Quantum Mechanics Notes

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1 Formalism

PHYS 6572 - Lectures 1-5; Sakurai ch.1

Kets represent a physical state - atom for example. They are represented by a vector in Hilbert space - a vector space with vectors and complex numbers. One example of such space is the space of square integrable functions, L_2. Such space is equipped with/closed under vector addition: $a\left|\alpha\right\rangle + b\left|\beta\right\rangle = \left|\gamma\right\rangle \in V$. This operation is:

1. Linear: $(a+b)\left|\alpha\right\rangle = a\left|\alpha\right\rangle + b\left|\alpha\right\rangle$; $a(\left|\alpha\right\rangle + \left|\beta\right\rangle) = a\left|\alpha\right\rangle + a\left|\beta\right\rangle$
2. Commutative: $\left|\alpha\right\rangle + \left|\beta\right\rangle = \left|\beta\right\rangle + \left|\alpha\right\rangle$
3. Associative: $(\left|\alpha\right\rangle + \left|\beta\right\rangle) + \left|\gamma\right\rangle = \left|\alpha\right\rangle + (\left|\beta\right\rangle + \left|\gamma\right\rangle)$.

Furthermore, the null vector ($\exists\left|0\right\rangle$ such that $\left|\alpha\right\rangle + \left|0\right\rangle = \left|\alpha\right\rangle$) and the inverse vector ($\left|\alpha\right\rangle + \left|-\alpha\right\rangle = \left|0\right\rangle$) exist.

Observables represent a physical quantity - spin of an atom, for example, are represented by an operator. Given an observable, there exists eigenstates that satisfy, for an operator,

$$A\left|\alpha'\right\rangle = \alpha'\left|\alpha'\right\rangle, \quad A\left|\alpha''\right\rangle = \alpha''\left|\alpha''\right\rangle,$$

where $\left|\alpha^n\right\rangle \in H$ are eigenkets and $\alpha^n \in \mathbb{C}$ are eigenvalues.

Generally, for an ordinary ket $\left|\alpha\right\rangle$ and observable A, we have completeness relation: $\left|\alpha\right\rangle = \sum_{\alpha'} c_{\alpha'}\left|\alpha'\right\rangle$.

Bras are the dual vector space to kets; there's a correspondance between bra and ket spaces. For example,

$$\begin{aligned}\left|\alpha\right\rangle, \left|\alpha'\right\rangle, \left|\alpha''\right\rangle, \cdots &\longleftrightarrow \left\langle\alpha\right|, \left\langle\alpha'\right|, \left\langle\alpha''\right|, \cdots \\ \left|\alpha\right\rangle + \left|\beta\right\rangle &\longleftrightarrow \left\langle\alpha\right| + \left\langle\beta\right| \\ c\left|\alpha\right\rangle &\longleftrightarrow c^*\left\langle\alpha\right|.\end{aligned}$$

An operator called the **inner product** exists in H; it's given $\langle\beta|\alpha\rangle = (\left\langle\beta\right|)\cdot(\left|\alpha\right\rangle)$.

There are two postulates regarding the inner product;

1. $\langle\beta|\alpha\rangle = \langle\alpha|\beta\rangle^*$
2. $\langle\alpha|\alpha\rangle \geq 0$.

Furthermore, $\left|\alpha\right\rangle$ and $\left|\beta\right\rangle$ are orthogonal if $\langle\alpha|\beta\rangle = 0 \implies \langle\beta|\alpha\rangle = 0$. For a nonzero ket, we can also normalize it; $\left|\tilde{\alpha}\right\rangle = \left(\frac{1}{\sqrt{\langle\alpha|\alpha\rangle}}\right)\left|\alpha\right\rangle$.

Operators are observables that work on kets. Addition operators are generally commutative, associative, and linear. Furthermore, we have

$$X\left|\alpha\right\rangle \longleftrightarrow \left\langle\alpha\right|X^\dagger,$$

where $X^\dagger$ is the Hermitian adjoint; X is Hermitian if $X = X^\dagger$.

Multiplication operators are, in gneral,

1. Noncommutative; $XY \neq YX$
2. Associative; $X(YZ) = (XY)Z = XYZ$; $(XY)^\dagger = Y^\dagger X^\dagger$.

The "associative axioms of multiplication" are

1. $\left|\beta\right\rangle\left\langle\alpha\right| \cdot \left|\gamma\right\rangle = \left|\beta\right\rangle \cdot \langle\alpha|\gamma\rangle$.
2. $\left|\alpha\right\rangle \longleftrightarrow \left\langle\alpha\right|$ and $X\left|\alpha\right\rangle \longleftrightarrow \left\langle\alpha\right|X^\dagger$.
   Then, $X = \left|\beta\right\rangle\left\langle\alpha\right| \implies X^\dagger = \left|\alpha\right\rangle\left\langle\beta\right|$ because $\beta\langle\alpha|\alpha\rangle = X\left|\alpha\right\rangle \longleftrightarrow \left\langle\alpha\right|X^\dagger = \langle\alpha|\alpha\rangle\left|\beta\right\rangle$.
3. $\left\langle\beta\right|\cdot X\left|\alpha\right\rangle = \left\langle\beta\right|X\cdot\left|\alpha\right\rangle = \left\langle\beta\right|X\left|\alpha\right\rangle$.
   Further, $\left\langle\beta\right|X\left|\alpha\right\rangle = \left\langle\beta\right|\cdot X\left|\alpha\right\rangle = \left(\left\langle\alpha\right|X^\dagger\cdot\left|\beta\right\rangle\right)^* = \left\langle\alpha\right|X^\dagger\left|\beta\right\rangle^*$.
   Hence, X is Hermitian iff $\left\langle\beta\right|X\left|\alpha\right\rangle = \left\langle\alpha\right|X\left|\beta\right\rangle^*$.

Proposition 1.1. Hermitian A has real, orthogonal eigenvalues.

For eigenkets α', α'', we have $A\left|\alpha'\right\rangle = \alpha'\left|\alpha'\right\rangle$ and $\left\langle\alpha''\right|A = a''^*\left\langle\alpha''\right|$. If we multiply by $\left\langle\alpha''\right|$ and $\left|\alpha'\right\rangle$ respectively, we get $\left\langle\alpha''\right|A\left|\alpha'\right\rangle = \alpha'\langle\alpha''|\alpha'\rangle$ and $\left\langle\alpha''\right|A\left|\alpha'\right\rangle = \alpha''^*\langle\alpha''|\alpha'\rangle$. Subtracting these gives

$$(\alpha' - \alpha''^*)\langle\alpha''|\alpha'\rangle = 0.$$

If $\alpha' = \alpha''$, then $\alpha' = \alpha'^*$ (realness). For $\alpha' \neq \alpha''$, we have $\langle\alpha''|\alpha'\rangle = 0$ (orthogonality).

For a complete set of eigenkets, we can use **vector expansion**; $\left|\alpha\right\rangle = \sum_{\alpha'}\left|\alpha'\right\rangle\langle\alpha'|\alpha\rangle$, which is analogous to the familiar form $\mathbf{v} = \sum\hat{e}_i(\hat{e}_i\cdot\mathbf{v})$. This also gives the **completeness relation**:

$$\sum_{\alpha'}\left|\alpha'\right\rangle\left\langle\alpha'\right| = 1.$$

We examine $\langle\alpha|\alpha\rangle$:

$$\langle\alpha|\alpha\rangle = \left\langle\alpha\right|\cdot\left(\sum_{\alpha'}\left|\alpha'\right\rangle\left\langle\alpha'\right|\right)\cdot\left|\alpha\right\rangle = \sum_{\alpha'}\left|\langle\alpha'|\alpha\rangle\right|^2.$$

We say $\left|\alpha\right\rangle$ is **normalized** if $\langle\alpha|\alpha\rangle = \sum_{\alpha'}\left|\langle\alpha'|\alpha\rangle\right|^2 = 1$.

It is often convenient to use **matrix representation** in quantum mechanics. To motivate, for an operator, we have, from completeness relations, $X = \sum_{a'}\sum_{a''}\left|a''\right\rangle\left\langle a''\right|X\left|a'\right\rangle\left\langle a'\right|$. From this expression, we define

$$X_{ij} = \left\langle a^i\right|X\left|a^j\right\rangle \implies X = \begin{pmatrix}\left\langle a^1\right|X\left|a^1\right\rangle & \left\langle a^1\right|X\left|a^2\right\rangle & \\ \left\langle a^2\right|X\left|a^1\right\rangle & \left\langle a^2\right|X\left|a^2\right\rangle & \\ & & \ddots\end{pmatrix}.$$

With this, we can represent matrix multiplication; for $Z = XY$,

$$Z_{ij} = \langle a''| Z |a'\rangle = \langle a''| XY |a'\rangle = \sum_{a'''} \langle a''| X |a'''\rangle \langle a'''| Y |a'\rangle = X_{ik}Y_{kj}.$$

In ket notation, if we let $|\gamma\rangle = X|a\rangle$ and $\langle a'|\gamma\rangle = \langle a'| X |a\rangle = \sum_{a''} \langle a'| X |a''\rangle \langle a''|a\rangle$, which is similar to multiplying a square matrix by a column vector. Hence, we have

$$|\alpha\rangle = \begin{pmatrix} \langle a^1|a\rangle \\ \langle a^2|a\rangle \\ \vdots \end{pmatrix}, \quad |\gamma\rangle = \begin{pmatrix} \langle a^1|\gamma\rangle \\ \langle a^2|\gamma\rangle \\ \vdots \end{pmatrix}.$$

Furthermore, for a bra relation, $\langle\gamma| = \langle a| X$, we have $\langle\gamma|a'\rangle = \sum_{a''} \langle a|a''\rangle \langle a''| X |a'\rangle$, which is similar to multiplying a row vector by a square matrix, giving us

$$\langle a| = \begin{pmatrix} \langle a^1|a\rangle^* & \langle a^2|a\rangle^* & \ldots \end{pmatrix}, \quad \langle\gamma| = \begin{pmatrix} \langle a^1|\gamma\rangle^* & \langle a^2|\gamma\rangle^* & \ldots \end{pmatrix}.$$

It is easy to see that

$$\langle\beta|\beta\rangle\, \alpha = \sum_{a'} \langle\beta|a'\rangle \langle a'|a'\rangle\, \alpha = \begin{pmatrix} \langle a^1|\beta\rangle^* & \langle a^2|\beta\rangle & \cdots \end{pmatrix} \begin{pmatrix} \langle a^1|\alpha\rangle \\ \langle a^2|\alpha\rangle \\ \vdots \end{pmatrix}.$$

Finally,

$$|\beta\rangle \langle\alpha| = \begin{pmatrix} \langle a^1|\beta\rangle \langle a^1|\alpha\rangle^* & \langle a^1|\beta\rangle \langle a^2|\alpha\rangle^* & \ldots \\ \langle a^2|\beta\rangle \langle a^1|\alpha\rangle^* & \langle a^2|\beta\rangle \langle a^2|\alpha\rangle^* & \ldots \\ \vdots & \vdots & \ddots \end{pmatrix}.$$

We define the **projection/measurement operator** as $\Lambda_{a'} = |a'\rangle \langle a'|$. Using the projection operator, we can write an operator A in terms of its eigenkets;

$$A = \sum_{a''} \sum_{a'} |a''\rangle \langle a''| A |a'\rangle \langle a'| = \sum_{a'} a' |a'\rangle \langle a'| = \sum_{a'} a' \Lambda_{a'}.$$

When a **measurement** is made, $|a\rangle$ collapses to $|a'\rangle$ - Copenhagen interpretation. Furthermore, the probability for measuring a' is $|\langle a'|a\rangle|^2$.

For an observable, the **expectation value** is defined

$$\langle A\rangle = \langle\alpha| A |\alpha\rangle = \sum_{a'} \sum_{a''} \langle\alpha|a''\rangle \langle a''| A |a'\rangle \langle a'|\alpha\rangle = \sum_{a'} a' \langle a'|\alpha\rangle^* \langle a'|\alpha\rangle = \sum_{a'} a' |\langle a'|\alpha\rangle|^2,$$

which can be interpreted as the average measured value.

For the **commutator** defined $[A, B] = AB - BA$, for compatible observables, we have $[A, B] = 0$, and for incompatible observables, we have $[A, B] \neq 0$. An observable is **degenerate** if it has the same eigenvalue for multiple eigenstates.

Theorem 1.1. Compatible $\implies$ nondegenerate $\implies$ diagonal matrices

For compatible observables, $[A, B] = 0 \implies \langle a''| AB - BA |a'\rangle = (a'' - a') \langle a''| B |a'\rangle = 0$. Unless $a'' = a'$, $\langle a''| B |a'\rangle = 0$, which implies diagonal B. Furthermore, since B is diagonal, $\langle a''| B |a'\rangle = \delta_{a'a''} \langle a'| B |a''\rangle$. Using identity relations,

$$B = \sum_{a'} \sum_{a''} |a''\rangle \langle a''| B |a'\rangle \langle a'| = \sum_{a''} |a''\rangle \langle a''| B |a''\rangle \langle a''|$$
$$\implies B |a'\rangle = \sum_{a''} |a''\rangle \langle a''| B |a''\rangle \langle a''|a'\rangle = (\langle a'| B |a'\rangle) |a'\rangle.$$

Therefore, $|a\rangle'$ is an eigenstate of B with eigenvalue $b' = \langle a'| B |a'\rangle$.

To prove the uncertainty relation, we first introduce three lemmas: **Schwartz Inequality**: $\langle\alpha|\alpha\rangle \langle\beta|\beta\rangle \geq |\langle\alpha|\beta\rangle|^2$. To prove this, consider the equality

$$(\langle\alpha| + \lambda^* \langle\beta|) \cdot (|\alpha\rangle + \lambda |\beta\rangle) = ||\alpha\rangle + \lambda |\beta\rangle|^2 \geq 0,$$

where $\lambda \in \mathbb{C}$. If we let $\lambda = -\frac{\langle\beta|\alpha\rangle}{\langle\beta|\beta\rangle}$,

$$\langle\alpha|\alpha\rangle + \lambda \langle\alpha|\beta\rangle + \lambda^* \langle\beta|\alpha\rangle + \lambda^*\lambda \langle\beta|\beta\rangle = \langle\alpha|\alpha\rangle - \frac{2|\langle\alpha|\beta\rangle|^2}{\langle\beta|\beta\rangle} + \frac{|\langle\alpha|\beta\rangle|^2}{\langle\beta|\beta\rangle} \geq 0 \implies \langle\alpha|\alpha\rangle \langle\beta|\beta\rangle - |\langle\alpha|\beta\rangle|^2 \geq 0.$$

Lemma 2. Hermitian operators have real expectation values. To see this,

$$\langle H\rangle = \langle a| H |a\rangle = \langle a| H^\dagger |a\rangle^* = \langle a| H |a\rangle^* \implies \langle H\rangle \in \mathbb{R}.$$

Lemma 3. Anti-Hermitian operators have imaginary expectation values. To see this, $\langle H\rangle = -\langle H\rangle^* \implies \langle H\rangle \in \mathbb{C}$.

Uncertainty relation We claim that $\langle\Delta a\rangle \langle\Delta b\rangle \geq \frac{1}{2}|\langle[A, B]\rangle|$. To prove this, let $|\alpha\rangle = \Delta A |\psi\rangle$ and $|\beta\rangle = \Delta B |\psi\rangle$. From Schwartz inequality,

$$\langle\alpha|\alpha\rangle \langle\beta|\beta\rangle \geq |\langle\alpha|\beta\rangle|^2 \implies \langle\psi| \Delta A^\dagger \Delta A |\psi\rangle \langle\psi| \Delta B^\dagger \Delta B |\psi\rangle \geq \left|\langle\psi| \Delta A^\dagger \Delta B |\psi\rangle\right|^2.$$

Furthermore, we claim $\Delta A \Delta B = \frac{1}{2}[\Delta A, \Delta B] + \frac{1}{2}\{\Delta A, \Delta B\}$. Also,

$$[\Delta A, \Delta B] = [A - \langle A\rangle, B - \langle B\rangle] = [A, B] - [\langle A\rangle, B] - [A, \langle B\rangle] + [\langle A\rangle, \langle B\rangle] \implies [\Delta A, \Delta B] = [A, B],$$

since $\langle A\rangle$ and $\langle B\rangle$ commute. Lastl,y

$$[A, B]^\dagger = (AB - BA)^\dagger = BA - AB = -[A, B]$$
$$\{A, B\}^\dagger = (AB + BA)^\dagger = BA + AB = \{A, B\}.$$

The commutators are anti-hermitian and hence imaginary, and anticommutators are hermitian and hence real. Lastly,

$$\langle\Delta A\rangle^2\langle\Delta B\rangle^2 \geq |\langle\Delta A\Delta B\rangle|^2 = \frac{1}{4}|\langle[A,B]\rangle|^2 + \frac{1}{4}|\langle\{A,B\}\rangle|^2 \geq \frac{1}{4}|\langle[A,B]\rangle|^2.$$

Change of basis. Given a two sets of orthonormal and complete basis (for some space), there exists U such that $|b^1\rangle = U|a^1\rangle, |b^2\rangle = U|a^2\rangle, \cdots, |b^n\rangle = U|a^n\rangle$ with U unitary. We explicitly construct:

$$U = \sum_k |b^k\rangle\langle a^k|.$$

Indeed, $U|a^l\rangle = \sum_k |b^k\rangle\langle a^k|a^l\rangle = |b^l\rangle$. Furthermore, From definition, $\langle a^k|b^l\rangle = \langle a^k|U|a^l\rangle$, and hence $U's$ elements are, for a change in basis in $\mathbb{R}^3$, $U \sim \begin{pmatrix}\hat{x}\cdot\hat{x}' & \hat{x}\cdot\hat{y}' & \hat{x}\cdot\hat{z}' \\ \hat{y}\cdot\hat{x}' & \hat{y}\cdot\hat{y}' & \hat{y}\cdot\hat{z}' \\ \hat{z}\cdot\hat{x}' & \hat{z}\cdot\hat{y}' & \hat{z}\cdot\hat{z}'\end{pmatrix}$.

Likewise, we can do a change in bra basis. $\langle b^k|\alpha\rangle = \sum_l \langle b^k|a^l\rangle\langle a^l|\alpha\rangle = \sum_l \langle a^k|U^\dagger|a^l\rangle\langle a^l|\alpha\rangle$, meaning $\langle b^k| = \langle a^k|U^\dagger|a^l\rangle\cdot\langle a^l|$.

We define the **translator** to be a operator defined as $I(\mathrm{d}x')|x'\rangle = |x'+\mathrm{d}x'\rangle$. Turns out, we have $I(\mathrm{d}x') = 1 - i\mathbf{k}\cdot\mathrm{d}\mathbf{x}'$, with $\mathbf{k}$ hermitian. We can see that four properties are satisfied:

1. Unity; $I^\dagger(\mathrm{d}x')I(\mathrm{d}x') = 1$
2. Composition; $I(\mathrm{d}x'')I(\mathrm{d}x') = I(\mathrm{d}x' + \mathrm{d}x'')$
3. Inverse; $I(-\mathrm{d}x') = I^{-1}(\mathrm{d}x')$
4. Continuity; $\lim_{\mathrm{d}x'\to 0} I(\mathrm{d}x') = 1$.

With this definition, we get two commutation relations: $[x, I(\mathrm{d}x')] = \mathrm{d}x'$, $\left[\hat{x}_i, \hat{k}_j\right] = i\delta_{ij}$. With the generating function $F(\mathbf{xP}) = \mathbf{x}\cdot\mathbf{P} + \mathbf{p}\cdot\mathrm{d}\mathbf{x} \implies \mathbf{X} = \mathbf{x} + \mathrm{d}\mathbf{x}, \quad \mathbf{P} = \mathbf{p}$. We claim that this is the translator; if we match up the units, $I(\mathrm{d}\mathbf{x}') = 1 - \frac{i\mathbf{p}\cdot\mathrm{d}\mathbf{x}'}{\hbar}$. For a finite translation, we have $I(\Delta x' e_x) = \lim_{N\to\infty}\left(1 - \frac{ip_x\Delta x'}{N\hbar}\right)^N = \exp\left(-\frac{ip_x\Delta x'}{\hbar}\right)$. Furthermore, we can derive the **commutation relations**:

$$[x_i, x_j] = 0, \quad [p_i, p_j] = 0, \quad [x_i, p_j] = i\hbar\delta_{ij}.$$

We define the **wavefunction** in position basis as $\psi_\alpha(x') = \langle x'|\alpha\rangle$. Evidently,

$$\langle\beta|\alpha\rangle = \int \mathrm{d}x'\langle\beta|x'\rangle\langle x'|\alpha\rangle = \int \mathrm{d}x'\psi^*_\beta(x')\psi_\alpha(x')$$

$$\langle\beta|A|\alpha\rangle = \int \mathrm{d}x'\int \mathrm{d}x''\psi^*_\beta(x')\langle x'|A|x''\rangle\psi_\alpha(x'').$$

Furthermore, we can represent the momentum operator:

$$\begin{aligned}\left(1 - \frac{ip\Delta x'}{\hbar}\right)|\alpha\rangle &= \int \mathrm{d}x' I(\Delta x')|x'\rangle\langle x'|x'\rangle\,\alpha = \int ddx'|x'\rangle\langle x' - \Delta x'|\alpha\rangle \\ &= \int \mathrm{d}x'|x'\rangle\langle x'|\alpha\rangle - \int \mathrm{d}x'|x'\rangle\left(\Delta x'\frac{\partial}{\partial x'}\right)\langle x'|\alpha\rangle \\ \implies p &= \int \mathrm{d}x'|x'\rangle\left(-i\hbar\frac{\partial}{\partial x'}\langle x'|\right).\end{aligned}$$

Likewise, we define the wavefunction in the momentum basis as $\phi_\alpha(p) = \langle p'|\alpha\rangle$.

From $\langle x'|p|p'\rangle = -i\hbar\frac{\partial}{\partial x'}\langle x'|p'\rangle = p'\langle x'|p'\rangle$, we obtian $\langle x'|p'\rangle = \frac{1}{\sqrt{2\pi\hbar}}\exp\left(\frac{ip'x'}{\hbar}\right)$. Hence,

$$\psi_\alpha(x') = \frac{1}{\sqrt{2\pi\hbar}}\int \mathrm{d}p'\exp\left(\frac{ip'x'}{\hbar}\right)\phi_\alpha(p'), \quad \phi_\alpha(p') = \frac{1}{\sqrt{2\pi\hbar}}\int \mathrm{d}x'\exp\left(\frac{-ip'x'}{\hbar}\right)\psi_\alpha(x').$$

2 Dynamics

Lectures 5-6, Sakurai ch.2.1-2.4 A **time-evolution** operator, satisfying similar conditions as the translator, has the form

$$U(t_0 + \mathrm{d}t, t_0) = 1 - \frac{iH\mathrm{d}t}{\hbar} = \exp\left(\frac{-iH(t-t_0)}{\hbar}\right).$$

From this, we find the Schrodinger equation:

$$i\hbar\frac{\partial}{\partial t}U(t,t_0) = HU(t,t_0) \implies i\hbar\frac{\partial}{\partial t}|\alpha, t_0 : t\rangle = H|\alpha, t_0 : t\rangle,$$

where $|\alpha, t_0 : t\rangle = U(t,t_0)|\alpha, t_0\rangle$.

For **energy eigenkets** defined $H|a'\rangle = E_{a'}|a'\rangle$, we have

$$\exp\left(\frac{-iHt}{\hbar}\right) = \sum_{a'}|a'\rangle\exp\left(\frac{-iE_{a'}t}{\hbar}\right)\langle a'|.$$

As an example, when this acts on an initial state $|\alpha, t_0\rangle$, we get the expansion coefficients change with time as $c_{a'}(t) = c_{a'}(t = 0)\exp\left(\frac{-iE_{a'}t}{\hbar}\right)$. Furthermore, if the initial state happens to be an energy eigenstate itself, it is a constant of the motion.

Consider an observable B. If it were to be measured with respect to an energy eigenket, $|a'\rangle$, we have $|a', t_0 = 0; t\rangle = U(t,0)|a'\rangle$ for the state ket; $\langle B\rangle$ is given by $\langle B\rangle = \langle a'|U^\dagger(t,0)BU(t,0)|a'\rangle = \langle a'|\exp\left(\frac{iE_{a'}t}{\hbar}\right)B\exp\left(\frac{-iE_{a'}t}{\hbar}\right)|a'\rangle = \langle a'|B|a'\rangle$, independent of t. This is referred as a **stationary state**. If we take the superposition of energy eigenstates, we get a **nonstationary state**: for $|\alpha, t_0 = 0\rangle = \sum_{a'} c_{a'}|a'\rangle$, we have

$$|B\rangle = \sum_{a'}\sum_{a''}c^*_{a'}c_{a''}\langle a'|B|a''\rangle\exp\left(\frac{-i(E_{a''} - E_{a'})t}{\hbar}\right).$$

2.1 Harmonic Oscillator

Let $V(x) = \frac{1}{2}m\omega^2 x^2$ and $\hat{H} = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$. In the position basis, we have

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) + \frac{1}{2}m\omega^2 x^2\psi(x) = E\psi(x).$$

We define the creation and annihilation operator to be

$$a^\dagger = \frac{1}{\sqrt{2m\hbar\omega}}(m\omega x - ip), \quad a = \frac{1}{\sqrt{2m\hbar\omega}}(m\omega x + ip).$$

From this, we can write the Hamiltonian operator:

$$H = \left(a^\dagger a + \frac{1}{2}\right)\hbar\omega.$$

The commutation relations state

$$\left[a, a^\dagger\right] = \mathbb{1}, \quad [H, a] = -\hbar\omega a, \quad \left[H, a^\dagger\right] = \hbar\omega a^\dagger.$$

Using the commutation relations, we have that for $\{|n\rangle\}$ eigenstates of H, $a\,|n\rangle$ is also an eigenstate with $\hbar\omega$ less energy. Likewise, $a^\dagger\,|n\rangle$ is an eigenstate with $\hbar\omega$ more energy.

For physical reasons, we claim that there's a ground state where $a\,|\psi_0\rangle = |0\rangle$. The energy is given as $H\,|\psi_0\rangle = \frac{\hbar\omega}{2}\,|\psi_0\rangle$.

Since the eigenstates are normalized, we can easily found the proportionality constant of the ladder operators from their definition:

$$a\,|n\rangle = \sqrt{n}\,|n-1\rangle, \quad a^\dagger\,|n\rangle = \sqrt{n+1}\,|n-1\rangle.$$

Furthermore, we can find the ground state wavefunction from the definition of the ground state, $a\,|\psi_0\rangle = |0\rangle$; we have

$$\frac{1}{\sqrt{2m\hbar\omega}}(m\omega x + \hbar\partial_x)\psi_0(x) = 0 \implies \psi_0(x) = \frac{1}{(\pi x_0^2)^{1/4}}e^{-\frac{x^2}{2x_0^2}}, \quad x_0 = \sqrt{\frac{\hbar}{m\omega}}.$$

Furthermore, from the recursion relation, we get

$$|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}}\,|\psi_0\rangle \implies \psi_n(x) = \frac{(m\omega x - \hbar\partial_x)^n}{(2m\hbar\omega)^{n/2}\sqrt{n!}}\psi_0(x).$$

2.2 Hydrogen Atom

Let the Hamiltonian be $H = -\frac{\hbar^2}{2m}\nabla^2 + V(r)$. The differential equation becomes

$$-\frac{\hbar^2}{2mr^2}\left[\partial_r(r^2\partial_r\psi_n) + \nabla^2_{\theta\psi}\psi_n\right] + V(r)\psi_n = E_n.$$

If we let $\psi_n(x) = R(r)Y(\theta,\phi)$, we get two differential equations:

$$\frac{1}{R}\partial_r(r^2\partial_r R) - \frac{2mr^2}{\hbar^2}(V(r) - E_n) = l(l+1)$$
$$\frac{1}{Y}\nabla^2_{\theta\phi}Y = -l(l+1).$$

If we let $Y = f(\theta)g(\phi)$, we get two differential equations:

$$\frac{1}{f}\sin\theta\partial_\theta(\sin\theta\partial_\theta f) + l(l+1)\sin^2\theta = m^2$$
$$\frac{1}{g}\partial_\phi^2 g = -m^2.$$

From periodicity $(g(\phi) = g(\phi + 2\pi))$, we get $m = 0, \pm1, \pm2, \pm3, \cdots$. and solution $g(\phi) = e^{\pm im\phi}$. Furthermore, for f, the solutions are the associated legendre function;

$$P_{lm}(x) = (1-x^2)^{m/2}\left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^{|m|}P_l(x); \quad P_l(x) = \frac{1}{2^l l!}\left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^l (x^2-1)^l.$$

There's two conditions;

1. $l \in \mathbb{N}$; since the Legendre polynomial has the lth derivative
2. $|m| \leq 1$, since otherwise, P_{lm} has more derivatives than polynomials.

Therefore,

$$Y_{lm}(\theta,\phi) = AP_{lm}(\cos\theta)e^{im\phi},$$

known as the spherical harmonics. They are orthonormal.

2.3 Angular Momentum

Turns out, $Y_{lm}(\theta,\phi)$ are eigenstates of $\mathbf{L} = \mathbf{x} \times \mathbf{p}$. As far as the angular momentum operators are concerned, we have two facts:

1. L_i and L_j, for $i \neq j$ are incompatible; $[L_i, L_j] = i\hbar\epsilon_{ijk}L_k$. In other words, we can't determine all components of $\mathbf{L}$.

   This is due to the fact that angular momenta are generators of rotations, which don't commute.

2. L^2 and L_i are compatible; $\left[L^2, L_i\right] = 0$.

From fact 2, we can find simultaneous eigenstates for L_z and L^2. We define

$$L_z |\lambda, \mu\rangle = \mu |\lambda, \mu\rangle, \quad L^2 |\lambda, \mu\rangle = \lambda |\lambda, \mu\rangle.$$

Furthermore, we define the ladder operators: $L_\pm = L_x \pm iL_y$. By definition,

$$L^2 = L_\pm L_\mp + L_z^2 \mp \hbar L_z,$$

which correspond to raising/lowering L_z by $\hbar$. The commutation relations for these ladder operators are:

$$\left[L^2, L_\pm\right] = 0, \quad [L_z, L_\pm] = \pm\hbar L_\pm.$$

To find the upper and lower bounds, we let $L_z |\lambda, l\rangle = l\hbar |\lambda, l\rangle$, $L_z |\lambda, l'\rangle = l'\hbar |\lambda, l'\rangle$, and $L^2 |\lambda, l\rangle = \lambda |\lambda, l\rangle$. Then, the upper and lower bounds, defined as $L_+ |\lambda l\rangle = L_- |\lambda l'\rangle\, 0$, gives $\lambda = l(l+1)\hbar^2 = l'(l'-1)\hbar^2$, and from the ordering of bounds, we have $l' = -l$, giving us $\lambda = l(l+1)\hbar^2$.

Now, we label $|\lambda, \mu\rangle$ as $|l, m\rangle$. We see that $(L_+)^N |l, -l\rangle = (-l+N)\hbar |lm\rangle$, meaning l has to be half-integers and $m \in [-l, l] \bigcap \mathbb{Z}$. Now,

$$L^2 |lm\rangle = l(l+1)\hbar^2 |lm\rangle, \quad L_z |lm\rangle = m\hbar |lm\rangle.$$

If we go back to the hydrogen atom, we can express:

$$L_z = \frac{\hbar}{i}\partial_\phi, \quad L^2 = -\hbar^2 \nabla^2_{\theta\phi}.$$

Therefore,

$$\langle x|lm\rangle = Y_{lm}(\theta, \phi).$$

3 Berry's Phase, Aharnov-Bohm Effect (Lecture 23)

Gauge Invariance We work in the Lorenz gauge:

$$\mathbf{E} = -\nabla\phi - \frac{\partial \mathbf{A}}{\partial t}, \quad \mathbf{B} = \nabla \times \mathbf{A}.$$

Recall that we can make a gauge transformation

$$\phi \to \phi - \frac{\partial \Lambda}{\partial t}, \quad \mathbf{A} \to \mathbf{A} + \nabla\Lambda.$$

Recall that the Hamiltonian of a charged particle in $\mathbf{E}$ and $\mathbf{B}$ is

$$H = \frac{1}{2m}(\mathbf{p} - q\mathbf{A})^2 + q\phi,$$

Note that $\mathbf{p}$, the canonical momentum is not gauge invariant; instead, we use $\mathbf{p} - q\mathbf{A}$ as our **kinematic momentum** (Sakurai 2.7)

Gauge invariance in QM We make the following transformations to promote the canonical momenta to the kinematic momenta:

$$\mathbf{p} \to \mathbf{p} - q\mathbf{A}, \quad \frac{\hbar}{i}\nabla \to \left(\frac{\hbar}{i}\nabla - q\mathbf{A}\right).$$

We claim that the Schrodinger's equation is gauge invariant if

$$|\psi\rangle \to e^{iq\Lambda/\hbar} |\psi\rangle, q \quad \phi \to \phi - \frac{\partial \Lambda}{\partial t}, \quad \mathbf{A} \to \mathbf{A} + \nabla\Lambda.$$

Aharnov-Bohm Effect Consider two paths around an infinitely long solenoid. Consider two gauges:

(a) $\mathbf{A} = 0$, with $|\psi\rangle_{\mathbf{A}=0}$.

(b) $\mathbf{A} = \nabla\Lambda \implies \Lambda = \int_{\mathbf{r}_0}^{\mathbf{r}} \mathrm{d}\mathbf{r}' \cdot \mathbf{A}$.

Since wavefunctions in different gauges are related by a phase factor given above, we can write

$$|\psi\rangle_{\mathbf{A}} = \exp\left[\frac{iq}{\hbar}\int_{r_0}^{r} \mathrm{d}\mathbf{r}' \cdot \mathbf{A}(\mathbf{r}')\right] |\psi\rangle_{\mathbf{A}=0}.$$

Hence, if we were to split the original beam and evolve, then recombine, the norm becomes

$$\langle\psi|\psi\rangle = \langle\psi_0|\psi_0\rangle \cos^2\left(\frac{q\Phi}{2\hbar}\right).$$