenient to analyse the motion of systems in the coordinate representation.

B. The Schrödinger equation becomes a second-order partial differential equation on the wave function, and is called the Schrödinger wave equation.

C. Consider a single spinless particle with, in general, time-dependent Hamiltonian

$$H = \frac{\vec{P}^{\,2}}{2m} + V(\vec{X}\,, t) \tag{131}$$

(i) In the Schrödinger picture a state vector $|\psi\rangle$ evolves as

$$\mathrm{i}\,\hbar \frac{d}{dt}|\psi(t)\rangle = \Big(\frac{\vec{P}^{\,2}}{2m} + V(\vec{X}\,, t)\Big)\,|\psi(t)\rangle \tag{132}$$

(ii) In the coordinate representation we get the Schrödinger wave equation

$$\mathrm{i}\,\hbar \frac{\partial\psi(\vec{x}, t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi(\vec{x}, t) + V(\vec{x}, t)\psi(\vec{x}, t) \tag{133}$$

where $\nabla^2 = \partial^2/\partial\vec{x}^{\,2}$ is the Laplacian.

(iii) If the potential is time-independent then the energy is conserved, and writing

$$\psi(\vec{x}, t) = e^{-\frac{\mathrm{i}}{\hbar}Et}\psi(\vec{x}) \tag{134}$$

we get the time-independent Schrödinger equation for stationary states

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{x}) + V(\vec{x}, t)\psi(\vec{x}) = E\,\psi(\vec{x}) \tag{135}$$

IV. **Probability current**

A. As was first suggested by Max Born, the mod-square of a particle's wave function,

$$\rho(\vec{x},t) \equiv |\psi(\vec{x},t)|^2 \tag{136}$$

(i) is the probability density of finding the particle near x at time t

(ii) it must satisfy $\int d^3\vec{x}\,\rho(\vec{x},t) = 1$ at any time.

B. We know it is the case because the evolution is governed by a unitary operator

C. It is instructive to prove it by using the Schrödinger wave equation.

(i) Differentiate the probability density (136) wrt time and use the wave equation

$$\begin{aligned}\frac{\partial\rho}{\partial t} &= \psi^*\frac{\partial\psi}{\partial t} + \frac{\partial\psi^*}{\partial t}\psi = \psi^*\Big(\mathrm{i}\,\frac{\hbar}{2m}\nabla^2\psi - \frac{\mathrm{i}}{\hbar}V\psi\Big) + \Big(-\mathrm{i}\,\frac{\hbar}{2m}\nabla^2\psi^* + \frac{\mathrm{i}}{\hbar}V\psi^*\Big)\psi \\ &= \frac{\mathrm{i}\,\hbar}{2m}\Big(\psi^*\nabla^2\psi - \nabla^2\psi^*\psi\Big) = \frac{\mathrm{i}\,\hbar}{2m}\vec{\nabla}\Big(\psi^*\vec{\nabla}\psi - \vec{\nabla}\psi^*\psi\Big)\end{aligned} \tag{137}$$

(ii) Introduce the **probability current**

$$\vec{J}(\vec{x},t) \equiv \frac{\mathrm{i}\,\hbar}{2m}\Big(\vec{\nabla}\psi^*\psi - \psi^*\vec{\nabla}\psi\Big) \tag{138}$$

(iii) Get the equation

$$\frac{\partial\rho}{\partial t} = -\vec{\nabla}\cdot\vec{J} \tag{139}$$

- It is the continuity equation implying the conservation of probability.

- Integrating both sides of eq.(139) through a volume $\mathcal{V}$, we obtain

$$\frac{d}{dt}\int_{\mathcal{V}} d^3x\,\rho(\vec{x},t) = -\int_{\mathcal{V}} d^3x\,\vec{\nabla}\cdot\vec{J} = -\int_{\partial\mathcal{V}} d^2\vec{S}\cdot\vec{J} \tag{140}$$

  where we use the divergence theorem and $\partial\mathcal{V}$ is the boundary of $\mathcal{V}$.
- The rate of change of the probability $P = \int_{\mathcal{V}} d^3\vec{x}\,\rho(\vec{x},t)$ of finding the particle in $\mathcal{V}$ is equal to minus the integral over the volume's bounding surface of the probability flux out of the volume.
- If $\mathcal{V}$ is the whole space, then ψ and $\vec{J}$ will vanish on the boundary, so P will be constant.
- The reality of the potential V is crucial in obtaining this result.

D. Since the momentum operator is $\vec{P} = -\mathrm{i}\,\hbar\vec{\nabla}$, the probability current integrated over the whole space is equal to the expectation value of the velocity of the particle

$$\int_{\mathcal{V}} d^3x\,\vec{J}(\vec{x},t) = \int_{\mathcal{V}} d^3x\,\frac{\mathrm{i}\,\hbar}{2m}\Big(\vec{\nabla}\psi^*\psi - \psi^*\vec{\nabla}\psi\Big) = \int_{\mathcal{V}} d^3x\,\frac{1}{2m}\Big((\vec{P}\psi)^*\psi + \psi^*(\vec{P}\psi)\Big) = \frac{\langle\vec{P}\rangle_t}{m} \tag{141}$$

where $\langle\vec{P}\rangle_t$ is the expectation value of the momentum at time t.

E. The wave function is complex and is characterised by its modulus and phase.

(i) Let us write it in the "polar" coordinates form

$$\psi(\vec{x},t) = \sqrt{\rho(\vec{x},t)}\,\exp\Big(\frac{\mathrm{i}}{\hbar}S(\vec{x},t)\Big) \tag{142}$$

where S is real and $\rho > 0$.

(ii) Express the probability current in terms of ρ and S

$$\vec{J}(\vec{x},t) = \frac{\mathrm{i}\,\hbar}{2m}\Big(\vec{\nabla}\psi^*\psi - \psi^*\vec{\nabla}\psi\Big) = \frac{\mathrm{i}\,\hbar}{2m}\Big(\vec{\nabla}(\sqrt{\rho(\vec{x},t)})\sqrt{\rho(\vec{x},t)} + \rho(\vec{x},t)\vec{\nabla}(-\frac{\mathrm{i}}{\hbar}S(\vec{x},t)) \\ - \sqrt{\rho(\vec{x},t)}\,\vec{\nabla}(\sqrt{\rho(\vec{x},t)}) - \rho(\vec{x},t)\vec{\nabla}(\frac{\mathrm{i}}{\hbar}S(\vec{x},t))\Big) \tag{143}$$

Thus,

$$\vec{J}(\vec{x},t) = \frac{\rho(\vec{x},t)}{m}\vec{\nabla}S(\vec{x},t) \tag{144}$$

- The spacial variation of the phase of the wave function characterises the probability flux; the stronger the phase variation, the more intense the flux.
- The direction of $\vec{J}$ at some point $\vec{x}$ is normal to the surface of constant phase that goes through that point.
- In particular if ψ is a plane wave

$$\psi(\vec{x},t) \sim \exp(\frac{\mathrm{i}}{\hbar}\vec{p}\cdot\vec{x} - \frac{\mathrm{i}}{\hbar}Et) \tag{145}$$

then

$$\vec{\nabla}S(\vec{x},t) = \vec{p} \tag{146}$$

and it is normal to the plane $\vec{p}\cdot\vec{x} = \mathrm{const}$

V. **The classical limit**

A. The polar form of the wave function is useful to discuss the classical limit of QM.

B. Rewrite the Schödinger equation in terms of ρ and S.

(i) The equation for ρ

$$\frac{\partial \log \sqrt{\rho}}{\partial t} = -\frac{1}{2m}\Big(\nabla^2(S) + 2\vec{\nabla}(\log\sqrt{\rho})\cdot\vec{\nabla}(S)\Big) \tag{147}$$

is just the continuity equation (139) for the probability density and current.

(ii) The equation for the phase S is

$$\frac{\partial S}{\partial t} + \frac{1}{2m}\vec{\nabla}(S)\cdot\vec{\nabla}(S) + V - \frac{\hbar^2}{2m}\frac{\nabla^2(\sqrt{\rho})}{\sqrt{\rho}} = 0 \tag{148}$$

C. Take the limit $\hbar \to 0$

$$\frac{\partial S(\vec{x},t)}{\partial t} + \frac{1}{2m}\vec{\nabla}S(\vec{x},t)\cdot\vec{\nabla}S(\vec{x},t) + V(\vec{x},t) = 0 \tag{149}$$

(i) It is the Hamilton-Jacobi equation for Hamilton's principal function $S(\vec{x},t)$.

(ii) Since Hamilton's principal function encodes full information about the motion, in the limit $\hbar \to 0$, classical mechanics is contained in Schrödinger wave mechanics.

D. Semiclassical interpretation of the phase of the wave function:
$\hbar$ times the phase is equal to Hamilton's principal function provided that $\hbar$ can be regarded as a small quantity.

E. The classical momentum is given by $p_{\rm cl} = \vec{\nabla}S$
generalising the observation made for a plane wave.

Symmetries

I. Classical canonical transformations and symmetries

A. In CM a canonical transformation preserves the Poisson structure

$$z^i \mapsto \tilde{z}^i = \tilde{z}^i(z)\,, \quad \{\tilde{z}^i\,,\,\tilde{z}^j\}_z = \omega^{ij}(\tilde{z})$$

B. It can be generated by a real-valued function $G(z,t)$

$$z^i \mapsto \tilde{z}^i = \tilde{z}^i(z) = e^{\{G,} \cdot z^i = z^i + \sum_{n=1}^{\infty} \frac{1}{n!} \underbrace{\Big\{G, \Big\{G, \cdots \Big\{}_{n} G\,,\, z^i\Big\} \cdots \Big\}\Big\} \tag{150}$$

C. Any function $a(z,t)$ on the phase space transforms in the same way

$$a(z,t) \mapsto a(\tilde{z}(z),t) = e^{\{G,} \cdot a(z,t) \tag{151}$$

D. If $G(z,t)$ and $a(z,t)$ Poisson-commute then $a(\tilde{z}(z),t) = a(z,t)$,
for example since any function Poisson-commutes with itself then $G(\tilde{z}(z),t) = G(z,t)$.

E. The canonically transformed coordinates of the phase space satisfy Hamilton's equations

$$\frac{d\tilde{z}^i}{dt} = \{\widetilde{H}\,,\,\tilde{z}^i\}\,, \quad \widetilde{H}(\tilde{z},t) = H(z(\tilde{z}),t) + e^{\{G,} \cdot \frac{\partial G}{\partial t} \tag{152}$$

$$\widetilde{H} = H + \frac{\partial G}{\partial t} + \sum_{n=1}^{\infty} \frac{1}{n!} \underbrace{\Big\{G, \Big\{G, \cdots \Big\{}_{n} G, \frac{\partial V}{\partial t}\Big\} \cdots \Big\}\Big\} \tag{153}$$

F. The motion itself can be thought of as a canonical transformation.
If H is time-independent then choosing $G = -H\,t$, one gets $\widetilde{H} = 0 \;\Rightarrow\; \tilde{z}^i(t) = \tilde{z}^i(t_0)$.

G. A transformation which maps a solution of the eom to another solution of the same eom is called a symmetry of the mechanical system.

- If the transformed Hamiltonian $\widetilde{H}$ has the same functional dependence of $\tilde{z}^i, t$ as H of z, t

$$\widetilde{H}(\tilde{z},t) = H(\tilde{z},t) = H(z(\tilde{z}),t) + e^{\{G,} \cdot \frac{\partial G}{\partial t} \quad \Leftrightarrow \quad H(\tilde{z}(z),t) = H(z,t) + e^{\{G,} \cdot \frac{\partial G}{\partial t} \tag{154}$$

then a canonical transformation generated by $G(z,t)$ is a symmetry of a mechanical system.

- If $G(z)$ is independent of time then $H(\tilde{z}(z),t) = H(z,t)$, and $G(z)$ Poisson-commutes with the Hamiltonian.

H. Important examples of canonical transformations generated by a function G are

(i) Translations of x by a

$$G = a\,p \quad \Rightarrow \quad \tilde{x} = x + a\,, \quad \tilde{p} = p \tag{155}$$

(ii) Counterclockwise rotations in the xy-plane through angle ϕ

$$G = \phi\,\ell_z = \phi\,(x\,p_y - y\,p_x) \quad \Rightarrow \quad \begin{aligned} &\tilde{x} = x\cos\phi - y\sin\phi\,, \quad \tilde{y} = y\cos\phi + x\sin\phi \\ &\tilde{p}_x = p_x\cos\phi - p_y\sin\phi\,, \quad \tilde{p}_x = p_x\cos\phi - p_y\sin\phi \end{aligned} \tag{156}$$

(iii) Clockwise rotations in the xp-plane through angle ψ

$$G = \frac{\psi}{2}\,(x^2 + p^2) \quad \Rightarrow \quad \tilde{x} = x\cos\psi + p\sin\psi\,, \quad \tilde{p} = p\cos\psi - x\sin\psi \tag{157}$$

(iv) Parity transformation or reflection of x and p is a particular case of the rotation in the phase plane where $\psi = \pi$

$$G = \frac{\pi}{2}(x^2 + p^2) \quad \Rightarrow \quad \tilde{x} = -x\,, \quad \tilde{p} = -p \tag{158}$$

- It is a discrete transformation.
- We could choose $\psi = -\pi$ and would get the same parity transformation.

(v) Rescaling of x by e^{λ} and p by $e^{-\lambda}$

$$G = \lambda\, x\, p \quad \Rightarrow \quad \tilde{x} = e^{\lambda}\, x\,, \quad \tilde{p} = e^{-\lambda}\, p \tag{159}$$

- It is not a symmetry of any interesting system
- It is useful to simplify description of some systems, e.g. a system of coupled oscillators.

II. Quantum canonical transformations and symmetries

To understand how canonical transformations and symmetries are implemented in QM we follow our postulates, and first use the Heisenberg picture because

- The coordinates of the phase space become operators.
- Operators transform while state vectors remain untouched.
- Transformations are passive in the Heisenberg picture
- They are active in the Schrödinger picture where state vectors transform but operators do not.

A. **Quantum canonical transformations are unitary**

(i) The real-valued function $G(z,t)$ becomes a Hermitian operator

$$\hat{G}(\hat{Z},t) = \frac{1}{2}\Big(G(\hat{Z},t) + G(\hat{Z},t)^\dagger\Big) \tag{160}$$

(ii) The Poisson brackets are replaced by commutators

$$\{\bullet\,,\,\bullet\} \;\mapsto\; \frac{\mathrm{i}}{\hbar}[\,\bullet\,,\,\bullet\,] \tag{161}$$

(iii) The operators $\hat{Z}^i$ transform as follows

$$\hat{Z}^i \;\mapsto\; \hat{\tilde{Z}}^i = \hat{Z}^i + \sum_{n=1}^{\infty}\frac{1}{n!}\,\underbrace{\Big[\frac{\mathrm{i}}{\hbar}\hat{G},\Big[\frac{\mathrm{i}}{\hbar}\hat{G},\cdots\Big[\frac{i}{\hbar}\hat{G}\,,\,\hat{Z}^i\Big]}_{n}\cdots\Big]\Big] = e^{\frac{\mathrm{i}}{\hbar}\hat{G}}\,\hat{Z}^i\,e^{-\frac{\mathrm{i}}{\hbar}\hat{G}} \tag{162}$$

(iv) $\hat{G}$ is Hermitian $\Rightarrow$ $\hat{U} \equiv e^{-\frac{i}{\hbar}\hat{G}}$ is unitary.

(v) The canonical transformation generated by G becomes the unitary similarity transformation

$$\hat{Z}^i \;\mapsto\; \hat{\tilde{Z}}^i = \hat{U}^\dagger\,\hat{Z}^i\,\hat{U}\,, \quad \hat{U}^\dagger\,\hat{U} = \hat{U}\,\hat{U}^\dagger = \hat{I}\,, \quad \hat{U} = e^{-\frac{i}{\hbar}\hat{G}} \tag{163}$$

- It preserves the commutation relations (3).
- Any other operator transforms under the unitary transformation generated by $\hat{G}$ in the same way (163).
- The spectra of the original and transformed operators are the same.

(vi) To find the Heisenberg eom for the transformed operators $\hat{\widetilde{Z}}^i$, we differentiate (163) wrt time

$$\begin{aligned} \frac{d\hat{\widetilde{Z}}^i}{dt} &= \frac{d\hat{U}^\dagger}{dt}\,\hat{Z}^i\,\hat{U} + \hat{U}^\dagger\,\frac{d\hat{Z}^i}{dt}\,\hat{U} + \hat{U}^\dagger\,\hat{Z}^i\,\frac{d\hat{U}}{dt} \\ &= -\hat{U}^\dagger\frac{d\hat{U}}{dt}\hat{U}^\dagger\,\hat{Z}^i\,\hat{U} + \hat{U}^\dagger\,\frac{\mathrm{i}}{\hbar}[\hat{H}\,,\,\hat{Z}^i]\,\hat{U} + \hat{U}^\dagger\,\hat{Z}^i\,\hat{U}\,\hat{U}^\dagger\,\frac{d\hat{U}}{dt} \\ &= -\hat{U}^\dagger\frac{d\hat{U}}{dt}\hat{\widetilde{Z}}^i + \frac{\mathrm{i}}{\hbar}[\hat{U}^\dagger\,\hat{H}\,\hat{U}\,,\,\hat{\widetilde{Z}}^i] + \hat{\widetilde{Z}}^i\,\hat{U}^\dagger\,\frac{d\hat{U}}{dt} \\ &= \frac{\mathrm{i}}{\hbar}\Big[\,\hat{U}^\dagger\,\hat{H}\,\hat{U} + \mathrm{i}\,\hbar\,\hat{U}^\dagger\,\frac{d\hat{U}}{dt}\,,\,\hat{\widetilde{Z}}^i\,\Big] = \frac{\mathrm{i}}{\hbar}\Big[\,\hat{\widetilde{H}}\,,\,\hat{\widetilde{Z}}^i\,\Big] \end{aligned} \tag{164}$$

where

$$\hat{\widetilde{H}} \equiv \hat{U}^\dagger\,\hat{H}\,\hat{U} + \mathrm{i}\,\hbar\,\hat{U}^\dagger\,\frac{d\hat{U}}{dt} \tag{165}$$

is the transformed Hamiltonian which governs dynamics of $\hat{\widetilde{Z}}^i$.

- This form of $\hat{\widetilde{H}}$ is not very useful because $\hat{U}$ depends on $\hat{Z}$, which depend on time, and it is difficult to compute the total time derivative of $\hat{U}$.
- We simplify $\hat{\widetilde{H}}$ by using

$$-e^{\hat{A}}\frac{d}{dt}e^{-\hat{A}} = \frac{d\hat{A}}{dt} + \sum_{n=1}^{\infty}\frac{1}{(n+1)!}\,\underbrace{\big[\hat{A},\big[\hat{A},\cdots\big[}_{n}\,\hat{A}\,,\,\frac{d\hat{A}}{dt}\big]\cdots\big]\big] \tag{166}$$

- $\hat{A}$ satisfies the Heisenberg eom, and therefore

$$
\begin{aligned}
-e^{\hat{A}}\frac{d}{dt}e^{-\hat{A}} &= \frac{\partial \hat{A}}{\partial t} - \frac{\mathrm{i}}{\hbar}[\hat{A},\hat{H}] + \sum_{n=1}^{\infty}\frac{1}{(n+1)!}\,\underbrace{\big[\hat{A},\big[\hat{A},\cdots\big[}_{n}\,\hat{A}\,,\,\frac{\partial\hat{A}}{\partial t} - \frac{\mathrm{i}}{\hbar}[\hat{A},\hat{H}]\big]\cdots\big]\big]\\
&= -e^{\hat{A}}\frac{\partial}{\partial t}e^{-\hat{A}} - \frac{\mathrm{i}}{\hbar}\sum_{n=1}^{\infty}\frac{1}{n!}\,\underbrace{\big[\hat{A},\big[\hat{A},\cdots\big[}_{n}\,\hat{A}\,,\,\hat{H}\big]\cdots\big]\big]\\
&= -e^{\hat{A}}\frac{\partial}{\partial t}e^{-\hat{A}} + \frac{\mathrm{i}}{\hbar}\hat{H} - \frac{\mathrm{i}}{\hbar}e^{\hat{A}}\,\hat{H}\,e^{-\hat{A}}
\end{aligned}
\tag{167}
$$

- Use the formula with $e^{\hat{A}} = \hat{U}^\dagger$

$$
\hat{\tilde{\hat{H}}} = \hat{U}^\dagger\,\hat{H}\,\hat{U} + \mathrm{i}\,\hbar\,\hat{U}^\dagger\,\frac{d\hat{U}}{dt} = \hat{H} + \mathrm{i}\,\hbar\,\hat{U}^\dagger\,\frac{\partial\hat{U}}{\partial t} \tag{168}
$$

(vii) This form of the transformed Hamiltonian is a quantum analog of the classical formula (153). If we know how $\hat{H}$ and $\hat{U}$ act in the Hilbert space then we know the action of $\hat{\tilde{\hat{H}}}$ too.

(viii) In (168) $\hat{\tilde{\hat{H}}}$ depends on $\hat{\tilde{\hat{Z}}}$ while operators on the r.h.s. depend on $\hat{Z}$

$$
\hat{\tilde{\hat{H}}}(\hat{\tilde{\hat{Z}}},t) = \hat{H}(\hat{Z},t) + \mathrm{i}\,\hbar\,\hat{U}^\dagger\,\frac{\partial\hat{U}}{\partial t}(\hat{Z},t) \tag{169}
$$

(ix) Taking into account that $\hat{\tilde{\hat{Z}}} = \hat{U}^\dagger\hat{Z}\hat{U}$, and therefore $\hat{\tilde{\hat{H}}}(\hat{\tilde{\hat{Z}}},t) = \hat{U}^\dagger\hat{\tilde{\hat{H}}}(\hat{Z},t)\hat{U}$, we get

$$
\hat{\tilde{\hat{H}}}(\hat{Z},t) = \hat{U}\,\hat{H}(\hat{Z},t)\,\hat{U}^\dagger + \mathrm{i}\,\hbar\,\frac{\partial\hat{U}}{\partial t}\,\hat{U}^\dagger(\hat{Z},t) \tag{170}
$$

(x) If $\hat{U} = e^{-\mathrm{i}\,t\,\hat{H}/\hbar}$, and , $\hat{H}$ is time-independent, then $\hat{U}$ is the evolution operator and $\hat{\widetilde{H}} = 0$. The time-independent $\hat{H}$ generates translations in time, e.i. quantum dynamics.

(xi) Let us see how (170) is reproduced in the Schrödinger picture where operators do not transform but state vectors do

$$|\psi(t)\rangle \;\mapsto\; |\tilde{\psi}(t)\rangle \equiv \hat{U}\,|\psi(t)\rangle \tag{171}$$

- Differentiate the transformed state $|\tilde{\psi}\rangle$ wrt t

$$\begin{aligned} \mathrm{i}\,\hbar\frac{d}{dt}|\tilde{\psi}(t)\rangle &= \mathrm{i}\,\hbar\frac{d}{dt}\Big(\hat{U}\,|\psi(t)\rangle\Big) = \hat{U}\,\hat{H}\,|\psi(t)\rangle + \mathrm{i}\,\hbar\frac{\partial\hat{U}}{\partial t}|\psi(t)\rangle \\ &= \hat{U}\,\hat{H}\,|\psi(t)\rangle + \mathrm{i}\,\hbar\frac{\partial\hat{U}}{\partial t}|\psi(t)\rangle = \hat{U}\,\hat{H}\,\hat{U}^\dagger\,\hat{U}\,|\psi(t)\rangle + \mathrm{i}\,\hbar\frac{\partial\hat{U}}{\partial t}\hat{U}^\dagger\,\hat{U}\,|\psi(t)\rangle \\ &= \Big(\hat{U}\,\hat{H}\,\hat{U}^\dagger + \mathrm{i}\,\hbar\frac{\partial\hat{U}}{\partial t}\,\hat{U}^\dagger\,\Big)|\tilde{\psi}(t)\rangle \end{aligned} \tag{172}$$

- In the Schrödinger picture the transformed Hamiltonian is given by (170) with the replacement $\hat{Z}(t) \to \hat{Z}_0 = \hat{Z}(0)$.

(xii) Not every classical canonical transformation can be quantised

- $\hat{G}$ may not be Hermitian for an arbitrary real-valued function $G(z,t)$ if it acts in an infinite dimensional Hilbert space, and therefore, the corresponding $\hat{U}$ may not be unitary.
- Consider the following classical canonical transformation

$$\tilde{x} = \arctan\frac{x}{p}\,, \quad \tilde{p} = \frac{1}{2}(p^2 + x^2)\,, \quad x = \sqrt{2\tilde{p}}\sin\tilde{x}\,, \quad p = \sqrt{2\tilde{p}}\cos\tilde{x} \tag{173}$$

- These transformed $\tilde{x}$ and $\tilde{p}$ are the action/angle variables for a harmonic oscillator.
- We do not need to know $G(z)$ to claim that there is no corresponding unitary operator.
- If there were one then
$$\hat{\tilde{P}} = \frac{1}{2}(\hat{P}^2 + \hat{X}^2) = \hat{U}^\dagger \, \hat{P} \, \hat{U} \tag{174}$$
and the spectra of $\hat{P}$ and $\hat{\tilde{P}}$ would have to be the same.
- The spectrum of $\hat{P}$ is continuous while the spectrum of $\hat{\tilde{P}} = \frac{1}{2}(\hat{P}^2 + \hat{X}^2)$ is discrete.

B. **Quantum symmetries**

If the quantum canonical transformation by the unitary operator $\hat{U}$ is a symmetry then the transformed Hamiltonian must have the same functional dependence of $\hat{\tilde{Z}}, t$ as $\hat{H}$ of $\hat{Z}, t$, and, as follows from (170), $\hat{U}$ must satisfy the equation

$$\hat{H} = \hat{U} \, \hat{H} \, \hat{U}^\dagger + \mathrm{i}\, \hbar \, \frac{\partial \hat{U}}{\partial t} \, \hat{U}^\dagger \tag{175}$$

(i) Given two symmetry unitary operators $\hat{U}_1$ and $\hat{U}_2$, their product $\hat{U}_1 \hat{U}_2$ is a symmetry unitary operator, too. The set of all symmetry unitary operators forms an infinite-dimensional group which is a subgroup of the group of all unitary operators.

(ii) If $\hat{U}$ has no explicit time dependence then it is a symmetry if it commutes with $\hat{H}$.

(iii) Any observable $\hat{G}$ compatible with $\hat{H}$ generates a continuous quantum symmetry because $\hat{U}(\alpha) = \exp(-\mathrm{i}\alpha\hat{G}/\hbar)$, where α is a continuous parameter, commute with $\hat{H}$ for any α.

(iv) Consider observables $\hat{G}_i$, $i = 1, \ldots, n$ compatible with $\hat{H}$ which form a Lie algebra

$$[\hat{G}_i\,,\,\hat{G}_j] = \sum_{k=1}^{n} f_{ij}^k \hat{G}_k \tag{176}$$

- Let $|\psi\rangle$ be an eigenvector of $\hat{H}$: $\hat{H}|\psi\rangle = E|\psi\rangle$.
- Let us act on $|\psi\rangle$ by any products of $\hat{G}$'s and get vectors such as $\hat{G}_i|\psi\rangle$, $\hat{G}_i\hat{G}_j|\psi\rangle \ldots$
- This produces an irrep of the Lie algebra, and all vectors of this irrep are eigenvectors of $\hat{H}$ with the same eigenvalue E. Indeed, if, for example, $|\psi_i\rangle \equiv \hat{G}_i|\psi\rangle$ then

$$\hat{H}|\psi_i\rangle = \hat{H}\hat{G}_i|\psi\rangle = \hat{G}_i\hat{H}|\psi\rangle = E\hat{G}_i|\psi\rangle = E|\psi_i\rangle \tag{177}$$

- The observables $\hat{G}_i$ compatible with $\hat{H}$ generate quantum symmetry transformations, and the spectrum of the Hamiltonian is degenerate.

III. **Translations in space**

To simplify the notations we drop the hats from operators.

A. Single out one of the coordinates of our system and denote it by X.

B. The momentum P conjugate to X generates translations along the x-direction.

C. The translation operator is given by

$$T(a) = \exp(-\mathrm{i}\, a\, P/\hbar) \tag{178}$$

D. In the Heisenberg picture it transforms the coordinate operator X as

$$X \;\mapsto\; \widetilde{X} = T^\dagger(a)\, X\, T(a) = e^{\mathrm{i}\, a\, P/\hbar}\, X\, e^{-\mathrm{i}\, a\, P/\hbar} = X + a \tag{179}$$

E. The expectation values of X and $\widetilde{X}$ are related in the same way

$$\langle\psi|\widetilde{X}|\psi\rangle = \langle\psi|X|\psi\rangle + a \tag{180}$$

Since nothing has been done to the system and therefore to $|\psi\rangle$, the formula means that the origin of our reference frame has been shifted in the x-direction by $-a$.

F. In the Schrödinger picture the translation operator translates the state vector $|\psi\rangle$ to

$$|\psi\rangle \;\mapsto\; |\tilde{\psi}\rangle = T(a)|\psi\rangle = e^{-\mathrm{i}\,a\,P/\hbar}\,|\psi\rangle \tag{181}$$

G. Let us see how wave functions in coordinate and momentum spaces transform

(i) The wave function in the momentum space is multiplied by $e^{-\mathrm{i}\,a\,P/\hbar}$

$$|\tilde{\psi}\rangle = \int dp\,|p\rangle\tilde{\psi}(p) = e^{-\mathrm{i}\,a\,P/\hbar}\,|\psi\rangle = \int dp\,e^{-\mathrm{i}\,a\,P/\hbar}\,|p\rangle\psi(p) = \int dp\,|p\rangle e^{-\mathrm{i}\,a\,p/\hbar}\,\psi(p) \tag{182}$$

$$\tilde{\psi}(p) = e^{-\mathrm{i}\,a\,p/\hbar}\,\psi(p) \tag{183}$$

(ii) To obtain the wave function in the coordinate space

- First find

$$\begin{aligned} e^{-\mathrm{i}\,a\,P/\hbar}\,|x\rangle &= e^{-\mathrm{i}\,a\,P/\hbar}\int dp\,|p\rangle\langle p|x\rangle = \int dp\,e^{-\mathrm{i}\,a\,p/\hbar}\,|p\rangle\,\frac{1}{\sqrt{2\pi\hbar}}e^{-\mathrm{i}\,p\,x/\hbar} \\ &= \int dp\,|p\rangle\,\frac{1}{\sqrt{2\pi\hbar}}e^{-\mathrm{i}\,p\,(x+a)/\hbar} = |x+a\rangle \end{aligned} \tag{184}$$

- Then

$$\begin{aligned} |\tilde{\psi}\rangle &= \int dx\,|x\rangle\tilde{\psi}(x) = e^{-\mathrm{i}\,a\,P/\hbar}\,|\psi\rangle = \int dx\,e^{-\mathrm{i}\,a\,P/\hbar}\,|x\rangle\psi(x) = \int dx\,|x+a\rangle\psi(x) \\ &= \int dx\,|x\rangle\,\psi(x-a) \end{aligned} \tag{185}$$

- Thus,

$$\tilde{\psi}(x) = e^{-a\partial/\partial x}\psi(x) = \psi(x-a) \tag{186}$$

(iii) This formula shows that in the Schrödinger picture the wave function, i.e. the system, is shifted in the x-direction by a.

(iv) The expectation value of X wrt the transformed state $|\psi\rangle$ is

$$\langle\tilde{\psi}|X|\tilde{\psi}\rangle = \int dx\, \psi^*(x-a)x\psi(x-a) = \langle\psi|X|\psi\rangle + a \tag{187}$$

(v) No matter which picture we use the expectation values are the same.

H. The consideration above applies to any system.

I. If H of our system is independent of X then P commutes with H, and one can choose a basis of simultaneous eigenvectors of H and P.

J. Since momenta conjugate to different coordinates commute, it is obvious how to generalise this discussion to a more general case.

K. The total momentum of a system is the translation generator of the whole system, and, if the space is homogeneous then the total momentum is conserved, and commutes H.

IV. **Rotations**

A. Single out a particle with coordinates and momenta $\vec{X} = (X, Y, Z)$ and $\vec{P} = (P^x, P^y, P^z)$.

B. Consider a spinless particle. The generator of rotations is its orbital angular momentum

$$\vec{L} = \vec{X} \times \vec{P}\,, \quad L^x = Y P^z - Z P^y\,, \quad L^y = Z P^x - X P^z\,, \quad L^z = X P^y - Y P^x \tag{188}$$

(i) L^x, L^y and L^z generate counterclockwise rotations in the yz-, zx- and xy-planes, i.e. around the positive direction of the x-, y- and z-axes.

(ii) Rotations around the direction of a unit vector $\vec{n}$ are generated by the operator

$$L^{\vec{n}} \equiv \vec{n} \cdot \vec{L} = n^x L^x + n^y L^y + n^z L^z\,, \quad \vec{n}^{\,2} = 1 \tag{189}$$

(iii) The angular momentum operators satisfy the commutation relations of the $\mathfrak{so}(3)$ algebra

$$[L^x, L^y] = \mathrm{i}\,\hbar\, L^z\,, \quad [L^y, L^z] = \mathrm{i}\,\hbar\, L^x\,, \quad [L^z, L^x] = \mathrm{i}\,\hbar\, L^y \quad \Leftrightarrow \quad [L^\alpha, L^\beta] = \mathrm{i}\,\hbar\,\epsilon^{\alpha\beta\gamma} L^\gamma \tag{190}$$

(iv) They have the following commutation relations with $\vec{X}$ and $\vec{P}$

$$\begin{aligned} &[L^x, X] = 0\,, \quad [L^x, Y] = \mathrm{i}\,\hbar\, Z\,, \quad [L^x, Z] = -\mathrm{i}\,\hbar\, Y \\ &[L^y, X] = -\mathrm{i}\,\hbar\, Z\,, \quad [L^y, Y] = 0\,, \quad [L^y, Z] = \mathrm{i}\,\hbar\, X \\ &[L^z, X] = \mathrm{i}\,\hbar\, Y\,, \quad [L^z, Y] = -\mathrm{i}\,\hbar\, X\,, \quad [L^z, Z] = 0 \end{aligned} \tag{191}$$

$$[L^\alpha, X^\beta] = \mathrm{i}\,\hbar\,\epsilon^{\alpha\beta\gamma} X^\gamma\,, \quad [L^\alpha, P^\beta] = \mathrm{i}\,\hbar\,\epsilon^{\alpha\beta\gamma} P^\gamma \tag{192}$$

(v) These relations can be combined into

$$[L^{\vec{m}}, L^{\vec{n}}] = \mathrm{i}\hbar\, L^{\vec{m}\times\vec{n}}\,, \quad [L^{\vec{n}}, \vec{X}] = \mathrm{i}\hbar\, \vec{X} \times \vec{n}\,, \quad [L^{\vec{n}}, \vec{P}] = \mathrm{i}\hbar\, \vec{P} \times \vec{n} \tag{193}$$

C. The rotation operator through an angle ϑ around the direction of the unit vector $\vec{n}$ is

$$R(\vec{\vartheta}) = \exp\Big(- \mathrm{i}\, \vec{\vartheta} \cdot \vec{L}/\hbar \Big) = \exp\Big(- \mathrm{i}\, \vartheta\, L^{\vec{n}}/\hbar \Big)\,, \quad \vec{\vartheta} = \vartheta\, \vec{n}\,, \quad \vec{n}^{\,2} = 1 \tag{194}$$

(i) It transforms $\vec{X}$ as

$$\vec{X}(\vec{\vartheta}) = R^{\dagger}(\vec{\vartheta})\, \vec{X}\, R(\vec{\vartheta}) = \vec{X}^{\parallel} + \vec{X}^{\perp} \cos\vartheta - \vec{X}^{\perp} \times \vec{n}\, \sin\vartheta \tag{195}$$

$\vec{X}^{\parallel}$ and $\vec{X}^{\perp}$ are the components of $\vec{X}$ parallel and orthogonal to $\vec{n}$

$$\vec{X} = \vec{X}^{\parallel} + \vec{X}^{\perp}\,, \quad \vec{X}^{\parallel} = (\vec{X} \cdot \vec{n})\, \vec{n}\,, \quad \vec{X}^{\perp} = \vec{n} \times (\vec{X} \times \vec{n}) \tag{196}$$

(ii) In particular, rotations around the z-axis ($\vec{n} = \vec{e}_z$) through the angle φ are given by

$$\begin{aligned} X(\varphi) &= \exp\Big(\mathrm{i}\, \varphi\, L^z/\hbar\Big)\, X\, \exp\Big(- \mathrm{i}\, \varphi\, L^z/\hbar\Big) = X \cos\varphi - Y \sin\varphi \\ Y(\varphi) &= \exp\Big(\mathrm{i}\, \varphi\, L^z/\hbar\Big)\, Y\, \exp\Big(- \mathrm{i}\, \varphi\, L^z/\hbar\Big) = Y \cos\varphi + X \sin\varphi \end{aligned} \tag{197}$$

Z does not transform.

(iii) The expectation values of $\vec{X}$ and $\vec{X}(\vartheta)$ are related in the same way (196)

(iv) In the Heisenberg picture state vectors do not change $\Rightarrow$ (196) implies that the axes of our reference frame have been rotated through an angle $-\vartheta$ around the direction of $\vec{n}$.

(v) Any vector of operators, e.g. $\vec{P}$ and $\vec{L}$. transforms in the same way.

D. In the Schrödinger picture the rotation operator transforms a state vector $|\psi\rangle$ to

$$|\psi\rangle \;\mapsto\; |\tilde{\psi}\rangle = R(\vec{\vartheta})|\psi\rangle = \exp\Big(-\mathrm{i}\,\vartheta\, L^{\vec{n}}/\hbar\Big)\,|\psi\rangle \tag{198}$$

(i) One can show that

$$R(\vec{\vartheta})\,|\vec{x}\rangle = |\vec{x}(\vec{\vartheta})\rangle\,, \quad R(\vec{\vartheta})\,|\vec{p}\rangle = |\vec{p}(\vec{\vartheta})\rangle \tag{199}$$

$\vec{x}(\vec{\vartheta})$ and $\vec{p}(\vec{\vartheta})$ are given by (196) with $\vec{X}$ and $\vec{P}$ replaced by lowercase $\vec{x}$ and $\vec{p}$.

(ii) Acting on $|\psi\rangle$ with $R(\vec{\vartheta})$, we get

$$\begin{aligned}|\tilde{\psi}\rangle &= \int d\vec{x}\,|\vec{x}\rangle\tilde{\psi}(\vec{x}) = R(\vec{\vartheta})\,|\psi\rangle = \int d\vec{x}\,R(\vec{\vartheta})\,|\vec{x}\rangle\psi(\vec{x}) = \int d\vec{x}\,|\vec{x}(\vec{\vartheta})\rangle\psi(\vec{x})\\ &= \int d\vec{x}\,|\vec{x}\rangle\,\psi(\vec{x}(-\vec{\vartheta}))\end{aligned} \tag{200}$$

- Thus,

$$\tilde{\psi}(\vec{x}) = \exp\Big(-\vec{\vartheta}\cdot(\vec{x}\times\frac{\partial}{\partial\vec{x}})\Big)\psi(\vec{x}) = \psi(\vec{x}(-\vec{\vartheta})) \tag{201}$$

- The operator acting on $\psi(\vec{x})$ is the rotation operator in the coordinate representation.
- In the Schrödinger picture the wave function, i.e. the system, is rotated through an angle $|\vec{\vartheta}|$ around the direction of the vector $\vec{\vartheta}$.

E. Since angular momenta of different particles commute, it is straightforward to generalise this discussion to a more general case.

(i) The total angular momentum of a system is the rotation generator of the whole system.

(ii) If the space is isotropic the total angular momentum is conserved, and commutes with H

(iii) Since $\vec{L}^2$ commutes with $\vec{L}$ and H, we have three compatible operators H, $\vec{L}^2$ and one component of $\vec{L}$, say L^z, and we can find a basis of their simultaneous eigenvectors.

F. If a particle has spin then its angular momentum is

$$\vec{J} = \vec{L} + \vec{S} \tag{202}$$

(i) $R(\vec{\vartheta})$ is given by (194) with $\vec{L}$ replaced by $\vec{J}$. Since $\vec{L}$ and $\vec{S}$ commute

$$R(\vec{\vartheta}) = R_\ell(\vec{\vartheta})R_s(\vec{\vartheta})\,, \quad R_\ell(\vec{\vartheta}) \equiv \exp\Big(-\mathrm{i}\,\vec{\vartheta}\cdot\vec{L}/\hbar\Big)\,, \quad R_s(\vec{\vartheta}) \equiv \exp\Big(-\mathrm{i}\,\vec{\vartheta}\cdot\vec{S}/\hbar\Big) \tag{203}$$

(ii) All vector operators continue to transform in the same way (196) as $\vec{X}$ does.
In the Heisenberg picture there is no difference in treating particles with or without spin.

(iii) In the Schrödinger picture eigenkets are characterised by additional indices which label eigenvectors of the $\mathfrak{su}(2)$ representations where spin operators act.

- For a single particle with spin s, a state vector in coordinate space has the decomposition

$$|\psi\rangle = \int d\vec{x} \sum_{m=-s}^{s} |\vec{x}, m\rangle \psi_m(\vec{x}) \tag{204}$$

  m is a spin label taking $2s+1$ discrete values, $-s, -s+1, \ldots, s$.

- $R(\vec{\vartheta})$ acts on both continuous coordinate label x and discrete spin label m.

G. Consider a spin 1/2 particle. Its state vector is

$$|\psi\rangle = \int d\vec{x}\,\Big(|\vec{x},\uparrow\rangle\psi_\uparrow(\vec{x}) + |\vec{x},\downarrow\rangle\psi_\downarrow(\vec{x})\Big) \tag{205}$$

and the spin operators are $S^\alpha = \hbar\,\sigma^\alpha/2$.

(i) The eigenkets $|x,\uparrow\rangle$ and $|x,\downarrow\rangle$ are simultaneous eigenkets of $\vec{X}$ and S^z.

(ii) The spin part of the rotation operator (203) is given by

$$R_s(\vec{\vartheta}) = \exp\Big(-\mathrm{i}\,\vec{\vartheta}\cdot\vec{S}/\hbar\Big) = e^{\frac{1}{2\mathrm{i}}\vartheta\,\vec{n}\cdot\vec{\sigma}} = I\cos\frac{\vartheta}{2} + \frac{1}{\mathrm{i}}\vec{n}\cdot\vec{\sigma}\,\sin\frac{\vartheta}{2} \tag{206}$$

(iii) It acts on the spin eigenkets as

$$\begin{aligned} R_s(\vec{\vartheta})|\uparrow\rangle &= (\cos\frac{\vartheta}{2} - \mathrm{i}\,n_z\sin\frac{\vartheta}{2})\,|\uparrow\rangle \;+\; (-\mathrm{i}\,n_x + n_y)\sin\frac{\vartheta}{2}\,|\downarrow\rangle \\ R_s(\vec{\vartheta})|\downarrow\rangle &= (\cos\frac{\vartheta}{2} + \mathrm{i}\,n_z\sin\frac{\vartheta}{2})\,|\downarrow\rangle \;+\; (-\mathrm{i}\,n_x - n_y)\sin\frac{\vartheta}{2}\,|\uparrow\rangle \end{aligned} \tag{207}$$

(iv) The rotation operator transforms $|\psi\rangle$ into

$$
\begin{aligned}
|\tilde{\psi}\rangle &= \int d\vec{x}\,\Big(|\vec{x},\uparrow\rangle\tilde{\psi}_\uparrow(\vec{x}) + |\vec{x},\downarrow\rangle\tilde{\psi}_\downarrow(\vec{x})\Big) = R(\vec{\vartheta})\,|\psi\rangle \\
&= \int d\vec{x}\,\Big(R_s(\vec{\vartheta})|\vec{x}(\vec{\vartheta}),\uparrow\rangle\psi_\uparrow(\vec{x}) + R_s(\vec{\vartheta})|\vec{x}(\vec{\vartheta}),\downarrow\rangle\psi_\downarrow(\vec{x})\Big) \\
&= \int d\vec{x}\,\Big(\big((\cos\frac{\vartheta}{2} - \mathrm{i}\,n_z\sin\frac{\vartheta}{2})\,|\vec{x},\uparrow\rangle \;+\; (-\mathrm{i}\,n_x + n_y)\sin\frac{\vartheta}{2}\,|\vec{x},\downarrow\rangle\big)\psi_\uparrow(\vec{x}(-\vec{\vartheta})) \\
&\qquad + \big((\cos\frac{\vartheta}{2} + \mathrm{i}\,n_z\sin\frac{\vartheta}{2})\,|\vec{x},\downarrow\rangle \;+\; (-\mathrm{i}\,n_x - n_y)\sin\frac{\vartheta}{2}\,|\vec{x},\uparrow\rangle\big)\psi_\downarrow(\vec{x}(-\vec{\vartheta}))\Big) \\
&= \int d\vec{x}\,\Big(|\vec{x},\uparrow\rangle\,\big((\cos\frac{\vartheta}{2} - \mathrm{i}\,n_z\sin\frac{\vartheta}{2})\psi_\uparrow(\vec{x}(-\vec{\vartheta})) \;+\; (-\mathrm{i}\,n_x - n_y)\sin\frac{\vartheta}{2}\psi_\downarrow(\vec{x}(-\vec{\vartheta}))\big) \\
&\qquad + \;|\vec{x},\downarrow\rangle\big((-\mathrm{i}\,n_x + n_y)\sin\frac{\vartheta}{2}\,\psi_\uparrow(\vec{x}(-\vec{\vartheta})) + \;(\cos\frac{\vartheta}{2} + \mathrm{i}\,n_z\sin\frac{\vartheta}{2})\psi_\downarrow(\vec{x}(-\vec{\vartheta}))\big)\Big)
\end{aligned} \tag{208}
$$

(v) The wave function components transform as

$$
\begin{aligned}
\tilde{\psi}_\uparrow(\vec{x}) &= (\cos\frac{\vartheta}{2} - \mathrm{i}\,n_z\sin\frac{\vartheta}{2})\psi_\uparrow(\vec{x}(-\vec{\vartheta})) \;+\; (-\mathrm{i}\,n_x - n_y)\sin\frac{\vartheta}{2}\psi_\downarrow(\vec{x}(-\vec{\vartheta})) \\
\tilde{\psi}_\downarrow(\vec{x}) &= (-\mathrm{i}\,n_x + n_y)\sin\frac{\vartheta}{2}\,\psi_\uparrow(\vec{x}(-\vec{\vartheta})) + \;(\cos\frac{\vartheta}{2} + \mathrm{i}\,n_z\sin\frac{\vartheta}{2})\psi_\downarrow(\vec{x}(-\vec{\vartheta}))
\end{aligned} \tag{209}
$$

- If $\vartheta = 2\pi$ then $\tilde{\psi}_m(\vec{x}) = -\psi_m(\vec{x})$, $m =\uparrow,\downarrow$
  After a complete rotation the wave function changes its sign.
- This anti-periodicity property is a feature of any fermion.

(vi) Combine the components into a column

$$\Psi(\vec{x}) \equiv \begin{pmatrix} \psi_\uparrow(\vec{x}) \\ \psi_\downarrow(\vec{x}) \end{pmatrix}, \quad \tilde{\Psi}(\vec{x}) \equiv \begin{pmatrix} \tilde{\psi}_\uparrow(\vec{x}) \\ \tilde{\psi}_\downarrow(\vec{x}) \end{pmatrix} \tag{210}$$

- The transformation takes the form

$$\tilde{\Psi}(\vec{x}) = \exp\Big(- \vec{\vartheta} \cdot (\vec{x} \times \frac{\partial}{\partial \vec{x}})\Big) R_s(\vec{\vartheta}) \Psi(\vec{x}) \tag{211}$$

- The same transformation rule applies to any wave function of a spin s particle combined into a $2s+1$-dimensional column.

V. Parity

Translations and rotations are continuous transformations.

The **parity transformation** $\mathcal{P}$ is discrete. It swaps the sign of all the coordinates and momenta

$$\vec{X}_a \mapsto -\vec{X}_a\,, \quad \vec{P}_a \mapsto -\vec{P}_a\,, \quad a = 1, \ldots, N \tag{212}$$

A. Consider a single particle – generalisation to a system of N particles is straightforward.

(i) The parity transformation is the multiplication of $\vec{X}$ and $\vec{P}$ by $-\mathbb{I}_3$

(ii) $\det(-\mathbb{I}_3) = -1 \;\Rightarrow\;$ it is not a rotation matrix.

(iii) Any 3×3 orthogonal matrix with determinant equal to -1 can be written as a product of $-\mathbb{I}_3$ and a rotation matrix.

B. $\mathcal{P}$ is a reflection about the origin, and it is a product of reflections about all the three coordinate planes (or axes).

(i) In CM a reflection about the x-axis can be thought of as the rotation in the phase xp^x-plane through the angle $\pm\pi$ which is a canonical transformation generated by $G_x = \pm\frac{\pi}{2}\,(x^2+(p^x)^2)$.

(ii) In QM the parity operator can be written as

$$\mathcal{P}_+ = \exp\Big(+\frac{\mathrm{i}\,\pi}{2\hbar}(\vec{X}^2+\vec{P}^2)\Big) \quad \text{or} \quad \mathcal{P}_- = \exp\Big(-\frac{\mathrm{i}\,\pi}{2\hbar}(\vec{X}^2+\vec{P}^2)\Big) \tag{213}$$

- The two operators are conjugate to each other
- Both operators satisfy the necessary relations

$$\mathcal{P}^\dagger\,\vec{X}\,\mathcal{P} = -\vec{X}\,, \quad \mathcal{P}^\dagger\,\vec{P}\,\mathcal{P} = -\vec{P} \tag{214}$$

(iii) (214) do not define $\mathcal{P}$ uniquely because it can be multiplied by any c: $|c| = 1$.

(iv) Since if we apply the parity transformation twice we get back to the original coordinates and momenta, we require

$$\mathcal{P}^2 = 1\,, \quad \mathcal{P}^\dagger = \mathcal{P} \tag{215}$$

- It is simultaneously unitary and Hermitian.
- We still have the freedom of multiplying the parity operator by -1.

(v) The operators (213) satisfy the opposite relations

$$\mathcal{P}_\pm^2 = -1\,, \quad \mathcal{P}_\pm^\dagger = \mathcal{P}_\mp = -\mathcal{P}_\pm \tag{216}$$

- To prove the relations we introduce the creation and annihilation operators

$$\vec{X} = \sqrt{\frac{\hbar}{2}}(\vec{a}^{\,\dagger} + \vec{a})\,, \quad \vec{P} = \mathrm{i}\sqrt{\frac{\hbar}{2}}(\vec{a}^{\,\dagger} - \vec{a})\,, \quad [a^{\alpha}\,,\, a^{\beta,\dagger}] = \delta^{\alpha\beta} \tag{217}$$

- Then,

$$\frac{1}{2\hbar}\big(\vec{X}^2 + \vec{P}^2)\big) = \vec{a}^{\,\dagger}\cdot\vec{a} + \frac{3}{2} = \hat{N} + \frac{3}{2} \tag{218}$$

- Thus,

$$\mathcal{P}_+ = e^{+\mathrm{i}\,\pi\,(\hat{N}+\frac{3}{2})} = -\mathrm{i}\,e^{+\mathrm{i}\,\pi\,\hat{N}}\,, \quad \mathcal{P}_- = e^{-\mathrm{i}\,\pi\,(\hat{N}+\frac{3}{2})} = \mathrm{i}\,e^{-\mathrm{i}\,\pi\,\hat{N}} \tag{219}$$

- Now,

$$\mathcal{P}_+^2 = -\,e^{+2\mathrm{i}\,\pi\,\hat{N}}\,, \quad \mathcal{P}_-^2 = -\,e^{-2\mathrm{i}\,\pi\,\hat{N}} \tag{220}$$

- Since the spectrum of the number operator consists of nonnegative integers, $\mathcal{P}_\pm^2$ acting on any state produces the same state with the minus sign, and therefore $\mathcal{P}_\pm^2 = -\hat{I}$.

(vi) It is now clear that the operator satisfying (214, 215) is

$$\mathcal{P} = e^{+\mathrm{i}\,\pi\,\hat{N}} = e^{-\mathrm{i}\,\pi\,\hat{N}} \tag{221}$$

- This definition of the parity operator also fixes the sign ambiguity mentioned above
- In practice it is much easier to use its defining relations (214, 215) together with specifying its action on eigenkets of the coordinate and momentum operators

$$\mathcal{P}\,|\vec{x}\rangle = |-\vec{x}\rangle\,, \quad \mathcal{P}\,|\vec{p}\rangle = |-\vec{p}\rangle \tag{222}$$

(vii) Let us show that the parity operator (221) satisfies (222)

- $\mathcal{P}$ anti-commutes with $\vec{X} \;\Rightarrow\; \mathcal{P}\,|\vec{x}\rangle$ is an eigenket of $\vec{X}$ with the eigenvalue $-\vec{x}$.
- $\mathcal{P}\,|\vec{x}\rangle$ may be equal to either $|-\vec{x}\rangle$ or $-|-\vec{x}\rangle$.
- To fix the sign, consider the wave function of $|0\rangle$

$$\psi(\vec{x}) = \langle \vec{x}|0\rangle \tag{223}$$

- $|0\rangle$ is destroyed by the annihilation operator $\Rightarrow$

$$\hat{a}\,\psi(\vec{x}) = \sqrt{\frac{2}{\hbar}}(\vec{X} + \mathrm{i}\,\vec{P})\,\psi(\vec{x}) = \sqrt{\frac{2}{\hbar}}(\vec{x} + \hbar\frac{\partial}{\partial\vec{x}})\,\psi(\vec{x}) = 0 \quad\Rightarrow\quad \psi(\vec{x}) = C\exp\Big(-\frac{\vec{x}^{\,2}}{2\hbar}\Big) \tag{224}$$

- Since $\psi(\vec{x})$ is even, $\mathcal{P}\,|\vec{x}\rangle = |-\vec{x}\rangle$

$$\psi(\vec{x}) = \langle\vec{x}|0\rangle = \langle\vec{x}|\mathcal{P}|0\rangle = \langle-\vec{x}|0\rangle = \psi(-\vec{x}) \tag{225}$$

(viii) The parity operator acts on wave functions as

$$|\tilde{\psi}\rangle = \int d\vec{x}\,|\vec{x}\rangle\tilde{\psi}(\vec{x}) = \mathcal{P}\,|\psi\rangle = \int d\vec{x}\,\mathcal{P}\,|\vec{x}\rangle\psi(\vec{x}) = \int d\vec{x}\,|-\vec{x}\rangle\psi(\vec{x}) = \int d\vec{x}\,|\vec{x}\rangle\,\psi(-\vec{x}) \tag{226}$$

$$\mathcal{P}\,\psi(\vec{x}) = \psi(-\vec{x})\,, \quad \mathcal{P}\,\psi(\vec{p}) = \psi(-\vec{p}) \tag{227}$$

The function $\psi(-\vec{x})$ is the mirror image of $\psi(\vec{x})$ about the origin.

C. Since $\mathcal{P}^2 = 1$ the eigenvalues of the parity operator can only be ±1.

(i) Eigenstates of $\mathcal{P}$ are said to have **definite parity**

- $|\psi_+\rangle = \mathcal{P}\,|\psi_+\rangle$ is a state of **even parity**
- $|\psi_-\rangle = -\mathcal{P}\,|\psi_-\rangle$ is a state of **odd parity**.

(ii) The wave function of an eigenstate of the number operator with an even eigenvalue has even parity and the one with odd eigenvalue has odd parity

$$\psi_n(\vec{x}) = \langle \vec{x}|n\rangle = (-1)^n \langle \vec{x}|\mathcal{P}|n\rangle = (-1)^n \langle -\vec{x}|n\rangle = (-1)^n \psi_n(-\vec{x}) \tag{228}$$

(iii) The expectation value of any operator A anti-commuting with the parity operator is 0

$$\langle \psi_\pm|A|\psi_\pm\rangle = \langle \psi_\pm|\mathcal{P}\, A\, \mathcal{P}|\psi_\pm\rangle = -\langle \psi_\pm|A|\psi_\pm\rangle = 0 \tag{229}$$

D. An operator $A(X, P)$ is compatible with the parity operator, and therefore in the Heisenberg picture does not change under the parity transformation, if

$$\mathcal{P}^\dagger\, A(X, P)\, \mathcal{P} = A(-X, -P) = A(X, P) \tag{230}$$

X and P denote the full set of coordinates and momenta.

(i) The angular momentum vector is invariant under the parity transformation.
By this reason it is called a **pseudovector** or an **axial vector**.

(ii) Vectors which change sign are called **polar vectors**.

E. Almost everything we have discuss applies to odd number of reflections about coordinate axes in space of any dimension.