Spring

Physics 661 Quantum Mechanics II

Review

The Postulates of Quantum Mechanics are

1) The set of all possible states of a physical system stand in 1-1 correspondence with the vector directions (rays) in a Hilbert space $\mathcal{H}$. Since the state is described by the entire ray, we have that $|\psi\rangle$ and $\lambda|\psi\rangle$ with $\lambda \in \mathbb{C}$ describe the same state.

2) The physical observables of a system stand in a 1-1 correspondence with the set of Hermitian operators on the state space $\mathcal{H}$. That is, to each measurable quantity $\mathcal{A}$, there corresponds a Hermitean operator A acting on $\mathcal{H}$. Out of the set of all Hermitean operators, there is a subset, which consists of mutually commuting operators and they are assumed to be complete (they form a CSCO).

3) Spectral Decomposition

a) The only possible result of the measurement of a physical observable $\mathcal{A}$ is one of the (real) eigenvalues of the corresponding Hermitian operator A.

b) Let $\{|\phi_k\rangle\}$ be the simultaneous eigenstates of a CSCO so that

$$A|\phi_k\rangle = a_k|\phi_k\rangle \text{ etc.}$$

These states form an orthonormal basis for the state space $\mathcal{H}$.

For a system in state $|\psi\rangle$ (with $\langle\psi|\psi\rangle = 1$) the probability of measuring the value a_k for the physical observable $\mathcal{A}$ is

$$P_k = |\langle\phi_k|\psi\rangle|^2 .$$

Immediately following the measurement, the system is in the state $|\phi_k\rangle$.

4) The time evolution of the physical states is given by the Schrödinger equation

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H(t) |\psi(t)\rangle ,$$

where $H = H(t)$ is the Hermitian Hamiltonian operator. $H(t)$ is the total energy of the system. (In general the observables may also have explicit time dependence, $A = A(t)$.)

For an isolated system, the observables including the Hamiltonian are independent of time $\frac{dA}{dt} = 0$ and H is a constant operator.

Comments: 1) We extend the Hilbert space of states to include generalized kets with infinite (continuum) norms but whose scalar product with every ket of $\mathcal{H}$ is finite. So doing, to every bra-vector $\langle\psi|$ there corresponds a ket-vector and vice-versa in the extended Hilbert space and its dual.

2) Then in postulate 3 we can have discrete as well as continuous (or even mixed) sets of basis vectors. That is if the orthonormal basis is a discrete basis, then the simultaneous eigenvectors, $|\phi_{ab\ldots}\rangle$, of the CSCO $\{A, B, \ldots\}$ obey

$$\langle \phi_{a'b'\ldots} | \phi_{ab\ldots} \rangle = \delta_{a'a}\, \delta_{b'b} \cdots$$

$$\mathbb{1} = \sum_{a,b,\ldots} |\phi_{ab\ldots}\rangle\langle \phi_{ab\ldots}|$$

where

$$A|\phi_{ab\ldots}\rangle = a|\phi_{ab\ldots}\rangle$$

$$B|\phi_{ab\ldots}\rangle = b|\phi_{ab\ldots}\rangle, \text{ etc.},$$

with the eigenvalues $\{a, b, \ldots\}$ taking discrete values (in 1-1 correspondence with the integers).

An arbitrary state vector $|\psi\rangle$ has the expansion in terms of the $|\phi_{ab\ldots}\rangle$ basis

$$|\psi\rangle = \sum_{a,b,\ldots} \psi_{ab\ldots} |\phi_{ab\ldots}\rangle$$

with

$$\psi_{ab\ldots} = \langle \phi_{ab\ldots} | \psi \rangle .$$

This implies

$$A|\psi\rangle = \sum_{a,b,\ldots}' a \, \psi_{ab\ldots} |\phi_{ab\ldots}\rangle$$

$$B|\psi\rangle = \sum_{a,b,\ldots}' b \, \psi_{ab\ldots} |\phi_{ab\ldots}\rangle, \text{ etc.}$$

The probability of finding the values $a, b, \ldots$ when $A, B, \ldots$ are measured when the system is in state $|\psi\rangle$ is

$$P_{ab\ldots} = |\langle \phi_{ab\ldots} | \psi \rangle|^2 .$$

Note that

$$\sum_{a,b,\ldots}' P_{ab\ldots} = \sum_{a,b,\ldots}' |\langle \phi_{ab\ldots} | \psi \rangle|^2$$

$$= \sum_{a,b,\ldots}' \langle \psi | \phi_{ab\ldots} \rangle \langle \phi_{ab\ldots} | \psi \rangle$$

$$= \langle \psi | \psi \rangle = 1$$ as required of a probability.

Finally, the expectation value of $A, B, \ldots$ in state $|\psi\rangle$ is

$$\langle\psi|A|\psi\rangle = \sum_{a,b,\ldots}{}' a \underbrace{\psi_{ab\ldots}}_{=\langle\phi_{ab\ldots}|\psi\rangle} \langle\psi|\phi_{ab\ldots}\rangle$$

$$= \sum_{a,b,\ldots}{}' a\, |\langle\phi_{ab\ldots}|\psi\rangle|^2$$

$$= \sum_{a,b,\ldots}{}' a\, P_{ab\ldots}$$, etc., again as expected for $P_{ab\ldots}$ a probability.

On the other hand, if the orthonormal basis is continuous, then

$$\langle\phi_{\alpha'\beta'\ldots}|\phi_{\alpha\beta\ldots}\rangle = \delta(\alpha'-\alpha)\,\delta(\beta'-\beta)\cdots$$

$$\mathbb{1} = \int d\alpha\, d\beta \cdots |\phi_{\alpha\beta\ldots}\rangle\langle\phi_{\alpha\beta\ldots}|$$

where

$$A|\phi_{\alpha\beta\ldots}\rangle = \alpha|\phi_{\alpha\beta\ldots}\rangle$$

$$B|\phi_{\alpha\beta\ldots}\rangle = \beta|\phi_{\alpha\beta\ldots}\rangle$$, etc.,

with the eigenvalues $\{\alpha, \beta, \ldots\}$ taking on a continuum of values.

An arbitrary state vector $|\psi\rangle$ has the expansion in terms of the continuous basis $\{|\phi_{\alpha\beta\ldots}\rangle\}$ given by

$$|\psi\rangle = \int d\alpha\, d\beta \ldots\, \psi(\alpha,\beta,\ldots)\, |\phi_{\alpha\beta\ldots}\rangle$$

with

$$\psi(\alpha,\beta,\ldots) = \langle \phi_{\alpha\beta\ldots}|\psi\rangle .$$

This implies

$$A|\psi\rangle = \int d\alpha\, d\beta \ldots\, \alpha\, \psi(\alpha,\beta,\ldots)\, |\phi_{\alpha\beta\ldots}\rangle$$

$$B|\psi\rangle = \int d\alpha\, d\beta \ldots\, \beta\, \psi(\alpha,\beta,\ldots)\, |\phi_{\alpha\beta\ldots}\rangle, \text{ etc.}$$

For the system in state $|\psi\rangle$, the probability of measuring $\mathcal{A}$ in the range α to $\alpha + d\alpha$, $\mathcal{B}$ in the range β to $\beta + d\beta$, etc. is

$$dP(\alpha,\beta,\ldots) = |\langle\phi_{\alpha\beta\ldots}|\psi\rangle|^2\, d\alpha\, d\beta \ldots .$$

Note, as required of a probability density

$$\int dP(\alpha,\beta,\ldots) = \int d\alpha\, d\beta \ldots |\langle\phi_{\alpha\beta\ldots}|\psi\rangle|^2$$

$$= \langle\psi| \int d\alpha\, d\beta \ldots\, |\phi_{\alpha\beta\ldots}\rangle\langle\phi_{\alpha\beta\ldots}|\psi\rangle$$

$$= \langle \psi | \psi \rangle = 1.$$

And finally the expectation value of A, B, ... in state $|\psi\rangle$ is

$$\langle \psi | A | \psi \rangle = \int d\alpha\, d\beta \cdots \alpha \underbrace{\psi(\alpha,\beta,\ldots)}_{= \langle \phi_{\alpha\beta\ldots} | \psi \rangle} \langle \psi | \phi_{\alpha\beta\ldots} \rangle$$

$$= \int d\alpha\, d\beta \cdots \alpha \, |\langle \phi_{\alpha\beta\ldots} | \psi \rangle|^2$$

$$= \int d\mathcal{P}(\alpha,\beta,\ldots)\, \alpha \, , \quad \text{etc.}.$$

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3) Further, immediately following the measurement of A, the state of the system is reduced to that part of $|\psi\rangle$ which is precisely that eigenvector of A. So if A is measured to yield a, the system immediately afterwards is in state

$$|\psi\rangle \longrightarrow \frac{\sum_{b,c,\ldots} \psi_{a,b,c\ldots} |\phi_{abc\ldots}\rangle}{\left(\sum_{b,c,\ldots} |\psi_{a,b,c\ldots}|^2\right)^{1/2}}$$

normalizes new state to 1.

In the case of continuous eigenvalues the state of the system reduces to the state

$$|\psi\rangle \longrightarrow \frac{\int_{\alpha-\frac{\Delta\alpha}{2}}^{\alpha+\frac{\Delta\alpha}{2}} d\alpha \int d\beta\, d\gamma \cdots \psi(\alpha,\beta,\gamma,\ldots)\,|\phi_{\alpha,\beta,\gamma,\ldots}\rangle}{\left(\int_{\alpha-\frac{\Delta\alpha}{2}}^{\alpha+\frac{\Delta\alpha}{2}} d\alpha \int d\beta\, d\gamma \cdots |\psi(\alpha,\beta,\gamma,\ldots)|^2\right)^{1/2}}$$

immediately after the measurement of A which yields α to within $\Delta\alpha$.

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4) The Hilbert space is completely characterized by giving all algebraic relations (commutation relations) among the elements of an irreducible set of linear operators. An irreducible set of operators is one such that the only operator to commute with all the members of the set is the identity. For the case of a single particle with no other internal degrees of freedom (ex. no spin) we had that the position operator $\underline{X}$ and its

canonically conjugate momentum operator P formed an irreducible set. Their CCR are

$$[X_i, P_j] = i\hbar\delta_{ij}$$

$$[X_i, X_j] = 0 = [P_i, P_j].$$

So if an operator commutes with X, it cannot be a function of P since they do not commute. If it also commutes with P likewise, it cannot be a function of X. Hence, the operator is independent of X and P, since there are no other degrees of freedom for the operator to act on, it must be a multiple of the identity. From the irreducible set we can extract a CSCO whose eigenvectors form a basis for the Hilbert space. Thus we are led to consider the coordinate basis and the momentum basis.

<u>Coordinate Representation</u>: Given a Cartesian coordinate system with the particle position denoted by vector $\vec{r}$ we have

$$X_i |\vec{r}\rangle = x_i |\vec{r}\rangle \quad ; \quad (x_1, x_2, x_3) \in \mathbb{R}^3$$

The states are continuum normalized

1) $$\langle \vec{r}' | \vec{r} \rangle = \delta^3(\vec{r}' - \vec{r})$$

and complete

2) $$\mathbb{1} = \int d^3r \, |\vec{r}\rangle\langle\vec{r}| .$$

Hence any state $|\psi\rangle$ has the expansion

$$|\psi\rangle = \int d^3r \, \psi(\vec{r}) \, |\vec{r}\rangle$$

with wavefunction $\psi(\vec{r}) = \langle \vec{r} | \psi \rangle$.

Any function of X_i has expectation value

$$\langle \psi | F(\vec{R}) | \psi \rangle = \int d^3r \, \psi^*(\vec{r}) F(\vec{r}) \psi(\vec{r})$$

since $$F(\vec{R}) |\vec{r}\rangle = F(\vec{r}) |\vec{r}\rangle .$$

Consider the unitary operator (translation operator)

$$\mathcal{U}(\vec{a}) \equiv e^{-\frac{i}{\hbar}\vec{P}\cdot\vec{a}}$$

$$\mathcal{U}^\dagger(\vec{a}) = \mathcal{U}(-\vec{a}) = \mathcal{U}^{-1}(\vec{a}) \quad \text{since } \vec{P}^\dagger = \vec{P}.$$

Since $[X_i, P_j] = i\hbar\delta_{ij}$ we have that

$$[X_i, \mathcal{U}(\vec{a})] = -\frac{i}{\hbar}(i\hbar a_i)\,\mathcal{U}(\vec{a})$$

$$= a_i\,\mathcal{U}(\vec{a})$$

Thus $\vec{R}\,\mathcal{U}(\vec{a}) = \mathcal{U}(\vec{a})(\vec{R}+\vec{a})$.

Applying this to the position eigenstates we find

$$\vec{R}(\mathcal{U}(\vec{a})\,|\vec{r}\rangle) = (\vec{r}+\vec{a})(\mathcal{U}(\vec{a})|\vec{r}\rangle)$$

Thus $\mathcal{U}(\vec{a})|\vec{r}\rangle = |\vec{r}+\vec{a}\rangle$.

Now

$$\langle\vec{r}|\,\mathcal{U}^\dagger(\vec{a})\,|\psi\rangle = \langle\vec{r}|\,\mathcal{U}(-\vec{a})\,|\psi\rangle$$

$$= \langle\vec{r}+\vec{a}|\psi\rangle = \psi(\vec{r}+\vec{a})$$

but for infinitesimal $\vec{a} = \vec{\epsilon}$ we have

$$U^{\dagger}(\vec{\epsilon}) = 1 + \frac{i}{\hbar}\vec{P}\cdot\vec{\epsilon} + O(|\vec{\epsilon}|^2)$$

So

$$\langle\vec{r}|U^{\dagger}(\vec{\epsilon})|\psi\rangle = \langle\vec{r}|\psi\rangle + \frac{i}{\hbar}\langle\vec{r}|\vec{P}\cdot\vec{\epsilon}|\psi\rangle$$

$$= \psi(\vec{r}) + \frac{i}{\hbar}\langle\vec{r}|\vec{P}\cdot\vec{\epsilon}|\psi\rangle$$

but this $= \psi(\vec{r}+\vec{\epsilon}) = \psi(\vec{r}) + \vec{\epsilon}\cdot\vec{\nabla}\psi(\vec{r})$

$\Rightarrow$

$$\langle\vec{r}|\vec{P}|\psi\rangle = -i\hbar\vec{\nabla}\psi(\vec{r})$$

$$= -i\hbar\vec{\nabla}\langle\vec{r}|\psi\rangle$$

Since $|\psi\rangle$ was arbitrary $\Rightarrow$

$\langle\vec{r}|\vec{P} = -i\hbar\vec{\nabla}_{\vec{r}}\langle\vec{r}|$, that is

$\vec{P}$ is represented by $\frac{\hbar}{i}\vec{\nabla}_{\vec{r}}$ in the $\{|\vec{r}\rangle\}$ basis.

Suppose $|\psi\rangle$ is a momentum eigenstate $|\vec{p}\rangle$

$$\vec{P}|\vec{p}\rangle = \vec{p}|\vec{p}\rangle \quad ; \quad \vec{p} \in \mathbb{R}^3$$

with continuum normalization

1) $$\langle \vec{p}\,' | \vec{p} \rangle = (2\pi\hbar)^3 \delta^3(\vec{p}\,' - \vec{p})$$

Then

$$\langle \vec{r} | \vec{P} | \vec{p} \rangle = -i\hbar \vec{\nabla}_r \langle \vec{r} | \vec{p} \rangle$$

$$= \vec{p} \langle \vec{r} | \vec{p} \rangle$$

$$\Rightarrow \boxed{\langle \vec{r} | \vec{p} \rangle = N e^{+\frac{i}{\hbar}\vec{p}\cdot\vec{r}}}$$

Since $\{|\vec{r}\rangle\}$ is complete we have

$$\langle \vec{p}\,' | \vec{p} \rangle = (2\pi\hbar)^3 \delta^3(\vec{p}\,' - \vec{p})$$

$$= \int d^3r \langle \vec{p}\,' | \vec{r} \rangle \langle \vec{r} | \vec{p} \rangle$$

$$= \int d^3r \, e^{\frac{i}{\hbar}(\vec{p} - \vec{p}\,')\cdot\vec{r}} \, |N|^2$$

$$= |N|^2 (2\pi\hbar)^3 \delta^3(\vec{p}\,' - \vec{p}),$$

thus we take $\boxed{N = 1.}$

Likewise the completeness relation for the momentum basis $\{|\vec{p}\rangle\}$ is

2) $$\mathbb{1} = \int \frac{d^3p}{(2\pi\hbar)^3} |\vec{p}\rangle\langle\vec{p}| \,.$$

Any state $|\psi\rangle$ has the expansion in terms of momentum eigenstates

$$|\psi\rangle = \int \frac{d^3p}{(2\pi\hbar)^3} \tilde{\psi}(\vec{p}) \, |\vec{p}\rangle$$

with $\tilde{\psi}(\vec{p}) = \langle\vec{p}|\psi\rangle$.

Thus

$$\psi(\vec{r}) = \int \frac{d^3p}{(2\pi\hbar)^3} e^{\frac{i\vec{p}\cdot\vec{r}}{\hbar}} \tilde{\psi}(\vec{p})$$

and

$$\tilde{\psi}(\vec{p}) = \int d^3r \, e^{-\frac{i\vec{p}\cdot\vec{r}}{\hbar}} \psi(\vec{r}) \,.$$

Finally for $H = \frac{1}{2m}\vec{P}^2 + V(\vec{R})$, the Schrödinger equation in the $\{|\vec{r}\rangle\}$-basis takes the form of the Schrödinger wave equation

$$i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t) = \left[-\frac{\hbar^2}{2m}\nabla_{\vec{r}}^2 + V(\vec{r})\right]\psi(\vec{r},t)$$

with $\psi(\vec{r},t) = \langle\vec{r}|\psi(t)\rangle$.

<u>Transformation Theory</u>: Suppose 2 observers O and O' describe the same system S. O associates the unit ray $|\Psi\rangle$ with S while O' associates the unit ray $|\Psi'\rangle$ with the same state of affairs S. We assume there is a 1-1 mapping of the unit rays onto each other so that the probability of O finding the system S in state ray $|\Phi\rangle$, $|\langle\phi|\psi\rangle|^2$ where $|\psi\rangle \in |\Psi\rangle$ and $|\phi\rangle \in |\Phi\rangle$, is the same as O' finding S in the corresponding state ray $|\Phi'\rangle$, $|\langle\phi'|\psi'\rangle|^2$ with

$$|\langle\phi|\psi\rangle|^2 = |\langle\phi'|\psi'\rangle|^2 .$$

This is the passive description of the transformation between equivalent observers. Alternatively we can transform the system, that is have one fixed observer and two systems which are transformed: translated rotated etc. with respect to eachother. Then the states and operators are transformed $|\psi\rangle \to |\psi'\rangle$ and $A \to A'$ with the following properties

1) if $A|\phi_n\rangle = a_n|\phi_n\rangle$ then after the transformation $A'|\phi'_n\rangle = a_n|\phi'_n\rangle$. The eigenvalues of A and A' are the same. A' afterall represents the same observable as A, only in a different frame. Hence they must have the same set of possible values.

2) as before, if $|\psi\rangle = \sum_n c_n|\phi_n\rangle$ then

$$|\psi'\rangle = \sum_n c'_n|\phi'_n\rangle \text{ and } |c_n|^2 = |c'_n|^2$$

that is $|\langle\phi_n|\psi\rangle|^2 = |\langle\phi'_n|\psi'\rangle|^2$.

The probabilities for equivalent events in the 2 frames must be the same.

Since the 1-1 mapping is between rays $|\Psi\rangle \leftrightarrow |\Psi'\rangle$ there corresponds infinitely many vector mappings compatible with the ray mapping,

$|\psi\rangle \rightarrow |\psi'\rangle$ with $|\psi'\rangle \in |\Psi'\rangle$ if $|\psi\rangle \in |\Psi\rangle$.

However Wigner showed that due to $|\langle\phi'|\psi'\rangle|^2 = |\langle\phi|\psi\rangle|^2$, there is a mapping among the infinite possible that can be represented by either a unitary operator or by an anti-unitary operator.

<u>Wigner's Theorem</u>: If U is an operator satisfying

$$|\langle\phi'|\psi'\rangle|^2 = |\langle\phi|\psi\rangle|^2 \quad \text{with}$$

$|\psi'\rangle = U|\psi\rangle$ for each vector $|\psi\rangle$ in $\mathcal{H}$,

then one may choose the arbitrary phases to define the operator U'

$$U'|\psi\rangle = e^{+i\alpha_\psi} U|\psi\rangle = e^{+i\alpha_\psi}|\psi'\rangle$$

So the U' is either <u>unitary</u> or <u>anti-unitary</u>.

(Note if $|\phi_n'\rangle = U|\phi_n\rangle$ then $A'U|\phi_n\rangle = a_n U|\phi_n\rangle$

$\Rightarrow U^{-1}A'U|\phi_n\rangle = a_n|\phi_n\rangle$. But $A|\phi_n\rangle = a_n|\phi_n\rangle$

So $U^{-1}A'U = A$; that is $A' = UAU^{-1}$!)

Further anti-linear operators will only come into play when we consider discrete time-reversal ~~transformations~~. Indeed, continuous transformations have a square-root, and so are represented by linear operators since the product of 2 linear or anti-linear operators is again linear.

A continuous transformation operator is one which depends continuously on a smoothly varying parameter. For transformations connected to the identity, so that when the parameter, call it s, is zero we have $U(s=0) = \mathbb{1}$, we can represent it as an exponential

$$U(s) = e^{-isQ}$$ where

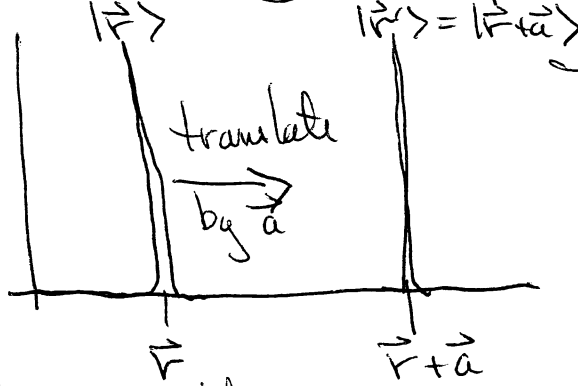
Q is called the <u>generator</u> of the transformation. Since $U^\dagger = U^{-1}$ $\Rightarrow Q = Q^\dagger$ is hermitian. Further when two consecutive transformations are made $|\psi\rangle \xrightarrow[U(s_1)]{} |\psi'\rangle \xrightarrow[U(s_2)]{} |\psi''\rangle$ which is physically equivalent to a single transformation $|\psi\rangle \xrightarrow[U(s_3)]{} e^{i\alpha}|\psi''\rangle$

we have that the final rays in both cases are the same. For vectors then they are equal up to a phase, hence

$$\mathcal{U}(s_3) = e^{i\alpha(s_2,s_1)}\,\mathcal{U}(s_2)\,\mathcal{U}(s_1)$$

where the phase $\alpha(s_2,s_1)$ depends on s_1 and s_2. If it depended also on the state $|\psi\rangle$ it would not be a linear operator contrary to Wigner's Theorem for continuous transformations.

For translations in space $\vec{r}\,' = \vec{r} + \vec{a}$ we have that a particle located precisely at $|\vec{r}\rangle$ upon translation is located at $|\vec{r}\,'\rangle = |\vec{r}+\vec{a}\rangle$



Thus $\mathcal{U}(\vec{a})|\vec{r}\rangle = |\vec{r}\,'\rangle$

$= |\vec{r}+\vec{a}\rangle$

Hence the wavefunction corresponding to state $|\psi'\rangle = \mathcal{U}|\psi\rangle$ becomes

$$\psi'(\vec{r}) = \langle\vec{r}|\psi'\rangle = \langle\vec{r}|\mathcal{U}(\vec{a})|\psi\rangle$$

$$= \langle \vec{r}\,|\,U^{\dagger}(-\vec{a})\,|\psi\rangle = \langle \vec{r}-\vec{a}\,|\psi\rangle$$

$$= \psi(\vec{r}-\vec{a}) = \psi'(\vec{r}) .$$

Also

$$\vec{R}\,U^{-1}(\vec{a})|\vec{r}\rangle = \vec{R}\,|\vec{r}-\vec{a}\rangle = (\vec{r}-\vec{a})|\vec{r}-\vec{a}\rangle$$

$$= (\vec{r}-\vec{a})\,U^{-1}(\vec{a})\,|\vec{r}\rangle$$

$$\Rightarrow \quad U(\vec{a})\,\vec{R}\,U^{-1}(\vec{a})|\vec{r}\rangle = (\vec{r}-\vec{a})|\vec{r}\rangle$$

$$= (\vec{R}-\vec{a})\,|\vec{r}\rangle$$

$$\Rightarrow \boxed{\vec{R}' = U(\vec{a})\,\vec{R}\,U^{-1}(\vec{a}) = \vec{R}-\vec{a}}$$

i.e. $[P_i, X_j] = -i\hbar\delta_{ij}$.

Note also that

$$\begin{tikzcd} \vec{r} \arrow[r, "U(\vec{a})"] \arrow[rr, bend right, "U(\vec{a}+\vec{b})"'] & \vec{r}+\vec{a} \arrow[r, "U(\vec{b})"] & \vec{r}+\vec{a}+\vec{b} \end{tikzcd}$$

So

$$U(\vec{a}+\vec{b})|\vec{r}\rangle = |\vec{r}+\vec{a}+\vec{b}\rangle$$

$$= U(\vec{a})\,U(\vec{b})\,|\vec{r}\rangle = |\vec{r}+\vec{a}+\vec{b}\rangle$$

Thus
$$\mathcal{U}(\vec{a}+\vec{b}) = \mathcal{U}(\vec{a})\,\mathcal{U}(\vec{b}) = \mathcal{U}(\vec{b})\,\mathcal{U}(\vec{a}).$$

Now let
$$\mathcal{U}(\vec{a}) = e^{-\frac{i}{\hbar}\vec{P}\cdot\vec{a}}$$
; then

$$\mathcal{U}(\vec{a}+\vec{b}) = \mathcal{U}(\vec{a})\,\mathcal{U}(\vec{b}) \Rightarrow [P_i, P_j] = 0.$$

Further $\mathcal{U}(\vec{a})|\vec{r}\rangle = |\vec{r}+\vec{a}\rangle$ or
$\psi'(\vec{r}) = \psi(\vec{r}-\vec{a}) \Rightarrow$

$$\langle\vec{r}|\,e^{-\frac{i}{\hbar}\vec{P}\cdot\vec{a}}\,|\psi\rangle = \psi(\vec{r}-\vec{a}) = \psi(\vec{r}) - \vec{a}\cdot\vec{\nabla}_{\vec{r}}\psi(\vec{r})$$

$$= \psi(\vec{r}) - \frac{i}{\hbar}\,\langle\vec{r}|\vec{a}\cdot\vec{P}|\psi\rangle$$

So $\langle\vec{r}|\vec{P}|\psi\rangle = -i\hbar\vec{\nabla}_{\vec{r}}\langle\vec{r}|\psi\rangle$

Thus $\langle\vec{r}|\vec{P} = \frac{\hbar}{i}\vec{\nabla}_{\vec{r}}\langle\vec{r}|$.

Finally suppose the Hamiltonian is invariant under a transformation
$$H' = \mathcal{U}H\mathcal{U}^{-1} = H$$
$$\Rightarrow [\mathcal{U}, H] = 0.$$

Then if
$$i\hbar \frac{\partial}{\partial t}|\psi\rangle = H|\psi\rangle$$
we have
$$i\hbar \frac{\partial}{\partial t} U|\psi\rangle = U H U^{-1} U|\psi\rangle$$
$\Rightarrow$
$$i\hbar \frac{\partial}{\partial t}|\psi'\rangle = H'|\psi'\rangle$$
$$= H|\psi'\rangle$$

The transformed state evolves in time according to the same dynamics H. It is a physically realizable state.

So if H has a symmetry i.e remains unchanged upon transformation of the system, there is conservation of the generator of the symmetry i.e.
$$U(s) = e^{-iQs}$$
$$[U(s), H] = 0 \Rightarrow [Q, H] = 0$$
by Heisenberg's eq. of motion
$$-i\hbar \frac{dQ}{dt} = [H, Q] = 0 \Rightarrow Q = \text{constant operator}$$

or hence by Ehrenfest's theorem $\langle Q \rangle = \text{constant}$.

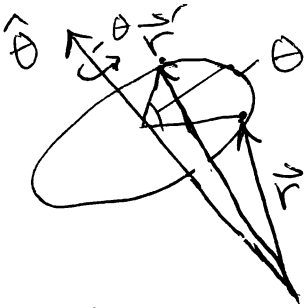
Besides translations in space, we are interested in time translations generated by the Hamiltonian, constant velocity boosts and spatial rotations. These set of geometric or space-time transformations between inertial frames form the Galilean group of transformations. These were studied carefully last semester. Let's now concentrate more depth on the spatial rotation subgroup and their generators, the angular momentum operators!

Rotations & Angular Momentum: Suppose the coordinate systems of 2 observers are related by a spatial rotation. Their coordinates are related by

$$x'_i = R_{ij} x_j \quad \text{with } R^T = R^{-1}$$

Characterizing the rotation by its axis of rotation and its angle of rotation about the axis, $\vec{\theta} = \theta\hat{\theta}$, the vector parameterizes the possible rotations $R_{ij} = R_{ij}(\vec{\theta})$. Further we have that

$$R_{ij}(\vec{\theta}) = \delta_{ij} + (\hat{\theta}_i \hat{\theta}_j - 1)(1-\cos\theta) + \epsilon_{ikj}\hat{\theta}_k \sin\theta$$



$$= \left(e^{\vec{\theta}\cdot\vec{I}}\right)_{ij} \quad \text{where } (I_k)_{ij} \equiv \epsilon_{ikj}$$
$$\Rightarrow [I_i, I_j] = \epsilon_{ijk} I_k$$

For consecutive rotations $R(\vec{\theta}_1)$, $R(\vec{\theta}_2)$

$$\vec{r} \xrightarrow{R(\vec{\theta}_1)} \vec{r}' \xrightarrow{R(\vec{\theta}_2)} \vec{r}''$$

$$\vec{r} \xrightarrow{R(\vec{\theta}_3)} \vec{r}''$$

$$R(\vec{\theta}_3) = R(\vec{\theta}_2) R(\vec{\theta}_1)$$
$$\Rightarrow \vec{\theta}_3 = \vec{\theta}_3(\vec{\theta}_1, \vec{\theta}_2)$$

we can always find an equivalent single composite rotation $R(\vec{\theta}_3)$ given the multiplication law of rotations.

O(3) group

For arbitrary rotations this is complicated so we equivalently considered the sequence of finite and infinitesimal rotations

$$\begin{tikzcd}
\vec{r} \arrow[r, "R^{-1}(\vec{\theta})"] \arrow[d, "R(\vec{\omega}')=(1+\omega')"'] & \vec{r}\,' \arrow[r, "\substack{R(\vec{\omega})\\ \shortparallel \\ (1+\omega)}"] & \vec{r}\,'' \arrow[dll, bend left, "R(\theta)"] \\
\vec{r}\,''' & &
\end{tikzcd}$$

Recall: $(\omega_{ij} = -\epsilon_{ijk}\omega_k)$

The infinitesimal angles ω' are found from

$$R(\vec{\omega}') = R(\vec{\theta})R(\omega)R^{-1}(\vec{\theta})$$

$$\Rightarrow \boxed{\omega'_{ij} = \left(R(\vec{\theta})\,\omega\, R^{-1}(\vec{\theta})\right)_{ij}}$$

According to Wigner's theorem the quantum mechanical state vectors these 2 observers use to describe the same system are related by a <u>unitary</u> transformation

$$|\psi'\rangle = U(R(\vec{\theta}))\,|\psi\rangle$$

$$U^{\dagger}(R(\vec{\theta})) = U^{-1}(R(\vec{\theta})).$$ Since

the state of the system is represented by a ray in $\mathcal{H}$, we have that the rotation group multiplication law need only be represented up to a phase

$$\vec{r} \xrightarrow{R(\vec{\theta}_1)} \vec{r}\,' \xrightarrow{R(\vec{\theta}_2)} \vec{r}\,''$$

$$R(\vec{\theta}_3) = R(\vec{\theta}_2)R(\vec{\theta}_1)$$

but

$$|\psi\rangle \xrightarrow{U(R(\vec{\theta}_1))} |\psi'\rangle \xrightarrow{U(R(\vec{\theta}_2))} e^{i\alpha(\vec{\theta}_2,\vec{\theta}_1)}|\psi''\rangle$$

$\to |\psi''\rangle$ same state of system

$$U(R(\vec{\theta}_3)) = e^{-i\alpha(\vec{\theta}_2,\vec{\theta}_1)}\,U(R(\vec{\theta}_2))\,U(R(\vec{\theta}_1))$$

Or for our infinitesimal transformation

$$|\psi\rangle \xrightarrow{U(R^{-1})} |\psi'\rangle \xrightarrow{U(1+\omega)} |\psi''\rangle$$

$$|\psi\rangle \xrightarrow{U(1+\omega')} |\psi'''\rangle \qquad |\psi''\rangle \xrightarrow{U(R)} e^{i\hat{\alpha}(\omega,\vec{\theta})}|\psi'''\rangle$$

$$\Rightarrow \boxed{e^{i\hat{\alpha}(\omega,\vec{\theta})}\,U(1+\omega') = U(R(\vec{\theta}))\,U(1+\omega)\,U(R^{-1}(\vec{\theta}))}$$

Since $U^\dagger = U^{-1}$ we can represent U by the exponential operator

$$U(R(\theta)) = e^{-\frac{i}{\hbar}\vec{\theta}\cdot\vec{J}}$$

where $J_i^\dagger = J_i$ and $\vec{J}$ is known as the generator of rotations or the total angular momentum operator.
Changing $\vec{J}$ by a phase $\vec{J} \to \vec{J} + \vec{F}$, $\vec{F} \in \mathbb{R}^3$, still leaves U unitary, $U^\dagger = U^{-1}$. We can use this phase to eliminate $\hat{\alpha}$. The multiplication law becomes

$$\omega^i\, U(R(\vec{\theta}))\, J_i\, U^{-1}(R(\vec{\theta})) = \omega'^i J_i + \omega^i f_i(\vec{\theta})$$

$\hbar\hat{\alpha}(\omega,\vec{\theta})$

$$= (R\omega R^{-1})^i J^i + \omega^i f^i$$

Now if $\vec{\theta}$ is also infinitesimal we have

$$[J_i, J_j] = i\hbar\,\epsilon_{ijk}(J_k + F_k)$$

Redefining $\vec{J} + \vec{F} \to \vec{J} \Rightarrow$

$$\boxed{[J^i, J^j] = i\hbar\,\epsilon_{ijk} J^k}$$ The angular momentum commutation relations

~~Standard Basis~~

Since $J_i = J_i^\dagger$, we can use J_i as part of our CSCO. In particular

$$[\vec{J}^2, J^i] = 0 \Rightarrow \{A, \vec{J}^2, J_z\} = \text{CSCO}$$

with simultaneous eigenvectors

$$A|k,j,m\rangle = a_k|k,j,m\rangle$$

$$\vec{J}^2|k,j,m\rangle = j(j+1)\hbar^2|k,j,m\rangle$$

$$J_z|k,j,m\rangle = m\hbar\,|k,j,m\rangle.$$

<u>Thm.</u> $j = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$

$$m = \underbrace{-j, -j+1, \ldots, j-1, +j}_{(2j+1)\text{ values}}.$$

Thus $\{|k,j,m\rangle\}$ is the Standard Basis for $\mathcal{H}$.

given $|k,j,m\rangle$ we can obtain all m by $J_\pm$.

1) Orthonormal

$$\langle k,j,m|k',j',m'\rangle = \delta_{kk'}\delta_{jj'}\delta_{mm'}$$

2) Complete

$$\sum_j \sum_{m=-j}^{+j} \sum_{k=1}^{g(j)} |k,j,m\rangle\langle k,j,m| = \mathbb{1}$$

$(2j+1)$ $\mathcal{H}(j,m)$ spaces each of dimension $g(j)$

$$\left\{\begin{array}{lll}
\mathcal{H}(j,j) & = & |1,j,j\rangle,\ |2,j,j\rangle,\ \ldots,\ |g(j),j,j\rangle \\
\mathcal{H}(j,j-1) & = & |1,j,j-1\rangle,\ |2,j,j-1\rangle,\ \ldots,\ |g(j),j,j-1\rangle \\
\vdots & & \vdots \\
\mathcal{H}(j,m) & = & |1,j,m\rangle,\ |2,j,m\rangle,\ \ldots,\ |g(j),j,m\rangle \\
\vdots & & \\
\mathcal{H}(j,-j) & = & |1,j,-j\rangle,\ |2,j,-j\rangle,\ \ldots,\ |g(j),j,-j\rangle
\end{array}\right.$$

$$\underbrace{\begin{array}{ccccc} \parallel & & \parallel & & \\ \mathcal{H}(1,j) & & \mathcal{H}(2,j) & \ldots & \mathcal{H}(g(j),j) \end{array}}_{g(j)\ \mathcal{H}(k,j)\ \text{spaces each of dimension } (2j+1)}$$

So we have 2 equivalent points of view

$$\mathcal{H} = \bigoplus_j \bigoplus_{m=-j}^{+j} \mathcal{H}(j,m)$$

$$= \bigoplus_j \bigoplus_{k=1}^{g(j)} \mathcal{H}(k,j)$$

$\mathcal{H}(k,j)$ is more convenient a labelling since

$$\vec{J} : \mathcal{H}(k,j) \longrightarrow \mathcal{H}(k,j)$$

due to

$$J_z |k,j,m\rangle = m\hbar |k,j,m\rangle$$

$$J_\pm |k,j,m\rangle = \hbar\sqrt{j(j+1)-m(m\pm 1)}\, |k,j,m\pm 1\rangle$$

So the matrix elements of $\vec{J}$ are block diagonal if we use the $\mathcal{H}(k,j)$ subspaces.

$$\langle\,|\vec{J}|\,\rangle = \begin{array}{c|ccc} & \mathcal{H}(k,j) & \mathcal{H}(k',j) & \mathcal{H}(k',j') \\ \hline \mathcal{H}(k,j) & \boxed{\begin{matrix} 2j+1 \\ \times 2j+1 \end{matrix}} & & 0 \\ \mathcal{H}(k',j) & & \boxed{\begin{matrix} 2j+1 \\ \times 2j+1 \end{matrix}} & \\ \mathcal{H}(k',j') & 0 & & \boxed{\begin{matrix} 2j'+1 \\ \times 2j'+1 \end{matrix}} \ \ldots \end{array}$$

Thus we found the ∡ momentum operator's matrix elements in the Standard Basis $\mathcal{H}(k,j)$. That is

$$\langle k,j,m|J_z|k',j',m'\rangle = m\hbar\,\delta_{kk'}\delta_{jj'}\delta_{mm'}$$

$$\langle k,j,m|J_\pm|k',j',m'\rangle = \hbar\sqrt{j(j+1)-m'(m'\pm1)}\;\delta_{m(m'\pm1)} \times \delta_{kk'}\delta_{jj'}.$$

Recall $J_\pm \equiv J_x \pm iJ_y \Rightarrow J_x = \frac{1}{2}(J_+ + J_-)$

and $J_y = -\frac{i}{2}(J_+ - J_-)$

$$\langle k,j,m|\vec{J}|k,j,m'\rangle \equiv \left(\vec{J}^{(j)}\right)_{mm'}$$

1) $j=0$; $\mathcal{H}(k,j=0)$ has dimension $2j+1=1$

since $j=0$, $m=0 \Rightarrow \boxed{\vec{J}^{(0)}=0}$

2) $j=\frac{1}{2}$: $\mathcal{H}(k,j=\frac{1}{2})$ has dimension $2j+1=2$ with $m=\pm\frac{1}{2} \Rightarrow$

$$\vec{J}^{(\frac{1}{2})} = \frac{\hbar}{2}\vec{\sigma}\quad;\quad \vec{\sigma} = \text{Pauli Matrices}$$

3) $j=1$: $\mathcal{H}(k, j=1)$ has dimension $2j+1=3$ with $m=+1, 0, -1$.

$$J_x^{(1)} = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \; ; \; J_y^{(1)} = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}$$

$$J_z^{(1)} = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

etc.

Spin $\vec{J} = \vec{L} + \vec{S}$; $\vec{L} \equiv \vec{R} \times \vec{P}$

$$\Rightarrow [S_i, S_j] = i\hbar\epsilon_{ijk} S_k$$

So we can introduce a standard spin basis

$$\vec{S}^2 |s, m_s\rangle = s(s+1)\hbar^2 |s, m_s\rangle$$
$$S_z |s, m_s\rangle = m_s\hbar \, |s, m_s\rangle$$

with $s = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$, $m_s = -s, \ldots, +s$.

and $S_\pm = S_x \pm i S_y$ with

$$S_\pm |s, m_s\rangle = \hbar\sqrt{s(s+1) - m_s(m_s \pm 1)} \, |s, m_s \pm 1\rangle$$
$$S_z |s, m_s\rangle = \hbar m_s |s, m_s\rangle$$

Thus in the $\{A, \vec{S}^2, S_z\}$ spin basis $\{|k, s, m_s\rangle\}$

we have

$$\langle k, s, m_s | \vec{S} | k, s, m_s' \rangle = \left(\vec{S}^{(s)}\right)_{m_s m_s'}$$

with $\left(\vec{S}^{(s)}\right)_{m_s m_s'} = \left(\vec{J}^{(s)}\right)_{m_s m_s'}$.

In particular for $s = \frac{1}{2}$ $\vec{S}^{(\frac{1}{2})} = \frac{\hbar}{2}\vec{\sigma}$ and we have 2 spin states a spin up $m_s = +\frac{1}{2}$ and a spin down $m_s = -\frac{1}{2}$. So using $\{\vec{R}, \vec{S}^2, S_z\}$ as a CSCO we have basis vectors $\{|\vec{r}, s, m_s\rangle\}$ for the Hilbert space. Since $\vec{R}$ commutes with $\vec{S}$ we have

$$|\vec{r}, s, m_s\rangle = |\vec{r}\rangle \otimes |s, m_s\rangle.$$

Any state of a <u>spin-s</u> system has the expansion

$$|\psi\rangle = \int d^3r \sum_{m_s=-s}^{+s} \psi^{(s)}_{m_s}(\vec{r})\, |\vec{r}, s, m_s\rangle$$

with the <u>multi-component wavefunction</u>

$$\psi^{(s)}_{m_s}(\vec{r}) = \langle \vec{r}, s, m_s | \psi \rangle.$$

Since $\vec{J} = \vec{L} + \vec{S}$ $\Rightarrow$

$$\langle \vec{r}, s, m_s | \vec{J} | \psi \rangle = \langle \vec{r}, s, m_s | \vec{L} | \psi \rangle + \langle \vec{r}, s, m_s | \vec{S} | \psi \rangle$$

$$= \left(\vec{r} \times \frac{\hbar}{i} \vec{\nabla}_{\vec{r}}\right) \langle \vec{r}, s, m_s | \psi \rangle + \sum_{m_s' = -s}^{+s} \left(\vec{S}^{(s)}\right)_{m_s m_s'} \langle \vec{r}, s, m_s' | \psi \rangle$$

$$= \left[\left(\vec{r} \times \frac{\hbar}{i} \vec{\nabla}_{\vec{r}}\right) \delta_{m m_s'} + \left(\vec{S}^{(s)}\right)_{m_s m_s'}\right] \psi^{(s)}_{m_s'}(\vec{r})$$

But $|\psi'\rangle = e^{-\frac{i}{\hbar}\vec{\theta}\cdot\vec{J}} |\psi\rangle$ so

$$\psi'^{(s)}_{m_s}(\vec{r}) = \langle \vec{r}, s, m_s | \psi' \rangle$$

$$= \langle \vec{r}, s, m_s | \mathbb{1} - \frac{i}{\hbar} \vec{\omega} \cdot \vec{J} | \psi \rangle$$

$$= \psi^{(s)}_{m_s}(\vec{r}) - \frac{i}{\hbar} \vec{\omega} \cdot \langle \vec{r}, s, m_s | \vec{J} | \psi \rangle$$

$$= \psi^{(s)}_{m_s}(\vec{r}) - \frac{i}{\hbar} \vec{\omega} \cdot \left[\left(\vec{r} \times \frac{\hbar}{i} \vec{\nabla}_{\vec{r}}\right) \delta_{m_s m_s'} + \left(\vec{S}^{(s)}\right)_{m_s m_s'}\right] \psi^{(s)}_{m_s'}(\vec{r})$$

Summing up the infinitesimal rotations to make ~~a~~ finite one, we find

$$\psi'^{(s)}_{m_s}(\vec{r}) = D^{(s)}_{m_s m_s'}(R(\vec{\theta}))\,\psi^{(s)}_{m_s'}(R^{-1}(\vec{\theta})\vec{r}),$$

with

$$D^{(s)}_{m_s m_s'}(R(\vec{\theta})) = \left(e^{-\frac{i}{\hbar}\vec{\theta}\cdot\vec{S}^{(s)}}\right)_{m_s m_s'} .$$

<u>Example</u>: $s=0$ subspace; i.e. spinless particles $\vec{J} = \vec{L}$ on this space. Since $\vec{L} = \vec{R}\times\vec{P}$ we have

$$\langle\vec{r}|\vec{L} = (\vec{r}\times\frac{\hbar}{i}\vec{\nabla}_{\vec{r}})\langle\vec{r}| \quad \text{which}$$

in spherical polar coordinates yields the usual angular differential operator representation of $\vec{L}$ as given on page -72- of the notes.
