Personal Notes on

Quantum Mechanics

Jeffrey Ming Han Li

jeffreyli2288@Outlook.com

Abstract

This note incorporates information from both Griffith's Introduction to Quantum Mechanics and Sakurai's Modern Quantum Mechanics.

Contents

1 Fundamentals

1.1 Rules of Operators

- **Ket Space:**
  The dimensionality of the vector space is determined by the number of alternatives in the physical experiment we discuss here. Let say a system of N-dimensional vector space spanned by the N eigenkets of observable A. Any arbitrary ket $|\alpha\rangle$(a physical state) can be written as
  $$|\alpha\rangle = \sum_{a'} c_{a'} |a'\rangle$$
  with $a', a''...$ up to $a^{(N)}$ and $c_{a'}$ is a complex coefficient.

- **Bra Space:**
  It is a **dual correspondence** space to the ket space, which is also spanned by eigenbras $\{\langle a'|\}$. For instance the bra dual to c$|\alpha\rangle$ is $c^* \langle\alpha|$

- **Inner Product:** The inner product between a bra and a ket states is denoted by
  $$\langle\beta \,|\, \alpha\rangle = \langle\alpha \,|\, \beta\rangle^*$$
  and
  $$\langle\alpha \,|\, \alpha\rangle \geq 0$$
  Two kets are said to be orthogonal if
  $$\langle\alpha \,|\, \beta\rangle = 0$$

- **Operators:** The operators applying on ket and bra are commutative and associative. When it acts on bra is acts from the right side. The dual of an operated state to another is that
  $$X \,|\alpha\rangle \overset{\text{DC}}{\leftrightarrow} \langle\alpha|\, X^\dagger.$$
  Some rules about Operators are that

  1. **Multiplication:**
     $$X(YZ) = (XY)Z = XYZ$$
  2. $$X(Y \,|\alpha\rangle) = (XY)\,|\alpha\rangle = XY \,|\alpha\rangle\,, \quad (\langle\beta|\, X)Y = \langle\beta|\,(XY) = \langle\beta|\, XY.$$
  3. $$(XY)^\dagger = Y^\dagger X^\dagger$$
     also
     $$XY \,|\alpha\rangle = X(Y \,|\alpha\rangle) \overset{\text{DC}}{\leftrightarrow} ((\langle\alpha|\, Y^\dagger)X^\dagger = \langle\alpha|\, Y^\dagger X^\dagger$$
  4. **Associative Axiom:**
     $$(|\beta\rangle\,\langle\alpha|) \cdot |\gamma\rangle = |\beta\rangle \cdot (\langle\alpha \,|\, \gamma\rangle)$$
     $$\underbrace{(\langle\beta|)}_{\text{bra}} \cdot \underbrace{(X \,|\alpha\rangle)}_{\text{ket}} = \underbrace{(\langle\beta|\, X)}_{\text{bra}} \cdot \underbrace{(|\alpha\rangle)}_{\text{ket}}$$
     Note that
     $$\begin{aligned}\langle\beta|\mathbf{X}|\alpha\rangle &= \langle\beta| \cdot (\mathbf{X}|\alpha\rangle) \\ &= \left\{\left(\langle\alpha|\mathbf{X}^\dagger\cdot\right)|\beta\rangle\right\}^* \\ &= \left(\langle\alpha|\mathbf{X}^\dagger|\beta\rangle\right)^* = \langle\beta|\mathbf{X}|\alpha\rangle\end{aligned}$$

1.1.1 EigenKets of Observables

There is a theorem to remember that

> **Theorem**: *The eigenvalues of a Hermitian Operator A are real; the eigenkets of A corresponding to different eigenvalues are orthogonal*

the result is that $\{|a'\rangle\}$ forms an orthonormal set:

$$\langle a'' \,|\, a' \rangle = \delta_{a''a'}$$

also be cause of this property any state in this ket space can be expressed by

$$|\alpha\rangle = \sum_{a'} |a'\rangle \langle a' \,|\, \alpha\rangle$$

which is analogous to an expansion of a vector $\mathbf{V}$ in real Euclidean Space

$$\mathbf{V} = \sum_i \hat{e}_i (\hat{e}_i \cdot \mathbf{V})$$

and we also have the **Completeness Relation or Closure** that

$$\sum_{a'} |a'\rangle \langle a'| = I = \sum_{a'} \Lambda_{a'} = 1$$

1.1.2 Matrix Representation of Operators

Given an operator X we can use the compleness properties twice to obtain the form

$$X = \sum_{a''} \sum_{a'} |a''\rangle \langle a''| \, X \, |a'\rangle \langle a'|$$

and in the a',a" basis, we may write X as a matrix

$$X = \begin{pmatrix} \langle a^{(1)}|X|a^{(1)}\rangle & \langle a^{(1)}|X|a^{(2)}\rangle & \cdots \\ \langle a^{(2)}|X|a^{(1)}\rangle & \langle a^{(2)}|X|a^{(2)}\rangle & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}$$

also here are few expressions to know

- When there are two operators we can express it as such

$$\begin{aligned} \langle a''| \, Z \, |a'\rangle &= \langle a''| \, XY \, |a'\rangle \\ &= \sum_{a'''} \langle a''| \, X \, |a'''\rangle \langle a'''| \, Y \, |a'\rangle \end{aligned}$$

- for a operator we might use its eigenkets to be the basis, we can expresss A as

$$\begin{aligned} A &= \sum_{a''} \sum_{a'} |a''\rangle \langle a''| \, A \, |a'\rangle \langle a'| \\ &= \sum_{a'} a' \, |a'\rangle \langle a'| = \sum_{a'} a' \Lambda_{a'} \end{aligned}$$

1.1.3 Spin 1/2 System

recall that in the spin 1/2 system the two basis are $|+\rangle, |-\rangle$, according to the equation above, we can write the Operator S_z as

$$S_z = (\hbar/2)[(|+\rangle \langle +|) - |-\rangle \langle -|]$$

also two other operators are $S_+ = \hbar \, |+\rangle \langle -|$ and $S_- = \hbar \, |-\rangle \langle +|$ where we can understand as a transformation between the $|-\rangle$ to $|+\rangle$ state and vice versa. by using the standard convention

$$|+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

we have the

$$S_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad S_+ = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad S_- = \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}.$$

1.1.4 Measurements, Observables, Uncertainties

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

Here is a definition to remember

- **Pure Ensemble:** When you have a collection of identically prepared physical systems all characterized by the same ket $|\alpha\rangle$.
- **Expectation Value:** of A taken with respect to state $|\alpha\rangle$ is

$$\langle A|A\rangle = \langle\alpha| A |\alpha\rangle$$

1.1.5 Compatible Observables

Observables A and B are considered **compatible** when the operators commute $[A, B] = 0$ and vice versa for **incompatible** scenario. Regarding the relationship of the eigenket space spanned by A and B, there is an important theory to remember

- *Suppose that A and B are compatible observables and the eigenvalues of A are non degenerate, Then the matrix elemtns* $\langle a''| B |a'\rangle$ *are all diagonal*

by some transformation

$$B|a'\rangle = \sum_{a''} |a''\rangle \langle a''| B |a''\rangle \langle a''|a'\rangle = (\langle a'| B |a'\rangle)|a'\rangle \tag{1}$$

but there is nothing other than the eigen value equation for the operator B with eigen value

$$b' = \langle a'| B |a'\rangle$$

and the ket $|a'\rangle$ is called a **simultaneous eigenket** of A and B. We use $|a', b'\rangle$ to describe this eigenket. This notation is powerful when there are degeneracies. Let say in the case of molecule orbit First using the orbital number l and m, we can uniquely characterize the orbital angular momentum state, and a **collective Index** K' is used to stand for (a',b') so that

$$|K'\rangle = |a', b'\rangle$$

lets assume several mutually compatible observables exist, and assume we found a maximal set of commuting observables when there is degeneracy presents, lets say the measurement A yields a'. The system is thrown into some linear combination

$$\sum_i^n c_{a'}^{(i)} \left|a', b^{(i)}\right\rangle$$

where n is the degree of degeneracy and the kets $\left|a', b^i\right\rangle$, the second B measurement may select of the terms in the linear combination.

1.1.6 Uncertainty

The uncertainty relation is the generalization of the well-known x-p uncertainty

$$\langle(\Delta A)^2\rangle\langle(\Delta B)^2\rangle \geq \frac{1}{4}|\langle[A, B]\rangle|^2 \tag{2}$$

1.1.7 Change of Basis

- There is a unitary operator that given two sets of base kets, both satisfying orthonormality and completeness.

$$|b^{(1)}\rangle = U|a^{(1)}\rangle,\ |b^{(2)}\rangle = U|a^{(2)}\rangle,\ \ldots,\ |b^{(N)}\rangle = U|a^{(N)}\rangle.$$

- The transformation matrix for this operator is interesting, this matrix is made up of $\left\langle a^{(k)}\right| U \left|a^{(l)}\right\rangle$ is the transformation matrix from the a' basis to the b' basis. By simple proof, we can show that the basis transformation goes by

$$\boxed{(new) = (U^\dagger)(old)}$$

  where the new column matrix $|\alpha\rangle$ can be obtained this way.

- The old matrix element and the new matrix element for an Operator X is described by the **similarity transformation**

$$\boxed{X' = U^\dagger X U}$$

- The **trace** of an operator X is defined as the sum of the diagonal elements

$$tr(X) = \sum_{a'} \langle a'| X |a'\rangle = \sum_{b'} \langle b'| X |b'\rangle$$

  indicating the trace of the operator is basis independent. here are also some operations that worth memorization

  1. $tr(XY) = tr(YX)$
  2. $tr(U^\dagger X U) = tr(X)$
  3. $tr(|a'\rangle \langle a''|) = \delta_{a'a''}$
  4. $tr(|b'\rangle \langle a'|) = \langle a'|b'\rangle$

1.1.8 Diagonalization

The eigenvalue problem to solve for b' can be expressed as such

$$\begin{pmatrix} B_{11} & B_{12} & B_{13} & \cdots \\ B_{21} & B_{22} & B_{23} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} C_1^{(l)} \\ C_2^{(l)} \\ \vdots \end{pmatrix} = b^{(l)} \begin{pmatrix} C_1^{(l)} \\ C_2^{(l)} \\ \vdots \end{pmatrix},$$

with

$$B_{ij} = \langle a^{(i)}|B|a^{(j)}\rangle,$$

and

$$C_k^{(l)} = \langle a^{(k)}|b^{(l)}\rangle,$$

One last concept to remember is the **Unitary Equivalent Observables** where it is defined by a theorem

> **Theorem**: *Consider two sets of orthonormal basis a' and b' connected by the U operator. Knowing U, we may construct a unitary transform of A UAU^{-1} are said to be unitary equivalent observables. The eigenvalue equation for A*
>
> $$A\left|a^{(l)}\right\rangle = a^{(l)}\left|a^{(l)}\right\rangle$$
>
> implies that
>
> $$(UAU^{-1})\left|b^{l}\right\rangle = a^{(l)}\left|b^{(l)}\right\rangle$$

This theorem tells us that the $\left|b^{(l)}\right\rangle$ are eigenkets of UAU^{-1} with exactly the same eigenvalues as the A eigenvalues.

1.1.9 Continuous Spectra

Now this section will quickly go through the observables.

- **Position Eigenkets and Position Measurements:** When performing a measurement to $|\alpha\rangle$, the state will fall into a narrow range of $(x' - \Delta/2, x' + \Delta/2)$, and the state collapse as

$$|\alpha\rangle = \int_{-\infty}^{\infty} dx'' \, |x''\rangle\langle x''|\alpha\rangle \xrightarrow{\text{measurement}} \int_{x'-\Delta/2}^{x'+\Delta/2} dx'' \, |x''\rangle\langle x''|\alpha\rangle.$$

The normalization also reads that

$$\langle\alpha\,|\,\alpha\rangle = 1 \rightarrow \int_{-\infty}^{\infty} dx'\langle\alpha\,|\,x'\rangle\langle x'\,|\,\alpha\rangle = 1$$

and in three dimension, we can find a simultaneous eigenket simply by replacing the $|x'\rangle \rightarrow |\mathbf{x}'\rangle = |x', y', z'\rangle$ and here are a few rules to remember from the discrete spectrum:

$$\langle a'|a''\rangle = \delta_{a'a''} \rightarrow \langle\xi'|\xi''\rangle = \delta(\xi' - \xi''),$$

$$\sum_{a'} |a'\rangle\langle a'| = 1 \quad \rightarrow \quad \int d\xi'\,|\xi'\rangle\langle\xi'| = 1,$$

$$|\alpha\rangle = \sum_{a'} |a'\rangle\langle a'|\alpha\rangle \quad \rightarrow \quad |\alpha\rangle = \int d\xi'\,|\xi'\rangle\langle\xi'|\alpha\rangle,$$

$$\sum_{a'} |\langle a'|\alpha\rangle|^2 = 1 \quad \rightarrow \quad \int d\xi'\,|\langle\xi'|\alpha\rangle|^2 = 1,$$

$$\langle\beta|\alpha\rangle = \sum_{a'}\langle\beta|a'\rangle\langle a'|\alpha\rangle \quad \rightarrow \quad \langle\beta|\alpha\rangle = \int d\xi'\,\langle\beta|\xi'\rangle\langle\xi'|\alpha\rangle,$$

$$\langle a''|A|a'\rangle = a'\delta_{a''a'} \quad \rightarrow \quad \langle\xi''|A|\xi'\rangle = \xi'\delta(\xi'' - \xi').$$

- **Translation:** A translation is simple, suppose the state is well localized around $\mathbf{x}'$, then there is an operation that transforms it into $\mathbf{x}' + d\mathbf{x}'$. This is called an **Infinitesimal Translation** by $d\mathbf{x}'$

$$\mathscr{J}\,(d\mathbf{x}')\,|\mathbf{x}'\rangle = |\mathbf{x}' + d\mathbf{x}'\rangle,$$

generalizing it to a $|\alpha\rangle$ state, we can write

$$|\alpha\rangle \rightarrow \mathscr{J}\,(d\mathbf{x}')\,|\alpha\rangle = \mathscr{J}\,(d\mathbf{x}')\int d^3x'\,|\mathbf{x}'\rangle\langle\mathbf{x}'|\alpha\rangle = \int d^3x'\,|\mathbf{x}' + d\mathbf{x}'\rangle\langle\mathbf{x}'|\alpha\rangle = \int d^3x'\,|\mathbf{x}'\rangle\langle\mathbf{x} - \mathbf{dx}''|\alpha\rangle$$

we also demand the translation operator to be unitary such that

$$\langle\alpha|\alpha\rangle = \langle\alpha|\,\mathscr{J}^{\dagger}(d\mathbf{x}')\,\mathscr{J}\,(d\mathbf{x}')|\alpha\rangle.$$

also a few properties to note are

- $\mathscr{J}\,(d\mathbf{x}')\mathscr{J}\,(d\mathbf{x}'') = \mathscr{J}\,(d\mathbf{x}' + d\mathbf{x}'')$
- $\mathscr{J}\,(-d\mathbf{x}') = \mathscr{J}^{-1}(d\mathbf{x}')$
- $\lim\limits_{d\mathbf{x}'\rightarrow 0} \mathscr{J}\,(d\mathbf{x}') = 1$
- $\mathscr{J}\,(d\mathbf{x}') = 1 - i\mathbf{K}\cdot d\mathbf{x}'$

which we can see that the difference between the operator and the identity be of first order in $d\mathbf{x}'$. where the components $\mathbf{K}, K_x, K_y, K_z$ are **Hermitian Operators**, this form satisfies all the properties above. But next the relationship of $\mathbf{K}$ and x worth investigation. First, by writing each part out, we can find the commutator of the expression

$$[\mathbf{x},\,\mathscr{J}\,(d\mathbf{x}')]\,|\mathbf{x}'\rangle = d\mathbf{x}'\,|\mathbf{x}' + d\mathbf{x}'\rangle \simeq d\mathbf{x}'\,|\mathbf{x}'\rangle,$$

The simplification is because of the second order of $d\mathbf{x}'$. Therefore

$$[\mathbf{x},\,\mathscr{J}\,(d\mathbf{x}')] = d\mathbf{x}'$$

or

$$-i\mathbf{x}\mathbf{K}\cdot d\mathbf{x}' + i\mathbf{K}\cdot d\mathbf{x}'\,\mathbf{x} = d\mathbf{x}',$$

and note that $d\mathbf{x}'$ on the RHS is the number multiplied by the identity operator (it is a matrix).

- **Momentum** The momentum is the generator of an infinitesimal translation, where the generating function is defined as

$$F(\mathbf{x}, \mathbf{P}) = \mathbf{x} \cdot \mathbf{P} + \mathbf{p} \cdot d\mathbf{x}$$

by which we can infer the relationship that $\mathbf{K} = p/constant$ and that constant actually makes K the quantum-mechanical operator that corresponds to the wave number. Therefore

$$\mathscr{J}(d\mathbf{x}') = 1 - i\mathbf{p} \cdot d\mathbf{x}'/\hbar,$$

indicating $K = i\mathbf{p}/\hbar$ and recall the commutation relation

$$[x_i, p_i] = i\hbar\delta_{ij}$$

Now what about a **finite Translation**, which can be obtained by compounding infinitesimal translations, consider that

$$\mathscr{J}(\Delta x'\,\hat{\mathbf{x}})\,|\mathbf{x}'\rangle = |\mathbf{x}' + \Delta x'\,\hat{\mathbf{x}}\rangle.$$

Consider N infinitesimal translations, which each is characterized by a spatial displacement $\Delta x'/N$ and letting $N \to \infty$ we obtain

$$\mathscr{J}(\Delta x'\,\hat{\mathbf{x}}) = \lim_{N\to\infty}\left(1 - \frac{ip_x\Delta x'}{N\hbar}\right)^N = \exp\left(-\frac{ip_x\Delta x'}{\hbar}\right).$$

Yet it is notable that rotation along different axes do not commute, but for translation it doesn't matter

$$\left[\mathscr{J}(\Delta y'\,\hat{\mathbf{y}}),\ \mathscr{J}(\Delta x'\,\hat{\mathbf{x}})\right] = \left[\left(1 - \frac{ip_y\Delta y'}{\hbar} - \frac{p_y^2(\Delta y')^2}{2\hbar^2} + \cdots\right), \left(1 - \frac{ip_x\Delta x'}{\hbar} - \frac{p_x^2(\Delta x')^2}{2\hbar^2} + \cdots\right)\right] \simeq -\frac{(\Delta x')(\Delta y')}{\hbar^2}[p_y$$

because the shift in x and y are arbitrary, we require that the two terms to be compatible, which leads to

$$[p_x, p_y] = 0$$

which is a property of the **Abelian** group.

- **Matrix Mechanics** Matrix Mechanics originates from Heisenberg's multiplication rules(Page 45 of Sakurai). Recall that classical Poisson brackets are defined as

$$[A(q,p),\ B(q,p)]_{\text{classical}} \equiv \sum_s \left(\frac{\partial A}{\partial q_s}\frac{\partial B}{\partial p_s} - \frac{\partial A}{\partial p_s}\frac{\partial B}{\partial q_s}\right)$$

It is a measurement of how much two variables influence each other, for instance when A has an infinitesimal change and how much would B changes, it is a value of 0 or 1. When it is 0 it means two variables are involutional(A = B) and vice versa.

an important thing to note is that we can obtain the quantum-mechanical relations by replacing classical Poisson brackets by commutators. For instance

$$[x_i, p_i]_{classical} = \delta_{ij} \to [x_i, p_i]_{quantum} = i\hbar\delta_{ij}$$

so called the **Dirac Rule**.

  - $[A, A] = 0$
  - $[A, B] = -[B, A]$
  - $[A, c] = 0$ (c is just a number)
  - $[A + B, C] = [A, C] + [B, C]$
  - $[A, BC] = [A, B]\,C + B\,[A, C]$
  - $[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0$ **Jacobi Identity**

1.2 Wave Functions

This section is now time for wave functions in both position and momentum space, which will be very quick. The notation in Sakurai is different from that of classical way we learn from Griffith, the wave function for state $|\alpha\rangle$ is defined as

$$\langle x' \,|\, \alpha\rangle = \psi_\alpha(x')$$

which unifies both the expansion factor and the classical wave function we talk about using the Dirac formalism. For instance consider the inner product of two states

$$\langle\beta|\alpha\rangle = \int dx' \,\langle\beta|x'\rangle\langle x'|\alpha\rangle = \int dx' \,\psi^*_\beta(x')\,\psi_\alpha(x'),$$

it is simple to make the correlation that we are just specifying the wave function to one of the eigenket, which makes no difference to the expansion coefficient. Now lets have another example with a generalized state

$$|\alpha\rangle = \sum_{a'} |a'\rangle \,\langle a' \,|\, \alpha\rangle$$

by multiply both sides by the position eigenbra we have

$$\langle x' \,|\, \alpha\rangle = \psi_\alpha(x') = \sum_{a'} c_{a'} u_{a'}(x')$$

where we introduced an eigen function of operator A with eigenvalue a'

$$u_{a'}(x') = \langle x' \,|\, a'\rangle$$

There are a few more examples on Page 48 of Sakurai 3rd Edition. What this essentially mean is that the notation of wave function tells us the square root of the probability at position x' given the system is at state $|\alpha\rangle$. Also that

$$\langle\beta|f(x)|\alpha\rangle = \int dx' \,\psi^*_\beta(x')f(x')\psi_\alpha(x').$$

and note that f(x) on the left is an operator.

- **Momentum:** by applying translation operator on a state we can obtain that

$$p|\alpha\rangle = \int dx' \,|x'\rangle \left(-i\hbar\frac{\partial}{\partial x'}\langle x'|\alpha\rangle\right),$$

$$\langle x'|p|\alpha\rangle = -i\hbar\frac{\partial}{\partial x'}\langle x'|\alpha\rangle,$$

  This gives the form for the momentum operator in position baiss by applying the orthonormal property

$$\langle x'|\, p\,|x''\rangle = -i\hbar\frac{\partial}{\partial x'}\delta(x' - x'')$$

  or we can also obtain the expected value form for it

$$\begin{aligned}\langle\beta|p|\alpha\rangle &= \int dx' \,\langle\beta|x'\rangle \left(-i\hbar\frac{\partial}{\partial x'}\langle x'|\alpha\rangle\right) \\ &= \int dx' \,\psi^*_\beta(x') \left(-i\hbar\frac{\partial}{\partial x'}\right)\psi_\alpha(x').\end{aligned}$$

  What about it in the p-basis, which is in the momentum representation, with all the properties same as the x-basis, the equation $\langle p' \,|\, \alpha\rangle$ is called the **momentum-space wave function**, and it is described by

$$\langle p' \,|\, \alpha\rangle = \phi_\alpha(p')$$

  Yet there is a matrix that can transform from x to p basis, which is simple to obtained by the matrix which we used to obtain the expression for p

$$p'\langle x'|p'\rangle = -i\hbar\frac{\partial}{\partial x'}\langle x'|p'\rangle.$$

which can be solved to be

$$\langle x'|p'\rangle = N \exp\left(\frac{ip'x'}{\hbar}\right),$$

where N is the normalization constant, which can be determined to be $1/\sqrt{2\pi\hbar}$, using this normalization factor, we can determine that

$$\psi_\alpha(x') = \left[\frac{1}{\sqrt{2\pi\hbar}}\right] \int dp' \, \exp\left(\frac{ip'x'}{\hbar}\right) \, \phi_\alpha(p'),$$

and

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

- **Gaussian Wave Packets:** the x-space wave function is given by

$$\langle x'|\alpha\rangle = \left[\frac{1}{\pi^{1/4}\sqrt{d}}\right] \exp\left[ikx' - \frac{x'^2}{2d^2}\right].$$

- **Generalization to Three dimensions** the generalization is the same and detailed derivation can be seen from page 53-54 of Sakurai
- **Correlation Amplitude:** It is the inner product that tells the extent to which the state ket at a later time t is similar to the state ket at t = 0.

$$C(t) = \langle \alpha \,|\, \alpha, t_0 = 0; t\rangle = \langle \alpha| \, \mathscr{U}(t,0) \, |\alpha\rangle$$

lets say the states are generalized to superposition of states, the correlation amplitude is then

$$C(t) = \left(\sum_{a'} c^*_{a'} \langle a'|\right) \left[\sum_{a''} c_{a''} \exp\left(-\frac{iE_{a''}t}{\hbar}\right) |a''\rangle\right]$$

$$= \sum_{a'} |c_{a'}|^2 \exp\left(-\frac{iE_{a'}t}{\hbar}\right).$$

which, lets assume a density of energy eigenstates $\rho(E)$ and a term representing the expansion coefficient $g(E)$ we then have

$$C(t) = \int dE \, |g(E)|^2 \, \rho(E) \, \exp\left(-\frac{iEt}{\hbar}\right),$$

where

$$\int dE \, |g(E)|^2 \, \rho(E) = 1.$$

the realistic condition is that $|g(E)|^2\rho(E)$ may be peaked around $E = E_0$ with width ΔE, so the equation might as well be written as

$$C(t) = \exp\left(-\frac{iE_0t}{\hbar}\right) \int dE \, |g(E)|^2 \, \rho(E) \, \exp\left[-\frac{i(E-E_0)t}{\hbar}\right],$$

one physical insight is that the oscillation term is determined by the exponent, if the interval for which $|E-E_0| \approxeq \hbar/t$ is much narrower than ΔE, then there is no contribution to C(t) because of the rapid oscillation and strong cancellations. This tells that the characteristic time at which the correlation amplitude starts becoming different from 1 is given by

$$t \approxeq \frac{\hbar}{\Delta E}$$

2 Quantum Dynamics

2.1 Time-Evolution Operator

The ket corresponding to the state at some later time is

$$|\alpha, t_0; t\rangle \quad (t > t_0)$$

which is describing a system that is at $|\alpha\rangle$ at t_0. The **time-evolution operator** is denoted as

$$|\alpha, t_0; t\rangle = \mathscr{U}(t, t_0)|\alpha, t_0\rangle.$$

which tells a time displacement $t_0 \to t$

- For a state is initially normalized to unity, it must remain normalized to unity at all later times.
- $$\mathscr{U}^\dagger(t, t_0)\mathscr{U}(t, t_0) = 1$$
- Compositttion Property:
$$\mathscr{U}(t_2, t_0) = \mathscr{U}(t_2, t_1)\mathscr{U}(t_1, t_0) \quad (t_2 > t_1 > t_0)$$
- Infinitsimal time Evolution:
$$\lim_{dt\to 0} \mathscr{U}(t_0 + dt, t_0) = 1$$
- Time evolution Expression:
$$\mathscr{U}(t_0 + dt, t_0) = 1 - i\Omega dt$$
where Ω is a Hermitian Operator.

The idea from classical mechancis is that *Hamiltonian is the generator of time evolution*, such that we can relate Ω to the Hamiltonian operator H

$$\Omega = \frac{H}{\hbar}$$

such that

$$\mathscr{U}(t_0 + dt, t_0) = 1 - i\Omega dt = 1 - \frac{iH dt}{\hbar}$$

2.2 Schrodinger Equation

Using the time evolution, we are able to deduce the Schrodinger Equation.

$$\mathscr{U}(t + dt, t_0) = \mathscr{U}(t + dt, t)\,\mathscr{U}(t, t_0) = \left(1 - \frac{iH\,dt}{\hbar}\right)\mathscr{U}(t, t_0),$$

where the time difference $t - t_0$ need not be infinitesimal. We have

$$\mathscr{U}(t + dt, t_0) - \mathscr{U}(t, t_0) = -i\left(\frac{H}{\hbar}\right) dt\,\mathscr{U}(t, t_0)$$

which can be written in differential equation form:

$$\boxed{i\hbar\frac{\partial}{\partial t}\mathscr{U}(t, t_0) = H\,\mathscr{U}(t, t_0)}$$

which is the **Schrodinger Equation for the time-evolution operator**, under different dependencies of H, there will be a different solution to the time-evolution operator

1. **H is Time Independent:**
$$\mathscr{U}(t, t_0) = \exp\left[\frac{-iH(t - t_0)}{\hbar}\right]$$

2. **H is time Dependent:**
$$\mathscr{U}(t,t_0) = \exp\Big[-(\frac{i}{\hbar})\int_{t_0}^{t} dt' H(t')\Big]$$
an example with this can be that the spin-magnetic moment subjected to a magnetic field with varying strength but directions remained unchanged.

3. **H is time Dependent, not time commutable:** Lets say the magnetic field direction is also changing with time. The solution must be described by the **Dyson Series** which is shown as
$$\mathscr{U}(t,t_0) = 1 + \sum_{n=1}^{\infty}\left(\frac{-i}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n\, H(t_1)H(t_2)\cdots H(t_n).$$
(Add prove here later)!!!!!

2.2.1 Energy Eigenkets

The definition for Energy eigenkets is simple
$$H\,|a'\rangle = E_{a'}\,|a'\rangle$$
and by expanding the time evolution operator, we can find the following relation
$$\exp\left(-\frac{iHt}{\hbar}\right) = \sum_{a'}\sum_{a''}|a''\rangle\langle a''|\exp\left(-\frac{iHt}{\hbar}\right)|a'\rangle\langle a'|$$
$$= \sum_{a'}|a'\rangle\exp\left(-\frac{iE_{a'}t}{\hbar}\right)\langle a'|.$$
with all the followed calculation assuming case 1(H is time independent). By showing the state under time evolution, we can also find the rate of change of the expansion coefficient corresponds to
$$c_{a'}(t=0) \to c_{a'}(t) = c_{a'}(t=0)\exp\left(\frac{-iE_{a'}t}{\hbar}\right)$$
However, in the case that there are multiple observables that commute with H, the time evolution operator becomes
$$\exp\left(-\frac{iHt}{\hbar}\right) = \sum_{K'}|K'\rangle\exp\left(-\frac{iE_{K'}t}{\hbar}\right)\langle K'|$$
where K' is the collective index notation, uniquely specified once $a', b', c'....$ Therefore, it is important to find a complete set of mutually compatible observables.

2.2.2 Time Evolution of Expectation Values

- A observable B that doesn't commute with A or H.
- The expectation of such an observable is
$$\langle B\rangle = \langle a'|\mathscr{U}^{\dagger}(t,0)\cdot B\cdot\mathscr{U}(t,0)|a'\rangle$$
$$= \langle a'|\exp\left(\frac{iE_{a'}t}{\hbar}\right)B\exp\left(-\frac{iE_{a'}t}{\hbar}\right)|a'\rangle$$
$$= \langle a'|B|a'\rangle,$$
which is independent of time, so *an energy eigenstate is often referred to as a* ***stationary state***. Suppose the initial state is not a single basis state but a superposition of basis, then we have
$$\langle B\rangle = \left[\sum_{a'} c^*_{a'}\langle a'|\exp\left(\frac{iE_{a'}t}{\hbar}\right)\right]\cdot B\cdot\left[\sum_{a''} c_{a''}\exp\left(-\frac{iE_{a''}t}{\hbar}\right)|a''\rangle\right]$$
$$= \sum_{a'}\sum_{a''} c^*_{a'}c_{a''}\langle a'|B|a''\rangle\exp\left(-\frac{i(E_{a''}-E_{a'})t}{\hbar}\right).$$
so now the expectation value consists of oscillating terms whose angular frequencies are determined by
$$\omega_{a''a'} = \frac{(E_{a''}-E_{a'})}{\hbar}$$
for a detailed example of the application of this, refer to page 69 of Sakurai

2.3 Heisenberg Picture

The **Schrodinger Picture** is considering the time-evolution of the state kets. Meanwhile the **Heisenberg Picture** is that the observables vary with time instead of the state kets. It can be explained in a few sentences

- Under a unitary operation to a state ket $|\alpha\rangle$, the inner product remains unchanged

$$\langle\beta\,|\,\alpha\rangle = \langle\beta|\,U^\dagger U\,|\alpha\rangle$$

- The observable will change as

$$\langle\beta|X|\alpha\rangle \;\rightarrow\; \left(\langle\beta|U^\dagger\right)\cdot X\cdot(U|\alpha\rangle) = \langle\beta|U^\dagger XU|\alpha\rangle.$$

which suggest two approaches, either $|\alpha\rangle \rightarrow U\,|\alpha\rangle$ with operators unchanged or $X \rightarrow U^\dagger XU$ with state kets unchanged. But note that for **Schrodinger Picture**, the base ket do not change while only the state ket changes. For **Heisenberg Picture**, the base eigenket is rotating by $\mathscr{U}^\dagger$ opposite to that of the Schrodinger picture state kets, while the eigenvalue remained unchanged and operator evolving. Another question is, suppose we have the state a with eigenvalue a' at time t: What is the probability amplitude known as **Transition amplitude**, for the system to be found in an eigenstate of observable B with eigenvalue b'. In **Schrodinger** picture, this amplitude is

$$\underbrace{\langle b'|}_{\text{base bra}}\cdot\underbrace{\mathscr{U}|a'\rangle}_{\text{state ket}}$$

and for the Heisenberg Picture:

$$\underbrace{(\langle b'|\mathscr{U})}_{\text{base bra}}\cdot\underbrace{|a'\rangle}_{\text{state ket}}\;.$$

For instance, the translation operator, if we implement the second approach, then the translation becomes

$$|\alpha\rangle \;\rightarrow\; |\alpha\rangle,$$

$$\begin{aligned}\mathbf{x} \;&\rightarrow\; \left(1+\frac{i\,\mathbf{p}\cdot d\mathbf{x}'}{\hbar}\right)\mathbf{x}\left(1-\frac{i\,\mathbf{p}\cdot d\mathbf{x}'}{\hbar}\right)\\ &=\; \mathbf{x}+\left(\frac{i}{\hbar}\right)[\mathbf{p}\cdot d\mathbf{x}',\,\mathbf{x}]\\ &=\; \mathbf{x}+d\mathbf{x}'.\end{aligned}$$

and for the expentation value

$$\langle\mathbf{x}\rangle \rightarrow \langle\mathbf{x}\rangle + \langle d\mathbf{x}'\rangle$$

note that we use $A^{(H)}(t)$ and $A^{(H)}$ to represent Heisenberg and Schrodinger picture observables, where

$$A^{(H)}(t_0) = A^{(S)}$$

and

$$|\alpha, t_0 = 0; t\rangle_H = |\alpha, t_0 = 0\rangle$$

which is independent of t, and so for the expectation value of an observable in both states.

2.3.1 Heisenberg Equation of Motion

We can relate the operators in Heisenberg pictures and Schrodinger Pictures by

$$A^{(H)}(t) = \mathscr{U}^\dagger(t)A^{(S)}\mathscr{U}(t) \tag{3}$$

and by differentiating this relation, we can obtain that

$$\frac{dA^{(H)}}{dt} = \frac{\partial\mathscr{U}^\dagger}{\partial t}A^{(S)}\mathscr{U} + \mathscr{U}^\dagger A^{(S)}\frac{\partial\mathscr{U}}{\partial t}$$

$$= -\frac{1}{i\hbar}\mathscr{U}^\dagger H\mathscr{U}\,\mathscr{U}^\dagger A^{(S)}\mathscr{U} + \frac{1}{i\hbar}\mathscr{U}^\dagger A^{(S)}\mathscr{U}\,\mathscr{U}^\dagger H\mathscr{U}$$

$$= \frac{1}{i\hbar}\left[A^{(H)},\, \mathscr{U}^\dagger H\mathscr{U}\right].$$

and we can write $H^{(H)} = \mathscr{U}^\dagger H\mathscr{U}$, and this leads to

$$\boxed{\frac{dA^{(H)}}{dt} = \frac{1}{i\hbar}[A^{(H)}, H]}$$

so called the **Heisenberg Equation of Motion**

2.4 Free Particle & Ehrenfest's Theorem

Starting from here, whenever an ambiguity arises because of noncommuting observables, we attempt to resolve it by requiring H to be Hermitian. For instance we write the quantum mechanical analogue of the classical product xp as $\frac{1}{2}(xp + px)$. Firstly

$$\boxed{[x_i, F(\mathbf{p})] = i\hbar\frac{\partial F}{\partial p_i}}$$

and

$$\boxed{[p_i, G(\mathbf{x})] = -i\hbar\frac{\partial G}{\partial x_i}}$$

we also define Hamiltonian as the same for mas in classical mechanics

$$\boxed{H = \frac{\mathbf{p}^2}{2m}}$$

also we have

$$\frac{dp_i}{dt} = \frac{1}{i\hbar}[p_i, H] = 0$$

because p_i commutes with any function of p_j. Thus for a free particle, the momentum operator is a constant of the motion. Also

$$\frac{dx_i}{dt} = \frac{1}{i\hbar}[x_i, H] = \frac{1}{i\hbar}\cdot\frac{1}{2m}\cdot i\hbar\,\frac{\partial}{\partial p_i}\left(\sum_{j=1}^{3} p_j^2\right)$$

$$= \frac{p_i}{m} = \frac{p_i(0)}{m},$$

which suggests that the commutator of the x_i at different times does not vanish. From which we can take the expectation values of both sides with respect to a Heisenberg state ket that does not move with time.

$$\boxed{m\frac{d^2}{dt^2}\langle\mathbf{x}\rangle = \frac{d\langle\mathbf{p}\rangle}{dt} = -\langle\nabla V(\mathbf{x})\rangle}$$

2.5 Simple Harmonic Oscillator

as in my another note *Quantum Optics*, I've included a lot of information about this section about using simple harmonic oscillator to quantize light, here I will go through some simple knowledge again but in a dot format.

- **Definitions:** The hamiltonian, non-hermitian annihilation, and creation Operators are defined as

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

  The operators follow the canonical commutation relations

$$[a, a^\dagger] = 1$$

The number operator is also

$$N = a^\dagger a = (\frac{m\omega}{2\hbar})(x^2 + \frac{p^2}{m^2\omega^2}) + (\frac{i}{2\hbar})[x,p] = \frac{H}{\hbar\omega} - \frac{1}{2}$$

where $N|n\rangle = n|n\rangle$, where n is a nonnegative integer. where it follows the relationship of

$$[N, a^\dagger] = a^\dagger$$
$$[N, a] = -a$$

from which the hamiltonian operator becomes

$$H = \hbar\omega(N + \frac{1}{2})$$

and the result of the commutation yields

$$Na^\dagger|n\rangle = \left([N, a^\dagger] + a^\dagger N\right)|n\rangle = (n+1)a^\dagger|n\rangle$$

and

$$Na|n\rangle = ([N, a] + aN)|n\rangle = (n-1)a|n\rangle$$

This tells that a$|n\rangle$ is also an eigenket but with n - 1 eigenvalue(or one unit of energy), which implies that $a|n\rangle$ and $|n-1\rangle$ are the same up to a multiplicative constant.

$$a|n\rangle = c|n-1\rangle, \quad n = |c|^2 \text{by normalization}$$

Therefore

$$\boxed{\begin{aligned} a|n\rangle &= \sqrt{n}|n-1\rangle \\ a^\dagger|n\rangle &= \sqrt{n+1}|n+1\rangle \end{aligned}}$$

and leading to our final conclusion that

$$\boxed{|n\rangle = [\frac{(a^\dagger)}{\sqrt{n!}}]|0\rangle}$$

- **Position:** The position operator is defined by

$$x = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger)$$

by solving the differential equation

$$\langle x'|a|0\rangle = \sqrt{\frac{m\omega}{2\hbar}}\langle x'|\left(x + \frac{ip}{m\omega}\right)|0\rangle = 0 = (x' + x_0^2\frac{d}{dx'})\langle x'|0\rangle$$

where $x_0 = \sqrt{\frac{\hbar}{m\omega}}$ which sets the length scale of the oscillator. The solution is

$$\langle x'|0\rangle = \left(\frac{1}{\pi^{1/4}\sqrt{x_0}}\right)\exp\left[-\frac{1}{2}\left(\frac{x'}{x_0}\right)^2\right].$$

and the generalized solution becomes

$$\boxed{\langle x'|n\rangle = \left(\frac{1}{\pi^{1/4}\sqrt{2^n n!}}\right)\left(\frac{1}{x_0^{n+1/2}}\right)\left(x' - x_0^2\frac{d}{dx'}\right)^n \exp\left[-\frac{1}{2}\left(\frac{x'}{x_0}\right)^2\right]}$$

from which we can find the expectation value using the expression

$$x^2 = \frac{\hbar}{2m\omega}(a^2 + a^{\dagger 2} + a^\dagger a + aa^\dagger) \rightarrow \langle x^2\rangle = \frac{\hbar}{2m\omega} = \frac{x_0^2}{2}$$

The probability amplitude of finding particle at any x' location

- **Momentum:**

$$p = i\sqrt{\frac{m\hbar\omega}{2}}(-a + a^\dagger)$$

The expectation value follows that

$$\langle p^2 \rangle = \frac{\hbar m\omega}{2}, \quad \langle p \rangle = \langle x \rangle = 0$$

- **Time Evolution: Sakurai P88** by taking derivative to momentum and position, we can find that

$$\frac{da}{dt} = \sqrt{\frac{m\omega}{2\hbar}}\left(\frac{p}{m} - i\omega x\right) = -i\omega a$$

and

$$\frac{da^\dagger}{dt} = i\omega a^\dagger,$$

By the **Baker-Hausdorff lemma**, we can use equation 42 to find the solution for position.

$$\begin{aligned} x(t) &= x(0)\cos(\omega t) + [\frac{p(0)}{m\omega}]\sin(\omega t) \\ &= \exp\left(\frac{iHt}{\hbar}\right)x(0)\exp\left(\frac{-iHt}{\hbar}\right) \\ &= x(0) + \left[\frac{p(0)}{m}\right]t - \left(\frac{1}{2!}\right)t^2\omega^2 x(0)` - \left(\frac{1}{3!}\right)t^3\omega^2\frac{p(0)}{m} + \cdots \\ &= x(0)\cos\omega t + \left[\frac{p(0)}{m\omega}\right]\sin\omega t \end{aligned}$$

Yet we can verify that $|\alpha\rangle = c_0|0\rangle + c_1|1\rangle$ the expectation value of x oscillate in a frequency of ω

- **Coherent State:**

1. the energy eigenstate do not behave like the classical oscillator, like a wave packet bouncing back and forth. Meanwhile, the energy of a Fork state might vanish with some probability. However, we can construct a superposition of energy state that closely imitates the classical oscillator defined by

$$a|\lambda\rangle = \lambda|\lambda\rangle = \lambda\sum_{n=0}^{\infty} f(n)|n\rangle$$

the distribution of $|f(n)|^2$ with respect to n is of the Poisson type about the mean value of $\bar{n}$

$$|f(n)|^2 = \left(\frac{\bar{n}^n}{n!}\right)\exp(-\bar{n})$$

2. It can be obtained by translating the oscillator ground state by some finite distance.
3. It satisfies the minimum uncertainty product relation at all times. The coherent state is essentially a ground state (gaussian) shifted in position and momentum.

2.6 Schrodinger's Wave Equation

2.6.1 Time-Dependent Wave Equation

Read through derivation on Sakurai P91. essentially, the result is the classical time-dependent Schrodinger Equation

$$i\hbar\frac{\partial}{\partial t}\langle \mathbf{x}'|\alpha, t_0; t\rangle = -\left(\frac{\hbar^2}{2m}\right)\nabla'^2\langle \mathbf{x}'|\alpha, t_0; t\rangle + V(\mathbf{x}')\langle \mathbf{x}'|\alpha, t_0; t\rangle,$$

2.6.2 Time-Independent Wave Equation

Recall that the time dependence of stationary state(H is independent of time) is given by

$$\langle \mathbf{x}'|a', t_0; t\rangle = \langle \mathbf{x}'|a'\rangle \exp\left(-\frac{iE_{a'}t}{\hbar}\right),$$

substituting it into the time-dependent wave equation we have

$$-\left(\frac{\hbar^2}{2m}\right)\nabla'^2\langle \mathbf{x}'|a'\rangle + V(\mathbf{x}')\langle \mathbf{x}'|a'\rangle = E_{a'}\langle \mathbf{x}'|a'\rangle.$$

Now we also need to introduce the **Probability Flux** given by

$$\begin{aligned}\mathbf{j}(\mathbf{x},t) &= -\left(\frac{i\hbar}{2m}\right)[\psi^*\nabla\psi - (\nabla\psi^*)\psi] \\ &= \left(\frac{\hbar}{m}\right)\mathrm{Im}(\psi^*\nabla\psi).\end{aligned}$$

which follows

- Continuity Equation:

$$\frac{\partial\rho}{\partial t} + \nabla\cdot\mathbf{j} = 0$$

  where ρ is the $|\psi|^2$

- Momentum:

$$\int d^3x\mathbf{j}(\mathbf{x},t) = \frac{\mathbf{p}_t}{m}$$

  where $\mathbf{p}_t$ is the expectation value of momentum operator at time t. Continue Reading page 95 Sakurai. By subbing in the ∇S form into the time-dependent wav equation we obtain

$$\frac{1}{2m}|\nabla S(\mathbf{x},t)|^2 + V(\mathbf{x}) + \frac{\partial S(\mathbf{x},t)}{\partial t} = 0. \tag{4}$$

  which is the **Hamilton-Jacobi Equation**, and it makes sense that the shcrodigner wave mechanics contain classical mechanics if we assume $\hbar \to 0$. This time the solution to this equation yields,

$$S(x,t) = W(x) - Et$$

  $W(x)$ is the **Hamilton's characteristic function**

2.7 Elementary Solutions to Schrodinger's Wave Equation

2.7.1 Free Particle in Three Dimensions

- The Schrodinger Equation at V = 0 becomes

$$\nabla^2 u_E(\mathbf{x}) = -\frac{2mE}{\hbar}u_E(\mathbf{x})$$

- By separation of variable, we found that the solution to be

$$u_E(\mathbf{x}) = Ce^{i\mathbf{k}\cdot\mathbf{x}} = \frac{1}{L^{3/2}}e^{i\mathbf{k}\cdot\mathbf{x}}$$

  by normalization, and letting the size $L \to \infty$, and impose the condition $u_x(x+L) = u_x(x)$ we have

$$\psi(\mathbf{x},t) = \frac{1}{L^{3/2}}\exp\left(\frac{i\mathbf{p}\cdot\mathbf{x}}{\hbar} - \frac{iEt}{\hbar}\right)$$

$$\text{in which case we find} \quad \mathbf{j}(\mathbf{x},t) = \frac{\hbar}{m}\mathrm{Im}(\psi^*\nabla\psi) = \frac{\hbar\mathbf{k}}{m}\cdot\frac{1}{L^3} = \mathbf{v}\rho$$

- Energy eigenvalue is

$$E = \frac{\mathbf{p}^2}{2m} = \frac{\hbar^2\mathbf{k}^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2\left(n_x^2 + n_y^2 + n_z^2\right). \tag{5}$$

- Density of state, is the number of combinations of n's having an energy between E and E + dE, so dN/dE is an important quantity, which we can imagine a spherical shell in $\mathbf{k}$ space with radius $|\mathbf{k}| = 2\pi|\mathbf{n}|/L$, the number of states dN within this shell is $4\pi\mathbf{n}^2 d|\mathbf{n}|$ Therefore,

$$\begin{aligned}\frac{dN}{dE} &= \frac{4\pi n^2 d|\mathbf{n}|}{\hbar^2|\mathbf{k}|d|\mathbf{k}|/m} = \frac{4\pi}{\hbar^2}m\left(\frac{L}{2\pi}\right)^2|\mathbf{k}|\frac{L}{2\pi} \\ &= \frac{m^{3/2}E^{1/2}L^3}{\sqrt{2}\pi^2\hbar^3}.\end{aligned}$$

2.7.2 Simple Harmonic Oscillator

- $V(x) = m\omega^2x^2/2$, $\epsilon = 2E/\hbar\omega$, $y = x/x_0$, $x_0 = \sqrt{\hbar/m\omega}$
- The differential equations become

$$\frac{d^2}{dy^2}u(y) + (\varepsilon - y^2)u(y) = 0. \tag{6}$$

and the solution is that

$$\boxed{u(y) = h(y)e^{-y^2/2}} \tag{7}$$

and by taking second derivative of the 6, we find that the $h(y)$ follows

$$\frac{d^2h}{dy^2} - 2y\frac{dh}{dy} + (\varepsilon - 1)h(y) = 0. \tag{8}$$

- This is the traditional solution of the SHO in many textbooks, and we expect to find a series solution for $h(y)$ and this series must terminate somewhere to ensure it is normalizable.
  1. One forces this termination is by imposing the condition that $\epsilon - 1$ be an even, positive integer 2n.

  we can understand the $h(y)$ **Hermite Polynomial** by taking a different approach, using the "generating function"

$$\begin{aligned}g(x,t) &\equiv e^{-t^2+2tx} \\ &\equiv \sum_{n=0}^{\infty} H_n(x)\frac{t^n}{n!}.\end{aligned}$$

  at x = 0 we can rewrite this into

$$g(0,t) = e^{-t^2} = \sum_{n=0}^{\infty}\frac{(-1)^n}{n!}t^{2n}$$

  which is clear that $H_n(0) = 0$ if n is odd. We can take derivatives of $g(x,t)$ to build the Hermite Polynomials using recursion relations between them and their derivatives like such.

$$\frac{\partial g}{\partial x} = 2tg(x,t) = \sum_{n=0}^{\infty}2H_n(x)\frac{t^{n+1}}{n!} = \sum_{n=0}^{\infty}2(n+1)H_n(x)\frac{t^{n+1}}{(n+1)!} = \sum_{n=0}^{\infty}H'(x)\frac{t^n}{n!}$$

  This brings us the following properties
  - $H_n(-x) = (-1)^nH_n(x)$
  - $H_n'(x) = 2nH_{n-1}(x)$
  - $H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x)$ if we differentiate with t instead.
  - $H_n''(x) - 2xH_n'(x) + 2nH_n(x) = 0$ which is the same as the Schrodinger equation

which is enough for us to build the Hermite Polynomials. Therefore, the final wave functions for the SHO are given by

$$\boxed{u_n(x) = c_n H_n(x\sqrt{\frac{m\omega}{\hbar}})e^{-m\omega x^2/2\hbar}} \tag{9}$$

this constant c can be determined from the orthogonality relationship.

$$\int_{-\infty}^{\infty} H_n(x)H_m(x)e^{-x^2} = \pi^{1/2}2^n n!\delta_{nm}$$

2.7.3 Linear Potential

- $V(x) = k|x|$, this potential has a classical turning point at a value x = a where E = ka.
- By symmatry ($u_E(-x) = -u_E(x)$) we need $u_E(0) = 0$, the other way around if ($u_E(-x) = +u_E(x)$) then we have $u'_E(0) = 0$.
- Some terms for definition are $x_0 = (\hbar^2/mk)^{1/3}$, $E_0 = kx_0 = (\hbar^2k^2/m)^{1/3}$, let $y = x/x_0$ and $\epsilon = E/E_0$
- With the definitions, we can rewrite the differential equations into

$$\frac{d^2u_E}{dy^2} - 2(y-\epsilon)u_E(y) = 0 \tag{10}$$

notice that when $y = \epsilon$ $x = E/k$. Lets define a translated position variable z = $2^{1/3}(y-\epsilon)$

$$\frac{d^2u_E}{dz^2} - zu_E(z) = 0 \tag{11}$$

which is the Airy equation Ai(z). This function has a behavior of oscillatory for negative values of the argument, and decreasing rapidly towards zero for positive values.

2.7.4 WKB(Semiclassical) Approximation

This approximation is used of regions where the wavelength is much shorter than the typical distance over which the potential energy varies. Such is the case of **never** near the classical turning point.

$$\frac{d^2u_E}{dx^2} + \frac{2m}{\hbar^2}(E - V(x))u_E(x) = \frac{d^2u_E}{dx^2} + [k(x)]^2u_E(x) = 0$$

The key is that *the V(x) varies only "slowly" with x*, then we are tempted to try a solution of the form.

$$u_E(x) = \exp[iW(x)/\hbar]$$

such that

$$i\hbar\frac{d^2W}{dx^2} - (\frac{dW}{dx})^2 + \hbar^2[k(x)]^2 = 0$$

and we also consider the condition that

$$\hbar|\frac{d^2W}{dx^2}| \ll |\frac{dW}{dx}|^2$$

which is the notion of a "slowly varying" potential V(x). We can also use this to write a lowest-order approximation for $W(x)$, namely,

$$W'_0(x) = \pm\hbar k(x)$$

leading to a first-order approximation for $W(x)$, based on

$$(\frac{dW_1}{dx})^2 = \hbar^2[k(x)]^2 + i\hbar W''_0(x) = \hbar^2[k(x)]^2 + i\hbar k'(x)$$

where the second term is much smaller than the first, so that

$$\begin{aligned} W(x) \approx W_1(x) &= \pm\hbar \int^x dx' \left[k^2(x') \pm ik'(x')\right]^{1/2} \\ &\approx \pm\hbar \int^x dx' k(x') \left[1 \pm \frac{i}{2}\frac{k'(x')}{k^2(x')}\right] \\ &= \pm\hbar \int^x dx' k(x') + \frac{i}{2}\hbar \ln[k(x)] \end{aligned}$$

The WKB approximation is given by

$$\boxed{u_E(x) \approx \exp[iW(x)/\hbar] = \frac{1}{[k(x)]^{1/2}} \exp\left[\pm i \int^x dx' k(x')\right]} \tag{12}$$

this choice of two solutions, is when in region where $E > V(x)$ or in the region where E < V(x). Continue Page 105 Sakurai. Also near the classical turning point, the solution follows the Airy FUnction as we assumed a linear regime at the boundary. Essentially following this form we can obtain some relationship

- From Region II to Region III and from Region II to Region I, the wave function in region II must be the same, which implies that the arguments of the cosine in the wave function must differ by at most by an integer multiple of π, and reason for not 2π is because the sign doesn't matter($|\psi|^2$ ignores the sign of the wave function).

$$\int_{x_1}^{x_2} dx \sqrt{2m[E - V(x)]} = (n + \frac{1}{2})\pi\hbar \quad (n = 0, 1, 2, 3...)$$

- This relationship can be used to approximate expressions for eneryg levels in a potential well, for instance

$$V = \begin{cases} mgx & \text{for} \quad x > 0 \\ \infty & \text{for} \quad x < 0 \end{cases}$$

  lets consider a ball bouncing up and down over a hard surface where x stands for the height of the ball measured from the hard surface. However, the WKB approximation is based on that the function leaked into the classically forbidden regime, so we need the *odd-parity solutions.*

- **Odd-Parity Solutions:** this is an approach that ensure at x = 0 the wave function vanishes we generalized the potential configuration above into

$$V(x) = mg|x| \quad (-\infty < x < \infty)$$

  whose turning points are now $x_1 = -E/mg$ and $x_2 = E/mg$, the cumulated phase shift becomes

$$\int_{-E/mg}^{E/mg} dx \sqrt{2m(E - mg|x|)} = (n_{odd} + \frac{1}{2})\pi\hbar \quad (n_{odd} = 1, 3, 5...) \tag{13}$$

  and equivalently since we want to study on x > 0 location, we can have that

$$\int_{0}^{E/mg} dx \sqrt{2m(E - mgx)} = (n - \frac{1}{4})\pi\hbar \quad (n = 1, 2, 3, 4...)$$

  Therefore, we can obtain the energy levels of the bouncing ball.

$$\boxed{E_n = \{\frac{[3(n - \frac{1}{4})\pi]^{2/3}}{2}\}(mg^2\hbar^2)^{1/3}} \tag{14}$$

Continue on page 108 Sakurai.

3 Angular Momentum

3.1 definition of rotation

- Rotation in two axis are not commutable. applying rotation around the z axis $R_z(\pi/2)$ and rotation by the x axis $R_x(\pi/2)$ are not commutable.
- **active rotation:** the angle ϕ is positive when counterclockwise rotation in the xy-plane. Therefore we define that the rotation operator around the z axis is

$$R_z(\phi) = \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix} \approx \begin{pmatrix} 1-\frac{\epsilon^2}{2} & -\epsilon & 0 \\ \epsilon & 1-\frac{\epsilon^2}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

the second matrix is an **infinitesimal form** of R_z, also noticing that

$$R_x(\epsilon)R_y(\epsilon) - R_y(\epsilon)R_x(\epsilon) = \begin{pmatrix} 0 & -\epsilon^2 & 0 \\ \epsilon^2 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = R_z(\epsilon^2) - 1 = R_z(\epsilon^2) - R_{any}(0)$$

- **passive rotation:**another convention is when the axis is rotating instead of the vector, the positive ϕ is then representing clockwise rotation.

3.2 Rotation in Quantum Mechanics

- **Infinitesimal rotation** So what about rotation in quantum-mechanical concepts, let's characterize the rotation to a state ket as such

$$|\alpha\rangle_R = \mathscr{D}(R)\,|\alpha\rangle \tag{15}$$

note the dimension of this operator is represented by 2x2 matrix for a spin half system and 3x3 unitary matrix for a spin 1 system. With similar approach as the translation and the evolution oeprators, we can write out the experiment for any operator.

$$U_\epsilon = 1 - iG\epsilon$$

with a Hermitian operator G such that $G \to \frac{p_x}{\hbar}, \epsilon \to dx'$ for translation in the x direction, and $G \to \frac{H}{\hbar}, \epsilon \to dt'$ for the evolution operator. This time we want an operator for the generator of rotation, which we can define the angular-momentum operator J_k in such a way that the operator for an infinitesimal rotation around the kth axis by angle $d\phi$ can be obtained by $G \to \frac{J_k}{\hbar}, \epsilon \to d\phi$, therefore we have the rotation operator as

$$\boxed{\mathscr{D}(\hat{\mathbf{n}}, d\phi) = 1 - i(\frac{\mathbf{J}\cdot\hat{\mathbf{n}}}{\hbar})d\phi} \tag{16}$$

- **Finite Rotation**

$$\begin{aligned} \mathscr{D}_z(\phi) &= \lim_{N\to\infty}[1 - i(\frac{J_z}{\hbar})(\frac{\phi}{N})]^N \\ &= \exp\left\{(-\frac{iJ_z\phi}{\hbar})\right\} \\ &= 1 - \frac{iJ_z\phi}{\hbar} - \frac{J_z^2\phi}{2\hbar^2} + ... \end{aligned}$$

Yet we need to mark the properties of the rotation orthogonal matrix R that

1. Identity: $R\cdot 1 = R \to \mathscr{D}(R)\cdot 1 = \mathscr{D}(R)$
2. Closure: $R_1R_2 = R_3 \to \mathscr{D}(R_1)\mathscr{D}(R_2) = \mathscr{D}(R_3)$
3. Inverses: $RR^{-1} = 1 \to \mathscr{D}(R)\mathscr{D}^{-1}(R) = 1 = \mathscr{D}^{-1}(R)\mathscr{D}(R)$

4. Associativity: $\mathscr{D}(R_1)[\mathscr{D}(R_2)\mathscr{D}(R_3)] = [\mathscr{D}(R_1)\mathscr{D}(R_2)]\mathscr{D}(R_3)$

- **Commutation Relations:** by ignoring higher order ϵ we can obtain the following commutator

$$[J_x, J_y] = i\hbar J_z$$

a more general form is

$$[J_i, J_j] = i\hbar\epsilon_{ijk}J_k$$

- **Operation on Expectation Value:** The effect of a rotation operator on the expectation value of angular momentum is

$$\langle J_x\rangle \to_R \langle\alpha| J_x |\alpha\rangle_R = \langle\alpha| \mathscr{D}_z^\dagger(\phi) J_x \mathscr{D}_z(\phi) |\alpha\rangle$$

using the Baker-Hausdorff lemma 42(do this proof as an exercise)

$$\begin{aligned}
\exp\left(\frac{iJ_z\phi}{\hbar}\right) J_x \exp\left(\frac{-iJ_z\phi}{\hbar}\right) &= J_x + \left(\frac{i\phi}{\hbar}\right)\underbrace{[J_z, J_x]}_{i\hbar J_y} \\
&\quad + \left(\frac{1}{2!}\right)\left(\frac{i\phi}{\hbar}\right)^2 \underbrace{[J_z,[J_z,J_x]]}_{\substack{i\hbar J_y \\ \Downarrow \\ \hbar^2 J_x}} \\
&\quad + \left(\frac{1}{3!}\right)\left(\frac{i\phi}{\hbar}\right)^3 \underbrace{[J_z,[J_z,[J_z,J_x]]]}_{\substack{\hbar^2 J_x \\ \Downarrow \\ i\hbar^3 J_y}} + \cdots \\
&= J_x\left[1 - \frac{\phi^2}{2!} + \cdots\right] - J_y\left[\phi - \frac{\phi^3}{3!} + \cdots\right] \\
&= J_x\cos\phi - J_y\sin\phi.
\end{aligned}$$

3.3 Spin $\frac{1}{2}$ system

- **Rotation Operator** From what we learned previously

$$\begin{aligned}
S_x &= \left(\frac{\hbar}{2}\right)\{|+\rangle\langle -| + |-\rangle\langle +|\}, \\
S_y &= \left(\frac{i\hbar}{2}\right)\{-|+\rangle\langle -| + |-\rangle\langle +|\}, \\
S_z &= \left(\frac{\hbar}{2}\right)\{|+\rangle\langle +| - |-\rangle\langle -|\},
\end{aligned}$$

satisfies the commutation relations for rotation operators, yet, we can also show that

$$\langle S_x\rangle \to_R \langle\alpha| S_x |\alpha\rangle_R = \langle S_x\rangle\cos(\phi) - \langle S_y\rangle\sin(\phi)$$

and similar for S_y and S_z Therefore, we can also write that the expectation value of the spin operator behaves as though it were a classical vector under rotation:

$$\langle S_k\rangle \to \sum_l R_{kl}\langle S_l\rangle \tag{17}$$

where R_{kl} stands for the elements of the 3x3 orthogonal matrix R. Also in Pauli Formalism, we can also write

$$\begin{aligned}
\exp\left(-i\frac{\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\,\phi}{2}\right) &= \left[1 - \frac{(\boldsymbol{\sigma}\cdot\hat{\mathbf{n}})^2}{2!}\left(\frac{\phi}{2}\right)^2 + \frac{(\boldsymbol{\sigma}\cdot\hat{\mathbf{n}})^4}{4!}\left(\frac{\phi}{2}\right)^4 - \cdots\right] \\
&\quad - i\left[(\boldsymbol{\sigma}\cdot\hat{\mathbf{n}})\frac{\phi}{2} - \frac{(\boldsymbol{\sigma}\cdot\hat{\mathbf{n}})^3}{3!}\left(\frac{\phi}{2}\right)^3 + \cdots\right] \\
&= \mathbb{1}\cos\left(\frac{\phi}{2}\right) - i(\boldsymbol{\sigma}\cdot\hat{\mathbf{n}})\sin\left(\frac{\phi}{2}\right).
\end{aligned}$$

- **Why Spin** 1/2**?**: when we apply the rotation operator on the state $|\alpha\rangle$ we can observe something interesting.

$$\exp\left(\frac{-iS_z\phi}{\hbar}\right)|\alpha\rangle = e^{-i\phi/2}|+\rangle\langle+|\alpha\rangle + e^{i\phi/2}|-\rangle\langle-|\alpha\rangle = \exp\left(\frac{-i\sigma\cdot\hat{\mathbf{n}}\phi}{2}\right)|\alpha\rangle$$

where we use

$$(\sigma\cdot\hat{\mathbf{n}})^n = \begin{cases} 1 & \text{for n even} \\ \sigma\cdot\hat{\mathbf{n}} & \text{for n odd} \end{cases}$$

considering a rotation by 2π we have

$$|\alpha\rangle_{R_z(2\pi)} \to -|\alpha\rangle$$

which is still differing from the orginal ket, and we need 4π to restore to original state. This can be explained by the **spin precession**

- **Spin Precession:** Recall the basic Hamiltonian of the problem is given by

$$H = -(\frac{e}{m_e c})\mathbf{S}\cdot\mathbf{B} = \omega S_z$$

and the time evolution operator of this hamiltonian is given by

$$\mathscr{U}(t,0) = \exp\left(\frac{-iS_z t}{\hbar}\right)$$

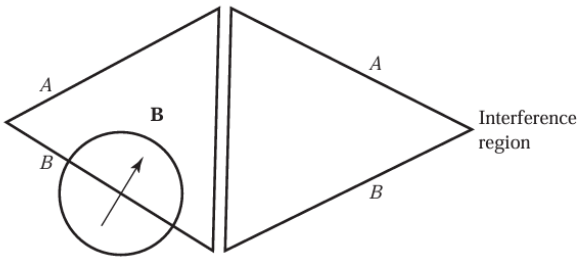
which is precisely the same as the rotation operator if we set $\phi = \omega t$, which shows a spin precession as such

$$\begin{aligned}\langle S_x\rangle_t &= \langle S_x\rangle_{t=0}\cos\omega t - \langle S_y\rangle_{t=0}\sin\omega t,\\ \langle S_y\rangle_t &= \langle S_y\rangle_{t=0}\cos\omega t + \langle S_x\rangle_{t=0}\sin\omega t,\\ \langle S_z\rangle_t &= \langle S_z\rangle_{t=0}.\end{aligned}$$

so here is an example to talk about 2π rotation

3.3.1 Neutron Interferometry Experiment to Study 2π Rotations

This experiment is used to *detect the minus sign in* 2π *rotation.* The only way to detect that is to make a comparison between an unrotated state and a rotated state. As shown in the figure below, we may use the art of neutrino interferometry to verify this difference. A monoenergetic beam of thermal neutrons is split into two parts, path A and path B; where path A goes through a region magnetic-field -free, and path B suffers a phase change $e^{\mp i\omega T/2}$,where T is the time spent in the $B \neq 0$ region where ω is the spin-precession frequency. where



$$\omega = \frac{g_n eB}{m_p c} \qquad (g_n \simeq -1.91)$$

why varying the magnetic field, we can see a sinusoidal variation

$$\cos\left(\frac{\mp\omega T}{2} + \delta\right)$$

(Prove 3.43)

3.3.2 Pauli Two-Component Formalism

Manipulations with the state kets of spin half system can be conviniently carried out using the two-component spinor formalism introduced by W.Pauli in 1926. In the spin half case, we have

$$|+\rangle = \begin{pmatrix}1\\0\end{pmatrix} = \chi_+ \quad |-\rangle = \begin{pmatrix}0\\1\end{pmatrix} = \chi_-$$
$$\langle +| = (1,0) = \chi_+^\dagger \quad \langle -| = (0,1) = \chi_-^\dagger$$

For an arbitrary state ket and the corresponding state bra, we have

$$|\alpha\rangle = |+\rangle\langle +\,|\,\alpha\rangle + |-\rangle\langle -\,|\,\alpha\rangle = \begin{pmatrix}\langle +\,|\,\alpha\rangle\\ \langle -\,|\,\alpha\rangle\end{pmatrix}$$

where this is also called the **two-component spinor** and can be written as

$$\chi = \begin{pmatrix}\langle +\,|\,\alpha\rangle\\ \langle -\,|\,\alpha\rangle\end{pmatrix} = \begin{pmatrix}c_+\\c_-\end{pmatrix} = c_+\chi_+ + c_-\chi_-$$

Yet some things we learned previous finally connect to a line. The matrix elements of the expectation value in the spin half system are also known as the **Pauli Matrices** ignoring the $\hbar/2$.

$$\langle \pm|S_k|+\rangle \equiv \left(\frac{\hbar}{2}\right)(\sigma_k)_{\pm,+}, \qquad \langle \pm|S_k|-\rangle \equiv \left(\frac{\hbar}{2}\right)(\sigma_k)_{\pm,-}.$$

We can now write the expectation value $\langle S_k\rangle$ in terms of χ and σ_k:

$$\begin{aligned}\langle S_k\rangle = \langle\alpha|S_k|\alpha\rangle &= \sum_{a'=+,-}\sum_{a''=+,-}\langle\alpha|a'\rangle\langle a'|S_k|a''\rangle\langle a''|\alpha\rangle\\ &= \left(\frac{\hbar}{2}\right)\chi^\dagger\sigma_k\chi,\end{aligned}$$

where the usual rule of matrix multiplication is used in the last line.

$$\sigma_1 = \begin{pmatrix}0&1\\1&0\end{pmatrix}, \quad \sigma_2 = \begin{pmatrix}0&-i\\i&0\end{pmatrix}, \quad \sigma_3 = \begin{pmatrix}1&0\\0&-1\end{pmatrix}.$$

Here are some properties of the Pauli Matrices

- $\sigma_i^2 = 1$
- $\sigma_i\sigma_j + \sigma_j\sigma_i = 0$ for $i \neq j$
- $\{\sigma_i, \sigma_j\} = 2\delta_{ij}$
- $[\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k$
- $\sigma_i^\dagger = \sigma_i$
- $\det(\sigma_i) = -1$
- $Tr(\sigma_i) = 0$
- consider a vector $\mathbf{a}$ a vector in three dimensions.

$$\begin{aligned}\sigma\cdot\mathbf{a} &= \sum_k a_k\sigma_k\\ &= \begin{pmatrix}a_3 & a_1 - ia_2\\ aa_1 + ia_2 & -a_3\end{pmatrix}\end{aligned}$$

there is an important identity

$$\boxed{(\sigma\cdot\mathbf{a})(\sigma\cdot\mathbf{b}) = \mathbf{a}\cdot\mathbf{b} + i\sigma\cdot(\mathbf{a}\times\mathbf{b})}$$

a specific case can be that $(\sigma\cdot\mathbf{a})^2 = |\mathbf{a}|^2$

- **EigenSpinor:** constructing the eigenspinor of $\sigma \cdot \hat{\mathbf{n}}$ can tell us information as an instructive application.

$$\sigma \cdot \hat{\mathbf{n}} \chi = \chi$$

In other word, in the spin half system, we look for the two-component column matrix of $|\mathbf{S} \cdot \hat{\mathbf{n}}; +\rangle$ defined by

$$\mathbf{S} \cdot \hat{\mathbf{n}} \, |\mathbf{S} \cdot \hat{\mathbf{n}}; +\rangle = (\frac{\hbar}{2}) \, |\mathbf{S} \cdot \hat{\mathbf{n}}; +\rangle$$

3.4 SO(3), SU(2), and Euler Rotations

- **Orthogonal Group:** for a rotational matrix, recall that $RR^T = I$ which is a symmetrical matrix. Also any orthogonal group is a length preserving operator. The set of all multiplication operations with orthogonal matrices forms a group, following the four requirements

1. The product of any two orthogonal matrices is another orthogonal matrix, which is satisfied because.

$$(R_1 R_2)(R_1 R_2)^T = R_1 R_2 R_2^T R_1^T = I$$

2. The associative law holds:

$$R_1(R_2 R_3) = (R_1 R_2) R_3$$

3. The identity matrix I, physically corresponding to no rotation, defined by

$$RI = IR = R$$

4. The Inverse of matrix R, physically corresponding to rotation in the opposite sense, defined by

$$RR^{-1} = R^{-1} R = I$$

This group is so called **SO(3)**, where S stands for special, O stands for orthogonal, 3 for three dimensions. Since we only consider Rotational operation, so it is SO(3) not O(3)

- **Unitary Unimodular Group:** A more well known name is unitary operator, and the most general unimodular matrix is defined by

$$U(a,b) = \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix}$$

where a and b are complex number known as **Cayley-Klein Parameters** satisfying the unimodular condition

$$|a|^2 + |b|^2 = 1$$

where $U(a,b)^\dagger U(a,b) = I$, a 2x2 matrix for rotation can also be characterized as this category. Also note that

$$U(a_1, b_1) U(a_2, b_2) = U(a_1 a_2 - b_1 b_2^*, a_1 b_2 + a_2^* b_1)$$

For the inverse of U we have

$$U^{-1}(a,b) = U(a^*, -b)$$

This group is known as **SU(2)** where U stands for Unitary and 2 for dimensionality 2. A more general unitary matrices for U(2), can be written as

$$U = e^{i\gamma} \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix}, \quad |a|^2 + |b|^2 = 1, \quad \gamma^* = \gamma$$

Note that we can characterize rotations using both SO(3) and SU(2) group, but they are not isomorphic.

3.4.1 Euler Rotations

Euler Rotations describe the rotation of a rigid object in three steps. It goes as follow

1. Rotate the rigid body counterclockwise about the z-axis by angle α, assume there is a body y-axis, that is initially coincides with the usual y-axis, but no longer after the rotation called y'.
2. Rotate around the y'-axis by angle β. The z' axis no longer points in the space fixed z-axis direction.
3. The Final Rotation is by the z'-axis by angle γ.

This process can be expressed by

$$R(\alpha,\beta,\gamma) = R_{z'}(\gamma)R_{y'}(\beta)R_z(\alpha) = R_z(\alpha)R_y(\beta)R_z(\gamma)$$

We need to express each of the body-axis rotation in terms of the space-fixed axis rotation, such that

$$R_{y'}(\beta) = R_z(\alpha)R_y(\beta)R_z^{-1}(\alpha)$$
$$R_{z'}(\gamma) = R_{y'}(\beta)R_z(\beta)R_{y'}^{-1}(\beta)$$

applying this to the spin half system, we can replace all the rotation matrix with rotation operator.

$$\mathscr{D}(\alpha,\beta,\gamma) = \mathscr{D}_z(\alpha)\mathscr{D}_y(\beta)\mathscr{D}_z(\gamma)$$

which is equivalent to

$$\exp\left(-i\frac{\sigma_3\alpha}{2}\right)\exp\left(-i\frac{\sigma_2\beta}{2}\right)\exp\left(-i\frac{\sigma_3\gamma}{2}\right) \tag{18}$$

$$= \begin{pmatrix} e^{-i\alpha/2} & 0 \\ 0 & e^{i\alpha/2} \end{pmatrix}\begin{pmatrix} \cos(\beta/2) & -\sin(\beta/2) \\ \sin(\beta/2) & \cos(\beta/2) \end{pmatrix}\begin{pmatrix} e^{-i\gamma/2} & 0 \\ 0 & e^{i\gamma/2} \end{pmatrix}$$

$$= \begin{pmatrix} e^{-i(\alpha+\gamma)/2}\cos(\beta/2) & -e^{-i(\alpha-\gamma)/2}\sin(\beta/2) \\ e^{i(\alpha-\gamma)/2}\sin(\beta/2) & e^{i(\alpha+\gamma)/2}\cos(\beta/2) \end{pmatrix},$$

This matrix is called the $j = \dfrac{1}{2}$ irreducible representation of the rotation operator $\mathscr{D}(\alpha,\beta,\gamma)$ with its matrix elements denoted by $\mathscr{D}^{1/2}_{m,m}(\alpha,\beta,\gamma)$. In terms of the angular momentum operator we have

$$\boxed{\mathcal{D}^{(1/2)}_{m'm}(\alpha,\beta,\gamma) = \left\langle j=\frac{1}{2},m' \middle| \exp\left(\frac{-iJ_z\alpha}{\hbar}\right)\exp\left(\frac{-iJ_y\beta}{\hbar}\right)\exp\left(\frac{-iJ_z\gamma}{\hbar}\right) \middle| j=\frac{1}{2},m \right\rangle} \tag{19}$$

3.5 Density Operators and Mixed Ensembles

- **Ensemble:** A collection of identically prepared physical systems. with all members the same ket state $|\alpha\rangle$
- **Incoherent Mixture:** When the ratio between two states are real without phase information.
- **Mixed Ensemble:** In a mixed ensemble a certain fraction, of the members are characterized by a state ket $|\alpha\rangle$ where the other are characterized by $|\beta\rangle$ such a beam is said to be **partially polarized**
- **Fractional Population:** The portion of the atoms that are in a state $|\alpha\rangle$ while the rest in $|\beta\rangle$.

Suppose we make a measurement of some observables A, we may ask the average measured value of A with large number of measurements are carried out so called the **ensemble average** of A

$$[A] = \sum_i w_i \left\langle \alpha^{(i)} \middle| A \middle| \alpha^{(i)} \right\rangle$$

$$= \sum_i \sum_{a'} w_i |\langle a' \,|\, \alpha^{(i)}\rangle|^2 a'$$

where $|a'\rangle$ is an eigenket of A. This also motivates us to define the density operator ρ as

$$\boxed{\rho = \sum_i w_i \left|\alpha^{(i)}\right\rangle \left\langle\alpha^{(i)}\right|} \tag{20}$$

Therefore, we can write the ensemble average as

$$[A] = \sum_{b'} \sum_{b''} \langle b''| \rho |b'\rangle \langle b'| A |b''\rangle = tr(\rho A)$$

4 Quantum Mechanics

4.1 Schrodinger equation

Schrodinger Equation:

$$ih\frac{\partial \psi}{\partial t} = -\frac{h^2}{2m}\frac{\partial \psi^2}{\partial t^2} + V\psi$$

Definition: The average value of j or the expectation value:

$$< j >= \frac{\sum jN(j)}{N} = \sum jjP(j)$$

for a continuous distribution we use probability density $\rho(x)$ so the probability of a particle between a and b is:

$$\int_b^a \rho(x)dx$$

here are a few equations to take note of:

- Expected Position:

$$< x >= \int_{+\infty}^{-\infty} x|\psi(x,t)|^2 dx$$

- Expected momentum:

$$< p >= \int_{+\infty}^{-\infty} -ih(\psi^* \frac{\partial \psi}{\partial x})dx$$

a few important things i learned:

- if LHS is dependent on t and RHS dependent on x, the only possibility is that both sides are constant.
- if we want an operator just sub in the form of the p - momentum
- c_n is the probability of measurement of the energy would return the value E_n

The Schrodinger equation can be solved by **seperation of variables**

$$\Psi(x,t) = \psi(x)\phi(t)$$

and by separating variables we got :

$$E = ih\frac{\partial \phi}{\partial t}$$

in other words:

$$-\frac{h^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V\psi = E\psi$$

There are 3 reasons to use separable solutions:

- Stationary States:
$$\Psi(x,t) = \psi(x)e^{-iEt/h}$$
where the wavefunction does not depend on time:
$$|\Psi(x,t)|^2 = |\psi(x)|^2$$

- States of Defined energy: Where the total Hamiltonian of the system is a constant:
$$H = \frac{p^2}{2m} + V(x)$$
where the hamiltonian operator is:
$$\hat{H} = -\frac{h^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$$
The time independent Schrodinger equation is:
$$\hat{H}\psi(x) = E\psi(x)$$
where the variance of H is 0 aka all the measurements should return the same energy E.

- General Solution is linear combination of separable solutions: A collection of solutions$(\psi_1(x), \psi_2(x), \psi_3(x))$ can be combined to form a general solution: each with a defined separation constant(E_1, E_2, E_3) thus there is a different wave function for each allowed energy.
$$\Psi(x,t) = \sum_n c_n\psi_n(x)e^{-iE_nt/h}$$
and every time dependent solution can be written in this form.

To solve schrodinger equation, with a given potential V and $\Psi(x,0)$ we can always fit the t = 0 state by:
$$\Psi(x,0) = \sum_n c_n\psi_n(x)$$
with an appropriate choise of c_n we can always fit the initial state.

and $|c_n|^2$ is the probability of measurement of the energy would return the value E_n and the sum should be equivalent to 1. With the expectation hamiltonian being:
$$< H >= \sum_n |c_n|^2 E_n$$

4.1.1 Infinite Square Well

suppose we need a boundary condition for the wave function to be 0 at the boundaries of the well.
$$V(x) = \begin{cases} 0, & 0 \le x \le a, \\ \infty, & \text{otherwise} \end{cases}$$
and the equation of time-independent schrodinger equation is:
$$-\frac{h^2}{2m}\frac{\partial^2\psi}{\partial x^2} = E\psi$$
which is a simple harmonic oscillator equation. and the solution is:
$$\psi(x) = A\sin(kx)$$
where k is the wave number: $k = \frac{\sqrt{2mE}}{h}$ since the boundary condition requires the wave function to be 0 at the boundaries. So ka must be a multiple of π: By subbing the new equation into the original time-independent schrodinger equatiom, the possible values of E in each mode is:
$$E_n = \frac{n^2\pi^2h^2}{2ma^2} = \frac{h^2k_n^2}{2m}$$

and the solutions is:

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$$

ψ_1 is called ground state and states with energies increase in proportion to n^2 is called excited States.

and here are a few interesting properties:

- They are alternately even and odd.
- each successive state has one more node.
- They are mutually orthogonal such that:

$$\int \psi_m(x)^* \psi_n(x) dx = \begin{cases} 0, & m \neq n \\ 1, & m = n \end{cases}$$

- They are complete, such that any other fucntion f(x) can be expressed as a linear combination of them.

To find c_n we can use fourier trick: let

$$\psi(x) = \sqrt{\frac{2}{a}} \sum_{n=1}^{\infty} c_n sin(\frac{n\pi}{a}x)$$

to find the probability factor for one state -m - is:

$$c_m = \int \psi_m^*(x)\psi(x)dx$$

in addition, the stationary states are:

$$\Psi_n(x,t) = \sqrt{\frac{2}{a}} sin(\frac{n\pi}{a}x) e^{-i(n^2\pi^2 h/2ma^2)t}$$

Therefore, the coefficient is:

$$c_n = \sqrt{\frac{2}{a}} \int_0^a sin(\frac{n\pi}{a}x)\Psi(x,0)dx$$

4.1.2 Harmonic Oscillator

Any simple harmonic oscillator can be approximated as:

$$V(x) = \frac{1}{2}V''(x_0)(x - x_0)^2$$

and for quantum problem we can further simplify it into:

$$V(x) = \frac{1}{2}mw^2x^2$$

and sub it into the time independent schrodinger equation:

$$-\frac{h}{2m}\frac{\partial\psi^2}{\partial x^2} + \frac{1}{2}mw^2x^2\psi = E\psi$$

and there are two solutions

- power series method
- Ladder operators method

Algebraic Method: Ladder Method we can rewrite time independent schrodinger equation into this form:

$$\frac{1}{2m}(\hat{p}^2 + m^2w^2\hat{x}^2)\psi = E\psi$$

and the basic idea is to factor the hamiltonian. here we have the famous **ladder operator**

$$\hat{a}_+ = \frac{1}{\sqrt{2m\hbar w}}(-i\hat{p} + mwx)$$

$$\hat{a}_- = \frac{1}{\sqrt{2m\hbar w}}(i\hat{p} + mwx)$$

and the relationship bewteen hamiltonian is:

$$\hat{a}_-\hat{a}_+ = \frac{1}{h\omega}\hat{H} + \frac{1}{2}$$

if we reverse the order of multiplication in the left hand side, the sign of that one have reverses. aka the **commutator** of the two operators is:

$$[\hat{a}_-, \hat{a}_+] = 1$$

by subbing the new hamiltonian equation into the solution we obtain:

$$h\omega(\hat{a}_+\hat{a}_- + \frac{1}{2})\psi = E\psi$$

Definition: If ψ satisfies the schrodinger equation with energy E, then $\hat{a}_+\psi$ also satisfies the schrodinger equation with energy E + hω

$$\hat{H}(a_+\psi) = (E + h\omega)(a_+\psi)$$

Idea: HOWEVER, it is not guaranteed that the new solution is normalize.

In practice, there is a lowest rung such that

$$\hat{a}_-\psi_0 = 0$$

so

$$\psi_0(x) = (\frac{m\omega}{\pi\hbar})^{1/4}e^{-\frac{m\omega}{2\hbar}x^2}$$

Therefore a generalized expression for the solutions of the Harmonic Oscillator is:

$$\boxed{\psi_n(x) = A_n(\hat{a}_+)^n\,\psi_0(x) \quad \text{with} \quad E_n = \left(n + \tfrac{1}{2}\right)\hbar\omega} \tag{21}$$

The relationship between n and n+1 stage is

$$\boxed{\hat{a}_+\,\psi_n = \sqrt{n+1}\,\psi_{n+1} \quad , \quad \hat{a}_-\,\psi_n = \sqrt{n}\,\psi_{n-1}} \tag{22}$$

Therefore, we can conclude that the expression for arbitrary mode is

$$\boxed{\psi_n = \frac{1}{\sqrt{n!}}\,(\hat{a}_+)^n\,\psi_0} \tag{23}$$

Yet in this harmonic oscillator the stationary states are still Orthogonal.

4.1.3 Hermite Polynomials

The time independent solution for Schrodinger Equation can be expressed as

$$\psi(\xi) = h(\xi)e^{-\xi^2/2}, \tag{24}$$

where as the $h(\xi)$ can be seek in the form of power series

$$h(\xi) = a_0 + a_1\xi + a_2\xi^2 + \cdots = \sum_{j=0}^{\infty} a_j\xi^j.$$

and

$$a_{j+2} = \frac{(2j+1-K)}{(j+1)(j+2)} a_j.$$

For the equation to be normalizable, the power series must terminate somewhere, this indicate that $a_{n+2} = 0$ which indicates that either the even or the odd terms must be zero from the start. This also indicates that $K = 2n+1$, and the solution for the harmonic oscillator are

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi) e^{-\xi^2/2}.$$

4.1.4 The Free Particle

The free particle should have been the simplest case (V(x) = 0 everywhere). It is just a motion at constant velocity. However it is kinda subtle. For the simplified Schrodinger Equation:

$$-\frac{h^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

The solution is simply a general solution for a second order ODE:

$$\psi(x) = Ae^{ikx} + Be^{-ikx}$$

where

$$k = \frac{\sqrt{2mE}}{\hbar}$$

Taking on the standard time dependent exponential term, the general solution for the time dependent free partical equation becomes:

$$\Psi(x,t) = Ae^{ik(x-\frac{\hbar k}{2m}t)} + Be^{-ik(x+\frac{\hbar k}{2m}t)}$$

Where the first term is a wave packet traveling to the right, and the second term is to the left. Since they are only differ by the the sign of k, we might as well write the equation in

$$\Psi_k(x,t) = Ae^{i\left(kx-\frac{\hbar k^2}{2m}t\right)}, \tag{25}$$

essentially if k is larger than 0 it is traveling to the right and vice versa. Therefore, the stationary states of these are simply free particles of propagating waves, they carry momentum

$$p = \hbar k$$

with a velocity of

$$v_{quantum} = \sqrt{\frac{E}{2m}} = v_{classical}/2$$

Yet as soon as we realized, this equation is not normalizable. In fact, *There is no such thing as a free particle with a definite energy.* Yet, it is still separable, but this time it is a continuous equation.

$$\boxed{\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) e^{i\left(kx-\frac{\hbar k^2}{2m}t\right)} dk.} \tag{26}$$

the $\frac{1}{\sqrt{2\pi}}\phi(k)$ is essentially c_n and now this equation is normalizable with a appropriate$\phi(k)$. Now everything that is left is how to determine $\phi(k)$, which is something fourier transform can handle.

$$\boxed{f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} F(k) e^{ikx} dk \iff F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(x) e^{-ikx} dx.} \tag{27}$$

Therefore,

$$\boxed{\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \Psi(x,0) e^{-ikx} dx.} \tag{28}$$

Note that for small a $\Psi(x,0)$ is narrow while $\phi(k)$ is broad and vice versa for large a. Physically, this is because forming a narrower wave requires more waves to superimpose, and mathematically we can explain by the uncertainty principles since k is directly related to momentum.

Now we shift our focus to deducing why the group velocity of the wave packet (quantum velocity) is twice of the phase velocity(particle velocity). By taking a fourier transform and taylor expand the function $\omega(k)$ we can obtain the relationships

$$v_{phase} = \frac{\omega}{k}$$

and the group velocity is

$$v_{group} = \frac{d\omega}{dk}$$

4.1.5 Bound States and Scattering States

The free particle and infinite squared well solutions perfectly correspond to the scattering and bound state of a particle. Defined as below.

$$\begin{cases} E < V(-\infty) \text{ and } V(+\infty) \implies \text{bound state}, \\ E > V(-\infty) \text{ or } V(+\infty) \implies \text{scattering state}. \end{cases} \tag{29}$$

Physically, bound state is defined as when E is smaller than the potential and it cannot escape, whereas the scattering state can be imagined as how an electron getting slowed in a potential field. However, since tunneling exists, so the particle can leak through any finite potential barrier so only thing that matters is the potential at infinity. In real life, most potentials go to zero at infinity.

4.1.6 The Delta-Function Well

The essence of this case is to use **Dirac Delta Function** to construct the potential of the system.

$$\delta(x) \equiv \begin{cases} 0, & \text{if } x \neq 0 \\ \infty, & \text{if } x = 0 \end{cases}, \quad \text{with } \int_{-\infty}^{+\infty} \delta(x)\, dx = 1.$$

Consider a potential of the form

$$V(x) = -\alpha\delta(x)$$

the solution yields 2 possibilities (bound states and scattering states) considering the bound states. In the region x < 0, V(x) $= 0$ so

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi = \kappa^2\psi,$$

where

$$\kappa \equiv \frac{\sqrt{-2mE}}{\hbar}.$$

the solution to this 2nd ODE is what we have learned before

$$\psi(x) = Ae^{-\kappa x} + Be^{\kappa x}$$

since the first term blows up as x goes to negative infinity, what is left is

$$\psi(x) = Be^{\kappa x}$$

Similar results can be obtained for x larger than 0

$$\psi(x) = Fe^{-\kappa x}$$

Yet, two important ideas for the wave function is that:

1.	ψ is always continuous;
2.	$\frac{d\psi}{dx}$ is continuous except at points where the potential is infinite.

The trick to find the solution is to integrate the schrodinger equation from $-\epsilon$ to $+\epsilon$ and take the limit as ϵ goes to 0.

$$\Delta(\frac{d\psi}{dx}) = -\frac{2m\alpha}{\hbar^2}\psi(0)$$

from the case at hand, we can tell that the first term is $-2B\kappa$ by taking direct derivative to the solutions we obtained before. Therefore, we can obtain that

$$\kappa = \frac{m\alpha}{\hbar^2}$$

making the allowed energy as

$$E = -\frac{m\alpha^2}{2\hbar^2}$$

We then normalize ψ yielding one bound state

$$\boxed{\psi(x) = \sqrt{\frac{m\alpha}{\hbar}}e^{-m\alpha|x|/\hbar^2}, \quad E = -\frac{m\alpha^2}{2\hbar^2}.}$$

Now we can discuss about **Scattering States** where E > 0 at ∞ where

$$k = \frac{\sqrt{2mE}}{\hbar}$$

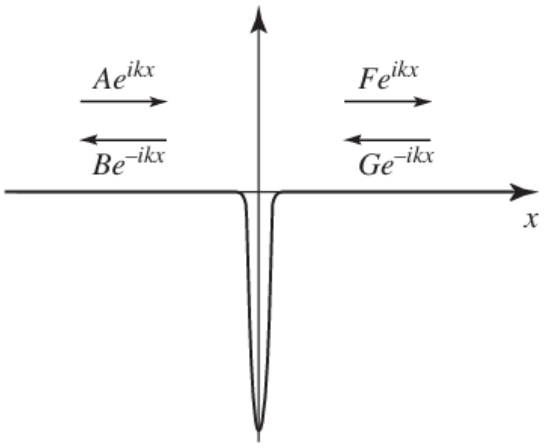
is real and positive, so the general solution is

$$\psi(x) = Fe^{ikx} + Ge^{-ikx} \quad x > 0$$

and

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \quad x < 0$$

by the continuity equations, we obtain In reality particles are fired from one direction, so G = 0 (since it is coming



from the right)

A is the amplitude of the **incident wave** and B is the amplitude of the **reflected wave**, and F is the amplitude of the transmitted wave. Using similar method as the Bound state, we can obtain

$$B = \frac{i\beta}{1-i\beta}A, \quad F = \frac{1}{1-i\beta}A. \tag{30}$$

where $\beta = \frac{m\alpha}{\hbar^2 k}$ Speaking in the language of probability, the relative probability that an incident particle would reflect is

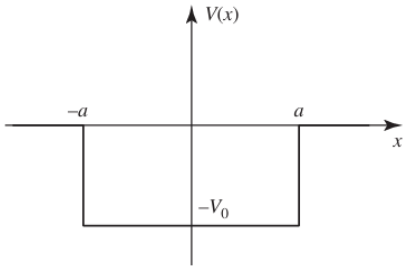
$$R = \frac{|B|^2}{|A|^2} = \frac{\beta^2}{1+\beta^2} \quad T = \frac{|F|^2}{|A|^2} = \frac{1}{1+\beta^2}$$

so

$$R = \frac{1}{1+\left(\frac{2\hbar^2 E}{m\alpha^2}\right)}, \quad T = \frac{1}{1+\left(\frac{m\alpha^2}{2\hbar^2 E}\right)}. \tag{31}$$

- The higher the energy, the greater the probability of transmission
- The only way to obtain a normalizable solution is similar to the free particle solution

4.2 Finite Square Well



For a finite square well as shown above we can find three expressions for the solutions. Since the potential is even, so the old theorem says that the bound state solution should be either even or odd. First, the Schrodinger equation looks as below within the well

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - V_0\psi = E\psi \quad \text{or} \frac{d^2\psi}{dx^2} = -l^2\psi \tag{32}$$

where $\mathrm{l} = \frac{\sqrt{2m(E+V_0)}}{\hbar}$ the solutions are

$$\psi(x) = \begin{cases} Fe^{-\kappa x}, & x > a, \\ D\cos(lx), & 0 < x < a, \\ \psi(-x), & x < 0. \end{cases}$$

lets first consider the even function. By the continuity of the wave function and the derivative, we find that

$$k = l\tan(la)$$

Since k and l are both functions of E, to find E we need some simplification and analytical solutions

$$z = la \quad and \quad z_0 = \frac{a}{\hbar}\sqrt{2mV_0}$$

and the equation becomes

$$\tan(z) = \sqrt{(z_0/z)^2 - 1}$$

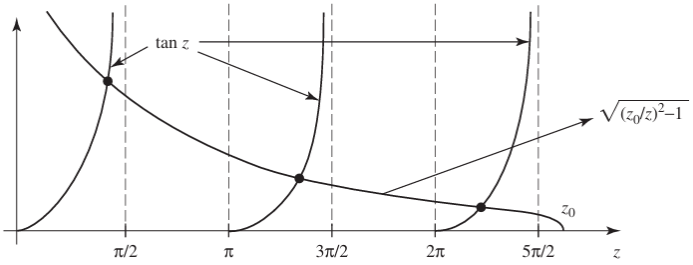
plotting them together we have the following diagram.

There are two major solutions we can draw from this diagram

- **Wide Deep wall**: For large z_0 the intersection goes very close to $z_n = n\pi/2$ with n odd; which follows that

$$E_n + V_0 = \frac{n^2\pi^2\hbar^2}{2m(2a)^2} \quad n = 1, 3, 5...$$

- **Shallow Narrow Wall**: as z_0 decreases, there are fewer and fewer bound states, until for $z_0 < \pi/2$ only one remains. There is always at least one bound state no matter how "weak" the well becomes.



5 Quantum Mechanics in Three Dimensions

5.1 3D Schrodinger Equation

Schrodinger Equation can be generalized as

$$i\hbar\frac{\partial\Psi}{\partial t} = \hat{H}\Psi$$

and the Hamiltonian is obtained by

$$\hat{H} = \frac{1}{2}mv^2 + V = \frac{1}{2m}(p_x^2 + p_y^2 + p_z^2) + V$$

In terms of operator languages, the equation then simplifies to

$$\boxed{i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi} \tag{33}$$

The normalization factor is by volume

$$\int |\Psi|^2 d^3r = 1$$

and if V is independent of time, the time dependent solution is

$$\Psi(r,t) = \psi_n(r)e^{-iE_nt/\hbar}$$

so the time independent Schrodinger Equation is

$$\boxed{-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi} \tag{34}$$

5.2 Two Dimensional Square Box

A simpler case is a two dimensional system such that

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} = \frac{2M}{\hbar^2}[U - E]\psi$$

considering the potential as a infinite square wall of width x. by separation of variables in X and Y coordinates, we see the solution

$$X(x) = B\sin\left(\frac{n_x\pi x}{a}\right)$$
$$Y(y) = C\sin\left(\frac{n_y\pi y}{a}\right)$$

The complete wave function becomes

$$\psi(x,y) = BC\sin\left(\frac{n_x\pi x}{a}\right)\sin\left(\frac{n_y\pi y}{a}\right)$$

The allowed energies of the states can be derived by subbing in the derived equations back into the original expression

$$E = E_{n_x,n_y} = \frac{\hbar^2\pi^2}{2Ma^2}(n_x^2 + n_y^2)$$

Degeneracy

One properties to mention is that there can be several different wave functions for which the particle has the same energy. In general, if there ar eN independent wave functions all with the same energy E, we say taht the energy level E is degenerate and has degeneracy N.

5.3 Two-Dimensional Central-Force

In terms of polar Coordinate, the LHS of Schrodinger Equation can be expressed as:

$$\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}=\frac{\partial^2\psi}{\partial r^2}+\frac{1}{r}\frac{\partial\psi}{\partial r}+\frac{1}{r^2}\frac{\partial^2\psi}{\partial\phi^2}=\frac{2m}{\hbar^2}(U-E)\psi$$

By separation of variables we can assume a constant M such that

$$\Phi''(\phi)=-M^2\Phi(\phi)$$

and

$$R''+\frac{R'}{r}-\left[\frac{M^2}{r^2}+\frac{2m}{\hbar^2}(U-E)\right]R=0$$

Which we can derive that

$$\Phi(\phi)=e^{iM\phi}$$

However, for this function to be periodic we realized that m must be an integer.

Angular Momentum

Using the expression we had above, we can draw an analogy by changing the form of the equation above

$$\psi(r,\phi)=R(r)e^{i(M/r)s}$$

where k = M/r and this gives us the expression for the tangential momentum as

$$p_{tang}=\hbar\frac{M}{r}$$

and the angular momentum is

$$L_z=M\hbar$$

just remember that M is essentially the wave number/ quantum number of the wave function.

The allowed energy for each M has multiple energy levels labeled by n = 1,2,3,4... Yet, since M is related to the energy by $\frac{m^2}{r^2}$ so there is degeneracy except when m = 0

$$E_{n,m}=E_{n,-m}$$

5.4 The Three-Dimensional Central-Force Problem

recalled that we need to express Schrodinger's Equation in spherical polar coodinate.

$$x=r\sin\theta cos\phi \quad y=r\sin\theta\sin\phi \quad z=r\cos\phi$$

which we obtained that

$$\frac{1}{r}\frac{\partial^2}{\partial r^2}(r\psi)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial\psi}{\partial\theta})+\frac{1}{r^2\sin\theta}\frac{\partial^2\psi}{\partial\phi^2}=\frac{2m}{\hbar^2}[U(r)-E]\psi \tag{35}$$

By the separation of variable, we can once again obtain the following equations

$$\Phi''(\phi)=-m^2\Phi(\phi)$$

Quantum number, l:	0	1	2	3	4	...
Magnitude:	0	$\sqrt{2}\hbar$	$\sqrt{6}\hbar$	$\sqrt{12}\hbar$	$\sqrt{20}\hbar$	...

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+\left(k-\frac{M^2}{\sin^2\theta}\right)\Theta=0 \tag{36}$$

and

$$\frac{d^2}{dr^2}(rR)=\frac{2m}{\hbar^2}\left[U(r)+\frac{k\hbar^2}{2Mr^2}-E\right](rR) \tag{37}$$

where k is the constant that $\frac{\Theta''}{\Theta}$ and the other function are equal to.

Note that ϕ and θ are not related to the potential energy function, this means that the solutions for these two won't apply to any central-force problem.

5.5 Quantization of Angular Momentum

the k term followed the Legendre's Polynomials. Yet we can discuss one of the acceptable solution

$$k=l(l+1)$$

where l is a positive integer greater than or equal in magnitude to m. $l \geq |m|$ such that the wavefunction is

$$\psi(r,\theta,\phi)=R(r)\Theta(\theta)e^{im\phi}$$

In reality, the angular momentum is

$$L=\sqrt{l(l+1)}\hbar$$

for large l we can approximate that $L \approx l\hbar$

5.6 Hydrogen Atom

- In any central-forcep roblem, a level with $L=\sqrt{l(l+1)}\hbar$ will always be at leaast $(2l+1)$ fold degenerate.

Consider a hydrogen atom having

$$U(r)=\frac{-ke^2}{r}$$

where we can find the equation to the corresponding Schrodinger's Equation must have the allowed energy of the form

$$E=-\frac{m_e(ke^2)^2}{2\hbar^2}\frac{1}{n^2}$$

where n is any integer greater than l. The first energy level is the Rydberg Energy 13.6 eV. This yield the Bohr model of energy levels.

Hydrogenic Wave Functions

Based on the spherical coordinate representation of Schrodinger's Equation, we can find that the ground state with n = 1, l =0 m = 0 of a hydrogen atom is

$$\psi_{1s}(r,\theta,\phi)=R_{1s}(r)$$

substituting the energy and the potential we have

$$R_{1s}(r)=Ae^{-r/a_B}$$

This represents the probability density of the electron around hydrogen.

- For any state with $l \neq 0$ $|\psi|^2$ is zero at the origin.

If we find the probability density of finding electron within a finite radial volume around the atom we have

$$P(r) = 4\pi r^2 |R(r)|^2$$

For non-Ground state(2s State) we have n = 2 with E = $-E_R/4$, which yields 4 independent wave functions to consider. Speaking of 2s state, it is only r dependent

$$R_{2s} = A(2 - \frac{r}{a_B})e^{-r/2a_B}$$

2p state has three directions to consider in x,y, and z directions. The z direction (l = 1) can be written as

$$\psi(r, \theta, \phi) = Are^{-r/2a_B}\cos(\theta) = Aze^{-r/2a_B}$$

therefore wave functions in other directions are

$$\psi_x = Axe^{-r/2a_B}$$

$$\psi_y = Aye^{-r/2a_B}$$

Electron Spin

The angular momentum of an electron spin is obtained by

$$S = \sqrt{s(s+1)\hbar}$$

where s always has a fixed value $s = \frac{1}{2}$, and similarly, the possible value of S_z is

$$S_z = m_s\hbar$$

where m_s can be either $\frac{1}{2}$ or $-\frac{1}{2}$.

- The energy is independent of electron spin, so a ground state can have 2 degeneracy, and therefore, the degeneracy of nth level is $2n^2$

Magnetic Moments

A few equations to remember are

- Potential Energy: $U = -\mu \cdot B$
- Gyromagnetic Ratio: $\mu = -\frac{e}{2m_e}L$
- Zeeman Effect: $\Delta E = -\mu \cdot B = (\frac{e}{2m_e})L_zB = m\mu_B B$
- Spin Magnetic Moment: $\mu_{spin} = -\frac{e}{m_e}S = \gamma S$

The total Magnetic Moment is the sum of the orbital magnetic moment and the spin magnetic moment

$$\mu_{tot} = -\frac{e}{2m_e}(L + 2S)$$

5.7 Multielectron Atoms

One method is to use IPA(independent-particle approximation) or Central-Field Approximation disregarding the forces from other electrons. Essentially using the potential energy function to solve the Schrodinger Equation and obtain a new set of potential function so called the **Hartree-Fock method** such that as the electron goes outside of other electrons

$$U(r) = -\frac{ke^2}{r}$$

and when the electron is close to nucleus

$$U(r) = -\frac{Zke^2}{r}$$

6 Quantum Formalism

6.1 Hilbert Space

Definition: Hilbert Space
a set of all square integrable functions on a specified interval f(x) such that

$$\int_a^b |f(x)|^2 dx < \infty \tag{38}$$

constitues a vector space of $L^2(a,b)$ namely **Hilbert Space**.
And for two functions that live in Hilbert Space, the inner product is defined as:

$$\langle f|g\rangle = \int_a^b f^*(x)g(x)dx \tag{39}$$

which follows the integral **Schwarz Inequality**:

$$|\langle f|g\rangle| \leq \sqrt{\langle f|f\rangle}\sqrt{\langle g|g\rangle} \tag{40}$$

a bit more definition for a terms:

- Normalized: if the inner project with itself is 1
- Orthogonal: if the inner product with another function is 0
- Orthonormal: if the inner product with itself is 1 and with another function is 0
- Complete: if any other function can be expressed as a linear combination of the existing functions
- **Hermitian Conjugate**: The Hermitian(adjoint) conjugate of an operator $\hat{Q}$ is $\hat{Q}^\dagger$

  $$\left\langle f\middle|\hat{Q}g\right\rangle = \left\langle \hat{Q}^\dagger g\middle|f\right\rangle$$

  an **Hermitian Operator** is equal to its adjoint $\hat{Q} = \hat{Q}^\dagger$
- **Determinate States**:
  The state observed is always $\langle Q|Q\rangle = q$ by computing the standard deviation of a determinate states $\sigma^2 = \left\langle (\hat{Q}-q)\Psi\middle|\hat{Q}-q)\Psi\right\rangle$, the only available solution is

  $$\hat{Q}\Psi = q\Psi$$

  Therefore, Determinate states of Q are eigenfunctions of $\hat{Q}$
- Spectrum: It is the list of eigenvalues that follow the eigenvalue problem in the determinate states of a system.
- Discrete Spectra: It is when the eigenvalues are
  1. Real
  2. Orthogonal for each corresponding eigenfunctions: However, degeneracy tells us that any linear combination of them is itself an eigenfunction with the same eigenvalue. Therefore we need to use **Gram-Schmidt Orthogonalization procedure** to construct orthogonal eigenfunctions within the degenerate subspace(Problem 3.7 Griffiths).
- Continuous Spectra: Momentum doesn't have a continuous spectra, and

  $$-i\hbar\frac{d}{dx}f_p(x) = pf_p(x) \rightarrow f_p(x) = Ae^{ipx/\hbar}$$

  Yet, we find the **Dirac Orthonormality**

  $$\left\langle f_{p'}\middle|f_p\right\rangle = \delta(p-p')$$

Any complete function associated to momentum can be written as

$$f(x) = \int_{-\infty}^{\infty} c(p)\, f_p(x)\, dp = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} c(p)\, e^{ipx/\hbar}\, dp$$

and the coefficients can be found by Fourier's Trick:

$$\langle f_{p'} \mid f \rangle = \int_{-\infty}^{\infty} c(p)\, \langle f_{p'} \mid f_p \rangle\, dp = \int_{-\infty}^{\infty} c(p)\, \delta(p - p')\, dp = c(p')$$

6.2 Statistical Interpretation

A general interpretation of is that

If you measure an observable Q on a particle in the state Ψ, you are certain to get one of the eigenvalues of the hermitian operator $\hat{Q}$, if the spectrum is

- **Discrete:** the probability of getting the particular eigenvalue is

$$|c_n|^2, \quad where \quad c_n = \langle f_n | \Psi \rangle$$

- **Continuous:** for eigenfunctions $f_z(x)$, the probability of getting a result in range dz is

$$|c(z)|^2 dz \quad where \quad c(z) = \langle f_z | \Psi \rangle$$

Another finding is related to the Uncertainty theorem: through sets of inequalities, you can obtain the relation that

$$\sigma_A^2 \sigma_B^2 \geq (\frac{1}{2i}[\hat{A}, \hat{B}])^2$$

The generalized Ehrenfest Theorem also reads

$$\frac{d}{dt}\langle \hat{Q} \rangle = \frac{i}{\hbar} \left\langle \left[\hat{H}, \hat{Q}\right] \right\rangle + \left\langle \frac{\partial \hat{Q}}{\partial t} \right\rangle \tag{41}$$

by directly taking derivative to the $\langle Q|Q\rangle = \left\langle \Psi \middle| \hat{Q}\Psi \right\rangle$

6.3 Bases and Operations

Griffiths P3.13

7 Appendix

7.1 A. Useful Formula

$$\exp(iG\lambda)\, A\, \exp(-iG\lambda) = A + i\lambda[G, A] + \frac{i^2\lambda^2}{2!}[G, [G, A]] + \cdots + \frac{i^n\lambda^n}{n!}[G, [G, \ldots [G, A]]] + \cdots \tag{42}$$

$$\mathrm{Ai}(z) \to \frac{1}{2\sqrt{\pi}} z^{-1/4} \exp\left(-\frac{2}{3} z^{3/2}\right) \quad \text{as } z \to +\infty$$
$$\mathrm{Ai}(z) \to \frac{1}{\sqrt{\pi}} |z|^{-1/4} \cos\left(\frac{2}{3}|z|^{3/2} - \frac{\pi}{4}\right) \quad \text{as } z \to -\infty$$

The first one is in the classically forbidden regime and the second one is in the classically allowed regime.

8 Measurements and Uncertainty Principles

8.1 Time-Energy Uncertainty Relation

We can derive the relationship between energy and time uncertainty using the general uncertainty principle.

Derivation

Starting with the general uncertainty relation for the Hamiltonian H and an observable Q:

$$\sigma_H^2 \sigma_Q^2 \geq \left(\frac{1}{2i} \langle [H, Q] \rangle \right)^2$$

Recall the Heisenberg equation of motion relating the commutator to the time derivative of the expectation value:

$$\langle [H, Q] \rangle = \frac{\hbar}{i} \frac{d}{dt} \langle Q \rangle$$

Substituting this back into the inequality:

$$\begin{aligned} \sigma_H^2 \sigma_Q^2 &\geq \left(\frac{1}{2i} \left(\frac{\hbar}{i} \frac{d}{dt} \langle Q \rangle \right) \right)^2 \\ &= \frac{1}{4} \hbar^2 \left(\frac{d}{dt} \langle Q \rangle \right)^2 \end{aligned}$$

We define the characteristic time scale Δt required for the expectation value of Q to change by one standard deviation σ_Q:

$$\Delta t = \frac{\sigma_Q}{|d\langle Q \rangle / dt|} \implies \sigma_Q = \Delta t \left| \frac{d\langle Q \rangle}{dt} \right|$$

Substituting σ_Q into the inequality yields:

$$\boxed{\Delta E \Delta t \geq \frac{\hbar}{2}} \tag{43}$$

8.2 Measurements Formalism

Definition: Measurement Types

- **POVM:** Positive Operator-Valued Measure.
- **PVM:** Projection Valued Measure (standard projective measurement).

8.2.1 Projectors

A projector P satisfies the property $P^2 = P$ and is Hermitian $P = P^\dagger$.

- **Rank 1 Projector:** Projects onto a single state, e.g., $|1\rangle\langle 1|$.
- **Rank 2 Projector:** Projects onto a subspace, e.g., $|1\rangle\langle 1| + |2\rangle\langle 2|$.

For a continuous basis:

$$\int_a^b |x\rangle\langle x| dx = P$$

Orthogonality condition:

$$P_i P_j = \delta_{ij} P_j$$

The probability of outcome i is given by:

$$\text{Probability } i = \langle \psi | P_i | \psi \rangle$$

8.3 Hermitian Operators and Degeneracy

Consider an operator Ω with eigenvalues w_i and a degeneracy parameter α (since multiple states might share the same eigenvalue w_i).

$$\Omega|w_i, \alpha\rangle = w_i|w_i, \alpha\rangle$$

The orthonormality condition involves both the eigenvalue index and the degeneracy label:

$$\langle w_i, \alpha|w_j, \beta\rangle = \delta_{ij}\delta_{\alpha\beta}$$

Example 1: Angular Momentum Degeneracy
Consider the spherical harmonics $Y_l^m(\theta, \phi)$, which are the coordinate representation of $|l, m\rangle$:

$$\langle \mathbf{n}|l, m\rangle = Y_l^m(\theta, \phi)$$

The operators act as follows:

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

$$L_z|l, m\rangle = m\hbar|l, m\rangle$$

If our observable is $\Omega = L^2$, then the eigenvalue depends only on l. The quantum number m acts as the **degeneracy label**.

8.3.1 Spectral Resolution

We can express the operator in terms of its projectors (Spectral Decomposition):

$$\Omega = \sum_{i,\alpha} w_i|w_i, \alpha\rangle\langle w_i, \alpha|$$

8.4 PVM and Expectation Values

For a Projection Valued Measure, we define the projector for eigenvalue w_i by summing over the degenerate subspace α:

$$P_i = \sum_{\alpha} |w_i, \alpha\rangle\langle w_i, \alpha|$$

The probability of obtaining result i is:

$$p_i = \langle\psi|P_i|\psi\rangle$$

Using the expansion $|\psi\rangle = \sum_{i,\alpha} c_{i\alpha}|w_i, \alpha\rangle$, the probability is also:

$$p_i = \sum_{\alpha} |c_{i\alpha}|^2$$

The expectation value is:

$$\langle\Omega\rangle = \sum_i w_i p_i = \sum_i w_i\langle\psi|P_i|\psi\rangle = \langle\psi|\Omega|\psi\rangle$$

8.5 Energy Measurement Example

Given the Hamiltonian eigenproblem $H|n\rangle = E_n|n\rangle$, the spectral resolution is:

$$H = \sum_{n=1}^{\infty} E_n|n\rangle\langle n|$$

Let the projector be $P_n = |n\rangle\langle n|$. The expectation value of energy is:

$$\langle H\rangle = \sum_n E_n\langle\psi|P_n|\psi\rangle = \sum_n E_n|c_n|^2$$

8.5.1 State Collapse

If a general observable $\Omega = \sum_i w_i P_i$ is measured and the result i is obtained, the state vector collapses to:

$$\boxed{|\psi'\rangle = \frac{P_i|\psi\rangle}{\sqrt{\langle\psi|P_i|\psi\rangle}}} \tag{44}$$