

# **Dr. Widom's Quantum Mechanics I Lectures**

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# Preface

These are my notes from the lecture series taught by Dr. Michael Widom at Carnegie Mellon University during the Fall of 2019. I hope these notes will prove useful to current and future students of the course. Please note that I am missing lecture 20, which I believe concerned quantum computing. Supplemental notes for this lecture were included online by Dr. Widom, so I did not feel the need to retype them here. I cannot guarantee the accuracy of these notes, as they were all typed (quickly) during class with very minimal proofreading afterwards. Additionally there may be some missing information towards the end of the first twelve lectures (which were originally typed in a different format and converted to L<sup>A</sup>T<sub>E</sub>X later). I have tried to organize the notes roughly into chapters, and these chapters do not reflect the sections in *Consistent Quantum Theory* (Robert B. Griffiths) or *Quantum Mechanics, Volume 1* (Claude Cohen-Tannoudji et al.), the textbooks used in this course.

- Dene Hoffman

# Chapter 1

# Quantum Mechanics Essentials

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LECTURE 1-12: REVIEW OF QUANTUM MECHANICS  
Monday, August 26, 2019

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## 1.1 Hilbert Space and Phase Space

For a 1-D system, phase space has two variables, position  $x$  and “conjugate” momentum  $p$ . For a particle at  $(x_0, p_0)$  at  $t_0$  the position in phase space evolves to a different position  $(x_1, p_1)$  at  $t_1$ . Position and momentum here are real numbers, and the evolution is continuous and deterministic.

For a quantum system, we use a Hilbert space. We will use the Hilbert space of a spin-1/2 particle, generally thought of as a two level system. The spin is thought of as a vector, and we will let this vector be aligned along the  $z$  axis. The Hilbert space is two dimensional, and the  $x$ -axis refers to  $|z+\rangle$  while the  $y$ -axis refers to  $|z-\rangle$ , which are vectors pointing in the + and -  $z$ -directions. Regardless of the position along the  $+z$  axis, the particle has its spin in the  $+z$  position. All the states along that line, except for the origin, refer to particles with  $+z$  polarization. We can use a coefficient  $\alpha$  to refer to the position along this axis, and all the  $+z$  polarized particles belong to the set  $\alpha_+ |z+\rangle$ . Likewise,  $\alpha_- |z-\rangle$  can take us along the  $z$ -axis.

In QM, we can have states which are off-axis, they have attributes of both properties. Let's call one such state  $|\psi_0\rangle$ . The set of equivalent vectors is a line in Hilbert space! It will evolve continuously in time to a state  $|\psi_1\rangle$ . Suppose  $|\psi_1\rangle$  is perpendicular to  $|\psi_0\rangle$ . This state is completely different from the original, it shares no attributes with the original like the two  $z$ -states. Such states are orthogonal.

The Hilbert space is a complex vector space:

- $c |\psi\rangle \in \mathcal{H}$
- $|\psi\rangle + |\phi\rangle \in \mathcal{H}$
- Inner product: ket notation
  - ket vectors are elements of the Hilbert space:  $|\psi\rangle \in \mathcal{H}$
  - bra vectors are elements of the adjoint/dual space:  $\langle\psi| \in \mathcal{H}^\dagger$
  - $\langle\psi| \equiv (\langle\psi|)^\dagger$
  - $\langle\psi| : |\phi\rangle \rightarrow c \in \mathbb{C}$
  - $\langle\psi| : |\psi\rangle \rightarrow \langle\psi|\psi\rangle = \|\psi\|^2$ , the squared norm of the vector

$$|\psi\rangle = a_+ |z+\rangle + a_- |z-\rangle$$

$$|\phi\rangle = b_+ |z+\rangle + b_- |z-\rangle$$

$$\langle\psi| = \langle z+| a_+^* + \langle z-| a_-^*$$

$$\langle\psi|\psi\rangle = |a_+|^2 + |a_-|^2 \text{ because}$$

$$\langle z+|z-\rangle = 0$$

$$\langle\psi|\phi\rangle = a_+^* b_+ + a_-^* b_- = \langle\phi|\psi\rangle^*$$

## 1.2 Operators

$$A: \mathcal{H} \rightarrow \mathcal{H}$$

$$A: |\psi\rangle \rightarrow |\phi\rangle \equiv |A\psi\rangle$$

It is sufficient to make a list of what operators do to orthogonal elements, which will be equivalent to the complete set of all possible inner products.

### 1.2.1 Matrix Element

$$\langle\chi| A |\psi\rangle = \langle\chi| A\psi\rangle = \langle\chi|\phi\rangle$$

( $A$  does not operate on  $\chi$ )

The adjoint operator  $A^\dagger$ :

$$A^\dagger: \langle\chi| \rightarrow \langle\chi| A^\dagger \equiv (\langle\chi| A)|^\dagger$$

$$\langle\chi| A^\dagger \psi\rangle = (\langle\chi| A^\dagger) \langle\psi\rangle = (\langle\chi| A)|^\dagger \psi = (\langle\psi| A)|^\dagger \chi = \langle\psi| A^\dagger \chi\rangle$$

We will (almost always) talk about “Normal” Operators. Say  $N$  is a normal operator:

$$N^\dagger N = NN^\dagger$$

Hermitian operators are normal:  $H = H^\dagger$  — associated with physical properties, eigenvalues are real

Unitary operators are normal:  $U^\dagger U = UU^\dagger = I$ , the identity—these are associated with time evolution of quantum systems. Their eigenvalues have unit magnitude, time evolution will keep states on the unit circle.

*Note: the unit complex “circle” is a 4-D sphere called the Bloch sphere*

- $N|\psi\rangle = \lambda|\psi\rangle \Rightarrow \langle\psi|N^\dagger = \lambda^*|\psi\rangle$
- $$\|(N - \lambda I)|u\rangle\|^2 = 0 = \langle u| (N^\dagger - \lambda^* I)(N - \lambda I)|u\rangle = \|\langle u| (N^\dagger - \lambda^* I)\|^2$$

- $N|u_i\rangle = \lambda_i|u_i\rangle$  and  $N|u_j\rangle = \lambda_j|u_j\rangle$ . Then  $\lambda_i \neq \lambda_j \Rightarrow \langle u_i|u_j\rangle = 0$

$$\begin{aligned}\langle u_i|N|u_j\rangle &= \lambda_j\langle u_i|u_j\rangle \\ &= (\langle u_i|N)|u_j\rangle \\ &= \lambda_i\langle u_i|u_j\rangle\end{aligned}$$

- $H$  (a Hermitian operator) has real eigenvalues
- Eigenvalues of  $U$  (a Unitary operator) have unit magnitude  
 $(\langle u|U^\dagger)(U|u\rangle) = \lambda^*\lambda\langle u|u\rangle = \langle u|u\rangle$  since  $U^\dagger U = I$

### 1.3 Projectors

Projectors are operators which project any state to the specified projection subspace. In general, a projector  $P = P^2$  can be defined using the inner product of two states:

$$\langle\psi|\phi\rangle|\psi\rangle = |\psi\rangle\langle\psi|\phi\rangle = P_\psi|\phi\rangle$$

if  $|\psi\rangle$  is normalized (in general,  $P_\psi = \frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle}$ ).

The dimension of the subspace onto which the state is being projected is the dimension of the projector, and  $\dim P = \text{Tr } P$ , the trace of the projector matrix (called a dyad).

Note: In the textbook, the projector of a given state is often denoted by  $[\psi]$ .

Say we are defining the usual spin-1/2 system on the basis  $z+$  and  $z-$ . The projectors onto those states are:

$$[z+] = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$$

and

$$[z-] = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$$

Note that trace of both of these projectors is equal to 1, meaning the projected subspaces are one-dimensional.

Suppose we had a Normal operator  $A$  with eigenvectors denoted by  $\alpha_i$  and eigenvalues  $a_i$ .

$$A|\alpha_i\rangle = a_i|\alpha_i\rangle.$$

We can define a projector for each eigenvector (assuming they are not degenerate/have different eigenvalues):

$$P_i = |\alpha_i\rangle\langle\alpha_i|$$

If  $\langle\alpha_i|\alpha_j\rangle = \delta_{ij}$ ,  $P_i P_j = \delta_{ij} P_i$ .

## 1.4 Spectral Decomposition

For any operator, we can find a decomposition based on the sum of projectors multiplied by the corresponding eigenvalues:

$$A = \sum_i a_i P_i$$

## 1.5 Physical Variables and Properties

In *Classical* phase space, we can have properties like the energy  $H(\gamma)$  at some point  $\gamma$  in phase space. We can also make claims like  $H(\phi) < E_0$  ( $\phi$  has this “property”). Physical properties in phase space are subsets of the phase space.

In the *Quantum* Hilbert space, we say that physical properties are *linear* subspaces of  $\mathcal{H}$ .  $S_z$  has value  $+\frac{\hbar}{2}$  for  $\{|\psi\rangle \mid |\psi\rangle = c|z+\rangle\}$ ,  $c \neq 0$ .

## 1.6 Review of Properties

*Classical*: “The energy is less than x” is a subset of the phase space. In particular, it’s the set of points in phase space such that the property is true. Alternatively, we could define a function  $P$  for a property  $\mathcal{P}$ . This “indicator” function is defined as:

$$P(\gamma) = \begin{cases} 1 & \mathcal{P} \text{ is true} \\ 0 & \mathcal{P} \text{ is false} \end{cases}$$

*Quantum*: A property  $\mathcal{P}$  is a linear subspace of the Hilbert space. Algebraically, we can also define:

$$\mathcal{P} = \{|\psi\rangle \in \mathcal{H} \mid P_{\mathcal{P}}|\psi\rangle = |\psi\rangle\}$$

Here, the projector acts like an indicator function, since if the system does not have the property, the projector will return zero.

$$I = P_{z+} + P_{z-}$$

### 1.6.1 Logical Reasoning

Classical:

Operation	Set	Algebraic	$\mathcal{P}$ Example
$\mathcal{P}$	$\mathcal{P} \subset \Gamma$	$P(\gamma)$	$H(\gamma) < E_0$
Negation $\neg\mathcal{P}$	$\mathcal{P}^C = \Gamma - \mathcal{P}$	$P^C = 1 - P(\gamma)$	$H(\gamma) \geq E_0$
Conjunction $\mathcal{P} \wedge \mathcal{Q}$	$\mathcal{P} \cap \mathcal{Q}$	$P(\gamma)Q(\gamma)$	$((H\gamma) < E_0) \wedge (x < 0)$
Disjunction $\mathcal{P} \vee \mathcal{Q}$	$\mathcal{P} \cup \mathcal{Q}$	$P(\gamma) + Q(\gamma) - P(\gamma)Q(\gamma)$	$((H\gamma) < E_0) \vee (x < 0)$

Identities:

- $\neg(\mathcal{P} \cap \mathcal{Q}) = (\neg\mathcal{P} \cup \neg\mathcal{Q})$

- $\neg(\mathcal{P} \cup \mathcal{Q}) = (\neg\mathcal{P} \cap \neg\mathcal{Q})$
- $\mathcal{P} \cup (\mathcal{Q} \cap \mathcal{R}) = (\mathcal{P} \cup \mathcal{Q}) \cap (\mathcal{P} \cup \mathcal{R})$
- $\mathcal{P} \cap (\mathcal{Q} \cup \mathcal{R}) = (\mathcal{P} \cap \mathcal{Q}) \cup (\mathcal{P} \cap \mathcal{R})$

This set of rules constitutes a “boolean algebra.”

Quantum:

Operation	Set	Algebraic	Example
$\mathcal{P}$	$\mathcal{P} \subset \mathcal{H}$	$P: \mathcal{H} \rightarrow \mathcal{P}$	$S_x = +\frac{\hbar}{2}$
Negation $\neg\mathcal{P}$	$\mathcal{P}^\perp = \{ \psi\rangle \mid P \psi\rangle =  0\rangle\}$	$I - P$	$S_x = -\frac{\hbar}{2}$
Conjunction $\mathcal{P} \wedge \mathcal{Q}$	???	$PQ$ or $QP$ (commutation?)	$(S_x = +\frac{\hbar}{2}) \wedge (S_z = +\frac{\hbar}{2})$ is undefined
Disjunction $\mathcal{P} \vee \mathcal{Q}$	???	$P + Q - PQ$ or $P + Q - QP$	$(S_x = +\frac{\hbar}{2}) \vee (S_x = -\frac{\hbar}{2})$

**Conditional Probabilities and the Born Rule** Conditional probability:  $0 \leq \Pr(\mathcal{P} \mid \psi) \leq 1$  is the probability that the state is in the subspace  $P$ . If  $|\psi\rangle \in \mathcal{P} \rightarrow \Pr = 1$  and  $|\psi\rangle \in \neg\mathcal{P} = \mathcal{P}^\perp \rightarrow \Pr = 0$ . Intermediate states (linear combinations of property states) could have a value between 0 and 1. For example, the probability for a particle in the state  $|x+\rangle$  to have the property  $|z+\rangle$  is  $\frac{1}{2}$ .

Suppose  $\langle\psi|\psi\rangle = 1$ . The Born rule states that  $\Pr(\mathcal{P} \mid \psi) = \|P|\psi\rangle\|^2 = \langle\psi|P^\dagger P|\psi\rangle = \langle\psi|P|\psi\rangle$ .

## 1.7 Density Operator (Matrix)

### 1.7.1 Pure State:

$$|\psi\rangle \rightarrow [\psi] = |\psi\rangle\langle\psi| = \rho.$$

$$\Pr(\mathcal{P} \mid \rho) = \langle\psi|P|\psi\rangle$$

Insert identities on either side of  $P$ :

$$\Pr(\mathcal{P} \mid \rho) = \langle\psi|(\sum_m|m\rangle\langle m|)P(\sum_n|n\rangle\langle n|)|\psi\rangle = \sum_{mn}\langle\psi|m\rangle\langle m|P|n\rangle\langle n|\psi\rangle$$

The outermost brackets are just complex numbers, so we can move them around. Also,  $\langle n|\psi\rangle\langle\psi|m\rangle = \langle n|\rho|m\rangle$ :

$$\Pr(\mathcal{P}|\rho) = \sum_n \sum_m \rho_{nm} P_{mn} = \sum_n (\rho P)_{nn} = \text{Tr}(\rho P)$$

**Example.**

$$|\psi\rangle = |x+\rangle = \frac{1}{\sqrt{2}}(|z+\rangle + |z-\rangle)$$

$$\rho = \frac{1}{2}(|z+\rangle\langle z+| + \dots)$$

In  $z\pm$  basis,

$$\rho = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$$

$$\text{In } x\pm \text{ basis, } \rho = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$$

◊

### 1.7.2 Mixed State

For example, take a state which is 75%  $|x+\rangle$  and 25%  $|x-\rangle$ :

$$\frac{3}{4}\rho_{x+} + \frac{1}{4}\rho_{x-} = \rho = \begin{bmatrix} \frac{1}{2} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{2} \end{bmatrix}$$

in the  $z$  basis ( $\rho = \begin{bmatrix} \frac{3}{4} & 0 \\ 0 & \frac{1}{4} \end{bmatrix}$  in the  $x$  basis)

$$\text{Pr}([z+] \mid \rho) = \text{Tr}(\rho[z+]) = \text{Tr}\left(\begin{bmatrix} \frac{1}{2} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{2} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}\right) = \frac{1}{2}$$

$$\text{Pr}([x+] \mid \rho) = \text{Tr}(\rho[x+]) = \text{Tr}\left(\begin{bmatrix} \frac{3}{4} & 0 \\ 0 & \frac{1}{4} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}\right) = \frac{3}{4}$$

In a pure state,  $\text{Tr}(\rho) = 1$  and  $\text{Tr}(\rho^2) = \text{Tr}(\rho) = 1$  since the density matrix for a pure state is a projector onto that state.

In a general density matrix,  $\text{Tr}(\rho) = 1$ , but  $\rho^2 \neq \rho$ , so  $\text{Tr}(\rho^2) = \text{Tr}(\sum_j p_j P_j \sum_k p_k P_k) = \sum_j p_j^2$ , so  $\sum_j p_j^2 < 1$  unless  $p_j = \delta_{jk}$ . The trace of the density matrix squared is always non-zero in finite-dimension Hilbert spaces (could be zero in a maximally-mixed infinite-dimensional space).

## 1.8 Average Value of an Observable

$$A = \sum_a a P_a$$

For a state  $|\psi\rangle$ , the expectation value of the operator  $A$  is  $\langle A \rangle_\psi = \sum_a a \text{Pr}(A = a \mid \psi) = \sum_a a |P_a|\psi\rangle||^2 = \sum_a a \langle\psi|P_a|\psi\rangle = \langle\psi|A|\psi\rangle$ .

**Example.** For a pure state  $\rho = |\psi\rangle\langle\psi|$ ,

$$\langle A \rangle_\rho = \langle\psi|A|\psi\rangle = \text{Tr}(\rho A)$$

For a mixed state  $\rho = \sum_j p_j P_j$ ,  $P_j |\psi_j\rangle\langle\psi_j|$ ,

$$\langle A \rangle_\rho = \sum_j p_j \langle A \rangle_{\psi_j} = \sum_j p_j \text{Tr}(P_j A) = \text{Tr}(\rho A)$$

◇

### 1.8.1 Classical Composite

$$(x, p) \in \Gamma, \quad \dim(\Gamma) = 2$$

$$(x_a, p_a) \in \Gamma_a$$

$$(x_b, p_b) \in \Gamma_b$$

$$(x_a x_b, p_a p_b) \in \Gamma_a \times \Gamma_b, \text{ so}$$

$$\dim(\Gamma_a \times \Gamma_b) = \dim \Gamma_a + \dim \Gamma_b$$

### 1.8.2 Quantum Composite

$$\mathcal{H}_a, \mathcal{H}_b \rightarrow \mathcal{H}_{ab} = \mathcal{H}_a \otimes \mathcal{H}_b$$

$$|a\rangle \in \mathcal{H}_a, |b\rangle \in \mathcal{H}_b \rightarrow |a\rangle \otimes |b\rangle \in \mathcal{H}_{ab}$$

(Product State)

$$\dim \mathcal{H}_a \otimes \mathcal{H}_b = \dim \mathcal{H}_a \cdot \dim \mathcal{H}_b$$

For a basis  $\{|a_j\rangle\}$  and  $\{|b_k\rangle\}$  for  $\mathcal{H}_a$  and  $\mathcal{H}_b$ , we can choose a basis  $\{|a_j\rangle \otimes |b_k\rangle\}$  for  $\mathcal{H}_{ab}$ . To simplify notation,  $|a_j\rangle \otimes |b_k\rangle = |j\rangle_a \otimes |k\rangle_b = |j\rangle_a |k\rangle_b = |jk\rangle$ .

For a system with two spin-1/2 particles, the standard basis is  $\{|++\rangle, |+-\rangle, |-+\rangle, |--\rangle\}$ .

## 1.9 Spinor Particle

Spinors are used to describe particles with position and spin.

Position:  $\psi(\vec{r}) = \langle \vec{r} | \psi \rangle$

Spin:  $\alpha |+\rangle + \beta |-\rangle$

Product state:  $(\alpha |+\rangle + \beta |-\rangle) \cdot \psi(\vec{r})$

General state is a sum of product states:

$$|\omega\rangle = \sum_j (\alpha_j |+\rangle + \beta_j |-\rangle) \psi_j(\vec{r}) = \begin{bmatrix} \omega_+(r) \\ \omega_-(r) \end{bmatrix}$$

$\omega_+(\vec{r}) = \langle \vec{r} | \omega \rangle$  and  $\omega_-(\vec{r}) = \langle \vec{r} | \omega \rangle$ , so

$$\omega_+(\vec{r}) = \sum_j \alpha_j \psi_j(\vec{r})$$

$$\omega_-(\vec{r}) = \sum_j \beta_j \psi_j(\vec{r})$$

## 1.10 Toy Models

**Example.** Say we have a 1D line upon which a particle can move, and suppose this is a discrete space, where the position is given by  $m = 0, 1, 2, 3$  (in solid state this is a tight-binding model).  $\dim(\mathcal{H}_m) = 4$  since there are four possible place the particle can be.

Add a detector with two states,  $n = 0$  and  $n = 1$ . If the detector finds a particle in the detector space, it is in state 1, otherwise

$$n = 0, \quad \dim(\mathcal{H}_n) = 2$$

For the combined particle + detector space,  $\dim(\mathcal{H}_{mn}) = 8$ . ◊

**Example.** Eight positions, four for spin up and four for spin down. A particle with spin has  $\dim = 8$  also. ◊

**Example.** Suppose we have four possible positions in the  $x$ -direction and two in the  $y$ -direction. This is a particle in 2D. There are eight possible positions for the particle, so the dimension of the product space is 8.

All of these spaces are isomorphic.  $\diamond$

Notation
$ \psi\rangle \in \mathcal{H}_{mn}$
$\psi_n(m) = \langle mn \psi\rangle$

## 1.11 Entangled States

We know that any  $|\psi\rangle \in \mathcal{H}_{ab}$  can be expanded in a basis  $\{|j\rangle_a \otimes |k\rangle_b\}$ :

$|\psi\rangle = \sum_{jk} \Psi_{jk} |jk\rangle$  where  $\Psi$  is just the coefficient of the basis.

$$\Psi = (\dim \mathcal{H}_a) \times (\dim \mathcal{H}_b)$$

The “rank” of an array is the number of independent rows which is equivalent to the number of independent columns.

### 1.11.1 Rank = 1

$\exists |a\rangle \in \mathcal{H}_a, |b\rangle \in \mathcal{H}_b$  such that  $|\psi\rangle = |a\rangle \otimes |b\rangle$

This is a product state

### 1.11.2 Rank > 1

There is no such state. This is an entangled state.

$$|a\rangle = \alpha_+ |+\rangle_a + \alpha_- |-\rangle_a, \\ |b\rangle = \beta_+ |+\rangle_b + \beta_- |-\rangle_b$$

$$|\psi\rangle = |a\rangle \otimes |b\rangle = \alpha_+ \beta_+ |++\rangle + \alpha_+ \beta_- |+-\rangle + \alpha_- \beta_+ |-+\rangle + \alpha_- \beta_- |--\rangle$$

Here,  $\Psi_{++} = \alpha_+ \beta_+$ ,  $\Psi_{+-} = \alpha_+ \beta_-$ , etc.

Note,  $\Psi_{++}\Psi_{--} = \alpha_+ \beta_+ \alpha_- \beta_- = \Psi_{-+}\Psi_{+-}$ , so  $\det\{\Psi\} = 0$ . If the determinant vanishes, the state is a product state, otherwise it is an entangled state. For example,

$$|\psi_0\rangle = \frac{1}{\sqrt{2}}(|+-\rangle - |--\rangle) \text{ (EPR State)}$$

$$\Psi_{++} = \Psi_{--} = 0 \text{ while } \Psi_{+-} = \frac{1}{\sqrt{2}} = -\Psi_{-+} \text{ so } \det\{\Psi\} = \frac{1}{2}.$$

## 1.12 Tensor Product Spaces

### 1.12.1 Review

$$|\psi\rangle = |a\rangle \otimes |b\rangle = |ab\rangle \in \mathcal{H}_{ab} = \mathcal{H}_a \otimes \mathcal{H}_b$$

$$(|a\rangle \otimes |b\rangle)^\dagger = \langle ab| \in \mathcal{H}_{ab}^\dagger = \mathcal{H}_a^\dagger \otimes \mathcal{H}_b^\dagger$$

$$|\psi'\rangle = |a'\rangle \otimes |b'\rangle$$

$$\langle\psi|\psi'\rangle = \langle a|a'\rangle \cdot \langle b|b'\rangle$$

Suppose we have an operator  $A$  acting in  $\mathcal{H}_a$  and  $B$  acting in  $\mathcal{H}_b$ . Then  $A \otimes B$  acts on states in  $\mathcal{H}_{ab}$ . In this case, the tensor product is equivalent to  $\sum_{jk} A_j \otimes B_k$ .

We can also have products of tensor products of operators:

$$(A \otimes B)(A' \otimes B') = (AA') \otimes (BB'). \text{ Additionally } (A \otimes I_b)(I_a \otimes B) = A \otimes B.$$

**Example.** Spin in a two-particle space

$$A = [z+]_a = |+\rangle_a \langle +|_a, I_b = |+\rangle_b \langle +|_b + |-\rangle_b \langle -|_b.$$

$$(A \otimes I_b) = |++\rangle_{ab} \langle ++|_{ab} + |+-\rangle_{ab} \langle +-|_{ab} = [z_a+]$$

You can check that this is in fact an operator by squaring it.  $\diamond$

## 1.13 Recitation

$$|\psi_0\rangle = \frac{1}{\sqrt{2}}(|+-\rangle - |--\rangle) \text{ "EPR State"}$$

$$[\psi_0] = \frac{1}{2}([++]+[--]+|+-\rangle\langle-+|-|+-\rangle\langle+-|)$$

$$[z_a+] \equiv [z+]_a \otimes I_b = [++]+|+-\rangle\langle-+|$$

$$[\psi_0][z_a+] = \frac{1}{2}(|+-\rangle\langle+-|-|+-\rangle\langle-+|)$$

$$[z_a+][\psi_0] = \frac{1}{2}(|+-\rangle\langle+-|-|+-\rangle\langle+-|)$$

What can we say about this system? Are the spins the same?

$$P = [++]+[--]$$

$$Q = [+-]+[-+]$$

$P[\psi_0] = [\psi_0]P = 0$  implies the spins are not the same.

Let's work with the "GHZ" state, a state of three particles.

$$|\phi\rangle = |(z_1+)(z_2+)(z_3+)\rangle - |(z_1-)(z_2-)(z_3-)\rangle$$

Define  $\sigma_x = \frac{2}{\hbar}S_x$  such that  $\sigma_x|z+\rangle = |z+\rangle$ , and  $\sigma_x|z-\rangle = -|z-\rangle$ . It can also be shown that:

$$\sigma_x|z+\rangle = |z-\rangle$$

and

$$\sigma_y|z-\rangle = -i|z+\rangle, \text{ and}$$

$$\sigma_y|z+\rangle = i|z-\rangle$$

Define  $X_1 = \sigma_x^1\sigma_y^2\sigma_y^2$ ,  $X_2 = \sigma_y^1\sigma_x^2\sigma_y^3$ , and  $X_3 = \sigma_y^1\sigma_y^2\sigma_x^3$ .

$$X_1|z+z+z+\rangle = i^2|z-z-z-\rangle = -|z-z-z-\rangle.$$

The GHZ state is an eigenstate of  $X_1$ ,  $X_2$  and  $X_3$ . Suppose we measure  $S_x^1$ , yielding  $\pm 1$ . Likewise, we could measure other components of other particles.

$X_1|\phi\rangle = |\phi\rangle \Rightarrow m_x^1m_y^2m_y^2 = +1$  (and similar for other the other two operators). Additionally, we can take the product of these three results to claim  $m_x^1m_x^2m_x^3 = +1$ . We claim this is an eigenvalue of an operator called  $X_{123} = \sigma_x^1\sigma_x^2\sigma_x^3$ . The associated eigenvalue is  $-1 = m_x^1m_x^2m_x^3 = +1$ . The error is trying to apply the three operators at the same time. We cannot simultaneously attribute x and y values of the spin of a particle. We can measure them, but we can't claim they are preexisting "real" quantities.

# Chapter 2

## The Schrödinger Equation

### 2.1 The Unitary Time-Development Operator

Classical Phase Space: Given an initial condition,  $\vec{F} = m\vec{a}$  implies the system evolves along some unique path which does not cross any other path.  $\gamma(t)$  is uniquely determined by its initial state  $\gamma(0)$ .

$$\frac{d}{dt}\vec{\gamma}(t) = \bar{J}\frac{\partial H}{\partial \vec{\gamma}}, \text{ where } \bar{J} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}.$$

Quantum Hilbert Space: Let  $|\psi_t\rangle$  represent a state at time  $t$  after some initial state  $|\psi_0\rangle$ .

$$i\hbar\frac{\partial}{\partial t}|\psi_t\rangle = H|\psi_t\rangle \text{ for a Hamiltonian } H.$$

$$\frac{d}{dt}\langle\phi_t|\psi_t\rangle = \langle\phi_t|\frac{d}{dt}\psi_t\rangle + \left(\frac{d}{dt}\langle\phi_t|\right)|\psi_t\rangle = 0$$

because

$$\frac{d}{dt}\langle\phi_t| = \left(\frac{d}{dt}|\phi_t\rangle\right)^\dagger = \left(-\frac{i}{\hbar}H|\phi_t\rangle\right)^\dagger$$

and  $|\frac{d}{dt}\psi_t\rangle = \left(-\frac{i}{\hbar}H|\psi_t\rangle\right)$ . This implies the inner product is invariant under time evolution given the same Hamiltonian. This also implies  $\frac{d}{dt}\|\psi_t\rangle\| = \frac{d}{dt}\langle\psi|\psi\rangle = 0$ . This is an analog of the Classical Liouville theorem involving preservation of phase space volume with time evolution.

Consider a mapping  $T$  (the time-evolution operator) which takes a state from an earlier time to a later time. This mapping should be independent of initial condition, mapping the entire Hilbert space to itself. Additionally, it should be linear to maintain completeness.

$$|\psi_t\rangle = T(t, t')|\psi_{t'}\rangle \text{ for any state.}$$

$$\langle\phi_t|\psi_t\rangle = \langle\phi_{t'}|T^\dagger(t, t')T(t, t')|\psi_{t'}\rangle$$

takes both the ket and bra vector from  $t' \rightarrow t$ . The inner product tells us that this is equal to  $\langle\phi_{t'}|\psi_{t'}\rangle$ , and this holds for any pair of vectors. This tells us that  $T^\dagger T = I$ , so  $T$  must be a unitary operator.

Say we knew how the system evolves from  $t' \rightarrow t$ , and we knew how things evolved from  $t'' \rightarrow t'$  (here  $t > t' > t''$ ). We can compose these operators to figure out how to get from  $t'' \rightarrow t$ .

N.B.

The Hamiltonian could be time-dependent, so the time evolution operator at later times might be different than the operator at earlier times (for example, a magnetic field switched on at a later time).

$$T(t, t')T(t', t'') = T(t, t'')$$

Also, if we look at the adjoint,  $T^\dagger(t, t') = T^{-1}(t, t')$ . If we say that  $T$  is a map from earlier times to later times, and we know the map is one-to-one, then  $T^\dagger(t, t') = T^{-1}(t, t') = T(t', t)$ .

Additionally,  $T(t, t) = I$

### Note

For a general unitary operator  $U$ , we can introduce an orthonormal basis  $\{|b_j\rangle\}$ . We can find the matrix elements from  $\langle b_j | U | b_k \rangle = U_{jk}$  and  $U = \sum_{jk} |b_j\rangle U_{jk} \langle b_k|$ . Additionally,  $UU^\dagger = U^\dagger U = I$ . This tells us that the rows and columns of  $U$  form a set of orthonormal vectors.

For a general 2x2 unitary matrix,  $U = \begin{bmatrix} \alpha & \beta \\ -\beta^* & \alpha^* \end{bmatrix}$  where  $|\alpha|^2 + |\beta|^2 = 1$ . There could have been other choices which preserve orthogonality, but that could violate normalization (unless our choice had unitary magnitude). Therefore,  $U$  is unique up to a phase,  $U = e^{i\phi} \begin{bmatrix} \alpha & \beta \\ -\beta^* & \alpha^* \end{bmatrix}$ . In general, we can represent  $U$  as  $U = e^{iK} = I + iK + \sum_{n=1}^{\infty} \frac{1}{n!} i^n K^n$ , where  $K^\dagger = K$  is also unitary.

$$i\hbar \frac{d}{dt} |\psi_t\rangle = i\hbar \frac{d}{dt} T(t, t') |\psi_{t'}\rangle = H |\psi_t\rangle = HT(t, t') |\psi_{t'}\rangle. \text{ Therefore}$$

$i\hbar \frac{\partial}{\partial t} T(t, t') = HT(t, t')$ . This is a first-order linear differential equation, so there is an exact formal solution. It can be evaluated if  $H$  is time dependent, but let's focus on the special case where it isn't.

$$\frac{1}{T} \frac{\partial T}{\partial t} = -\frac{i}{\hbar} H = \frac{\partial}{\partial t} \ln T,$$

where  $S = \ln T \Rightarrow e^S = T$ . If  $H$  is time-independent,

$$\ln T = \frac{-i}{\hbar} H \cdot (t - t'), \text{ imposing the initial condition where } T(t, t) = I. \text{ Therefore, } T(t, t') = T(t - t') = e^{-\frac{i}{\hbar} H \cdot (t - t')}.$$

Suppose we knew the eigenvectors and eigenvalues of the Hamiltonian. We could then take the spectral decomposition of the Hamiltonian,

$$H = \sum_j E_j P_j, \text{ where } P_j = |\psi_j\rangle \langle \psi_j|.$$

$$H^2 = \sum_{jk} E_j E_k P_j P_k = \sum_{jk} E_j E_k \delta_{jk} P_j, \text{ so}$$

$$T(t - t') = \sum_j e^{-\frac{i}{\hbar} E_j \cdot (t - t')} P_j.$$

$$e^{-\frac{i}{\hbar} H \cdot (t - t')} |\psi_j\rangle = (I - \frac{i}{\hbar} H \cdot (t - t') - \frac{1}{2} \frac{1}{\hbar^2} H^2 \cdot (t - t')^2 + \dots) |\psi_j\rangle = (I - \frac{i}{\hbar} E_j \cdot (t - t') - \dots) |\psi_j\rangle$$

## 2.2 Multi-time Born Rule

$\Pr(P_t | |\psi_{t'}\rangle) = \Pr(P_t | |\psi_t\rangle)$  where  $|\psi_t\rangle = T(t - t') |\psi_{t'}\rangle$ . This is equivalent to  $\|P_t T(t, t') |\psi_{t'}\rangle\|^2$ .

### N.B.

$$\Pr(|\psi_t\rangle | |\psi_{t'}\rangle) = \|\langle \psi_t | T(t, t') |\psi_{t'}\rangle\|^2 = \|\langle \psi_t | \psi_{t'}\rangle\|^2 = 1$$

assuming we are working with normalized vectors. This is a demonstration of the determinism of time-evolution.

### 2.2.1 Bloch Sphere

“A handy way to relate ket vectors in Hilbert space to spin orientations in physical space”  
 - Dr. Widom

General spin- $\frac{1}{2}$ :

$$|\psi\rangle = \alpha|z+\rangle + \beta|z-\rangle$$

Normalize:  $|\alpha|^2 + |\beta|^2 = 1$

We can use a phase choice:  $\alpha \geq 0$

This gives us another way to write the general ket vector:

$$|\psi\rangle = \cos \frac{\theta}{2}|z+\rangle + \sin \frac{\theta}{2}e^{i\phi}|z-\rangle$$

with  $0 \leq \theta \leq \pi$ ,  $0 \leq \phi \leq 2\pi$ . Define  $\cos \theta = z_c$ ,  $\sin \theta \cos \phi = x_c$ , and  $\sin \theta \sin \phi = y_c$ . If we do this,  $|\alpha|^2 + |\beta|^2 = x_c^2 + y_c^2 + z_c^2 = 1$ , so we can represent spin vectors as locations on a sphere (the Bloch sphere).

The vector  $|z+\rangle$  sits at the top of the sphere and  $|z-\rangle$  on the bottom.  $|x\pm\rangle$  and  $|y\pm\rangle$  similarly sit on their corresponding axes.

$\langle z-|z+\rangle = 0$ , but on the Bloch sphere, these points are not perpendicular.

### 2.2.2 Pauli Matrices

$S_x = \frac{\hbar}{2}\sigma_x$ , where  $\sigma_x$  is now a dimensionless spin operator, called a Pauli matrix.

$S_x|x\pm\rangle = \pm\frac{\hbar}{2}|x\pm\rangle$ , so  $\sigma_x|x\pm\rangle = \pm|x\pm\rangle$ , therefore

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \text{ and } \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The Pauli matrices with the identity form a basis of any  $2 \times 2$  matrix. If we choose  $M = a_0I + a_X\sigma_x + a_y\sigma_y + a_z\sigma_z$ , we find that  $M = \begin{pmatrix} a_0 + a_z & a_x - ia_y \\ a_x + ia_y & a_0 - a_z \end{pmatrix} = a_0I + \vec{a} \cdot \vec{\sigma}$ .

## 2.3 Hermitian Matrices

$$M^\dagger = M \implies a_j \in \mathbb{R}$$

Let us define  $\hat{n} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$ , so  $S_n \equiv \hat{n} \cdot \vec{S} = \frac{\hbar}{2}\hat{n} \cdot \vec{\sigma} = \frac{\hbar}{2} \begin{pmatrix} \cos \theta & \sin \theta e^{-i\phi} \\ \sin \theta e^{i\phi} & -\cos \theta \end{pmatrix}$ .

You can apply trig identities to show that  $S_n|\hat{n}\pm\rangle = \pm\frac{\hbar}{2}|\hat{n}\pm\rangle$ .

### 2.3.1 Other Useful Facts

$\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = I$ , and  $\sigma_j\sigma_k = i\epsilon_{jkl}\sigma_l$ . We can also exponentiate the matrices:

$e^{i\theta\hat{n} \cdot \vec{\sigma}} = I + i\theta\hat{n} \cdot \vec{\sigma} + \frac{1}{2}(i\theta)^2(\hat{n} \cdot \vec{\sigma})^2 + \dots = I \cos \theta + i\hat{n} \cdot \vec{\sigma} \sin \theta$ . This is a generalization of the De Moivre formula to the space of operators.

## 2.4 Density Operator

$$\text{Tr}\rho = 1$$

For pure states,  $\text{Tr}\rho^2 = 1$ , and for mixed states, it is  $< 1$ .

General spin- $\frac{1}{2}$ :

$$\rho = \frac{1}{2}(I + \rho_x\sigma_x + \rho_y\sigma_y + \rho_z\sigma_z)$$

The trace of this must be less than or equal to 1 if we want it to be a density matrix.

$$\langle S_x \rangle = \frac{\hbar}{2} \text{Tr}(\rho\sigma_x) = \frac{\hbar}{2} \frac{1}{2} 2\rho_x = \frac{\hbar}{2}\rho_x, \text{ so } \langle \vec{S} \rangle = \frac{\hbar}{2}\vec{\rho}$$

Is  $\rho$  a pure or mixed state?

$$\text{Tr}\rho^2 = \text{Tr}\frac{1}{4}(I^2 + \rho_x I\sigma_x + \rho_y I\sigma_y + \rho_z I\sigma_z + \rho_x\sigma_x I + \rho_x^2\sigma_x^2 + \dots)$$

This is just  $\frac{1}{2}(1 + \rho_x^2 + \rho_y^2 + \rho_z^2) \leq 1$ .

If a single  $\rho_j = 1$ , the others are zero, so you would have a pure state. On the other hand, if multiple  $\rho_j$  are nonzero, this would be a mixed state. Pure states are on the surface of the Bloch sphere, whereas mixed states are points in its interior.

### Spin-1/2 in a Constant Magnetic Field

$$\vec{B} = B\hat{n}$$

$$H = -\vec{\mu} \cdot \vec{B}$$

$$\vec{\mu} = \gamma\vec{S} = \frac{1}{2}\hbar\gamma\vec{\sigma}$$

Define Armor frequency  $\omega = -\gamma B$

Let  $\vec{B} = B\hat{z}$ :

$$H = \frac{1}{2}\hbar\omega\sigma_z = \frac{1}{2}\hbar\omega \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$T(t) = e^{-itH/\hbar} = \begin{bmatrix} e^{-it\omega/2} & 0 \\ 0 & e^{it\omega/2} \end{bmatrix}$$

Let's start with the state  $|\psi_0\rangle = \begin{pmatrix} 1 \\ \beta \end{pmatrix}$ . Acting with the time operator, we see that  $|\psi_t\rangle = e^{-i\omega t/2} \begin{pmatrix} 1 \\ \beta e^{i\omega t} \end{pmatrix}$ . We can see that the spin-up component stays constant in time relative to the phase, but the other component rotates around the Bloch sphere at the Larmor frequency.

Take an arbitrary magnetic field in direction  $\hat{n}$ . Now  $T(t) = e^{i\hat{n} \cdot \vec{\sigma}\omega t/2} = \cos \frac{\omega t}{2} I - i \sin \frac{\omega t}{2} \hat{n} \cdot \vec{\sigma}$ .

Now suppose  $\hat{n} = \hat{y}$ , and  $\sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$ , so  $T(t) = \begin{bmatrix} \cos \frac{\omega t}{2} & -\sin \frac{\omega t}{2} \\ \sin \frac{\omega t}{2} & \cos \frac{\omega t}{2} \end{bmatrix}$ . Starting in the state  $|\psi_0\rangle = |z+\rangle$ , we find  $|\psi_t\rangle = \begin{pmatrix} \cos \frac{\omega t}{2} \\ \sin \frac{\omega t}{2} \end{pmatrix}$ . Let's calculate  $\text{Pr}([z+]_t | |\psi_t\rangle) = \langle \psi_t | z+ \rangle \langle z+ | \psi_t \rangle = \cos^2 \frac{\omega t}{2}$ . We can also see that  $\text{Pr}([x+]_t | |\psi_t\rangle) = \frac{1}{2} \cos \frac{\omega t}{2} \sin \frac{\omega t}{2}$ . The spin projection is rotating around the  $\hat{y}$  axis at the Larmor frequency.

### Generalization of Time-Dependent Spin Hamiltonian

$$H = \frac{1}{2} \hbar \vec{\omega}(t) \cdot \vec{\sigma}$$

$$\vec{\omega}(t) = \omega(t) \hat{n}(t)$$

$$T(t + \Delta t, t) \approx e^{-i(\omega(t)\hat{n}(t) \cdot \vec{\sigma}/2)\Delta t}$$

If  $|\vec{\omega}|$  is constant and  $\hat{n}$  rotates around a fixed axis at a fixed rate, we can find the exact solution. For instance, we could have  $\vec{\omega}(t) = \omega_z \hat{z} + \omega_p (\cos(\omega_r t) \hat{x} + \sin(\omega_r t) \hat{y})$ . In NMR,  $\omega_z$  is related to the large polarizing magnet while  $\omega_p$  is related to the RF pulse.

Let us now look at this in a co-rotating coordinate system.

$$|\psi\rangle = \sum_j \langle b_j | \psi \rangle |b_j\rangle = \sum_j |b_j\rangle \langle b_j| |\psi\rangle$$

$$\{|b_j\rangle\} \rightarrow \{|\bar{b}_j\rangle\}$$

$$\langle \bar{b}_k | \psi \rangle = \langle \bar{b}_k \sum_j |b_j\rangle \langle b_j| \psi \rangle = \sum_j U_{kj} \langle b_j | \psi \rangle$$

For our system, suppose

$$|\psi\rangle \rightarrow |\bar{\psi}\rangle = S(t) |\psi\rangle$$

so

$$i \frac{d}{dt} |\bar{\psi}\rangle = i \dot{S} |\psi\rangle + S i \frac{d}{dt} |\psi\rangle = i \dot{S} S^\dagger |\bar{\psi}\rangle + S H S^\dagger |\bar{\psi}\rangle$$

is the equation of motion in our rotating coordinate system. We can re-characterize this as the combination of two Hamiltonians,  $\bar{H}_1 = i \dot{S} S^\dagger$  and  $\bar{H}_0 = S H S^\dagger$ . Our old Hamiltonian was

$$H_0 = \frac{1}{2} \omega_z \sigma_z + \frac{1}{2} \omega_p \begin{pmatrix} 0 & \cos \omega_r t - i \sin \omega_r t \\ \cos \omega_r t + i \sin \omega_r t & 0 \end{pmatrix}$$

$$S(t) = \begin{pmatrix} e^{i\omega_r t/2} & 0 \\ 0 & e^{-i\omega_r t/2} \end{pmatrix}$$

$\bar{H}_1 = -\frac{1}{2} \omega_r \sigma_z$  and

$$\bar{H}_0 = \frac{1}{2} \omega_z \sigma_z + \frac{1}{2} \omega_p \sigma_x$$

The net result

$$\bar{H} = \bar{H}_0 + \bar{H}_1 = \frac{1}{2}(\omega_z - \omega_r)\sigma_z + \frac{1}{2}\omega_p\sigma_x$$

This is time-independent so we can use our solution from earlier. Note that if  $\omega_z = \omega_r$ , the effective field in the  $z$ -direction can be eliminated, meaning that if we match the frequency of our RF signal to the effect of the large super-conducting magnet, we can cancel its effect. Now the states will progress in the order

$$|\bar{z}+\rangle \rightarrow |\bar{y}-\rangle \rightarrow |\bar{z}-\rangle \rightarrow |\bar{y}+\rangle \rightarrow -|\bar{z}+\rangle$$

where we pick up a phase after one complete rotation. The first motion is a “ $\pi/2$  pulse”, where the characteristic time scale is  $t = \frac{\pi}{2}\frac{1}{\omega_p}$ . If we start with the state  $|\bar{z}+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ , we can write the other states as column vectors,  $|\bar{y}-\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix}$ ,  $|\bar{z}-\rangle = \begin{pmatrix} 1 \\ -i \end{pmatrix}$ ,  $|\bar{y}+\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ -i \end{pmatrix}$ . The motion from  $|\bar{z}+\rangle \rightarrow |\bar{z}-\rangle$  is a “ $\pi$  pulse” with characteristic time scale  $t = \frac{\pi}{\omega_p}$ . The time evolution operator is  $T = e^{-i\frac{1}{2}\omega_p t \sigma_x}$ .

This was in the “on resonance” condition, where  $\omega_r = \omega_z$ . In the “off resonance” condition, let’s call the distance off of the resonant condition  $\delta = \omega_z - \omega_r$ .

Now,

$$H = \frac{1}{2}\delta\sigma_z + \frac{1}{2}\omega_p\sigma_x = \frac{1}{2} \begin{pmatrix} \delta & \omega_p \\ \omega_p & -\delta \end{pmatrix}$$

Eigenstates and eigenvalues are:

$$|\phi\rangle = (\dots) \begin{pmatrix} \delta \pm \sqrt{\delta^2 + \omega_p^2} \\ -\omega_p \end{pmatrix}$$

$$\lambda = \pm \frac{1}{2}\Omega = \pm \frac{1}{2}\sqrt{\delta^2 + \omega_p^2}$$

$$\bar{T} = e^{-i\bar{H}t} = e^{i\Omega t/2} |\phi_+\rangle \langle \phi_+| + e^{i\Omega t/2} |\phi_-\rangle \langle \phi_-|$$

$$\text{Pr}([z-]_t) = \|[\bar{z}-]_t \bar{T}(t) |\bar{z}+\rangle_0\|^2$$

So the maximum probability of being flipped into the  $|z-\rangle$  state decreases the further off-resonance you are.

### 2.4.1 Sample Spaces

Take some space of samples  $\mathcal{S}$  with samples  $s \in \mathcal{S}$  with probability  $p_s$  of occurring. For some random variable on the samples  $V(s)$ , we can find the average value of the outcome as

$$\langle V \rangle = \sum_s p_s V(s).$$

For some indicator  $E(s)$ , we are defining a subspace of the sample space (all the dice rolls that turn up even, for example). The probability of getting a state with that particular indicator is

$$\text{Pr}(E) = \sum_{s \in E} p_s.$$

Say we have two random variables  $V(s)$  and  $W(s)$ . We can now talk about joint probabilities. For instance, let’s create two events,  $E$  is the event where  $V = v$  and  $F$  is the event where  $W = w$ :

$$\text{Pr}(V = v, W = w) = \sum_{s \in E \cap F} p_s = \langle EF \rangle.$$

**Example.** Fair 6-sided Die

$$\mathcal{S} = \{1, 2, 3, 4, 5, 6\}, \quad p_s = \frac{1}{6}$$

$V(s)$  = “parity”

$$W(s) = (s - 3)^2$$

v \ w	w = 0	w = 1	w = 4	w = 9	TOTALS
v = even	0	2/6	0	1/6	1/2
v = odd	1/6	0	2/6	0	1/2
TOTALS	1/6	2/6	2/6	1/6	1

Marginal probabilities: If you start with the joint probabilities for many variables and sum over all the probabilities for one of them, you get the marginal probability (the probabilities in the “TOTALS” rows and columns).  $\diamond$

## 2.5 Conditional Probability

$\Pr(A | B) = \Pr(A, B) / \Pr(B)$  reads as “the probability of A given B”

### 2.5.1 Examples

$$\Pr(v = \text{odd} | w = 4) = \Pr(\text{odd}, 4) / \Pr(4) = \frac{1}{3} / \frac{1}{3} = 1$$

$$\Pr(w = 4 | v = \text{odd}) = \Pr(4, \text{odd}) / \Pr(\text{odd}) = \frac{2}{6} / \frac{1}{2} = \frac{4}{6}$$

## 2.6 Statistical Independence

If we have a joint probability of two events,

$$\Pr(A, B) = \Pr(A) \cdot \Pr(B)$$

and

$$\Pr(\neg A, B) = \Pr(\neg A) \cdot \Pr(B) \text{ etc.}$$

are conditions which must be met for the events to be statistically independent.

**Example.**

$$\Pr(s = 1 \text{ or } 6, s = \text{even}) = \sum_{s \in \{1, 6\} \cap \{2, 4, 6\}} p_s = p_6 = \frac{1}{6}$$

$$\Pr(s = 1 \text{ or } 6) = \frac{2}{6}$$

$$\Pr(s = \text{even}) = \frac{3}{6}$$

We can continue through the other conditions to show that these events are independent. However, if we had the probability of rolling 2 or 6 instead of 1 or 6, we would find that these conditions are not satisfied, since all 2 and 6 rolls will also be even rolls.  $\diamond$

## 2.7 Quantum Statistics

We want this to be the same as the Classical case. However, there must be some differences (for instance, non-commuting operators). Our method to avoid these difficulties is called the “single framework rule”. Suppose  $V = v_1P_1 + v_2P_2 + v_3P_3$  and  $W = w_1P_1 + w_2Q_2 + w_3Q_3$ . Let’s imagine  $P_2Q_2 \neq Q_2P_2$  and  $P_3Q_3 \neq Q_3P_3$ . If we were to talk about values of  $V$  and  $W$ , we are forbidden from making statements about joint probabilities for all values of the operators. However, some statements can still be made. For example, if we took, as our sample space,  $\mathcal{P} = \{P_1, I - P_1\}$  (note  $I - P_1 = P_2 + P_3 = Q_2 + Q_3$ ) we can say things like  $\Pr(v_1, w_1)$ ,  $\Pr(v_1, \neg w_1)$ , etc. as long as we only talk about things in commuting subspaces.

Can we say that  $\neg(V = v_1) = (V = v_2)$  or  $(V = v_3)$ ? No, we cannot interpret this in such a way if we include  $W$  in our space of operators.

## 2.8 Sequences of Outcomes

Suppose we have a sequence of values  $\{s_0, s_1, \dots, s_f\}$  in a particular order. We can write this as a vector  $\vec{s}$  if we want.

$$\vec{s} \in \mathcal{S} \times \mathcal{S} \times \dots \times \mathcal{S} = S^f$$

is a cartesian product. We could use different sample spaces if we want. We require  $0 \leq \Pr(\vec{s}) \leq 1$  and  $\sum_{\vec{s}} \Pr(\vec{s}) = 1$ .

We can also calculate marginal probabilities

$$\Pr_j(s_j) = \sum_{s_0, s_1, \dots, s_{j-1}} \sum_{s_{j+1}, \dots, s_f} \Pr(s_0 s_1 \dots s_{j-1} s_j s_{j+1} \dots s_f)$$

These can tell us about any particular instance, but they won’t tell us anything about correlations.

## 2.9 Markov Process

This occurs when  $s_{j+1}$  is correlated with  $s_j$  but not  $s_{j-i}$  where  $i > 0$ . In this case,  $\Pr(s_0, s_1) = \Pr(s_1 | s_0)\Pr(s_0)$ ,  $\Pr(s_0, s_1, s_2) = \Pr(s_2 | s_1)\Pr(s_0, s_1)$ . This is sometimes true in general cases but it is always true in Markov processes.

# Chapter 3

## Multiple Time Histories

LECTURE 13: INTRODUCTION TO CONSISTENT HISTORIES  
 Wednesday, September 18, 2019

Classical Case:

$$\mathcal{S}_0, \mathcal{S}_1, \dots, \mathcal{S}_f$$

$$\vec{s} = (s_0, s_1, \dots, s_f) \in \mathcal{S}_0 \times \mathcal{S}_1 \times \dots \times \mathcal{S}_f = \tilde{\mathcal{S}}$$

The dimension of the total space is just the dimensions of each time step added together.

In Quantum, we have

$$\tilde{\mathcal{H}} = \mathcal{H}_0 \odot \mathcal{H}_1 \odot \dots \odot \mathcal{H}_f$$

with a basis

$$\{|\alpha_i\rangle \odot |\beta_j\rangle \odot \dots \odot |\omega_k\rangle\}$$

for  $\alpha_i$  at time  $t_0$ ,  $\beta_j$  at  $t_1$ , etc. We can form a “history”

$$Y = \sum_{ij\dots k} c_{ij\dots k} |\alpha_i\rangle \odot |\beta_j\rangle \odot \dots \odot |\omega_k\rangle$$

We can also have a product history for multiple states:

$$Y^{\vec{\alpha}} = P_0^{\alpha_0} \odot P_1^{\alpha_1} \odot \dots \odot P_f^{\alpha_f}$$

This means we have some certain property  $\alpha_0$  at time 0, another at time 1, etc.

The histories are mutually exclusive.

$$Y^{\vec{\alpha}} Y^{\vec{\beta}} = \delta_{\vec{\alpha}\vec{\beta}} Y^{\vec{\alpha}}$$

where the  $\delta$  vanishes if the vectors are different at any instant in time (any component is different).

$$\sum_{\vec{\alpha}} Y^{\vec{\alpha}} = \tilde{I} = I_0 \odot I_1 \odot \dots \odot I_f$$

**Example.** Product Space

$$\begin{aligned} Y_1 &= [z+]_0 \odot [x+]_1 \\ Y_2 &= [z+]_0 \odot [x-]_1 \\ Y_3 &= [z-]_0 \odot [x+]_1 \\ Y_4 &= [z-]_0 \odot [x-]_1 \end{aligned}$$

Check mutual exclusivity: For the first two, at time 0, we get  $[z+][z+]$  which is okay, but at time 1, we have  $[x+][x-]$ , which means the whole product vanishes.

$$Y_1 + Y_2 = [z+]_0 \odot I_1$$

$$Y_3 + Y_4 = [z-]_0 \odot I_1$$

and

$$Y_1 + Y_2 + Y_3 + Y_4 = I_0 \odot I_1 = \tilde{I}$$

◇

**Example.** Non-Product Space

$$Y_1 = [z+]_0 \odot [x+]_1$$

$$Y_2 = [z+]_0 \odot [x-]_1$$

$$Y_3 = [z-]_0 \odot [y+]_1$$

$$Y_4 = [z-]_0 \odot [y-]_1$$

This forms a complete and orthonormal set of histories.

◇

**Example.** Specified Initial Condition Suppose we specify that we are initially in state  $|\psi_0\rangle$ :

$$|\psi_0\rangle \implies I_0 = [\psi_0] + (I_0 - [\psi_0])$$

$$Y^{\vec{\alpha}} = [\psi_0] \odot P_1^{\alpha_1} \odot \cdots \odot P_f^{\alpha_f}$$

$$Z = (I - [\psi_0]) \odot I_1 \odot \cdots \odot I_f$$

◇

Single Time Born Rule:

$$Pr(P_0^{\alpha_0} | \psi_0) = |P_0^{\alpha_0} |\psi_0\rangle|^2 = \langle \psi_0 | P_0^{\alpha_0} |\psi_0\rangle$$

Time Evolution

$$\begin{aligned} |\psi_1\rangle &= T_{10} |\psi_0\rangle \\ Pr(P_1^{\alpha_1} | \psi_0) &= Pr(P_1^{\alpha_1} | \psi_1) \\ &= \langle \psi_1 | P_1^{\alpha_1} |\psi_1\rangle = \langle \psi_0 | T_{10} P_1^{\alpha_1} T_{10} |\psi_0\rangle \end{aligned}$$

### 3.0.1 Two-time history family

$$Y^k = [\psi_0] \odot [\phi_1^k]$$

means we start in the state  $\psi_0$  and end up in the state  $\phi_1^k$ . We can now discuss the probability of ending up in that state.

$$Z = (I - 0 - [\psi_0]) \odot I_1$$

$$\begin{aligned} Pr(Y^k) &= Pr(\phi_1^k | \psi_0) \\ &= \langle \psi_0 | T_{01} |\phi_1^k\rangle \langle \phi_1^k | T_{10} | \psi_0 \rangle \\ &= |\langle \phi_1^k | T_{10} | \psi_0 \rangle|^2 = |\langle \phi_1^k | \psi_1 \rangle|^2 \end{aligned}$$

Check  $\sum_k Pr(Y^k) + Pr(Z) = 1$

**Example.** Spin- $\frac{1}{2}$  in  $\vec{B} = B\hat{z}$

$$T(t) = \begin{bmatrix} e^{i\omega t/2} & 0 \\ 0 & e^{-i\omega t/2} \end{bmatrix}$$

$$Y^+ = [x+]_0 \odot [x+]_1$$

$$Y^- = [x+]_0 \odot [x-]_1$$

$$Z = [x-]_0 \odot I_1$$

$$\Pr(Y^+) = \cos^2(\omega t/2)$$

$$\Pr(Y^-) = \sin^2(\omega t/2)$$

The Born rule here allows us to talk about probabilities without invoking the notion of measurement. We are not thinking about collapsing wavefunctions. There is no notion of it in this formulation.  $\diamond$

## LECTURE 14: COMPATIBLE PROPERTIES IN HISTORIES

Fri Sep 20 2019

We don't want to make the mistake of discussing incompatible properties. To do this with histories, we start with some family of histories  $\{Y^\alpha\}$  and we require  $Y^\alpha Y^\beta = Y^\beta Y^\alpha, \forall \alpha, \beta$ . This is a complete family of histories, so  $\sum_{\vec{\alpha}} Y^{\vec{\alpha}} = \tilde{I}$ . Therefore, **logical negation** is  $\neg Y^{\vec{\alpha}} = \tilde{I} - Y^{\vec{\alpha}}$ .

**Example.** Coin toss:  $\{(H, H), (H, T), (T, H), (T, T)\}$ . The negation of  $(H, H)$  is  $\neg(H, H) = \{(H, T), (T, H), (T, T)\}$   $\diamond$

**Example.**

$$\neg[z+] \odot [x+] = [z-] \odot [x+] + [z+] \odot [x-] + [z-] \odot [x-]$$

$\diamond$

We can also have **conjunction**,  $Y \wedge Y' = YY'$ .

**Example.**

$$Y = [z+]_0 \odot I_1$$

$$Y' = I_0 \odot [x+]_1$$

$$YY' = [z+] \odot [x+]$$

$\diamond$

Additionally, **disjunction** is defined by  $Y \vee Y' = Y + Y' - YY'$ .

### 3.1 Chainket

If we start in a pure state, we can define a product history

$$Y^{\vec{\alpha}} = [\psi_0] \odot P_1^{\alpha_1} \odot \dots \odot P_f^{\alpha_f} \in \tilde{\mathcal{H}}$$

**Definition 3.1.1.** A **chainket** is defined by

$$|\vec{\alpha}\rangle = P_f^{\alpha_f} T_{f,f-1} \dots T_{21} P_1^{\alpha_1} T_{10} |\psi_0\rangle$$

**Theorem 3.1.1.** *Generalized Born Rule:*

$$\Pr(\vec{\alpha}) = \langle \vec{\alpha} | \vec{\alpha} \rangle$$

Is it correct? Let's check some cases.

### 3.1.1 Two-Time History

$$Y^k = [\psi_0] \odot [\phi_1^k]$$

All of our states start at  $|\psi_0\rangle$ , so we need to define a complete set of histories by adding all the things that don't start there:

$$Z = (I - [\psi_0]) \odot I_1$$

The chainket for this state is

$$\begin{aligned} |k\rangle &= [\phi_1^k] T_{10} |\psi_0\rangle \\ \langle k|k\rangle &= \langle \psi_0 | T_{01} | \phi_1^k \rangle \langle \phi_1^k | T_{10} | \psi_0 \rangle = |\langle \phi_1^k | \psi_1 \rangle|^2 = \text{Pr}([\phi_1^k] | \psi_0) \end{aligned}$$

N.B.

$$|\langle \phi_1^k | \psi_1 \rangle|^2 = \langle \phi_1^k | \psi_1 \rangle \langle \psi_1 | \phi_1^k \rangle = \langle \psi_1 | (\phi_1^k)^2 | \psi_1 \rangle = \langle \psi_1 | [\phi_1^k] | \psi_1 \rangle$$

### 3.1.2 Unitary History

$$\begin{aligned} |\psi_0\rangle &\rightarrow |\psi_1\rangle = T_{10} |\psi_0\rangle \rightarrow |\psi_2\rangle = T_{21} |\psi_1\rangle = T_{20} |\psi_0\rangle \\ U &= [\psi_0] \odot [\psi_1] \odot [\psi_2] \end{aligned}$$

$$|U\rangle = |\psi_2\rangle \langle \psi_2 | T_{21} |\psi_1\rangle \langle \psi_1 | T_{10} |\psi_0\rangle$$

There's another way of thinking about this:

$$|U\rangle = |\psi_2\rangle \xrightarrow{\langle \psi_2 | T_{21}} |\psi_1\rangle \xrightarrow{\langle \psi_1 | T_{10}} |\psi_0\rangle$$

so

$$\text{Pr}(U) = \langle U | U \rangle = \langle \psi_2 | \psi_2 \rangle = 1$$

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LECTURE 15: HISTORY SAMPLE SPACE  
Fri Sep 20 2019

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## 3.2 Consistent Histories

$$\begin{aligned} Y^1 &= [z+] \odot [x+] \odot [z+] \\ Y^2 &= [z+] \odot [x+] \odot [z-] \\ Y^3 &= [z+] \odot [x-] \odot [z+] \\ Y^4 &= [z+] \odot [x-] \odot [z-] \\ Z &= [z-] \odot I \odot I. \end{aligned}$$

**Definition 3.2.1.** The **History Sample Space** of a group of histories is  $Y^{\vec{\gamma}} = Y^{\vec{\alpha}} + Y^{\vec{\beta}}$ , where  $Y^{\vec{\alpha}} Y^{\vec{\beta}} = 0$ .

Because of this second condition,  $|\vec{\gamma}\rangle = |\vec{\alpha}\rangle + |\vec{\beta}\rangle$ , and  $\text{Pr}(\vec{\gamma}) = \text{Pr}(\vec{\alpha}) + \text{Pr}(\vec{\beta})$ , but when we actually compute  $\text{Pr}(\vec{\gamma})$ , we find that  $\text{Pr}(\vec{\gamma}) = \langle \vec{\gamma} | \vec{\gamma} \rangle = \langle \vec{\alpha} | \vec{\alpha} \rangle + \langle \vec{\beta} | \vec{\beta} \rangle + \langle \vec{\alpha} | \vec{\beta} \rangle + \langle \vec{\beta} | \vec{\alpha} \rangle$ . It seems like our Generalized Born Rule has failed, due to these last two cross-terms! How can we get around this? If we require "consistency", the Rule still works. Consistency is simply demanding that these inner products are zero:

**Definition 3.2.2.** A History Sample Space is **consistent** if

$$\langle \vec{\alpha} | \vec{\beta} \rangle = 0, \forall \vec{\alpha} \neq \vec{\beta}.$$

With these dynamics, the chainket for history 1 is  $|Y^1\rangle = \frac{1}{2}|z+\rangle$ :

$$|Y^1\rangle = |z+\rangle z+ |I| x+ \rangle x+ |I| z+\rangle$$

$$\langle Y^1 | Y^3 \rangle = \frac{1}{2} \langle z+ | z+ \rangle = \frac{1}{2} \neq 0$$

Ergo, these histories are not consistent.

Let's imagine a system in a magnetic field  $\vec{B} = B\hat{y}$ :

$$T: |z+\rangle \rightarrow |x+\rangle \rightarrow |z-\rangle \rightarrow |x-\rangle \rightarrow -|z+\rangle$$

Under this dynamic(s)?, we find  $|Y^1\rangle = |Y^3\rangle = |Y^4\rangle = 0$ ,  $|Y^2\rangle = |z-\rangle$ , so these histories are consistent in the dynamics of a constant magnetic field.

### 3.3 Beam Splitter

We will again use a discrete toy model space. Say we have three branches on a beam splitter, the branch  $a$  incoming,  $c$  outgoing perpendicular to  $a$ , and  $d$  outgoing parallel to  $a$ . We will call states in  $a$   $\{\dots, -2a, -1a, 0a\}$  going toward the beam splitter from left to right. Similarly,  $\{1c, 2c, 3c, \dots\}$  and  $\{1d, 2d, 3d, \dots\}$  go away from the beam splitter from left to right.

Our basis is  $\mathcal{B} = \{|mz\rangle : z \in a, c, d, m \in \mathbb{Z}\}$

$$T = S \implies S|mz\rangle = |(m+1)z\rangle$$

$$S|0a\rangle = \frac{1}{\sqrt{2}}(|1c\rangle + |1d\rangle)$$

For consistency, we also require a  $b$  branch with states labeled  $\{\dots, -2b, -1b, 0b\}$  going parallel to  $c$  moving towards the beam splitter from left to right.

$$S|0b\rangle = \frac{1}{\sqrt{2}}(-|1c\rangle + |1d\rangle)$$

Our histories are then

$$[0a] \odot \{[1c], [1d]\} \odot \{[2c], [2d]\}$$

$$t=0, |\psi_0\rangle = |0a\rangle$$

$$t=1, |\psi_1\rangle = \frac{1}{\sqrt{2}}(|1c\rangle + |1d\rangle)$$

$$t=2, |\psi_2\rangle = \frac{1}{\sqrt{2}}(|2c\rangle + |2d\rangle)$$

$$|(0a, 1c, 2c)\rangle = \frac{1}{\sqrt{2}}|2c\rangle$$

$$|(0a, 1d, 2d)\rangle = \frac{1}{\sqrt{2}}|2d\rangle$$

$$Pr([1c]_1, [2c]_2 \mid [0a]_0) = \frac{1}{2} = Pr([1d]_1, [2d]_2 \mid [0a]_0)$$

Additionally, we can calculate marginal probabilities from these:

$$Pr([1c]_1 \mid [0a]_0) = \frac{1}{2} = Pr([2c]_2 \mid [0a]_0)$$

$$Pr([1c]_1 \mid [2c]_2) = \frac{Pr([1c]_1, [2c]_2)}{Pr([2c]_2)} = 1$$

$$Pr([2c]_2 \mid [1d]_1) = 0$$

because that chainket would vanish:

$$|(0a, 1d, 2c)\rangle = [2c]_2 T_{21} [1d]_1 T_{10} |0a\rangle = 0$$

In the coming lecture, we will introduce a measurement device on the  $c$ -branch, called  $\hat{c}$ . This device sits in the path and has two states,  $0\hat{c}$  and  $1\hat{c}$ . Now our Hilbert space will have a basis  $\{|mz\hat{c}\rangle\}$ , so the whole space will be  $\mathcal{H} = \mathcal{H}_p \otimes \mathcal{H}_d$ , the product of the particle and detector spaces. Now our time evolution operator becomes  $T = SR$ ,  $R = I \otimes I$  except  $R|2c, 0\hat{c}\rangle = |2c, 1\hat{c}\rangle$ , switching the measurement device from the “ready” state to the “triggered” state. Acting  $R$  on a triggered state resets it to the ready state.

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## LECTURE 16: MEASUREMENT DEVICES

Mon Sep 23 2019

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### 3.4 Beam Splitter Example, Continued

From before, we have a four-port system with a shift operator  $S$  which takes  $|mz\rangle$  to  $|(m+1)z\rangle$ . It takes branch  $a$  to a superposition of branches  $c$  and  $d$ :  $S|0a\rangle = \frac{1}{\sqrt{2}}(|1c\rangle + |1d\rangle)$ . We also have a detector operator  $R$  which adds another dimension to the Hilbert space.  $R|2c, n\hat{c}\rangle = |2c, (1-n)\hat{c}\rangle$ . Therefore, the time evolution operator is  $T = SR$  and  $|\psi_0\rangle \xrightarrow{T} |\psi_1\rangle = \frac{1}{\sqrt{2}}(|1c, 0\hat{c}\rangle + |1d, 0\hat{c}\rangle) \xrightarrow{T} |\psi_2\rangle = \frac{1}{\sqrt{2}}(|2c, 02c, 0\hat{c}\rangle + |2d, 0\hat{c}\rangle) \xrightarrow{T} |\psi_3\rangle = \frac{1}{\sqrt{2}}(|3c, 1\hat{c}\rangle + |3d, 0\hat{c}\rangle)$ .

We can think of the family of histories as a subset of  $\{[mz, n\hat{c}]\}$ :

$$Y^c = [\psi_0]_0 \odot [1c, 0\hat{c}]_c \odot [2c, 0\hat{c}]_c \odot [3c, 1\hat{c}]$$

We claim the chainket for this is nonzero. If we were to apply the projector  $[3c, 0\hat{c}]$  instead, it would vanish.

$$|Y^c\rangle = [3c, 1\hat{c}]T_{32}[2c, 0\hat{c}]T_{21}[1c, 0\hat{c}]T_{09}|\psi_0\rangle = \frac{1}{\sqrt{2}}|3c, 1\hat{c}\rangle$$

There's another history with a non-vanishing chainket:

$$Y^d = [\psi_0]_0 \odot [1d, 0\hat{c}]_1 \odot [2d, 0\hat{c}]_2 \odot [3d, 0\hat{c}]_3$$

$$Pr([1\hat{c}]_3 \mid [2c]_2) = Pr(Y^c) / Pr(Y^d) = 1$$

We could also ask

$$Pr([2c]_2 \mid [1\hat{c}]_3) = 1$$

### 3.4.1 Measurement of Spin- $\frac{1}{2}$

A Stern-Gerlach apparatus allow us to split a beam of electrons (or any spin- $\frac{1}{2}$  particle) into two branches, one for each spin. Let's imagine we start in position  $w$ , go to  $w'$  right before the apparatus,  $w+$  after the detector in the spin-up branch, and  $w-$  after the detector in the spin-down branch. We also have a screen behind the apparatus, so when the electron passes through the device, we can see which branch it went through, but the electron state is destroyed.

$$|z+, w\rangle \rightarrow |z+, w'\rangle \rightarrow |z+, w_+\rangle$$

and

$$|z-, w\rangle \rightarrow |z-, w'\rangle \rightarrow |z-, w_-\rangle$$

Suppose we started in the  $x+$  state:

$$\begin{aligned} |\psi_0\rangle &= |x+, w\rangle = \frac{1}{\sqrt{2}}(|z+, w\rangle + |z-, w\rangle) \\ |x+, w\rangle &\rightarrow |x+, w'\rangle \rightarrow \frac{1}{\sqrt{2}}(|z+, w_+\rangle + |z-, w_-\rangle) \end{aligned}$$

The unitary history is

$$U = [\psi_0]_0 \odot [\psi_1]_1 \odot [\psi_2]_2$$

What can we “discuss” in this unitary history? What makes sense within our framework?

- $[I_s \otimes w_+]$
- $[I_s \otimes w_-]$

where  $I_s$  is the local spin operator. These topics are incompatible with the unitary history because  $[\psi_2][I_s \otimes w_+] \neq [I_s \otimes w_+][\psi_2]$  (remember,  $\psi_0$  is the  $x$ -polarized spin state). Let's then imagine a new family of histories for this state:

$$[\psi_0]_0 \odot [\psi_1]_1 \odot \begin{cases} |z+, w_+\rangle_2 \\ |z-, w_-\rangle_2 \end{cases}$$

along with  $I - [\psi_1]_1$  and  $I - [\psi_0]_0$ , to complete the history. Now surely, while we measure the state on the screen, it must have been measured in the Stern-Gerlach apparatus itself, so we believe we are detecting the state of the particle at time 1. We need a “new” new family of histories:

$$[\psi_0] \odot \begin{cases} |z+, w'\rangle_1 \odot |z+, w_+\rangle_2 \leftarrow Y_+ \\ |z-, w'\rangle_1 \odot |z-, w_-\rangle_2 \leftarrow Y_- \end{cases}$$

Now we can ask about some probabilities:

$$Pr(|z+\rangle_1 | |w_+\rangle_2) = Pr(Y_+)/Pr(Y_+) = 1$$

$$Pr(|z-\rangle_1 | |w_+\rangle_2) = 1$$

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LECTURE 17: MULTIPLE DETECTORS  
Wed Sep 25 2019

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## 3.5 Multiple Detectors on a Beam Splitter

Suppose we have detectors  $C$  between  $1c$  and  $2c$  on a beam splitter path,  $\hat{c}$  between  $2c$  and  $3c$ , and  $\hat{D}$  between  $2d$  and  $3d$ .  $|1c, C^0\rangle \rightarrow |2c, C^*\rangle$ , etc. Our evolution of states is:

$$\begin{aligned}
 |\psi_0\rangle &= |0a\rangle \\
 |\psi_1\rangle &= \frac{1}{\sqrt{2}} \left( |1cC^0\hat{C}^0\hat{D}^0\rangle + |1dC^0\hat{C}^0\hat{D}^0\rangle \right) \\
 |\psi_2\rangle &= \frac{1}{\sqrt{2}} \left( |2cC^*\hat{C}^0\hat{D}^0\rangle + |2dC^0\hat{C}^0\hat{D}^0\rangle \right) \\
 |\psi_3\rangle &= \frac{1}{\sqrt{1}} \left( |3cC^*\hat{C}^*\hat{D}^0\rangle + |3dC^0\hat{C}^0\hat{D}^*\rangle \right)
 \end{aligned}$$

Let's define a family of histories  $F$ :

$$Y^c = [\psi_0] \odot [1cC^0\hat{C}^0\hat{D}^0] \odot [2cC^*\hat{C}^0\hat{D}^0] \odot [3cC^*\hat{C}^*\hat{D}^0]$$

$$Y^d = [\psi_0] \odot [1dC^0\hat{C}^0\hat{D}^0] \odot [2dC^0\hat{C}^0\hat{D}^0] \odot [3dC^0\hat{C}^0\hat{D}^*]$$

These are the only nonzero chainkets in this family.

$$Pr([1c]_1 | C_2^*) = 1$$

$$Pr([1d]_1 | C_2^0) = 1$$

$$Pr([2d]_2 | C_2^0) = 1$$

$$Pr(D_3^* | C_2^0) = 1$$

### 3.5.1 Wave Function Collapse

How would this look if we interpreted it as a wave function collapsing?

$$|\psi_0\rangle \xrightarrow{T} |\psi_1\rangle \xrightarrow{\text{collapse}} \begin{cases} |2cC_2^*\hat{C}_2^0\hat{D}_2^0\rangle & \text{if } C_2^* \\ |2dC_2^0\hat{C}_2^0\hat{D}_2^0\rangle & \text{if } C_2^0 \end{cases} \xrightarrow{T} \begin{cases} |3cC_3^*\hat{C}_3^*\hat{D}_3^0\rangle & \text{Probability } = 1 \\ |3dC_3^0\hat{C}_3^0\hat{D}_3^*\rangle & \text{Probability } = 1 \end{cases}$$

The wave function “collapses” before the second state because of the  $C$  detector. However, if that detector is turned off, does that wave function still collapse? We know the state of that detector even if it's turned off!

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LECTURE 18: INTERFERENCE  
Mon Sep 30 2019

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## 3.6 Interference

Imagine we are throwing baseballs at a wall with two slits (yes, we're just rehashing the double-slit experiment). With baseballs, we notice two things. The baseballs are caught one at a time (they are discrete events), and there is a smooth distribution for where the balls land when they reach the “catcher”. If we take the distributions for balls which go through each slit, the total distribution is equal to the sum of both distributions ( $P_{12} = P_1 + P_2$ ). The conditional probability  $P_1$  is the same whether or not slit 2 is open or closed.

Now let's imagine the same scenario with water waves. We can imagine these waves passing through slits in the wall, and the wave crests coming out of both slits will interfere with each other. If one slit is open and the other closed, we would see some sort of unimodal distribution, but if both are open, we see that  $I_{12} \neq I_1 + I_2$  ( $I$  for “intensity”). The arrival of the wave is continuous (no discrete events for detection). With the waves, there is no analog of conditional probability. Manifestly, if both slits are open, the wave goes through both slits simultaneously, so the conditional probability is meaningless here. We could also

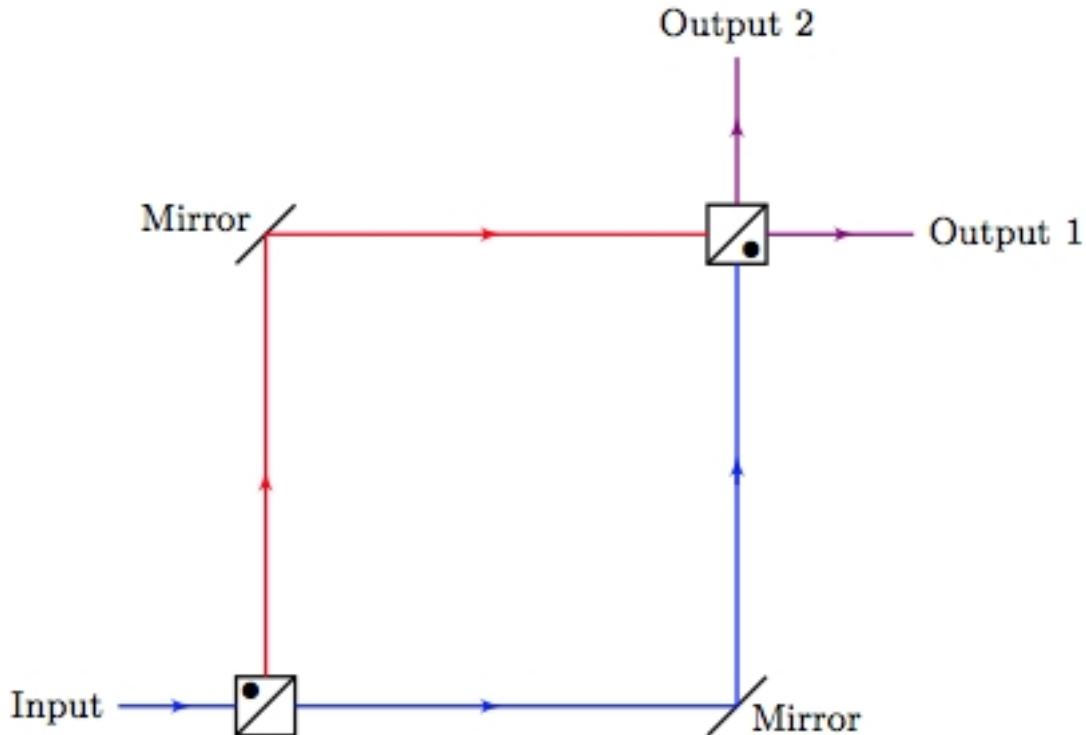
put a phase-shifter behind one or both of the slits (something that slows the wave temporarily). If we put it behind one, we would see the pattern shifted one way or the other, and if we put it behind both, nothing would change. The position of the largest peak depends on the phase difference between the waves leaving both slits.

What would we see if we did this experiment with electrons? Every item of this list has been experimentally verified:

1. Electrons arrive as individual events.
2. Probabilities  $P_{12} \neq P_1 + P_2$ . We see an interference pattern similar to the water waves example.
3. We can detect if a particle goes through the slit by scattering short wavelength photons. However, when we do this,  $P_{12} = P_1 + P_2$ .
4. We can detect if the particle passes through either slit with long wavelength photons (although you wouldn't be able to see which slit the particle goes through. Under this condition, the interference pattern is preserved.
5. If we "weakly" detect the slit (short wavelength, but low intensity, many electrons are not detected at all), we see a partial interference pattern.

Now we can start asking questions. Does the electron go through both slits? The final events are localized, unlike water waves. We detect singular events with definite position on the screen. If we say that the electron is localized, it can't go through both slits. However, there is an interference pattern, which would seem to require that the electron did go through both holes. However, when we use intense, short wavelength light to see which hole the electron passes through, we clearly only detect it going through one or the other.

### 3.6.1 Mach-Zehnder Interferometer



**Figure 3.6.1:** A Mach-Zehnder Interferometer

We will label the following paths. The input in the bottom right of the diagram will be path  $a$ , the downward path from here will be  $b$ , the upward path will go from  $1c$  between the beam splitter and mirror,  $2c$  at the mirror,  $3c$  between the mirror and the second beam splitter, and then  $4f$  after the second beam splitter. The same will follow for the other branch using the labels  $d$  and  $e$ . Our time evolution operator is our shift operator ( $T = S$ ). Here

$$\begin{aligned} S|mz\rangle &= |(m+1)z\rangle \\ S|0a\rangle &= \frac{1}{\sqrt{2}}(|1c\rangle + |1d\rangle) \\ S|0b\rangle &= \frac{1}{\sqrt{2}}(-|1c\rangle + |1d\rangle) \\ S|3c\rangle &= \frac{1}{\sqrt{2}}(|4e\rangle + |4f\rangle) \\ S|3d\rangle &= \frac{1}{\sqrt{2}}(-|4e\rangle + |4f\rangle) \end{aligned}$$

We see that, for the two paths,

$$\begin{aligned} |m\bar{a}\rangle &\equiv \frac{1}{\sqrt{2}}(|mc\rangle + |md\rangle) \\ |m\bar{b}\rangle &\equiv \frac{1}{\sqrt{2}}(-|mc\rangle + |md\rangle) \end{aligned}$$

For example

$$T|3\bar{a}\rangle = \frac{1}{\sqrt{2}}(|4c\rangle + |4d\rangle)$$

Imagine we now have phase shifters  $\phi_{c,d}$  between points 2 and 3 in the respective channels. We say the phase shifters operate as:

$$S|2x\rangle = e^{i\phi_x}|3x\rangle$$

for channel  $x$ .

$$|0a\rangle \rightarrow |1\bar{a}\rangle \rightarrow |2\bar{a}\rangle \rightarrow \frac{1}{\sqrt{2}}(e^{i\phi_c}|3c\rangle + e^{i\phi_d}|3d\rangle) \rightarrow \frac{1}{2}(e^{i\phi_c}(|4e\rangle + |4f\rangle) + e^{i\phi_d}(-|4e\rangle + |4f\rangle))$$

Let's write down the nonzero chainkets for this scenario:

$$Y^e = [0a]_0 \odot [4e]_4$$

$$Y^f = [0a]_0 \odot [4f]_4$$

since

$$|Y^e\rangle = [4e]T^4|0a\rangle = \frac{1}{2}(e^{i\phi_c} - e^{i\phi_d})|4e\rangle$$

and

$$|Y^f\rangle = [4f]T^4|0a\rangle = \frac{1}{2}(e^{i\phi_c} + e^{i\phi_d})|4f\rangle$$

We can also work out

$$\Pr(Y^e) = \frac{1}{4}\|e^{i\phi_c} - e^{i\phi_d}\|^2 = \sin^2(\Delta/2)$$

and

$$\Pr(Y^f) \cos^2(\Delta/2)$$

where

$$\Delta = \phi_c - \phi_d \in [0, 2\pi]$$

On Wednesday, we will start asking the question of which path the photon took if we know where it exited. This will be equivalent to asking which slit an electron goes through the double slit experiment when it creates the interference pattern.

### 3.7 Interference, Cont.

From the same interferometer we had before (using a different labeling from Monday, we now have the channels maintaining their names the whole way through both beam splitters, with 0 before the first, 1 before the mirror, 2 after the mirror, and 3 after the last beam splitter. The phase shifters are right in front of the mirrors),

$$\begin{aligned}
 S|0a\rangle &= \frac{1}{\sqrt{2}}(|1a\rangle + |1b\rangle) \\
 S|0b\rangle &= \frac{1}{\sqrt{2}}(-|1a\rangle + |1b\rangle) \\
 S|1a\rangle &= e^{i\phi_a}|2a\rangle \\
 S|1b\rangle &= e^{i\phi_b}|2b\rangle \\
 S|2a\rangle &= \frac{1}{\sqrt{2}}(|3a\rangle + |3b\rangle) \\
 S|2b\rangle &= \frac{1}{\sqrt{2}}(-|3a\rangle + |3b\rangle) \\
 |\psi_0\rangle &= |0a\rangle \rightarrow |\psi_1\rangle = \frac{1}{\sqrt{2}}(|1a\rangle + |1b\rangle) \rightarrow |\psi_2\rangle = \frac{1}{\sqrt{2}}(e^{i\phi_a}|2a\rangle + e^{i\phi_b}|2b\rangle) \\
 |\psi_3\rangle &= \frac{1}{2}(e^{i\phi_a} - e^{i\phi_b})|3a\rangle + \frac{1}{2}(e^{i\phi_a} - e^{i\phi_b})|3b\rangle
 \end{aligned}$$

so with no detector,

$$\text{Pr}([3a]_3) = \langle \psi_3 | [3a] | \psi_3 \rangle = \sin(\Delta/2)$$

where  $\Delta$  is the difference in phase.

If there is a detector  $\hat{a}$  before the phase shifter on the  $a$  path,

$$\begin{aligned}
 \mathcal{H} &= \mathcal{H}_p \otimes \mathcal{H}_{\hat{a}} \\
 |\Psi_0\rangle &= |\psi_0, 0\hat{a}\rangle \\
 |\Psi_3\rangle &= \frac{1}{2} [e^{i\phi_a}(|3a, 1\hat{a}\rangle + |3b, 1\hat{a}\rangle) + e^{i\phi_b}(-|3a, 0\hat{a}\rangle + |3b, 0\hat{a}\rangle)]
 \end{aligned}$$

Therefore,

$$\text{Pr}([3a]_3 \otimes I_{\hat{a}}) = \langle \Psi_3 | [3a]_3 \otimes I_{\hat{a}} | \Psi_3 \rangle = \underbrace{\frac{1}{4}}_{(0\hat{a})} + \underbrace{\frac{1}{4}}_{(1\hat{a})} = \frac{1}{2}$$

Notice we lose the  $\Delta$  relationship, so detection on channel  $a$  causes a loss of the interference pattern.

We can imagine a third case where there is a detector on  $a$  and  $b$  simultaneously (so we know when a particle goes through but we don't know which path):

$$\begin{aligned}
 \mathcal{H} &= \mathcal{H}_p \otimes \mathcal{H}_{\hat{a}} \\
 |\Psi_2\rangle &= \frac{1}{\sqrt{2}}(e^{i\phi_a}|2a, 1\hat{a}\rangle + e^{i\phi_b}|2b, 1\hat{a}\rangle) \\
 |\Psi_3\rangle &= e^{i\phi_a}(|3a, 1\hat{a}\rangle + |3b, 1\hat{a}\rangle) e^{i\phi_b}(-|3a, 1\hat{a}\rangle + |3b, 1\hat{a}\rangle) \\
 \text{Pr}([3a]_3) &= \sin^2(\Delta/2)
 \end{aligned}$$

In a fourth case, we have two detectors,  $\hat{a}$  and  $\hat{b}$ .

$$\begin{aligned}
 \mathcal{H} &= \mathcal{H}_p \otimes \mathcal{H}_{\hat{a}} \otimes \mathcal{H}_{\hat{b}} \\
 |\Psi_3\rangle &= \frac{1}{\sqrt{2}}(e^{i\phi_a}|2a, 1\hat{a}, 0\hat{b}\rangle + e^{i\phi_b}|2b, 0\hat{a}, 1\hat{b}\rangle)
 \end{aligned}$$

$$Pr([3a]_3) = \frac{1}{2}$$

In the fifth case, we have detectors  $\hat{c}$  and  $\hat{d}$  on the  $a$  and  $b$  channels respectively **after** the second beam splitter.

$$[\Phi_0] \odot \begin{cases} [1a] \\ [1b] \end{cases} \odot I_2 \odot I_3 \odot \begin{cases} [0\hat{c}] \\ [1\hat{c}] \end{cases}$$

Let's label the histories  $Y^{a0}, Y^{a1}, Y^{b0}, Y^{b1}$  corresponding to the branch and whether or not the detector was triggered. This family is NOT consistent. If we were to form the chainket for  $\langle Y^{a0} | Y^{b0} \rangle \neq 0$ . This is due to the fact that we can't tell which branch we had gone through, because the beam splitters create superpositions of the states. A particle going through either branch has some probability to exit to either detector. Any sort of  $[0\hat{c}]$  or  $[1\hat{d}]$  (and other) combinations in the final state of this history will result in inconsistencies.

A consistent history could be

$$[\Psi_0] \odot \begin{cases} [1a] \\ [1b] \end{cases} \odot I_2 \odot I_3 \odot \begin{cases} [\hat{c}+] \\ [\hat{c}-] \end{cases}$$

where

$$\hat{c}\pm = \frac{1}{\sqrt{2}}(|0\hat{c}\rangle \pm |1\hat{c}\rangle)$$

We can show that going through one branch makes the final state  $[\hat{c}\pm]$ , but from this we can't tell which path was taken.

In the sixth (and final) case, we have weak detection on each channel:

$$S |1a, 0\hat{a}, 0\hat{b}\rangle = \alpha e^{i\phi_a} |2a, 1\hat{a}, 0\hat{b}\rangle + \beta e^{i\phi_a} |2a, 0\hat{a}, 0\hat{b}\rangle$$

The other channel would have the same scenario, for some nonzero  $\beta$  corresponding to the chance to miss a detection.

$$Pr([3a]_3) = \|\beta\|^2 \sin^2(\Delta/2) + \frac{1}{2} \|\alpha\|^2$$

# Chapter 4

## Position and Momentum

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LECTURE 21: UNCOUNTABLE BASIS SETS  
Mon Oct 7 2019

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$l^2$  (Review)

- Countable Basis:  $\{|m\rangle, m \in \mathbb{Z}\}$
- Orthonormality:  $\langle m | m' \rangle = \delta_{mm'}$
- Completeness:  $I = \sum_m |m\rangle \langle m|$
- For any  $|\psi\rangle \in \mathcal{H}$ ,  $|\psi\rangle = \sum_m |m\rangle \langle m| |\psi\rangle$
- $|\psi\rangle = \sum_m C_m |m\rangle$

$L^2[a, b]$

- Uncountable Basis:  $\{|x\rangle, x \in [a, b]\}$
- Completeness:  $I = \int_a^b dx |x\rangle \langle x|$
- Component:  $\varphi(x) = \langle x | \varphi \rangle$
- $\varphi(x) = \langle x | \int_a^b dx' \underbrace{\langle x' |}_{\delta(x-x')} \underbrace{\langle x' |}_{\delta(x-x')} \varphi \rangle$
- $\langle \chi | \varphi \rangle = \int_a^b dx \chi^*(x) \varphi(x)$
- $\|\varphi\|^2 = \int_a^b dx |\varphi(x)|^2 < \infty$

$L^2(\mathbb{R})$

- Separability:

Fourier basis of  $L^2[a, b]$   $\{\varphi_n(x) = \frac{1}{\sqrt{b-a}} e^{i2\pi nx/(b-a)}\}$  Any  $\varphi$  can be written as a sum of basis elements with coefficients  $c_n = \langle n | \varphi \rangle = \frac{1}{\sqrt{b-a}} \int dx e^{-i2\pi nx/(b-a)}$

- $\|\varphi - \sum_n C_n \varphi_n\|^2 = 0$

Operators:

$$A: |\varphi\rangle \in \mathcal{H} \rightarrow A|\varphi\rangle \stackrel{?}{\in} \mathcal{H}$$

Typically, operators in uncountable bases will map to elements outside the basis:

**Example.**

$$|\varphi\rangle \in \mathcal{H}$$

$$\sum_{n=1}^{\infty} |C_n|^2 < \infty$$

$$\sum_{n=1}^{\infty} |nC_n|^2 \text{ diverges}$$

◊

For a bounded space,  $(X\varphi)(x) = \langle x| X |\varphi\rangle = x\varphi(x)$ ,  $L^2[0, 1]$  ( $X$  is the position operator). However, if we look at an unbounded space,

$$(x \frac{d}{dx} \varphi)(x) = x\varphi'(x)$$

Many functions will have an unbounded result, particularly any discontinuous  $\varphi$ .

The idea that operators can map outside of the basis becomes a problem when we want to find eigen-systems. The eigenvectors of an operator might not be in the original Hilbert space. To solve this, we will look at “pseudoeigenvectors”:

## 4.1 Pseudoeigenvectors

$$A = X, \quad \varphi_a(x) = \delta(x - a)$$

$$(X\varphi_a)(x) = x\varphi_a(x) = x\delta(x - a) = a\delta(x - a)$$

$$\langle \varphi_b | \varphi_a \rangle = \int dx \delta(x - a)\delta(x - b) = \delta(a - b)$$

$$A = -i \frac{d}{dx}$$

$$\varphi_k(x) = \frac{1}{\sqrt{2\pi}} e^{ikx}$$

$$A\varphi_k(x) = k\varphi_k(x)$$

$$\langle \varphi_k | \varphi_{k'} \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ikx} e^{ik'x} dx = \delta(k - k')$$

For any  $|\psi\rangle \in \mathcal{H}$ ,

$$\langle x | \psi \rangle = \psi(x) = \int dk \tilde{\psi}_k e^{ikx}$$

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### 4.1.1 Spectral Decomposition in Uncountable Spaces

$$I = \sum_n |n\rangle\langle n| + \int d\nu |\nu\rangle\langle\nu|$$

$$A = \sum_n |n\rangle a\langle n| + \int d\nu |\nu\rangle a(\nu)\langle\nu|$$

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## LECTURE 22: INFINITE DIMENSION HILBERT SPACES, CONTINUED

Wed Oct 9 2019

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Recall the position basis  $\{|x\rangle\}$  and the position operator  $X|x\rangle = x|x\rangle$ . We are going to use these to represent an arbitrary function on the real line:

$$|\varphi\rangle = \int dx \varphi(x) |x\rangle$$

or

$$\varphi(x) = \langle x| |\varphi\rangle$$

Let us now introduce a translation operator  $U$ . There could be many different transformations, so we will label ours  $U(\alpha)$  such that  $U(\alpha)|x\rangle = |x + \alpha\rangle$ . We have chosen to symbolize this with a capital “U” because we suspect it’s unitary. Unitary transformations transform orthonormal bases to orthonormal bases.  $\{|x\rangle\}$  is orthonormal, and the operator maps to states  $\{|x + \alpha\rangle\} = \{|x\rangle\}$ .

Let us translate the state  $|\varphi\rangle$  from above. We want to evaluate some  $\varphi(x)$  so we put the bra for the  $x$  states on each side. This shows that  $U: \varphi(x) \rightarrow \varphi(x - \alpha)$ :

$$\begin{aligned} \langle x| U(\alpha) |\varphi\rangle &= \langle x| \int dx' \varphi(x') |x' + \alpha\rangle \\ &= \int dx' \varphi(x') \delta(x - (x' + \alpha)) \\ &= \varphi(x - \alpha) \end{aligned}$$

What if we want to translate an operator? We say that  $A: |\varphi\rangle \rightarrow |\chi\rangle = A|\varphi\rangle$ . We want the following to happen

$$A': U|\varphi\rangle \rightarrow U|\chi\rangle = UA|\varphi\rangle$$

We know for a fact (from one line above) that  $A': U|\varphi\rangle \rightarrow A'U|\varphi\rangle$ . These must be equal, so

$$A' = UAU^\dagger$$

Now let us consider “infinitesimal” transformation. We consider a small  $\delta$  such that  $U(\delta)$  can be written as some Taylor series:

$$\begin{aligned} U(\delta) &\approx U(0) + \delta \frac{\partial U(\alpha)}{\partial \alpha} \Big|_{\alpha=0} \\ &= I - i\delta T \end{aligned}$$

where

$$T \equiv i \frac{\partial U}{\partial \alpha} \Big|_{\alpha=0}$$

Additionally,

$$U^\dagger = I + i\delta T^\dagger + \dots$$

Together

$$UU^\dagger = I = I + i\delta(T^\dagger - T) + \mathcal{O}(\delta^2)$$

This order of  $\delta$  must vanish, so  $T = T^\dagger$ , or  $T$  is hermitian.

Let us combine a finite and an infinitesimal transformation:

$$U(\alpha + \delta) = U(\delta)U(\alpha) = (I - i\delta T)U(\alpha)$$

Therefore,

$$\frac{\partial U}{\partial \alpha} = -iTU(\alpha)$$

We can solve this:

$$U(\alpha) = e^{-i\alpha T}$$

Now consider the infinitesimal operator acting on an arbitrary function

$$U(\delta)\varphi(x) = \varphi(x - \delta) \approx \varphi(x) - \delta\varphi'(x)$$

so

$$T = -i\frac{d}{dx}$$

so in general,

$$U(\alpha) = e^{-\alpha \frac{d}{dx}}$$

We say that the derivative is the “generator” for the transformation group. This can be brought into three dimensions. Define  $\vec{P} = -i\hbar\nabla$  such that  $E^{-i\vec{\alpha} \cdot \vec{P}/\hbar}$ .

$$\begin{aligned} X &\xrightarrow{U} X' \implies X' = (I - i\delta P/\hbar)X(I + i\delta P/\hbar) \\ &= X + (i\delta/\hbar)(XP - PX) + \mathcal{O}(\delta^2) \\ &= X - \delta I \implies [X, P] \equiv XP - PX = i\hbar I \end{aligned}$$

or by components,

$$[\vec{R}_j, \vec{P}_k] = i\hbar I \delta_{jk}$$

**Theorem 4.1.1. Ehrenfest Theorem:** Property  $A = A(t)$  in  $|\varphi(t)\rangle$ . We want to look at

$$\langle A \rangle_\varphi(t) = \langle \varphi(t) | A(t) | \varphi(t) \rangle$$

$$\frac{d}{dt} \langle \varphi | A | \varphi \rangle = \left( \frac{d}{dt} \langle \varphi | \right) A | \varphi \rangle + \langle \varphi | \frac{d}{dt} A | \varphi \rangle + \langle \varphi | A \frac{d}{dt} | \varphi \rangle$$

This is equivalent to

$$\frac{1}{i\hbar} \langle \varphi | [A, H] | \varphi \rangle + \langle \varphi | \frac{d}{dt} A | \varphi \rangle$$

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## LECTURE 23: THE MOMENTUM OPERATOR

Fri Oct 11 2019

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## 4.2 The Momentum Operator

From last lecture, we said

$$\vec{P} = -i\hbar\nabla$$

We believe this is the momentum operator because

$$[\vec{R}_j, \vec{P}_k] = i\hbar I \delta_{jk}$$

Recall Ehrenfest's theorem from the previous lecture:

$$\frac{d}{dt} \langle A \rangle_\varphi = \frac{1}{i\hbar} \langle \varphi | [A, H] | \varphi \rangle + \langle \varphi | \frac{\partial A}{\partial t} | \varphi \rangle$$

If

$$H = \frac{P^2}{2m}$$

Recall that we take the unitary operator for position to be

$$U(\vec{a}) = e^{-i\vec{a} \cdot \vec{P}/\hbar}$$

we can show that, for  $A = X$ ,  $U(\vec{a}) = e^{-i\vec{a} \cdot \vec{P}/\hbar}$

$$H' = UHU^\dagger = UU^\dagger H = H$$

so

$$\frac{d}{dt} \langle X \rangle = \frac{1}{i\hbar} \langle [X, H] \rangle$$

Note that

$$[X, P^2] = XP^2 - P^2X + (PXP - PXP) = P[X, P] + [X, P]P = 2i\hbar P$$

therefore

$$[X, H] = \frac{2i\bar{P}}{2m} = i\hbar P_x/m$$

so

$$[\vec{R}, H] = i\hbar \vec{P}/m$$

What we find from Ehrenfest's theorem is that

$$\frac{d}{dt} \langle \vec{R} \rangle = \vec{P}/m$$

which is the velocity. Therefore, it makes sense that this  $P$  operator is momentum because, for a massive Hamiltonian, it is mass times velocity. There's a third reason to call this operator momentum. Note that it commutes with the Hamiltonian and lacks any explicit time dependence. Therefore if we look at

$$\frac{d}{dt} \langle \vec{P} \rangle = 0$$

we discover this conservation law, particularly the conserved property whose conservation is associated with the invariance of the Hamiltonian under translation.

### 4.2.1 Position Basis

Recall that

$$e^{-iaP/\hbar} |x\rangle = |x+a\rangle$$

What does the momentum operator do to this basis?

$$e^{-i\delta P/\hbar} |x\rangle = (I - i\delta P/\hbar) |x\rangle = |x\rangle - \frac{i\delta}{\hbar} P |x\rangle = |x+\delta\rangle$$

where the last line comes from us knowing what this infinitesimal position operator must do. Therefore

$$P |x'\rangle = \lim_{\delta \rightarrow 0} \frac{i\hbar}{\delta} (|x'+\delta\rangle + |x'\rangle)$$

What does this look like in position space?

$$\begin{aligned} \langle x | (P |x'\rangle) &= \lim_{\delta \rightarrow 0} \frac{i\hbar}{\delta} (\langle x' + \delta | + \langle x' |) \\ &= \lim_{\delta \rightarrow 0} \frac{i\hbar}{\delta} (\langle x | |x' + \delta\rangle + \langle x | |x'\rangle) \\ &= i\hbar \delta'(x - x') \end{aligned}$$

What does this operator do to an arbitrary function on  $x$ ? Recall that

$$\langle x| (X |\varphi\rangle) = x\varphi(x)$$

Now with momentum:

$$\langle x| (P |\varphi\rangle) = \langle x| PI |\varphi\rangle$$

we insert an identity:

$$I = \int dx' |x'\rangle\langle x'|$$

so

$$\begin{aligned} \langle x| P |\varphi\rangle &= \int dx' \langle x| P |x'\rangle \langle x'| |\varphi\rangle \\ &= \int ddx' i\hbar\delta'(x - x')\varphi(x') \\ &= i\hbar \left( \delta(x - x')\varphi(x') \Big|_{x'=-\infty}^{\infty} - \int dx' \delta(x - x')\varphi'(x') \right) \\ &= -i\hbar\varphi'(x) \end{aligned}$$

The cancellation occurs because  $\varphi$  is an element of the Hilbert space and is thus square integrable, so it vanishes at infinity. Therefore the evaluation of the  $\varphi(x)$  at infinity will vanish.

### 4.2.2 Eigenstates of Momentum

$$P |p\rangle = p |p\rangle$$

what is  $|p\rangle$ ?

$$\begin{aligned} \langle x| |p\rangle &= \chi_p(x) \\ \langle x| P |p\rangle &= p\chi_p(x) \\ &= \langle p| P |x\rangle^* \\ &= \left[ \int dx' \langle p| |x'\rangle \langle x'| P |x\rangle \right]^* \\ &= -i\hbar\chi'_p(x) = p\chi_p(x) \end{aligned}$$

This last line is a differential equation, which we can solve:

$$\chi_p(x) = \frac{1}{2\pi\hbar} e^{ipx/\hbar}$$

In other words, the eigenstates of the momentum operators are plane waves. We can also use this as a basis:

$$I = \int dp |p\rangle\langle p|$$

$$\int dx \chi_p^*(x)\chi_{p'}(x) = \delta(p - p')$$

$$|\varphi\rangle \rightarrow \langle x| |\varphi\rangle = \varphi(x)$$

$$|\varphi\rangle \rightarrow \langle p| |\varphi\rangle = \tilde{\varphi}(p)$$

We can see that position and momentum are Fourier conjugates:

$$\tilde{\varphi}(p) = \langle p | \varphi \rangle = \langle p | \int dx |x\rangle \langle x| \varphi \rangle = \frac{1}{\sqrt{2\pi\hbar}} \int dx e^{-ipx/\hbar} \varphi(x)$$

and

$$\varphi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int dp e^{ipx/\hbar} \tilde{\varphi}(p)$$

$$\begin{aligned} \langle p | (P | \varphi \rangle) &= p \tilde{\varphi}(p) = P \tilde{\varphi}(p) \\ P \varphi(x) &= -i\hbar \frac{\partial}{\partial x} \varphi(x) \end{aligned}$$

What happens when we act the position operator on the Fourier transformed function of  $p$ ?

$$\begin{aligned} X \tilde{\varphi}(p) &= \langle p | X | \varphi \rangle \\ &= \langle p | \int dx |x\rangle \langle x| X | \varphi \rangle \\ &= \frac{1}{\sqrt{2\pi\hbar}} \int dx x e^{-ipx/\hbar} \varphi(x) \\ &= i\hbar \frac{\partial}{\partial p} \phi(p) \end{aligned}$$

We can see that this is just like acting the momentum operator on a function of position. We could imagine doing this to the Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} |\varphi\rangle = \left\{ \frac{p^2}{2m} + V(X) \right\} |\varphi\rangle$$

Let's project this onto  $\langle x |$ :

$$\begin{aligned} |x\rangle i\hbar \frac{\partial}{\partial t} |\varphi\rangle &= \left\{ \frac{p^2}{2m} + V(X) \right\} |\varphi\rangle \\ i\hbar \frac{\partial}{\partial t} \varphi(x, t) &= -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \varphi(x, t) + V(x) \varphi(x, t) \end{aligned}$$

and now onto  $\langle p |$ :

$$\begin{aligned} |p\rangle i\hbar \frac{\partial}{\partial t} |\varphi\rangle &= \left\{ \frac{p^2}{2m} + V(X) \right\} |\varphi\rangle \\ i\hbar \frac{\partial}{\partial t} \tilde{\varphi}(p, t) &= -\frac{\hbar^2}{2m} \tilde{\varphi}(p, t) + V \left( i\hbar \frac{\partial}{\partial p} \right) \tilde{\varphi}(p, t) \end{aligned}$$

What do we mean by the potential energy evaluated as a function of the derivative?

$$V(x) = \sum_n V_n x^n \rightarrow \sum_n V_n (\iota\hbar)^n \frac{\partial^n}{\partial p^n}$$

## 4.3 Heisenberg Uncertainty Relation

Suppose we have Hermitian operators  $A$  and  $B$  such that

$$[A, B] = AB - BA \equiv iC$$

and

$$\{A, B\} = AB + BA \equiv D$$

$$\langle A \rangle_\varphi = \langle \varphi | A | \varphi \rangle$$

and

$$\langle A^2 \rangle_\varphi = \langle \varphi | A^2 | \varphi \rangle$$

We will define

$$(\Delta A)^2 = \langle \varphi | \underbrace{A - \langle A \rangle_\varphi}_{\tilde{A}} | \varphi \rangle = \langle A^2 \rangle_\varphi - \langle A \rangle_\varphi^2$$

Similarly,  $\tilde{B} = B - \langle B \rangle_\varphi$ .

We say that

$$\langle \tilde{A} \rangle = \langle A - \langle A \rangle \rangle = \langle A \rangle - \langle A \rangle = 0$$

**Theorem 4.3.1.** *Schwarz Inequality:*

$$\|f\|^2 \|g\|^2 \geq |\vec{f} \cdot \vec{g}|, \quad (= \iff \vec{f} \parallel \vec{g})$$

Let  $\vec{f} = \tilde{A} | \varphi \rangle$  and  $\vec{g} = \tilde{B} | \varphi \rangle$ . Using this inequality,

$$(\Delta A)^2 = \|f\|^2$$

$$(\Delta B)^2 = \|g\|^2$$

$$(\Delta A)^2 (\Delta B)^2 \geq \left| \langle \tilde{A} \tilde{B} \rangle_\varphi \right|^2$$

where

$$\tilde{A} \tilde{B} = \frac{\tilde{A} \tilde{B} + \tilde{B} \tilde{A}}{2} + i \frac{\tilde{A} \tilde{B} - \tilde{B} \tilde{A}}{2i} = \frac{1}{2} \tilde{D} + \frac{1}{2} i C$$

What is the expectation value of this?

$$\begin{aligned} \left| \langle \tilde{A} \tilde{B} \rangle_\varphi \right|^2 &= \left| \frac{1}{2} \langle \tilde{D} \rangle + \frac{1}{2} i \langle C \rangle \right|^2 = \frac{1}{4} \left| \langle \tilde{D} \rangle \right|^2 + \frac{1}{4} \left| \langle C \rangle \right|^2 \\ &\geq \frac{1}{4} \left| \langle C \rangle \right|^2 \end{aligned}$$

Back to the original Schwarz Inequality:

$$(\Delta A)(\Delta B) \geq \left| \langle \tilde{A} \tilde{B} \rangle \right| \geq \frac{1}{2} | \langle [A, B] \rangle |$$

To show an example, let's use  $A = X$ ,  $B = P$ , and  $C = \hbar I$  as we have found before. This implies that

$$\Delta X \Delta P \geq \frac{\hbar}{2}$$

### 4.3.1 Temporal Heisenberg Relation

It can be shown that

$$\Delta H \Delta \tau \geq \frac{\hbar}{2}$$

What does it mean? Recall that in general

$$\Delta A \Delta H \geq \frac{1}{2} | \langle [A, H] \rangle |$$

From Ehrenfest's theorem,

$$\frac{d}{dt} \langle A \rangle = \frac{1}{i\hbar} \langle [A, H] \rangle$$

so

$$\Delta A \Delta H = \frac{1}{2} \hbar \frac{d}{dt} \langle A \rangle$$

Therefore, if we define

$$\Delta\tau \equiv \frac{\Delta A}{\frac{d\langle A \rangle}{dt}}$$

we can say that our  $\Delta\tau$  is really referring to the timescale or lifetime of some observable rather than an uncertainty in time.

**Example.** These Energy-Time relations are very useful in particle phenomenology. Imagine a  $Z^0$  boson that appears to have a Gaussian energy distribution centered at  $mc^2$  with a width  $\hbar\Gamma$ . We can say that the “lifetime” of the particle is  $\tau = \frac{1}{\Gamma}$ . In reality,  $mc^2 = 91.188\text{GeV}$  while  $\hbar\gamma = 2.5\text{GeV}$   $\diamond$

## LECTURE 25: FREE PARTICLE MOTION

Monday, October 14, 2019

The behavior of a particle in a potential is described by

$$H = \frac{P^2}{2m} + V(x)$$

In free motion,  $V(x) \rightarrow 0$ , so our states are eigenstates of the momentum states:

$$P |p\rangle = p |p\rangle$$

and

$$H |p\rangle = \underbrace{\frac{P^2}{2m}}_{E(p)} |p\rangle$$

If we want to see the time evolution, we use the Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} |\varphi\rangle = H |\varphi\rangle$$

$$|p\rangle(t) = e^{-iE(p)t/\hbar} |p\rangle(t=0)$$

We can also look at the state in terms of a wave packet:

$$\begin{aligned} |\varphi\rangle &= \int dp \tilde{\varphi}(p) |p\rangle \\ \varphi(x) &= \langle x | \varphi \rangle = \frac{1}{\sqrt{2\pi\hbar}} \int dp \tilde{\varphi}(p) e^{ipx/\hbar} \\ \varphi(x, t) &= \frac{1}{\sqrt{2\pi\hbar}} \int dp \tilde{\varphi}(p, t=0) e^{i(px - E(p)t)/\hbar} \end{aligned}$$

Let's write the momentum as  $p = \hbar k$  such that  $k$  is the wave number. We will also rescale  $E = \hbar\omega$ , where  $\omega = \omega(k)$ . Finally, we will define  $\sqrt{\hbar}\tilde{\varphi}(\hbar k) \equiv A(k)$ . Finally, we have

$$\varphi(x, t) = \frac{1}{2\pi} \int dk A(k) e^{i(kx - \omega t)}$$

If the phase is zero,  $x(t) = \underbrace{\frac{\omega}{k}}_{v_p} t$  where  $v_p$  is the phase velocity. Let's construct a wave packet by making

$A(k)$  a Gaussian about  $\bar{k}$ . In real space, this means that  $x(t)$  is a wave of a frequency  $\bar{k}$  with a Gaussian envelope. The wave inside the envelope moves at the phase velocity, but the envelope itself will move at

$v_g$ , the group velocity. To see what this means, let's imagine  $A(k)$  is two  $\delta$  functions,  $\delta(\bar{k} + \delta k) + \delta(\bar{k}) - \delta k$ . Now the Fourier transform is relatively simple. We will expand  $\omega(\bar{k} + \delta k) \approx \omega(\bar{k}) + \delta k \frac{d\omega}{dk}|_{\bar{k}} = \bar{\omega} + \delta\omega$ :

$$\begin{aligned}\varphi(x, t) &= \frac{1}{2} e^{i[(\bar{k} + \delta k)x - (\bar{\omega} + \delta\omega)t]} + \frac{1}{2} e^{i[(\bar{k} - \delta k)x - (\bar{\omega} - \delta\omega)t]} \\ &= e^{i(\bar{k}x - \bar{\omega}t)} \cos(\delta kx - \delta\omega t)\end{aligned}$$

The crests of the wave (the exponential) move at phase velocity  $v_p = \omega/k$ . However, the envelope (the cosine) moves at the group velocity  $v_g \equiv \frac{d\omega}{dk}|_{\bar{k}}$ .

Recall that  $\omega = E/\hbar = \frac{\hbar k^2}{2m}$  is nonlinear in  $k$ . Therefore,  $v_p = \frac{\hbar k}{2m}$  and  $v_g = \frac{\hbar k}{m}$ . Notice that in general, these are not the same number. The fact that  $v_p = v_p(k)$  will lead to a spreading of the group, which we call “wave packet spreading.” Note that we are talking about particles with mass. For massive particles, there is this phenomenon of dispersion  $\omega(k)$ . Massive particles have nontrivial dispersion relations.

Recall from last week that

$$(\Delta X)^2 = \langle X^2 \rangle - \langle X \rangle^2$$

and Ehrenfest’s theorem:

$$\frac{d}{dt} \langle A \rangle = \frac{1}{i\hbar} \langle [A, H] \rangle$$

If  $H = \frac{P^2}{2m}$ ,  $[X, P^2] = 2i\hbar P$ . Also,  $[X^2, P^2] = 2i\hbar\{X, P\}$  and  $[\{X, P\}, P^2] = 4i\hbar P^2$ .

$$\begin{aligned}\frac{d\langle X \rangle}{dt} &= \frac{\langle P \rangle}{m} = v_0 \implies \langle X \rangle = v_0 t + \langle X \rangle_0 \\ \frac{d\langle X^2 \rangle}{dt} &= \frac{\langle \{X, P\} \rangle}{m} \implies \frac{d^2\langle X^2 \rangle}{dt^2} = \frac{1}{i\hbar m} \langle [\{X, P\}, H] \rangle = \frac{2\langle P^2 \rangle}{m^2}\end{aligned}$$

Therefore

$$\frac{d\langle X^2 \rangle}{dt} = \frac{2\langle P^2 \rangle_0 t}{m^2} + \xi_0$$

where  $\xi_0 \equiv \left. \frac{d\langle X^2 \rangle}{dt} \right|_{t=0} \propto 2v_0 x_0$  in the classical limit.

$$\langle X^2 \rangle = \frac{\langle P^2 \rangle t^2}{m^2} + \xi_0 t + \langle X^2 \rangle_0$$

Finally we can write

$$(\Delta X)^2 = (\Delta v)_0^2 t^2 + 2\Delta(v_0 x_0) + (\Delta X)_0^2$$

Taking the square root, we can get  $\Delta X$ , which is like the width of the wave packet as a function of time. It rests on diagonal asymptotes with slope  $\pm(\Delta v)_0$ , and it intersects  $t = 0$  at  $(\Delta X)_0$ . The initial slope at  $t = 0$  is proportional to  $\xi_0$ .

## LECTURE 26: THE FEYNMAN PATH INTEGRAL

Wednesday, October 16, 2019

## 4.4 Feynman Path Integrals

Recall the double slit experiment. If we add up the possible paths the particle could take to get to a particular point, labeling the distance from the source to the slits as  $L_1$  and  $L_2$  respectively, priming the lengths after the slits, we find that at a point  $x$  on the screen,  $L_j + L'_j(x) \implies A_j(x) = e^{i(k(L_j + L'_j(x)))}$  and  $A(x) = \sum_j A_j(x)$ . For a massive particle, we suppose we have a unitary time operator  $U(t)$ :

$$U(t): |\psi(t=0)\rangle \rightarrow |\psi(t)\rangle = U(t)|\psi(0)\rangle$$

$$U(x, t; x_0) \equiv \langle x | U(t) | x_0 \rangle$$

We define the “propagator” as:

$$\psi(x, t) = \int dx_0 U(x, t; x_0) \psi_0(x)$$

since

$$\langle x | \left( |\psi(t)\rangle = \int dx_0 U(t) |x_0\rangle \langle x_0| |\psi(t=0)\rangle \right)$$

Let

$$H = \frac{P^2}{2m} + V(x) \implies U(t) = e^{-\imath H t / \hbar}$$

Let us separate the time axis into  $N$  discrete portions ( $\epsilon = t/N$ ). Doing this, we can write the unitary time operator in the following form:

$$U(t) = \overbrace{e^{-\imath H \epsilon / \hbar} e^{-\imath \epsilon / \hbar} \cdots e^{-\imath H \epsilon / \hbar}}^N$$

Next, we insert the identity:

$$U(t) = \underbrace{e^{-\imath H \epsilon / \hbar} e^{-\imath \epsilon / \hbar}}_{I_{N-1}} = \overbrace{\int dx_{N-1} |x_{N-1}\rangle \langle x_{N-1}| \cdots \underbrace{e^{-\imath H \epsilon / \hbar} e^{-\imath H \epsilon / \hbar}}_{I_1 = \int_{-\infty}^{\infty} dx_1 |x_1\rangle \langle x_1|}}^N$$

This is similar to a unitary history. We start at  $x_0$ . At time  $t = 1$  we could be anywhere in space, so we evolve unitarily in time from time 0 to 1, projecting into a generic state  $|x_1\rangle$ . From here, we find

$$\langle x | U(t) | x_0 \rangle = \int \prod_{j=1}^{N-1} dx_j \langle x_j | U_\epsilon | x_{j-1} \rangle$$

is the propagator. For each term in this product, what is

$$\langle x_j | e^{-\imath \left( \frac{P^2}{2m} + V \right) \epsilon / \hbar} | x_{j-1} \rangle?$$

### Operator Exponentials

$$e^A e^B = e^{A+B+\frac{1}{2}[A,B]}$$

We can make use of this identity, supposing that, with a potential  $V$  and kinetic term  $K$ ,

$$e^{V+K} = e^V e^K e^{-\frac{1}{2}[V,K]}$$

To order  $\mathcal{O}(\epsilon^1)$  (we will later take  $\epsilon \rightarrow 0$  we can ignore the last term:

$$\langle x_j | e^{-\imath H \epsilon / \hbar} | x_{j-1} \rangle = e^{-\frac{i}{\hbar} V(x_j)} \langle x_j | e^{-\frac{i}{\hbar} \frac{P^2}{2m} \epsilon} | x_{j-1} \rangle$$

We insert the identity (using now the momentum basis):

$$e^{-\frac{i}{\hbar} V(x_j)} \langle x_j | \left( I = \int dp |p\rangle \langle p| \right) e^{-\frac{i}{\hbar} \frac{P^2}{2m} \epsilon} | x_{j-1} \rangle = e^{-\frac{i}{\hbar} V(x_j)} \int dp \frac{1}{2\pi\hbar} e^{\frac{i}{\hbar} \left[ p(x_j - x_{j-1}) - \frac{p^2 \epsilon}{2m} \right]}$$

Now we need to evaluate this integral. It looks like a Gaussian integral, and we can evaluate it by completing the square. Recall that if (in the exponent) we have the following form:  $ap^2 + bp = (\sqrt{a}p + \sqrt{c})^2 - c$  where  $c = b^2/4a$ . Let  $a = \epsilon/2m$  and  $b = (x_j - x_{j-1})$

$$\implies e^{im(x_j - x_{j-1})^2/(2\epsilon\hbar)} \int dp e^{(\sqrt{a}p + \sqrt{c})^2}$$

where the integral evaluates to

$$\sqrt{\frac{m}{2\pi\imath\hbar\epsilon}}$$

Finally, we can write out our short time propagator as

$$U(x_j, \epsilon, x_{j-1}) = \sqrt{\frac{m}{2\pi\imath\hbar\epsilon}} e^{\frac{i}{\hbar} L_j \epsilon}$$

where

$$L_j = \frac{1}{2} m \dot{x}_j^2 - V(x_j)$$

where

$$\dot{x}_j \equiv \frac{x_j - x_{j-1}}{\epsilon}$$

which we will call the velocity, so we see that  $L_j$  is the Lagrangian.

Now let's get rid of the  $\epsilon$  terms.

$$U(x, t; x_0) = \int \mathcal{D}[x(t)] e^{\underbrace{\int_0^t dt' L(x(t'), \dot{x}(t'))}_{\text{action } S[x(t)]}}$$

and

$$\sqrt{\frac{m}{2\pi\imath\hbar\epsilon}} \rightarrow \sqrt{\frac{m}{2\pi\imath\hbar t}}$$

where we are integrating over all possible positions at all possible times (which we've done) in a continuum of both (which we haven't).

**Example.** Free Particle ( $v = 0$ ): Around the path of least action, the complex exponentials will not cancel against each other, and the dominant feature will result from this path. The path in general is  $x(t)$ :  $x(t=0) = x_0$ ,  $x(t_{\text{final}}) = x$ ,  $x = x_0 + vt$  where  $v = \frac{x-x_0}{t}$ .

$$U(x, t; x_0) = \sqrt{\dots} e^{\frac{i}{\hbar} m(x-x_0)^2 / (2t)}$$

Using this, we can work out the wave function at any position by

$$\psi(x, t) = \int dx_0 U(x, t; x_0) \psi_0(x) U(x, t; x_0)$$

As time goes to 0, the propagator becomes the  $\delta$  function at  $x_0$ , and as time goes toward  $\infty$ , the propagator spreads like a Gaussian.  $\diamond$

# Chapter 5

## Potential Scattering

LECTURE 27: MOTION IN CONTINUOUS SPACES  
Monday, October 21, 2019

The probability density for a particle to be found in some position  $\vec{r}$  is

$$\rho(\vec{r}) = \text{Pr}([\vec{r}]) = \langle \psi | |\vec{r}\rangle \langle \vec{r}| \psi \rangle = |\psi(r)|^2$$

Assuming continuous motion in time and space, the only way a probability of a single point can change is if it flows from nearby points. This leads to the continuity condition:

$$\frac{\partial}{\partial t} \rho(\vec{r}, t) + \vec{\nabla} \cdot \vec{J} = 0$$

Substituting in  $\psi$  for  $\rho$  from above, we can write this as

$$\frac{\partial}{\partial t} |\psi|^2 = \psi^* \frac{\partial \psi}{\partial t} + \psi \frac{\partial \psi^*}{\partial t}$$

From the Schrödinger equation (in free space), we have  $\vec{P} = -i\hbar \vec{\nabla}$ ,  $H = \frac{P^2}{2m}$ , so  $i\hbar \frac{\partial \psi}{\partial t} = H\psi$ :

$$\frac{\partial}{\partial t} |\psi|^2 = -\frac{\hbar}{2mi} \left\{ \psi^* \nabla^2 \psi - \psi \nabla^2 \psi^* + \vec{\nabla} \psi^* \cdot \vec{\nabla} \psi - \vec{\nabla} \psi \cdot \vec{\nabla} \psi^* \right\} = -\frac{\hbar}{2mi} \vec{\nabla} \cdot \underbrace{\left\{ (\psi^* \vec{\nabla} \psi - \psi \vec{\nabla} \psi^*) \right\}}_{\propto \vec{J}}$$

so

$$\vec{J} = \frac{\hbar}{2mi} \left\{ \psi^* \vec{\nabla} \psi - \psi \vec{\nabla} \psi^* \right\} = \text{Re} \left\{ \psi^* \left( \frac{\hbar}{im} \vec{\nabla} \psi \right) \right\} \propto \rho v$$

### 5.1 The Potential Step

Let's set up a potential which is zero for negative  $x$  and  $V_0$  for positive  $x$ . We will send a wave packet  $\varphi$  from negative to positive  $x$ :

$$i\hbar \frac{\partial}{\partial t} \varphi(x, t) = \left\{ -\frac{\hbar^2}{2m} \nabla^2 + V(x) \right\} \varphi(x, t)$$

Instead of thinking of this wave packet as a single particle, imagine there is a source sending many particles. We want to find the steady state (time independent) solutions to this equation to study things like reflection and transmission. The generic steady state wave packet is

$$\varphi(x, t) = e^{-iEt/\hbar} \varphi(x)$$

which keeps  $\varphi$  at a constant magnitude in time. The other way we get a steady state is if we are in an energy eigenstate. In either case, we can now write this in terms of the time independent Schrödinger equation

$$E\varphi(x) = H\varphi(x)$$

Let's now solve for  $x < 0$ , which is where  $V(x) = 0$ :

$$-\frac{\hbar^2}{2m}\varphi''(x) = E\varphi(x)$$

We know how to solve this differential equation. In general,

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

Points of constant phase for the first term move to the right, while the second term describes left-moving packets. In this case,  $E = \frac{\hbar^2}{2m}k^2 > 0$ . We assume the energy is positive. If we didn't, we would see that the solutions are now exponentials, so coming from  $-\infty$ , we would either have infinite or zero probability density at  $x = 0$ , which does not represent our system properly. Therefore,  $k = \sqrt{2mE/\hbar^2} \in \mathbb{R}$ .

Now let's look on the other side, where  $x > 0$  and  $V > 0$ :

$$\varphi(x) = Ce^{ik'x} + De^{-ik'x}$$

We see here that  $k' = \sqrt{2m(E - V_0)/\hbar^2}$ . If  $E > V_0$ , then  $k' \in \mathbb{R}$ , so we get oscillating solutions. However, if  $E < V_0$ ,  $k' \in \mathbb{I}$ , so we get decaying and growing exponentials. To make further progress, we need to look at the step boundary condition. We can start by writing the Schrödinger equation:

$$\left( \frac{\partial^2}{\partial x^2} + \frac{2m(E - V_0)}{\hbar^2} \right) \varphi(x) = 0$$

We will now integrate this over a small region  $[-\epsilon, \epsilon]$ :

$$\begin{aligned} & \int_{-\epsilon}^{\epsilon} \left\{ \left( \frac{\partial^2}{\partial x^2} + \frac{2m(E - V_0)}{\hbar^2} \right) \varphi(x) \right\} dx \\ &= \varphi'(\epsilon) - \varphi'(-\epsilon) + \int_{-\epsilon}^{\epsilon} \frac{2m(E - V_0)}{\hbar^2} \varphi(x) dx \end{aligned} \tag{5.1.1}$$

In this second integral, everything is a constant except for  $\varphi(x)$ , which is of order  $\mathcal{O}(\epsilon)$ , and as  $\epsilon \rightarrow 0$ , this integral also vanishes, so both  $\varphi(x)$  and  $\varphi'(x)$  are continuous over the boundary. For example, if  $0 < E < V_0$ , defining  $\imath k' \equiv \kappa \in \mathbb{R}_+$ :

$$\varphi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x < 0 \\ Ce^{-\kappa x} + De^{\kappa x} & 0 < x \end{cases}$$

Continuity of  $\varphi(x)$  tells us that  $A + B = C + D$ . Continuity of  $\varphi'(x)$  tells us that  $\imath kA - \imath kB = -\kappa C + \kappa D$ . Now we want to solve for these coefficients.  $k$  and  $\kappa$  are properties of the source particles, so we actually don't have to solve for them since they are considered "known" in this scenario. Additionally,  $A$  is set by properties of the source, since it represents the incoming wave. For now, let's just choose  $A = 1$ . The magnitude of  $A$  gives us the magnitude of the incident flux, while the phase of  $A$  gives us the phase of the incident flux, which we really don't care about right now. Additionally,  $e^{\kappa x}$  is growing exponentially with  $x$ , so  $D = 0$  due to divergence as  $x \rightarrow \infty$ . The only unknowns now are  $B$  and  $C$ , which we can solve as:

$$B = -\frac{\kappa + ik}{\kappa - ik}, \quad C = -\frac{2ik}{\kappa - ik}$$

What is the incident flux now?

$$J_{\text{inc}} = \underbrace{|A|^2}_{1} \frac{\hbar b a k}{m} = \rho v$$

What about the reflected flux?

$$J_{\text{refl}} = - \underbrace{|B|^2}_{1} \frac{\hbar k}{m} = \rho v_{\text{refl}} = -J_{\text{inc}}$$

Every particle which hits the barrier is reflected, but there is a nonzero probability to find a particle in the “classically forbidden” region, since  $C \neq 0$ . This is called “tunneling” and the probability is constant with time.

What happens as the energy of the incident particle approaches  $V_0$  from below? Now  $\kappa = \sqrt{2m(V_0 - E)/\hbar^2}$ , so the wave oscillates faster before the barrier (because it has greater energy) and it tunnels farther into the barrier.

What if  $V_0 \rightarrow \infty$ ? If we go back to that infinitesimal integral in equation (5.1.1), we no longer have a converging integral, so we no longer require the wave function to have a continuous derivative at the barrier. In this case, the wave function will vanish at the barrier.

Now let's see what happens if  $E > V_0$ . Now, there is a probability that the waves are transmitted. However, we know the transmitted waves will travel from left to right, so  $D = 0$  still. If we maintain the incident density with  $A = 1$ , we now have oscillating solutions in the positive  $x$  region. Here, the coefficients are

$$B = \frac{k - k'}{k + k'}, \quad C = \frac{2k}{k + k'}$$

Again, let's look at the currents:

$$\begin{aligned} J_{\text{inc}} &= |A|^2 \frac{\hbar k}{m} = \rho v \\ -J_{\text{refl}} &= -|B|^2 \frac{\hbar k}{m} = \left( \frac{k - k'}{k + k'} \right)^2 \frac{\hbar k}{m} < J_{\text{inc}} \end{aligned}$$

Let us define  $\left( \frac{k - k'}{k + k'} \right)^2 \equiv R$ . The remainder of the current must be transmitted, so  $T = 1 - R = \frac{4kk'}{(k+k')^2} = \frac{k'}{k} |C|^2 = \rho' v' / v_{\text{inc}} < |C|^2$ .

$$J_{\text{trans}} = |C|^2 \frac{\hbar k'}{m}$$

Because  $k' < k$  with positive  $V_0$ , we see that the transmitted velocity is less than the incident velocity.

### Exam

The upcoming exam will cover the notes up till this coming Wednesday (next lecture) and the homework due this Friday.

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## LECTURE 28: SQUARE WELL POTENTIAL

Wednesday, October 23, 2019

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Let's examine the steady state wave function solutions for a square well:

$$V = \begin{cases} V_0 & x < -a/2 \\ 0 & -a/2 < x < a/2 \\ V_0 & a/2 < x \end{cases}$$

For a steady state, recall that we generally want

$$\varphi(x, t) = e^{-iEt/\hbar} \varphi(x)$$

Now we can use the time independent Schrödinger equation:

$$H\varphi = E\varphi$$

where

$$H = \frac{P^2}{2m} + V(x)$$

so

$$-\partial_x^2 \varphi(x) = \left( \frac{2m}{\hbar^2} \right) (E - V(x)) \varphi(x)$$

In the regions with a nonzero potential, recall that we say the solution looks like  $e^{\pm \kappa x}$ . On the left side, we want this to be  $+$  and on the right we want  $-$  so that we don't get wave functions which diverge at infinity. In the middle, the wave function looks like  $e^{\pm i k x}$ .

Our potential is symmetric under parity:  $V(x) = V(-x)$ , so the parity operator  $\Pi$  commutes with the Hamiltonian:  $[H, \Pi] = 0$ . The parity operator forms a group with two elements,  $G = \{e, \Pi\}$ , where  $e$  is the identity. Applying the group operator twice returns us to the original state. One of the consequences of this symmetry is that, when we solve the Schrödinger equation and find some solution,

$$H |\varphi\rangle E |\varphi\rangle$$

because  $\Pi H \Pi^\dagger = H$ , we know that

$$\begin{aligned} \Pi H \Pi^{-1} \Pi |\varphi\rangle &= \Pi E |\varphi\rangle \\ H(\Pi |\varphi\rangle) &= E(\Pi |\varphi\rangle) \end{aligned}$$

This means that if we find an eigenstate of the Hamiltonian, we can apply the parity operator to our solution and get another solution with the same energy. Sometimes these will be the same solution.

#### Important Idea

We can do this same trick with *any* operator which commutes with the Hamiltonian. Eigenfunctions of the Hamiltonian are “basis” functions of representation of  $G$ , the symmetry group of the Hamiltonian.

For this group  $G$ ,  $\Pi = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$ , and  $\Pi^2 = e$  so the eigenvalues must be  $\pm 1$ . This means there is a basis where the parity operator is

$$\Pi = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

so there exist eigenstates  $|\varphi_{\pm}\rangle$  such that

$$\Pi |\varphi_+\rangle = |\varphi_+\rangle$$

and

$$\Pi |\varphi_-\rangle = -|\varphi_-\rangle$$

Unfortunately, applying the operator in our case will not give us a new solution, but it does tell us that we must have one even solution and one odd solution. Let's look at  $\varphi_+(x)$ :

$$\varphi_+(x) = \begin{cases} Ae^{-\kappa x} & a/2 < x \\ B \cos(kx) & -a/2 < x < a/2 \\ Ae^{+\kappa x} & x < -a/2 \end{cases}$$

Note the symmetry in coefficients. Now let's look at the other solution:

$$\varphi_-(x) = \begin{cases} Ae^{-\kappa x} & a/2 < x \\ B \sin(kx) & -a/2 < x < a/2 \\ -Ae^{+\kappa x} & x < -a/2 \end{cases}$$

Putting these solutions back into the Schrödinger equation, we find that  $k = \sqrt{2mE/\hbar^2}$  and  $\kappa = \sqrt{2m(V_0 - E)/\hbar^2}$ . Now we know almost everything about our solutions except for  $A$  and  $B$ . The

important condition is at the boundaries, where we must preserve continuity of the wave function and its derivative. For  $\varphi_+$ , we find that, at the right-hand boundary,

$$B \cos(ka/2) = Ae^{-\kappa a/2}$$

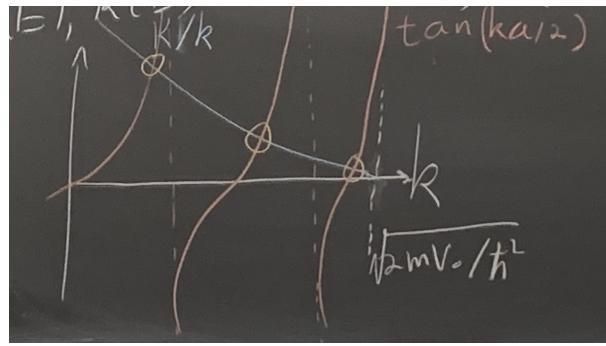
For the derivative,

$$-kB \sin(ka/2) = -\kappa A e^{-\kappa a/2}$$

Let's divide the bottom equation by the top equation. This gives us

$$\tan(ka/2) = \frac{\kappa}{k}$$

We were trying to find a relation between  $A$  and  $B$ , but we have now found a relationship between  $k$  and  $\kappa$ ! Notice as we vary the energy  $E$ , both  $k$  and  $\kappa$  vary continuously. The tangent equation does not hold for every  $k$  and  $\kappa$ , but we can imagine that there will be some values which work. Let's try to figure out what this means. Notice on the left-hand side, the function is transcendental, so this will be a difficult equation to solve. We look for a graphical solution:



**Figure 5.1.1:**  $\tan(ka/2)$  and  $\kappa/k$  plotted as functions of  $k$

Notice an upper bound on  $k$ , implying that these are bound states with energy less than  $V_0$ .

As  $V_0 \rightarrow \infty$ ,  $k \rightarrow \infty$  and  $\tan(ka/2) \rightarrow \infty$  since  $\cos(ka/2) \rightarrow 0$ . Now the upper bound on  $k$  vanishes, so there will be an infinite number of solutions,

$$k_n = \frac{(2n+1)\pi}{a} \implies E_n = \frac{\hbar^2}{2m} k_n^2$$

If we look at the boundary condition on  $\varphi_-$ , we get a cotangent function, which gives the form  $k_n = \frac{2n\pi}{a}$ . If we look at both even and odd solutions, we get that  $k_m = \frac{m\pi}{a}$ .

Let's now look in the limit where  $E \rightarrow 0$ ,  $k \rightarrow 0$  and  $\kappa \rightarrow 0$  accordingly.

$$\tan(ka/2) \approx ka/2 = \kappa/k$$

so (if we let  $a/2 = 1$  and  $\hbar^2/2m = 1$ )

$$E = \sqrt{V_0 - E}$$

which comes from  $k^2 = \kappa$ .

$$E = V_0 - E^2 < V_0$$

so at least one solution always exists no matter how small  $V_0$  is. Graphically, the leftmost solution will slide down the tangent curve toward 0. For example, if we have a one-dimensional wire, if there is a defect, no matter how small, we will have a state trapped at the defect. This tells us that there is no true electrical conductivity in one dimension.

First, some review of the exam:

$$|\psi_0\rangle = \frac{1}{\sqrt{3}}(|A\rangle + |B\rangle + |C\rangle)$$

and

$$|F\rangle = \frac{1}{\sqrt{3}}(|A\rangle + |B\rangle - |C\rangle)$$

$$Y^1 = [\psi_0] \odot [A] \odot [F]$$

so

$$|\psi^1\rangle = [F][A]|\psi_0\rangle = [F]\frac{1}{\sqrt{3}}|A\rangle = \frac{1}{3}|F\rangle$$

Next,

$$Y^2 = [\psi_0] \odot [A] \odot (I - [F])$$

so

$$|Y^2\rangle = (I - [F])[A]|\psi_0\rangle = (I - [F])\frac{1}{\sqrt{3}}|A\rangle$$

Instead of writing out  $I - [F]$ , we can just distribute:

$$|Y^2\rangle = \frac{1}{\sqrt{3}}|A\rangle - \frac{1}{3}|F\rangle$$

Let's look at one of the probability questions now:

$$\Pr([A]_1 \mid [\psi_0][F_1]) = \frac{\Pr(\psi_0, A_1, F_2)}{\Pr(\psi_0, F_1)} = \frac{\Pr(Y^1) = \frac{1}{9}}{\Pr(Y^1) + \Pr(Y^3) = \frac{1}{9} + 0} = 1$$

Now back to potential scattering:

### 5.1.1 Square Well Scattering

$$V(x) = \begin{cases} -V_0 & |x| > a/2 \\ 0 & |x| < a/2 \end{cases}$$

We know solutions are exponential, proportional to  $e^{\pm ikx}$  with  $k = \sqrt{E}$  outside the well and  $e^{\pm ik'x}$  with  $k' = \sqrt{V_0 + E} > k$  inside the well.

$$\phi = \begin{cases} Ae^{ikx} + Be^{-ikx} & x < -a/2 \\ Ce^{ik'x} + De^{-ik'x} & -a/2 < x < a/2 \\ Fe^{ikx} + Ge^{-ikx} & a/2 < x \end{cases}$$

Boundary conditions at  $-a/2$  give us

$$Ae^{-ika/2} + Be^{ika/2} = Ce^{-ik'a/2} + De^{ik'a/2}$$

and

$$\underbrace{kAe^{-ika/2} - kB e^{ika/2}}_{P\begin{pmatrix} A \\ B \end{pmatrix}} = \underbrace{k'Ce^{-ik'a/2} - k'D e^{ik'a/2}}_{Q\begin{pmatrix} C \\ D \end{pmatrix}}$$

so

$$\begin{pmatrix} A \\ B \end{pmatrix} = P^{-1}Q \begin{pmatrix} C \\ D \end{pmatrix}$$

where  $P^{-1}Q = R$ .

By time reversal symmetry (taking the complex conjugate of  $\varphi$  and noting that the Schrödinger equation is invariant under this operation), we can conclude that

$$\begin{pmatrix} A^* \\ B^* \end{pmatrix} = R \begin{pmatrix} C^* \\ D^* \end{pmatrix}$$

so  $R_{11}^* = R_{22}$  and  $R_{12}^* = R_{21}$

$$R = \sqrt{\frac{k'}{k}} \begin{pmatrix} \alpha & \beta \\ \beta^* & \alpha^* \end{pmatrix}$$

The incident current is

$$J_{\text{inc}} = k(|A|^2 - |B|^2) = J_{\text{transf}} = k'(|C|^2 - |D|^2)$$

therefore,

$$|\alpha|^2 - |\beta|^2 = 1$$

or

$$\det \left\{ \begin{pmatrix} \alpha & \beta \\ \beta^* & \alpha^* \end{pmatrix} \right\} = 1$$

Applying the same method of time-reversal and current conservation to the other boundary. We can reuse  $R$  evaluated at any other point in space (called  $\tilde{R}$ ). Therefore

$$\begin{bmatrix} A \\ B \end{bmatrix} = \underbrace{R\tilde{R}}_M \begin{bmatrix} F \\ G \end{bmatrix}$$

$$M = \begin{bmatrix} \gamma & \delta \\ \delta^* & \gamma^* \end{bmatrix}$$

$$|\gamma|^2 - |\delta|^2 = 1$$

so

$$\gamma = \alpha^2 - \beta^2 = e^{ik'a} \left[ \cos(k'a) - i \frac{k^2 + k'^2}{2kk'} \sin(k'a) \right]$$

is the reflection coefficient.

For transmission, set  $A = 1$ , and we want  $G = 0$ . Our equation now becomes

$$\begin{bmatrix} 1 \\ B \end{bmatrix} = M \begin{bmatrix} F \\ 0 \end{bmatrix}$$

so

$$F = \frac{1}{M_{11}}$$

and

$$T = |F|^2 = \frac{1}{|\gamma|^2} = \frac{1}{1 + \frac{(k^2 - k'^2)^2}{2k^2 k'^2} \sin^2(k'a)}$$

Recall that  $k' = \sqrt{V_0 + k^2}$ , so plotting the coefficients as a function of  $k$ , we see the following result:

### LECTURE 30: SCATTERING CONTINUED

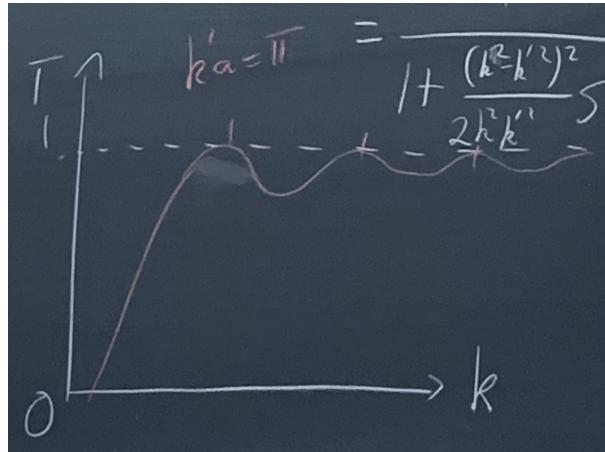
Friday, November 01, 2019

Recall the solutions for a square well:

$$\varphi = \begin{cases} Ae^{ikx} + Be^{-ikx} & x < -a/2 \\ Ce^{ik'x} + De^{-ik'x} & -a/2 < x < a/2 \\ Fe^{imathkx} + Ge^{-ikx} & a/2 < x \end{cases}$$

If we imagine there is some matrix  $M$  such that

$$\begin{bmatrix} A \\ B \end{bmatrix} = M \begin{bmatrix} F \\ G \end{bmatrix}$$


 Figure 5.1.2: Graph of  $k$  vs  $T$ 

then the  $M_{11}$  element is

$$M_{11} = e^{ika} \left[ \cos(k'a) - i \frac{k^2 + k'^2}{2kk'} \sin(k'a) \right]$$

For transmission,  $G = 0$  so  $T = \frac{1}{|M_{11}|^2}$ , for  $E > 0$ .

For bound states,  $-V_0 < E < 0$ ,  $k' = \sqrt{V_0 + E}$ ,  $\kappa = \sqrt{-E}$ , and  $A = G = 0$ , so

$$\begin{bmatrix} 0 \\ B \end{bmatrix} = M \begin{bmatrix} F \\ 0 \end{bmatrix}$$

so  $M_{11} = 0$ , meaning  $T$  diverges.

Let's look at resonances now. The bound states occur at certain energies. For a given depth of the potential well, there will be a certain number of bound states. Let's try to count how many bound states there are. We could imagine adjusting the depth of the potential well, and as it got deeper there would be more bound states, but as we made the well shallower, we would lose states. How do we lose a state? While decreasing the depth, the topmost state will be pushed up closer and closer to the top of the well to the point where the energy will be  $E = 0$ . Let's examine those states. As  $E \rightarrow 0$ ,  $\kappa \rightarrow 0$ , so the wave function will propagate infinitely far into the Classically forbidden region. The solution for this is

$$\tan\left(\frac{k'a}{2}\right) = \frac{\kappa}{k'} = 0$$

Recall that this was our even-state relation from when we solved this earlier. The odd states use cot and the sign on the right side is flipped. The even states occur when  $k' = \frac{2\pi n}{2a}$  and the odd states occur at  $k' = \frac{2n+1\pi}{2a}$ , so in general  $k' = l\frac{\pi}{a}$ . We know that  $k' = \sqrt{V_0}$ , so the bound state  $l$  has zero energy when  $V_l = l^2 \frac{\pi^2}{a^2}$ . These are the special potential depths where a  $E = 0$  state exists. There are  $l + 1$  bound states total including the  $E = 0$  state.

Let's now back off a bit so the bound state reappears. Set  $V_0 = V_l + \delta$ ,  $\delta \gtrsim 0$ . The highest  $E_n \lesssim 0$ ,  $\rightarrow 0^-$  as  $\delta \rightarrow 0^+$ .

Now set  $V_0 = V_l + \delta$ ,  $\delta \lesssim 0$ . Let's look at the lowest scattering resonance.

$$T = \frac{1}{1 + B^2 \sin^2(k'a)}$$

where  $k = \sqrt{V_0 + E} = \sqrt{l^2 \frac{\pi^2}{a^2} + \delta + E}$ . We see that the resonance occurs at  $k' = l\frac{\pi}{a}$ , or when  $E = -\delta \gtrsim 0$ .  $E \rightarrow 0^+$  as  $\delta \rightarrow 0^-$ . The transmission coefficient of the traveling wave goes to 1 as  $\delta \rightarrow 0$ . In the moment this happens, the wave number in the forbidden region goes from imaginary to real.

Let's now look at the same problem, but instead of a well, let's use a square step potential:

$$E = \begin{cases} 0 & x < -a/2 \\ +V_0 & -a/2 < x < /a2 \\ 0a/2 < x \end{cases}$$

Let's look at the case of tunneling. The wave function when  $E < V_0$  will now be oscillating in the outside regions and decaying in the Classically forbidden region.  $k' \rightarrow i\kappa$  where  $\kappa = \sqrt{V_0 - E}$ . Now,  $T = \frac{1}{1+B^2 \sinh^2(\kappa a)}$ . Lets imagine that we are sufficiently far below the top of the barrier such that  $\kappa a \gg 1$ . In this case,  $\sinh(x) = \frac{e^x + e^{-x}}{2} \sim \frac{1}{2}e^x$ , so  $T \approx e^{-2\kappa a}$ . If we look at the ratio of the amplitude of the wave function on either side of the step, that ratio must be about  $e^{-\kappa a}$ , since the amplitude is exponentially decaying in that regime. In the other direction, as the energy approaches the top of the well,  $\kappa \rightarrow 0$  so tunneling becomes easier.

We can extend this discussion to barriers of arbitrary shape. Let's focus on barriers which vanish at  $\pm\infty$ . We can approximate such a barrier into a collection of square barriers with width  $\Delta x$ ,  $0 \cdots x \cdots x_{N+1}$ , and the transmission coefficient for  $T(x_1, x_1 + \Delta x) = e^{-2\kappa(x_1)\Delta x}$ . Therefore,

$$T(x_1, x_{N+1}) \approx \prod_{i=1}^N T(x_i, x_i + \Delta x) = e^{-2\Delta x \sum_i \kappa(x_i)} \approx e^{-2 \int_{x_1}^{x_{N+1}} \kappa(x) dx}$$

This is the “WKB” or “semiclassical” approximation. We can use this to model things like nuclear decay, where there is some potential barrier  $V(r)$  caused by the nucleus which a particle has to tunnel through to decay. Another example is a scanning-tunneling microscope (STM). These work by measuring the tunneling current between a sharp metal tip and a potential below the surface you want to measure.

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## LECTURE 31: PERIODIC POTENTIALS

Friday, November 01, 2019

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Suppose  $V(x+a) = V(x)$ . From a previous lecture, we introduced a translation operator  $(T_a V)(x) = V(x-a) = V(x)$  for periodic potentials, where  $T_a = e^{a \frac{d}{dx}}$ .

We can see that the discrete translation over the period of the potential commutes with the Hamiltonian,  $[T_a, H] = 0$ . Recall that when we have an operator which commutes with the Hamiltonian, there exists a conserved charge. When we did this with infinitesimal translations, we found that the invariance leads to conservation of momentum. We can find the conserved charge here through Ehrenfest’s theorem:

$$\partial_t \langle T_a \rangle = \frac{1}{i\hbar} \langle [T_a, H] \rangle = 0$$

Notice that our infinitesimal translation no longer commutes with the Hamiltonian, since  $(T_\epsilon V)(x) = V(x-\epsilon) \neq V(x)$ . Momentum is no longer conserved in this case (not a free particle anymore). Something is still conserved here, but that thing is not momentum.

Let's see what happens when we have a plane wave in this periodic potential.

$$\varphi(x, t=0) \equiv \varphi_0 = e^{iqx}$$

If we translate the initial plane wave,

$$(T_a \varphi_0)(x) = e^{-iqa} \varphi_0(x)$$

we can look at the expectation value of the translation operator:

$$\langle \varphi_0 | T_a | \varphi_0 \rangle = e^{-iqa}$$

If we look at the wave function at time  $t$ , we know that this matrix element is time-invariant from Ehrenfest’s theorem, so

$$\langle \varphi_t | T_a | \varphi_t \rangle = \langle \varphi_0 | T_a | \varphi_0 \rangle$$

Therefore,  $e^{-\imath qa}$  is conserved! Note this doesn't imply that  $q$  is conserved. The exponential is invariant under  $q \rightarrow q + 2n\pi/a$ . Any function that varies by  $e^{-\imath qa}$  under this translation must be periodic with a frequency of  $q + 2n\pi/a$ . We claim this function has a Fourier series:

$$\varphi(x, t) = \sum_k C_k(t) e^{\imath kx}$$

where  $k = q + \frac{2\pi}{a} n$ . To clarify, an arbitrary wave function can be represented as a Fourier sum:

$$\varphi(x, t) = \int dk C(k, t) e^{\imath kx}$$

However, only discrete  $k$  values will result in a wave function that transforms with this conserved charge.

What we discover then is that  $\hbar q$ , the momentum, is not conserved, but the set  $\{q + \frac{2\pi}{a} n\}$  is conserved. This is related to Bragg scattering. If an electron entered a crystal with momentum  $q$ , it could exit with a momentum  $q + \frac{2\pi}{a} n$ , where  $a$  relates to the spacing of the crystal lattice. If we start with an initial plane wave, the thing that emerges after time evolution will be a function of the above form. There are non-vanishing Fourier modes for other values of  $k$ , but they always belong to the conserved set. This is a weak conservation law, since a discrete periodic potential is actually a reduction of symmetry from a constant potential, which has a continuous symmetry. The higher symmetry of the constant potential conserves momentum absolutely while the discrete periodic potential allows for finite variations in the momentum. In terms of groups, we would say that the symmetry group for such a crystal is  $G = \{T_a^n, n \in \mathbb{Z}\}$ . For the continuous symmetry group, we have  $\tilde{G} = \{T_a, a \in \mathbb{R}\}$ .

This is a derivation of a more general statement called the Bloch Theorem:

## 5.2 The Bloch Theorem

**Theorem 5.2.1.**

$$[T_a, H] = 0 \implies \exists \text{ simultaneous eigenfunctions}$$

Let's look at the translation of a more general function:

$$\begin{aligned} T_a [e^{\imath qx} U(x)] &= e^{-\imath qa} [e^{\imath qx} U(x - a)] \\ &= e^{-\imath qa} [e^{\imath qx} U(x)] \end{aligned}$$

if  $U(x - a) = U(x)$  is periodic. Therefore, the eigenstates of the Hamiltonian are of the form  $e^{\imath qx} U(x)$ .

For our previous example, we had

$$\varphi(x, t) = e^{\imath qx} \underbrace{\sum_j C_j(t) e^{\frac{2\pi\imath jx}{a}}}_{U(x)}$$

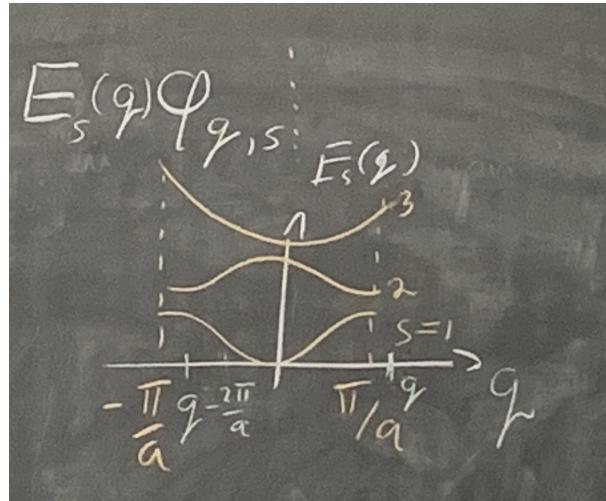
Typically there is dependence of  $U(x)$  on  $q$ , so  $U(x) = U(x, q) = U_q(x)$ . Because they are eigenstates,

$$H\varphi_q = E(q)\varphi_q$$

and for a given  $q$  there could be more than one such function that gives an eigenstate of the Hamiltonian. We will add another index  $s$  which we will call the "band" index in addition to  $q$  which we call the "Bloch" index:

$$H\psi_{q,s} = E_s(q)\psi_{q,s}$$

Below is a plot of the energy eigenstates as functions of  $q$ . This is called the band structure of the eigenstate:



**Figure 5.2.1:** Example Band Structure

Monday, November 04, 2019

From the last lecture, we found that a potential with  $V(x + a) = V(x)$  gave solutions of the form

$$\psi_q(x) = e^{iqx} U_q(x)$$

where  $U_q(x + a) = U_q(x)$ . Suppose we were in a region where  $V(x) = 0$ . We would then have left and right-going solutions like

$$\psi = A_0 e^{ikx} + B_0 e^{-ikx}$$

If we imagine the potential as having some shape which we are transmitting through or reflecting against centered about  $x = 0$ , we can say that to the left of this potential we have the above solution and to the right of the potential we have a similar solution

$$\psi = A_1 e^{ikx} + B_1 e^{-ikx}$$

Now we need to find the relationship between each coefficient and the coefficient in the next valley:

$$\begin{bmatrix} A_n \\ B_n \end{bmatrix} = M \begin{bmatrix} A_{n+1} \\ B_{n+1} \end{bmatrix}$$

where

$$M = \begin{bmatrix} \gamma & \delta \\ \delta^* & \gamma^* \end{bmatrix}$$

where  $|\gamma|^2 - |\delta|^2 = 1$ .

By the Bloch theorem from last lecture, we had  $\psi(x + a) = e^{iqa} \psi(x)$ , so

$$A_{n+1} e^{ik(x+a)} + B_{n+1} e^{-ik(x+a)} = e^{iqa} (A_n e^{ikx} + B_n e^{-ikx})$$

so

$$e^{iqa} \begin{bmatrix} A_n \\ B_n \end{bmatrix} = \begin{bmatrix} e^{ika} & 0 \\ 0 & e^{-ika} \end{bmatrix} \underbrace{\begin{bmatrix} A_{n+1} \\ B_{n+1} \end{bmatrix}}_{M^{-1} \begin{bmatrix} A_n \\ B_n \end{bmatrix}}$$

**Example.** Let's look at a specific example of periodic  $\delta$ -functions.

$$V(x) = \sum_{n=-\infty}^{\infty} \left( \frac{\hbar^2}{2m} \right) g \delta(x - na)$$

By continuity at  $x = 0$ , we have

$$A_0 \left[ 1 - e^{i(q-k)a} \right] + B_0 \left[ 1 - e^{i(q+k)a} \right] = 0$$

and by continuity of the derivative at  $x = 0$ ,

$$A_0 \left[ g + ik \left( 1 - e^{i(q-k)a} \right) \right] + B_0 \left[ g - ik \left( 1 - e^{i(q+k)a} \right) \right] = 0$$

We can't solve this system of equations since there are too many unknowns, but we can find a relation which will give us a relation for the allowed energy values. Note that the system can be put into matrix form over  $A_0$  and  $B_0$  and the determinant of this matrix is zero. Solving this gives

$$\cos(qa) = \cos(ka) + \frac{\alpha}{2ka} \sin(ka) = F(ka)$$

We won't allow solutions where  $|F(ka)| > 1$ , since this would require an imaginary  $q$ , which would cause diverging solutions in the original wave function. We can find allowed values of  $k$  by choosing values of  $q$ , for example, finding solutions of

$$\cos(k_0 a) + \frac{\alpha}{2k_0 a} \sin(k_0 a) = 1$$

when  $q = 0$ . These allowed and forbidden regions correspond to bands in  $k$ , which means there are allowed and forbidden bands in energy as well, since  $k \sim \sqrt{E}$ .

Near the band edge where  $q \approx 0$ ,

$$\begin{aligned} F(qa) &= F(ka) + (k - k_0)aF'(k_0 a) + \dots \\ &= 1 + (k - k_0)aF'(k_0 a) \approx 1 - \frac{(qa)^2}{2} \end{aligned}$$

so

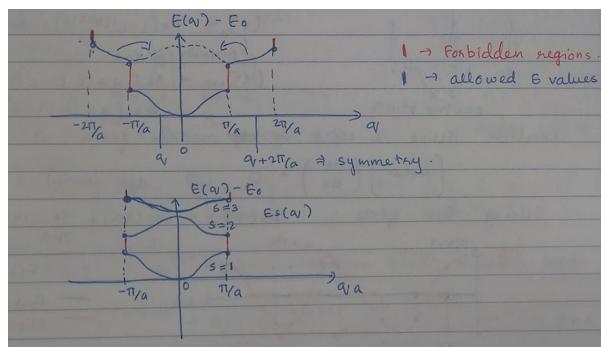
$$k - k_0 = \frac{q^2 a}{2|F'(k_0 a)|}$$

We can also expand this in  $E$ :

$$\begin{aligned} E(k) &= \frac{\hbar^2}{2mc^2} = E(k_0) + \frac{\hbar^2(k^2 - k_0^2)}{2m} \\ &\approx E(k_0) + \frac{\hbar^2 k (k - k_0)}{2m} \\ &\approx E_0 + \frac{\hbar^2 k_0}{m} \frac{q^2 a}{2|F'|} \end{aligned}$$

Plotting this band structure as a function of  $q$  gives us:

◇



**Figure 5.2.2:** Band Structure for Dirac Comb

# Chapter 6

## The Harmonic Oscillator

LECTURE 33: HARMONIC OSCILLATOR  
Wednesday, November 06, 2019

If our potential is  $V = \frac{1}{2}kx^2$ , we can write our Hamiltonian as

$$\mathbf{H} = \frac{\mathbf{P}^2}{2m} + \frac{1}{2}k\mathbf{X}^2 = \frac{\mathbf{P}^2}{2m} + \frac{1}{2}m\omega^2\mathbf{X}^2$$

where  $\omega = \sqrt{\frac{k}{m}}$ . We expect the eigenfunctions should have definite parity, since  $[\mathbf{H}, \mathbf{\Pi}] = 0$  so  $\mathbf{\Pi}|\varphi\rangle = \pm|\varphi\rangle$ . We also know  $[\mathbf{X}, \mathbf{P}] = i\hbar$  and  $\mathbf{H}|\varphi\rangle = E|\varphi\rangle$ . If we were to imagine differentiating the Schrödinger equation from  $-\infty$ , only a few miraculous values of  $E$  will solve this equation so that it vanishes at  $+\infty$ . We can make live a bit easier by getting rid of every quantity with physical dimensions. Let's introduce  $\hat{\mathbf{X}} = \sqrt{\frac{m\omega}{\hbar}}\mathbf{X}$  and  $\hat{\mathbf{P}} = \sqrt{\frac{1}{m\hbar\omega}}\mathbf{P}$  such that  $[\hat{\mathbf{X}}, \hat{\mathbf{P}}] = i$ . Therefore

$$\hat{\mathbf{H}} = \frac{1}{\hbar\omega}\mathbf{H} = \frac{1}{2}(\hat{\mathbf{P}}^2 + \hat{\mathbf{X}}^2)$$

We solve this by introducing two new operators, called “raising” and “lowering” operators:

$$\mathbf{a} \equiv \frac{1}{\sqrt{2}}(\hat{\mathbf{X}} + i\hat{\mathbf{P}})\mathbf{a}^\dagger = \frac{1}{\sqrt{2}}(\hat{\mathbf{X}} - i\hat{\mathbf{P}})$$

so  $[\mathbf{a}, \mathbf{a}^\dagger] = 1$  and we define  $\mathbf{N} = \mathbf{a}^\dagger\mathbf{a} = \frac{1}{2}(\hat{\mathbf{P}}^2 + \hat{\mathbf{X}}^2 - 1)$ . Therefore

$$\hat{\mathbf{H}} = \mathbf{a}^\dagger\mathbf{a} + \frac{1}{2} = \mathbf{N} + \frac{1}{2}$$

so  $[\mathbf{H}, \mathbf{N}] = 0$ .

$$\mathbf{N}|\varphi_\nu^{(i)}\rangle = \nu|\varphi_\nu^{(i)}\rangle$$

and

$$\hat{\mathbf{H}}|\varphi_\nu^{(i)}\rangle = \left(\nu + \frac{1}{2}\right)|\varphi_\nu^{(i)}\rangle$$

where  $(i)$  is an additional degree of freedom that we will find is not important.

$$\nu \geq 0$$

$$\nu = \nu \langle \varphi_\nu | \varphi_\nu \rangle = \langle \varphi_\nu | \mathbf{N} | \varphi_\nu \rangle = (\langle \varphi_\nu | \mathbf{a}^\dagger) (\mathbf{a} | \varphi_\nu \rangle) = \|\mathbf{a} | \varphi_\nu \rangle\|^2 \geq 0$$

$$\nu = 0$$

$$\implies \mathbf{a} | \varphi_\nu \rangle = 0$$

$$\nu > 0$$

$$\implies \mathbf{N}\mathbf{a}|\varphi_\nu\rangle = (\nu - 1)\mathbf{a}|\varphi_\nu\rangle$$

This is because  $[\mathbf{N}, \mathbf{a}] = -\mathbf{a}$ , so  $\mathbf{N}(\mathbf{a}|\varphi_\nu\rangle) = \mathbf{a}\mathbf{N}|\varphi_\nu\rangle - \mathbf{a}|\varphi_\nu\rangle = (\nu - 1)\mathbf{a}|\varphi_\nu\rangle$ .

$$\mathbf{a}^\dagger|\varphi_\nu\rangle \neq 0$$

$$\mathbf{N}\mathbf{a}^\dagger|\varphi_\nu\rangle = (\nu + 1)\mathbf{a}^\dagger|\varphi_\nu\rangle$$

**$\nu$  is a non-negative integer** Assume  $n < \nu < n + 1$ .  $\mathbf{a}^{n+1}|\varphi_\nu\rangle = 0$ , therefore  $\nu - (n + 1) = 0$  so  $\nu \in \mathbb{Z}$ .

$|\varphi_\nu\rangle$  is non-degenerate

$|\varphi_0\rangle$  Lowering this state must give us zero, so

$$\mathbf{a}|\varphi_0\rangle = 0 = \frac{1}{\sqrt{2}}(\hat{\mathbf{X}} + i\hat{\mathbf{P}})|\varphi_0\rangle$$

In  $x$ -space,

$$\left(x + \frac{d}{dx}\right)\varphi_0(x) = 0 \implies \varphi_0(x) = C_0 e^{-\frac{x^2}{2}}$$

$|\varphi_n\rangle$  non-degenerate implies  $|\varphi_{n+1}\rangle$  is non-degenerate

$$\begin{aligned} \mathbf{a}^\dagger[\mathbf{a}|\varphi_{n+1}^{(i)}\rangle] &= C^{(i)}|\varphi_n\rangle \\ \mathbf{N}|\varphi_{n+1}^{(i)}\rangle &= (n+1)|\varphi_{n+1}^{(i)}\rangle = C^{(i)}\mathbf{a}^\dagger|\varphi_n\rangle \\ |\varphi_{n+1}^{(i)}\rangle &= \frac{C^{(i)}}{n+1}\mathbf{a}^\dagger|\varphi_n\rangle \end{aligned}$$

### 6.0.1 Eigenfunctions of the Harmonic Oscillator

We start by normalizing the ground state wave function:

$$\varphi_0(x) = \frac{1}{\sqrt[4]{\pi}}e^{-\frac{x^2}{2}}$$

The other eigenfunctions can be found by raising the ground state:

$$|\varphi_n\rangle = \frac{1}{\sqrt{n!}}(\mathbf{a}^\dagger)^n|\varphi_0\rangle$$

so

$$\varphi_1(x) = \sqrt[4]{\frac{4}{\pi}}xe^{-\frac{x^2}{2}}$$

and

$$\varphi_2(x) = \sqrt[4]{\frac{1}{4\pi}}[2x^2 - 1]e^{-\frac{x^2}{2}}$$

where the polynomials in front of the exponential are the Hermite polynomials  $H_n(x)$ . The energy levels are evenly spaced by  $\hbar\omega$  (so that the energy difference between the energy of the ground state is  $\hbar\omega$  away from the first state, and the same with the first and second state). The space between the ground state and the  $x$ -axis is  $\frac{1}{2}\hbar\omega$ , so the energy eigenvalues are  $\hbar\omega(n + \frac{1}{2})$ .

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## LECTURE 34: THE SEMICLASSICAL (WKB) APPROXIMATION

Friday, November 08, 2019

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Start with the time-independent Schrödinger equation:

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + U(x) \right] \psi(x) = E\psi(x)$$

Let's assume solutions have the form

$$\psi(x) = e^{\frac{i}{\hbar} \sigma(x)}$$

such that

$$-\frac{i\hbar}{2m} \nabla^2 \sigma + \frac{1}{2m} (\vec{\nabla} \sigma)^2 = E - U(x) \equiv \frac{p^2(x)}{2m}$$

Now let's take  $\hbar \rightarrow 0$  and expand around  $\sigma$ :

$$\sigma = \sigma_0 + \frac{\hbar}{i} \sigma_1 + \dots$$

$$\sigma'_0 = \pm \sqrt{2m(E - U(x))} = \pm p(x)$$

and

$$\sigma_0 = \pm \int p(x) dx$$

so

$$\psi(x) = e^{\pm \frac{i}{\hbar} \int p(x) dx}$$

We believe this is proportional to  $e^{-ikx}$ , a plane wave solution where  $k = k(x) = p(x)/\hbar$ .

If the potential is slowly varying,

$$\hbar \sigma'' << (\sigma')^2 \implies \hbar \frac{d\hbar/\sigma'}{dx} << 1$$

We define  $\hbar/\sigma' = \lambda(x)$ , and  $\lambda = \frac{2\pi}{k} = \frac{2\pi\hbar}{p} = \frac{2\pi}{\sigma'}$  so  $\frac{d}{dx}\lambda(x) << 2\pi$ .

Now let's introduce the first-order  $\sigma_1$  correction. Then we take only the terms which are first-order in  $\hbar$ . There will be a second-order term, but we are only looking at the first-order correction and those terms are smaller than the ones we are looking at.

$$\begin{aligned} \sigma''_0 + 2\sigma'_0\sigma'_1 &= 0 \\ \sigma'_1 &= -\frac{\sigma''_0}{2\sigma'_0} = -\frac{p'}{2p} \\ \sigma_1 &= -\frac{1}{2} \ln p(x) \end{aligned}$$

so

$$\psi(x) = \frac{1}{\sqrt{p}} \left( C_1 e^{(\frac{i}{\hbar}) \int p dx} + C_2 e^{-(\frac{i}{\hbar}) \int p dx} \right)$$

We cannot use the WKB approximation in some region around the classical turning point because the potential will be varying too fast. However, if the function at this barrier is sufficiently smooth, we can approximate it as linear in this region and match up the wave function on either side of these areas.

We will use Airy functions as solutions to the Schrödinger equation. See Landau and Lifshitz for a detailed derivation of this. If we do this matching, we find that  $C_1 \sim Ae^{i\frac{\pi}{4}}$  and  $C_2 \sim Ae^{-im\frac{\pi}{4}}$ . In order to properly match up with this Airy function,  $\frac{C_1}{C_2} = i$ .

Suppose we are looking at the region around a point  $a$ , where the classically forbidden region is to the right of  $a$ :

$$\psi_{<a}(x) = \frac{C}{\sqrt{p}} \cos \left( \frac{1}{\hbar} \int_a^x p(x') dx' + \frac{\pi}{4} \right)$$

---

If we matched at  $b$ , the other turning point, we find that  $C_1 \sim A'e^{-im\frac{\pi}{4}}$  and  $C_2 \sim A'e^{i\frac{\pi}{4}}$  so

$$\psi_{>b}(x) = \frac{C'}{\sqrt{p}} \cos\left(\frac{1}{\hbar} \int_b^x p(x') dx' - \frac{\pi}{4}\right)$$

We want these functions to be the same in the inside region, so either  $C = C'$  and the phases differ by  $2\pi m$  or  $C = -C'$  and the phases differ by  $(2m+1)\pi$ . We can capture both of these at the same time by saying that

$$C' = (-1)^n C$$

and

$$\left[ \frac{1}{\hbar} \int_b^x p dx' - \frac{\pi}{4} \right] - \left[ \frac{1}{\hbar} \int_a^x p dx' + \frac{\pi}{4} \right] = n\pi$$

or

$$\frac{1}{\hbar} \int_b^a p dx' = \left(n + \frac{1}{2}\right) \pi$$

If we now add the contribution going from  $a$  to  $b$ , we can integrate over the entire path  $\Gamma = a \rightarrow b \rightarrow a$ :

$$\oint_{\Gamma} p dx = \left(n + \frac{1}{2}\right) h$$

The action is therefore quantized in multiples of  $h$  (Planck's constant) and we also have the "zero point" action  $\frac{1}{2}h$ . This exists because we are confining the wave function in space, so by the Heisenberg relation, there must be some nonzero momentum.

We can apply this approximation to systems other than bounded motion on a line. For instance, look at rotational motion. The action must be

$$S = \oint L_z d\varphi = nh$$

### 6.0.2 Energy Level Spacing

$$\Delta \oint p dx = 2\pi\hbar \approx \Delta E \oint \frac{\partial}{\partial E} p dx = \Delta E \oint \frac{dx}{v} = \Delta ET$$

We can write the period as  $T = \frac{2\pi}{\omega}$  so  $\Delta E = \hbar\omega(E)$ . Again, note that this is just an approximation.

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## LECTURE 35: HARMONIC OSCILLATORS, CONTINUED

Friday, November 08, 2019

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Let's return to the raising and lowering operator solution to the problem. Recall that

$$\hat{\mathbf{H}} = \frac{\hat{\mathbf{P}}^2}{2m} + \frac{1}{2}m\omega^2 \hat{\mathbf{X}}^2$$

where

$$\hat{\mathbf{X}} = \sqrt{\frac{\hbar}{m\omega}} \frac{1}{\sqrt{2}} (\hat{\mathbf{a}}^\dagger + \hat{\mathbf{a}})$$

and

$$\hat{\mathbf{P}} = \sqrt{m\hbar\omega} \frac{i}{\sqrt{2}} (\hat{\mathbf{a}}^\dagger - \hat{\mathbf{a}})$$

where  $[\hat{\mathbf{a}}, \hat{\mathbf{a}}^\dagger] = 1$ . We defined the number operator as  $\hat{\mathbf{N}} = \hat{\mathbf{a}}^\dagger \hat{\mathbf{a}}$  such that  $\hat{\mathbf{N}} |\varphi_n\rangle = n |\varphi_n\rangle$ .

We can build all the eigenstates by starting with the ground state and applying the raising operator:

$$|\varphi_n\rangle = \frac{(\hat{\mathbf{a}}^\dagger)^n}{\sqrt{n!}} |\varphi_0\rangle$$

We can show that  $\langle \varphi_n | X | \varphi_n \rangle = \langle \varphi_n | P | \varphi_n \rangle = 0$ .

Let's represent an arbitrary wave function as an expansion around eigenstates of the number operator:

$$|\psi(0)\rangle = \sum_n c_n(0) |n\rangle$$

such that

$$|\psi(t)\rangle = \sum_n c_n(0) e^{-iE_n t/\hbar} |\psi_n\rangle$$

In general,

$$\langle A \rangle_t = \langle \psi(t) | A | \psi(t) \rangle = \sum_{mn} c_m^* c_n e^{i(E_m - E_n)t/\hbar} A_{mn}$$

where we can define  $\omega_{mn} = (E_m - E_n)/\hbar$  as the Bohr frequencies. Here,  $A_{mn} = \langle \psi_m | A | \psi_n \rangle$ .

Let's look at what this means for the expectation value of the position.

$$X_{mn} = \sqrt{\frac{\hbar}{2m\omega}} \langle \varphi_m | (\hat{a}^\dagger + \hat{a}) | \varphi_n \rangle = \sqrt{\frac{\hbar}{2m\omega}} \begin{cases} \sqrt{m} & m = n+1 \\ \sqrt{n} & m = n-1 \end{cases}$$

so

$$\langle \hat{X} \rangle \sim e^{\pm i\omega t}$$

Let's now use Ehrenfest's theorem to see how the expectation values change in time:

$$\frac{d}{dt} \langle \hat{X} \rangle = \frac{d}{dt} x = \frac{1}{i\hbar} \langle [\hat{X}, \hat{H}] \rangle = \frac{1}{m} \langle \hat{P} \rangle$$

and

$$\frac{d}{dt} \langle \hat{P} \rangle = \frac{d}{dt} p = \frac{1}{i\hbar} \langle [\hat{P}, \hat{H}] \rangle = -\langle \hat{V}'(x) \rangle = -m\omega^2 \langle \hat{X} \rangle$$

so

$$\dot{x} = \frac{p}{m} \quad \text{and} \quad \dot{p} = -m\omega^2 x$$

Now lets look at the RMS position:

$$(\Delta \hat{X})^2 \equiv \langle \hat{X}^2 \rangle - \langle \hat{X} \rangle^2$$

where

$$\hat{X}^2 = \frac{\hbar}{2m\omega} \left( \langle (\hat{a}^\dagger)^2 \rangle + \overbrace{\langle \hat{a}^\dagger \hat{a} \rangle}^{\hat{N}} + \overbrace{\langle \hat{a} \hat{a}^\dagger \rangle}^{\hat{N}+1} + \langle \hat{a}^2 \rangle \right)$$

where the raising and lowering operators have no expectation value because the eigenstates of  $\hat{N}$  are orthogonal. Therefore,

$$(\Delta \hat{X})^2 = \frac{\hbar}{m\omega} \left( n + \frac{1}{2} \right)$$

We can also show that

$$\langle \hat{V} \rangle = \frac{1}{2} \left( n + \frac{1}{2} \right) \hbar\omega = \frac{1}{2} E_n$$

when we are in an energy eigenstate, and

$$\langle \hat{K} \rangle = \frac{1}{2} E_n = \langle \hat{V} \rangle$$

which is expected. This is the quantum virial theorem.

## H

ow do physicists actually produce band structure diagrams? One way is with “tight-binding” models, where  $\hat{\mathbf{H}} = -t \sum_n (|n\rangle\langle n+1| + |n+1\rangle\langle n|)$ . Solutions for this will be of the form  $|\psi\rangle = \sum_n e^{ikn} |n\rangle$ . This particular example would be a model for s-orbitals, and you could do similar things for other orbitals, adding all of the properties of the system to develop the band structure. Another model is the “nearly free electron” model. Solutions here are derived from quantum mechanical perturbation theory. You start with a Hamiltonian whose solutions you know (like a harmonic oscillator) and add a potential which you don’t know. You then take solutions to the known Hamiltonian and let the potential act on them. You end up mixing together the different eigenstates of the unperturbed Hamiltonian in order to see the states of the perturbed Hamiltonian.

Finally, you could use “density functional theory” to model all of the parts of the system using a complicated Hamiltonian which depends on a spatially varying electron density, act it on an electron to find a particular electron energy, and do this for all the electrons:  $\hat{\mathbf{H}}[\rho(x)]\psi_i = E_i\psi_i$  where  $\rho(x) = \sum_i |\psi_i(x)|^2$ .

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## LECTURE 36: CHARGED HARMONIC OSCILLATOR IN ELECTRIC FIELD

Monday, November 11, 2019

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### 6.1 Charged Harmonic Oscillator in Electric Field

Let  $V(x) = \frac{1}{2}m\omega^2x^2$  be a harmonic oscillator and  $W(x) = -q\mathcal{E}x$  be the potential of an electric field. We are basically imagining a particle with charge  $q$  on a spring with spring constant  $k = m\omega^2$  and an electric field of strength  $\mathcal{E}$  pulling the particle outwardly away from the spring surface. The minimum of the harmonic oscillator will be displaced. The new minimum energy will be at  $E = \frac{-q^2\mathcal{E}^2}{2m\omega^2}$  and the new equilibrium position will be  $x = \frac{q\mathcal{E}}{m\omega^2}$ . The new Hamiltonian will be

$$\hat{\mathbf{H}}_{\mathcal{E}} = \frac{\hat{\mathbf{P}}^2}{2m} + \frac{1}{2}m\omega^2 \left( \hat{\mathbf{X}} - \frac{q\mathcal{E}}{m\omega^2} \right)^2 - \frac{q^2\mathcal{E}^2}{2m\omega^2}$$

The eigenstates will have wave functions

$$\psi_n^{\mathcal{E}}(x) = \psi_n \left( x - \frac{q\mathcal{E}}{m\omega^2} \right)$$

with energy

$$E_n^{\mathcal{E}} = \left( n + \frac{1}{2} \right) \hbar\omega - \frac{q^2\mathcal{E}^2}{2m\omega^2}$$

#### 6.1.1 Dielectric Susceptibility

We can think of this system in terms of a dipole moment:

$$\hat{\mathbf{D}} = q\hat{\mathbf{X}}$$

The expectation of this operator is

$$\begin{aligned} \langle \hat{\mathbf{D}} \rangle_{\mathcal{E}} &= q \langle \psi_n^{\mathcal{E}} | \hat{\mathbf{X}} | \psi_n^{\mathcal{E}} \rangle \\ &= q \int_{-\infty}^{\infty} dx x \left| \psi_n^{\mathcal{E}} \left( x - \frac{q\mathcal{E}}{m\omega^2} \right) \right|^2 \\ &= q \int_{-\infty}^{\infty} du \left( u + \frac{q\mathcal{E}}{m\omega^2} \right) |\psi_n^{\mathcal{E}}(u)|^2 \\ &= \frac{q^2\mathcal{E}}{m\omega^2} \end{aligned}$$

The susceptibility is defined as

$$\chi \equiv \frac{\langle \hat{\mathbf{D}} \rangle_{\mathcal{E}}}{\mathcal{E}} = \frac{q^2}{m\omega^2}$$

### 6.1.2 Energy Shift or Electric Energy

This will be the size of the electric field times the displacement:

$$-q\mathcal{E} \cdot \delta x = \frac{-q^2\mathcal{E}^2}{m\omega^2}$$

### 6.1.3 Elastic Energy

The elastic energy is the energy stored in the spring, or

$$\frac{1}{2}m\omega^2(\delta x)^2 = \frac{q^2\mathcal{E}^2}{2m\omega^2}$$

Adding these together give us  $\frac{-q^2\mathcal{E}^2}{2m\omega^2}$ .

Let's now look at this as an example of spectroscopy. We are using the Born-Oppenheimer Approximation, treating the ionic cores of atoms classically, but solving the electrons quantum mechanically. Because we are going to treat the atoms classically, we can specify their positions. Imagine a molecule composed of two atoms of different elemental species. This means there is likely some difference in electrons between them and some charge imbalance. Let's say the separation between the atoms is  $r$ . Let  $r_0$  be the preferred separation (the equilibrium position) with an energy  $-V_0$ .

$$V_{eff}(r) \approx -V_0 + \frac{1}{2}V''(r_0)(r - r_0)^2 + \dots$$

We are approximating the potential as a parabola here, while we know that as  $r \rightarrow \infty$  the potential must really go to zero, so this shape is not useful far away from equilibrium.

The molecule can rotate, vibrate, or translate, and at room temperature, translational and rotational modes will likely be excited (vibration modes will be weakly excited). As long as the vibrations of the molecule are not extreme, we will ignore rotation. Let's focus on the small vibrational modes.

$$m\omega^2 = V''(r_0)$$

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega - V_0$$

Let's talk about two different types of spectroscopy. The first is infrared absorption. We imagine the molecules as a dipole with dipole moment

$$\hat{\mathbf{D}}(r) = d_0 + d_i(r - r_0)$$

where  $d_i$  is an additional dipole moment introduced by stretching bonds during vibrations. Recall that the dipole moment is like the harmonic oscillator position variable is like a raising and lowering operator,  $\hat{\mathbf{D}} \sim \hat{\mathbf{X}} \sim \hat{\mathbf{a}}^\dagger + \hat{\mathbf{a}}$ . Because of this,  $D_{n-1,n} \neq 0$  and  $D_{n+1,n} \neq 0$  and these elements are like  $\sim e^{\pm i\omega t}$ . The state of the molecule can change by absorbing or emitting photons of energy  $\hbar\omega$ , so there will be some absorption spectrum which we can plot as a function of  $\Omega$ , the frequency of incident radiation. There will be some peak in absorption around the resonant frequency of the molecule. In order to have this effect, recall that there had to be an existing dipole  $d_0$  to be able to activate the absorption and emission.

The other popular type of molecular spectroscopy uses the Raman Effect. This occurs if we have a homopolar molecule, where the two chemical species are identical ( $H^2$  for example). Without radiation, there will be no dipole moment. Suppose we have incident radiation  $\sim \mathcal{E}e^{\pm i\Omega t}$  where  $\Omega \gg \omega$ . Therefore,

$\hat{\mathbf{D}} = \chi(r)\mathcal{E}e^{i\Omega t}$ . The susceptibility will be some function of  $r$ . Let's let  $r = r_0 + \delta r$  and let the molecule vibrate such that  $r = r_0 + \delta \cos(\omega t)$  where  $\omega$  is the resonant frequency of the molecule, so  $\hat{\mathbf{D}}(t) = \underbrace{\hat{\mathbf{D}}_0(t)}_{\mathcal{E}\chi_0(r_0)e^{i\Omega t}} + \delta(\partial_r \chi)\mathcal{E} \underbrace{e^{\pm i\omega t} e^{i\Omega t}}_{\sim e^{i(\Omega \pm \omega)t}}$ .

When we do the experiment, we will hit the molecules with radiation of a certain frequency. We should see a main peak in outgoing intensity around  $\Omega$ , but we will also see two side bands (called Stokes and Anti-Stokes bands). These side bands will be displaced by  $\omega$  and will tell us about the structure of the molecule.

On Wednesday, we will discuss phonons and blackbody radiation.

### LECTURE 37: COUPLED OSCILLATORS

Wednesday, November 13, 2019

## 6.2 Coupled Oscillators

Suppose we have two oscillators coupled with strength  $\lambda$ . Essentially we are modeling two wells at  $\pm a$  containing particles which have some spring force proportional to  $\lambda$  between them:

$$\hat{\mathbf{U}}(x_1, x_2) = \frac{1}{2}m\omega^2(x_1 - a)^2 + \frac{1}{2}m\omega(x_2 + a)^2$$

and

$$\hat{\mathbf{V}}(x_1, x_2) = \lambda m\omega^2(x_1 - x_2)^2$$

so

$$\hat{\mathbf{H}} = \frac{\hat{\mathbf{P}}_1^2}{2m} + \frac{\hat{\mathbf{P}}_2^2}{2m} + \hat{\mathbf{U}} + \hat{\mathbf{V}}$$

Let's introduce some relative coordinates:

$$\begin{aligned} x_G &= \frac{x_1 + x_2}{2} & x_R &= x_1 - x_2 \\ \hat{\mathbf{P}}_G &= \hat{\mathbf{P}}_1 + \hat{\mathbf{P}}_2 & \hat{\mathbf{P}}_R &= \frac{\hat{\mathbf{P}}_1 + \hat{\mathbf{P}}_2}{2} \\ \mu_G &= 2m & \mu_R &= \frac{m}{2} \end{aligned}$$

Now

$$\hat{\mathbf{H}} = \frac{\hat{\mathbf{P}}_G^2}{2\mu_G} + \frac{1}{2}\mu_G\omega_G^2x_G^2 + \frac{\hat{\mathbf{P}}_R^2}{2\mu_R} + \frac{1}{2}\mu_R\omega_R^2x_R^2 + m\omega^2a^2\frac{4\lambda}{1+\lambda}$$

where  $\omega_G = \omega$  and  $\omega_R = \omega\sqrt{1+4\lambda}$ .

Now that we have decoupled the parts of the Hamiltonian, we can solve the equations of motion:

$$x_G = x_G^0 \cos(\omega_G t + \theta_G) \quad x_R = x_R^0 \cos(\omega_R t + \theta_R)$$

and

$$x_{1,2} = x_G \pm \frac{1}{2}x_R$$

This is the solution to the classical problem. Now let's look at it from a quantum mechanical perspective, where position and momentum don't commute. However, note that  $[x_1, x_2] = [x_1, p_2] = \dots = 0$ , and additionally  $[x_G, P_G] = [x_R, P_R] = i\hbar$  and the opposite pairings commute. Note that the Hilbert space is equivalent to the product space of the center-of-mass Hilbert space and the reduced-mass Hilbert space:

$$\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 = \mathcal{H}_G \otimes \mathcal{H}_R$$

We can define the raising and lowering operators in the following way:

$$\hat{\mathbf{a}}_G = \frac{1}{\sqrt{2}} \left( \sqrt{\frac{\mu_G \omega_G}{\hbar}} \hat{\mathbf{X}}_G + i \frac{\hat{\mathbf{P}}}{\sqrt{\mu_G \hbar \omega_G}} \right)$$

so

$$\hat{\mathbf{H}} = \left( \hat{\mathbf{a}}_G^\dagger \hat{\mathbf{a}}_G + \frac{1}{2} \right) \hbar \omega_G + \left( \hat{\mathbf{a}}_R^\dagger \hat{\mathbf{a}}_R + \frac{1}{2} \right) \hbar \omega_R + m \omega^2 a^2 \frac{4\lambda}{1+\lambda}$$

which has solutions

$$E_{np} = \left( n + \frac{1}{2} \right) \hbar \omega_G + \left( p + \frac{1}{2} \right) \hbar \omega_R + m \omega^2 a^2 \frac{4\lambda}{1+\lambda}$$

with

$$|\psi_{np}\rangle = |\psi_n^G\rangle |\psi_p^R\rangle$$

### 6.3 Harmonic Chain

Now let's imagine an infinite chain of coupled harmonic oscillators with

$$U = \sum_j \frac{1}{2} m \omega^2 x_j^2$$

and

$$V = \sum_j \frac{1}{2} m \omega_1^2 (x_{j+1} - x_j)^2$$

where the coupling is now  $\omega_1$ . Note that this is a periodic potential, so there is some symmetry. We should be able to simultaneously diagonalize the translation operator and Hamiltonian. We can use Bloch Theorem here to say that the solutions must be of the form

$$x_j^{(k)}(t) = A e^{i(kjl - \Omega t)}$$

Plugging this into our Hamiltonian, we find

$$-m\Omega^2 = -m\omega^2 - m\omega_1^2 [2 - e^{ikl} - e^{-ikl}]$$

so

$$\Omega = \Omega(k) = \pm \sqrt{\omega^2 + 4\omega_1^2 \sin^2\left(\frac{kl}{2}\right)}$$

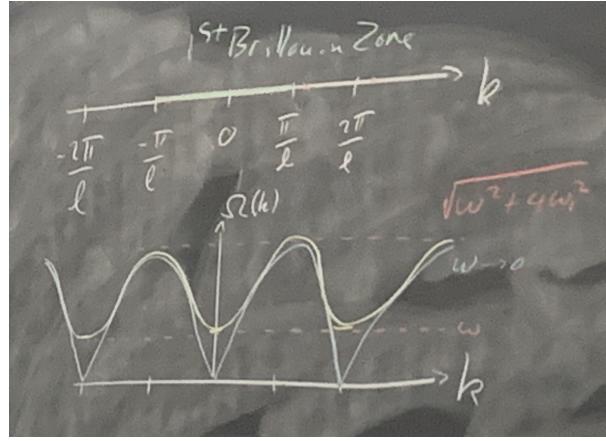
so each  $k$  is a normal mode of the system. For instance,  $k = 0$  represents uniform motion of all masses, while  $k = \frac{\pi}{l}$  represents each mass moving opposite to the next. There is some symmetry in  $k$  since

$$x_j^{(k')}(t) = k_j^{(k)}(t)$$

where  $k' = k + \frac{2\pi}{l}n$

Therefore, if we know what happens in the region  $k \in [-\frac{\pi}{l}, \frac{\pi}{l}]$ , we can figure out what happens for any other  $k$ . We call this region the first Brillouin zone.

In solids, we can imagine phonon interactions as just the coupling part, so  $\omega \rightarrow 0$ . Then,  $\Omega$  becomes proportional to  $|\sin(\frac{kl}{2})|$ . See figure 6.3.1.



**Figure 6.3.1:**  $\Omega(k)$  in the first Brillouin zone.

### The Classical Case, Continued

Recall our Hamiltonian:

$$H = \sum_j \left( \frac{p_j^2}{2m} \frac{1}{2} m\omega^2 x_j^2 + \frac{1}{2m\omega_j^2} (x_j - x_{j+1})^2 \right)$$

When we looked at the Classical case, we introduced normal modes:

$$x_j^{(k)}(t) = A e^{i(kjl - \omega t)}$$

Now let's introduce “normal coordinates”:

$$\xi(k, t) = \sum_j x_j(t) e^{-ikjl}$$

We also need to introduce a similar transformation of momentum variables:

$$\pi(k, t) = \sum_j p_j(t) e^{-ikjl}$$

These are the Fourier transforms of the position and momentum coordinates, so we can alternatively write those as

$$x_j(t) = \frac{l}{2\pi} \int_{-\frac{\pi}{l}}^{\frac{\pi}{l}} \xi(k, t) e^{ikjl} dk$$

$$p_j(t) = \frac{l}{2\pi} \int_{-\frac{\pi}{l}}^{\frac{\pi}{l}} \pi(k, t) e^{ikjl} dk$$

**Theorem 6.3.1. Parseval Theorem** The norm of a function equals the norm of its Fourier transform.

$$\sum_{j=-\infty}^{\infty} x_j^2 = \frac{l}{2\pi} \int_{-\frac{\pi}{l}}^{\frac{\pi}{l}} \|\xi(k, t)\|^2 dk$$

$$\sum_{j=-\infty}^{\infty} p_j^2 = \frac{l}{2\pi} \int_{-\frac{\pi}{l}}^{\frac{\pi}{l}} \|\pi(k, t)\|^2 dk$$

We can also find

$$\begin{aligned}\sum_j(x_j - x_{j+1})^2 &= \frac{l}{2\pi} \int (1 - e^{ikl}) \|\xi(k, t)\|^2 dk \\ &= \frac{l}{2\pi} \int dk 4 \sin^2\left(\frac{kl}{2}\right) \|\xi(k, t)\|^2\end{aligned}$$

We can now rewrite the Hamiltonian as

$$H = \frac{l}{2\pi} \int dk \left\{ \frac{1}{2m} \|\pi(k, t)\|^2 + \frac{1}{2} m\Omega^2 \|\xi(k, t)\|^2 \right\}$$

where  $\Omega^2 = \Omega^2(k) = \omega^2 + 4\omega_1^2 \sin^2\left(\frac{kl}{2}\right)$ .

Let's introduce a complex variable  $\alpha(k, t) = \frac{1}{\sqrt{2}} \left[ \sqrt{\frac{m\Omega}{\hbar}} \xi(k, t) + i \frac{1}{\sqrt{m\hbar\Omega}} \pi(k, t) \right]$  (reminiscent of the creation and annihilation operators in a quantum space):

$$H = \frac{l}{2\pi} \int dk \frac{1}{2} \hbar\Omega(k) [\alpha(k, t)\alpha^*(k, t) + \alpha(-k, t)\alpha^*(-k, t)]$$

### The Quantum Case

We now have to worry about non-commutation of the position and momentum variables, which are now promoted to quantum operators.

$$\begin{aligned}[\hat{\mathbf{X}}_{j_1}, \hat{\mathbf{P}}_{j_2}] &= i\hbar\delta_{j_1, j_2} \\ \hat{\Xi}(k) &= \sum_j \hat{\mathbf{X}}_j e^{-ik_j l} = \hat{\Xi}^\dagger(-k) \\ \hat{\Pi}(k) &= \sum_j \hat{\mathbf{P}}_j e^{-ik_j l} = \hat{\Pi}^\dagger(-k) \\ [\hat{\Xi}(k), \hat{\Pi}^\dagger(k')] &= i\hbar \frac{2\pi}{l} \delta(k - k')\end{aligned}$$

We can now define a ladder operator similar to  $\alpha$  in the classical case:

$$\hat{\mathbf{a}}(k) = \frac{1}{\sqrt{2}} \left[ \sqrt{\frac{m\Omega(k)}{\hbar}} \hat{\Xi}(k) + i \frac{1}{\sqrt{m\hbar\Omega}} \hat{\Pi}(k) \right]$$

so the quantum Hamiltonian can be written

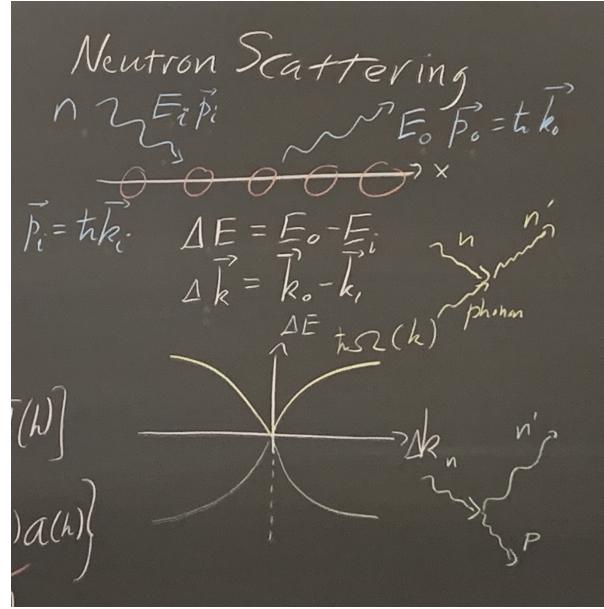
$$\hat{\mathbf{H}} = \frac{l}{2\pi} \int dk \underbrace{\frac{1}{2} \hbar\Omega(k) \{ \hat{\mathbf{a}}(k) \hat{\mathbf{a}}^\dagger(k) + \hat{\mathbf{a}}^\dagger(k) \hat{\mathbf{a}}(k) \}}_{\hat{\mathbf{H}}(k)}$$

or

$$\hat{\mathbf{H}} = \frac{l}{2\pi} \int dk \hat{\mathbf{H}}(k)$$

We see that this Hamiltonian in  $k$ -space is equivalent to  $\hat{\mathbf{H}}(k) = \hbar\Omega \left( \overbrace{\hat{\mathbf{a}}^\dagger(k) \hat{\mathbf{a}}(k)}^{\hat{\mathbf{N}}(k)} + \frac{1}{2} \right)$ .

We say that this number operator counts the number of phonons, where each phonon just refers to the number of times the system has been excited. One practical application of this is neutron scattering, where a neutron with some incident energy and momentum is scattered off of a crystal lattice. If we label the incident energy  $E_i$  and momentum  $\vec{p}_i = \hbar\vec{k}_i$  and the outgoing energy and momentum  $E_o$  and  $\vec{p}_o = \hbar\vec{k}_o$ , we can create a plot, for different incoming momenta,  $\Delta E = E_o - E_i$  and  $\Delta\vec{k} = \vec{k}_o - \vec{k}_i$  (see Figure 6.3.2)



**Figure 6.3.2:** Plot of  $\hbar\Omega(k)$  illustrating the interaction of neutrons with a crystal lattice. Negative values correspond to the creation of a phonon while positive values mean a phonon has been absorbed by the scattered neutron, giving it more energy when it leaves the system.

## 6.4 Thermal Equilibrium

Let's create a density operator  $\hat{\rho} = \frac{1}{Z} e^{-\frac{\hat{H}}{kT}}$  where  $\hat{Z} = \text{Tr}\left[e^{-\frac{\hat{H}}{kT}}\right]$ . For a simple harmonic oscillator, we had  $E_n = (n + \frac{1}{2}\hbar\omega)$  for eigenstates  $|n\rangle$ . Here,

$$\begin{aligned}
 \hat{Z} &= \sum_n \langle n | e^{-\frac{\hat{H}}{kT}} | n \rangle \\
 &= e^{-\frac{\hbar\omega}{2kT}} \sum_{n=0}^{\infty} (e^{-\frac{\hbar\omega}{kT}})^n \\
 &= \frac{e^{-\frac{\hbar\omega}{2kT}}}{1 - e^{-\frac{\hbar\omega}{kT}}} \\
 &= \text{Tr}\left[\hat{\rho}\hat{H}\right] \\
 &= \frac{1}{\hat{Z}} \sum_n \left(n + \frac{1}{2}\right) \hbar\omega e^{-E_n} \\
 &= \langle \hat{H} \rangle \quad = \frac{\hbar\omega}{2} + \frac{1}{e^{\frac{\hbar\omega}{kT}} - 1}
 \end{aligned}$$

The expectation value of the Hamiltonian here includes the zero-point energy.

We can also see that the expectation value of the number operator is

$$\langle \hat{N} \rangle = \frac{1}{e^{\frac{\hbar\omega}{kT}} - 1}$$

Note that at low temperature,  $\langle \hat{N} \rangle = 0$  while at high temperature,  $\langle \hat{N} \rangle \sim T$ .

Allow me to restate the Hamiltonian, dropping the harmonic oscillator part, which isn't physical in real atomic structures:

$$\hat{\mathbf{H}} = \sum_j \left( \frac{1}{2} m \dot{x}_j^2 + \frac{1}{2} m \omega_1^2 (x_{j+1} - x_j)^2 \right)$$

and

$$\Omega(k) = 2\omega_1 \left| \sin\left(\frac{kl}{2}\right) \right| = (\omega_1 l)k$$

where  $m\omega_1^2$  is the strength of the atomic bond, roughly modeled as a spring.

When we go to the continuum limit, our discrete sum becomes an integral  $\sim \int \frac{dx}{l}$ . Now our discrete  $x_j$  should also be replaced by some continuous function  $u(x)$ , so  $x_{j+1} - x_j \approx l \frac{\partial u(x)}{\partial x}$ . If  $k$  corresponds to a length scale much larger than the size of the atoms, we no longer care about the mass of the atoms, but rather the mass density  $\mu = \frac{m}{l}$ . Of course,  $\dot{x}_j \rightarrow \frac{\partial u(x)}{\partial t}$  and we will assign a new variable  $m\omega_1^2 l^2 \rightarrow K$  such that  $\omega_1 = \sqrt{\frac{K}{\mu}} - l$ .  $K$  is an elastic constant.

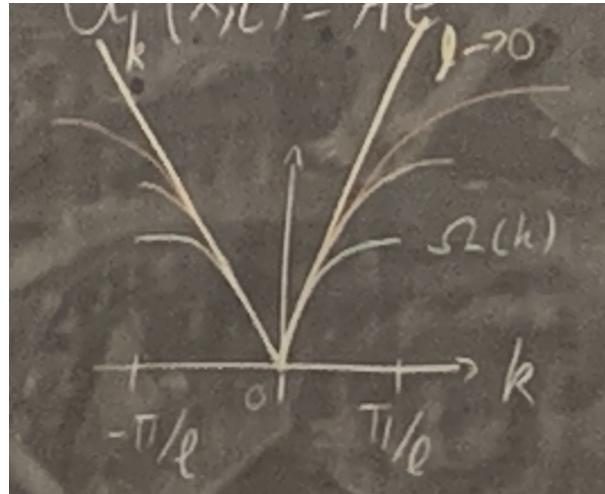
$$H = \int dx \left\{ \frac{1}{2} \mu \left( \frac{\partial u}{\partial t} \right)^2 + \frac{1}{2} K \left( \frac{\partial u}{\partial x} \right)^2 \right\}$$

Solutions to this equation are

$$u_k(x, t) = A e^{i(kx - \omega t)}$$

where  $\omega = vk$  with  $v = \sqrt{\frac{K}{\mu}}$ .

As  $l$  grows smaller,  $\frac{\pi}{l}$  grows bigger—the Brillouin zone gets larger, and the dispersion relation grow as shown in Figure 6.4.1.



**Figure 6.4.1:** Dispersion relation as  $l \rightarrow 0$

## 6.5 Blackbody Radiation

Think of a blackbody as a box of photons. Photons are allowed to leave (radiate) if they are excited.

Say we have a 1-D box which ranges from  $[0, L]$  with boundary conditions where the field vanishes at the boundaries. We see that the set of wavenumbers which conform to these conditions are  $k_j = \frac{\pi}{L} j$  and the allowed frequencies are  $\omega_j = ck_j$ . Call the density of states  $D(\omega)$  and we can define the number of states in an interval  $(\omega, \omega + d\omega)$  as  $D(\omega) d\omega$ . The number of modes with frequency less than  $\omega$  is  $\mathcal{N}(\omega) = \frac{L\omega}{\pi c}$ . Therefore,

$$D(\omega) = \frac{d\mathcal{N}}{d\omega} = \frac{L}{\pi c}$$

In 3-D,

$$\mathcal{N}(\omega) = \frac{4\pi}{3} \left( \frac{\omega L}{2\pi c} \right)^3$$

The values of allowed  $k$  form a discretely spaced set. If we then choose an  $\omega$ , we can see how many  $k$  values lie in the dispersion band for a particular  $\omega$  (again, see Figure 6.4.1).

For photons in 3-D space, we actually need to multiply this value by two, since we can have two different polarized states:

$$\mathcal{N}(\omega) = \frac{4\pi}{3} \left( \frac{\omega L}{2\pi c} \right)^3 \times 2$$

Given this  $\mathcal{N}$ ,

$$D(\omega) = \frac{\omega^2}{\pi^2} \frac{1}{c^3} V$$

where  $V$  is the volume of the box.

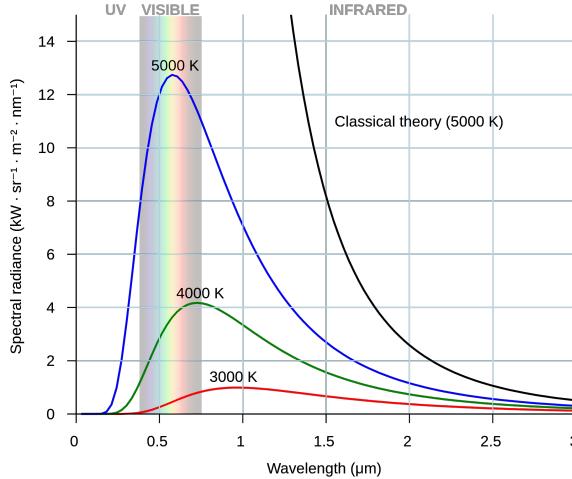
Recall from this morning we discussed the expectation value of the Hamiltonian for a particular temperature and value of  $\omega$ :

$$\hat{\mathbf{H}} = \int dk \hat{\mathbf{H}}(k)$$

so

$$\langle \hat{\mathbf{H}} \rangle(\omega) - \frac{1}{2}\hbar\omega = \frac{\omega^2}{\pi^2} \frac{1}{c^3} V \frac{\hbar\omega}{e^{\frac{\hbar\omega}{kT}} - 1}$$

because many of the modes in the 3-D box are degenerate (just in different directions). The spectral energy density is the famous blackbody spectrum (see Figure 6.5.1)



**Figure 6.5.1:** The Blackbody Energy Density Spectrum

We can see that the spectrum increases with  $\omega^2 T$  at low  $\omega$ , but at some point ( $\omega = \frac{kT}{\hbar}$ ) we leave this Classical behavior and the spectrum changes like  $e^{-\frac{\hbar\omega}{kT}}$ .

## 6.6 Heat Capacity

We can describe a characteristic called heat capacity which corresponds to the way the heat contained in an object changes with temperature:

$$C_v = \frac{\partial U(T)}{\partial T}$$

For a harmonic solid (something with quadratic terms in the Hamiltonian, no higher-order terms), the total energy constant is proportional to the total number of atoms present and the average amount of energy per atom:

$$U = 3N \langle \hat{\mathbf{H}} \rangle$$

Note that phonon modes have three polarizations (degenerate eigenstates in 3-D). Let's examine the Einstein model, where the density of states is described by

$$D(\omega) = 3N\delta(\omega - \omega_E)$$

This is equivalent to bringing back the local harmonic oscillators which we threw away in the continuum limit, and it removes the interaction between nearby atoms. It's not a great model. For this model,

$$C_v \sim e^{-\frac{\hbar\omega_E}{k_B T}}, \quad T \rightarrow 0$$

This explains nicely why heat capacity vanishes at low  $T$  and approaches  $3k_B$  as  $T \rightarrow \infty$ , the Classical limit. The Classical (high temp) and quantum (low temp) regions are separated by characteristic temperature  $\frac{\hbar\omega_E}{k_B}$ .

There is another model by Debye which takes into account the low frequency modes:

$$D(\omega) = \frac{\omega^2}{\pi^2} \frac{1}{c^3} V \div 2 \times 3$$

Note that  $c$  here is the speed of sound, not light.

We divide by 2 to eliminate the degeneracy of photon polarizations which was present in the blackbody derivation, but multiply by 3 to reintroduce the degeneracy of the phonon states.

While both models behave the same way in their extremes, the Debye model varies like  $T^3$  at low temperatures while Einstein's model varies like  $e^{-\frac{\hbar\omega_E}{kT}}$ .

# Chapter 7

## Angular Momentum

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LECTURE 40: ANGULAR MOMENTUM  
Monday, November 18, 2019

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In Classical mechanics, we know that the orbital angular momentum is  $\vec{L} = \vec{r} \times \vec{p}$ . We can examine components of this using the cross product and cyclic permutations ( $L_x = yp_z - zp_y$ ).

In Quantum mechanics, we promote position and momentum to operators.  $L_x$  contains two terms and so does  $L_y$  so any commutator will contain four terms:

$$[\hat{L}_x, \hat{L}_y] = [\hat{Y}\hat{P}_z - \hat{Z}\hat{P}_y, \hat{Z}\hat{P}_x - \hat{X}\hat{P}_z] = \underbrace{[\hat{Y}\hat{P}_z, \hat{Z}\hat{P}_x]}_{\hat{Y}[\hat{P}_z, \hat{Z}]\hat{P}_x} + \underbrace{[\hat{Z}\hat{P}_y, \hat{X}\hat{P}_z]}_{\hat{X}[\hat{Z}, \hat{P}_z]\hat{P}_{uy}} = -i\hbar\hat{Y}\hat{P}_x + i\hbar\hat{X}\hat{P}_y = i\hbar\hat{L}_z$$

This is the orbital angular momentum for a single particle, but we might have many particles. Let's call total angular momentum  $\vec{L} = \sum_{i=1}^N \hat{L}^{(i)}$ . We can also have the total angular momentum, which includes the spin:  $\vec{J} = \vec{L} + \vec{S}$ .

Additionally,  $[\hat{J}_x, \hat{J}_y] = i\hbar\hat{J}_z$  (along with the other cyclic permutations).

There is another operator we want to look at:

$$\hat{J}^2 = \vec{J} \cdot \vec{J} = \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2$$

This total angular momentum squared has interesting commutation relations:

$$[\hat{J}^2, \hat{J}_x] = [\hat{J}_y^2, \hat{J}_x] + [\hat{J}_z^2, \hat{J}_x] = 0$$

We see that  $\hat{J}^2$  commutes with  $\hat{J}_x$ , and it can be shown that it commutes with the other two components also. We are looking for a complete commuting set of observables (CCSO). Customarily, we choose this to be  $\{\hat{J}_z, \hat{J}^2\}$  (because 20th century physicists love Jay-Z according to Dr. Widom).

Let's define

$$\hat{J}_\pm = \hat{J}_x \pm i\hat{J}_y$$

such that we can redefine

$$\hat{J}^2 = \frac{1}{2}(\hat{J}_+ \hat{J}_- + \hat{J}_- \hat{J}_+) + \hat{J}_z^2$$

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We can show that

$$[\hat{\mathbf{J}}_z, \hat{\mathbf{J}}_{\pm}] = \pm \hbar \hat{\mathbf{J}}_{\pm},$$

$$[\hat{\mathbf{J}}_+, \hat{\mathbf{J}}_-] = 2\hbar \hat{\mathbf{J}}_z,$$

and

$$[\hat{\mathbf{J}}^2, \hat{\mathbf{J}}_{\pm}] = 0$$

Let's now talk about the eigenstates of angular momentum. Since  $\langle \psi | \hat{\mathbf{J}}^2 | \psi \rangle \geq 0$ , we know that its eigenvalues must be non-negative. Note that  $\hat{\mathbf{J}}$  is Hermitian, so the eigenvalues are real, therefore squaring them will result in non-negative numbers.

Let's call the eigenstates  $|j\rangle$  and say that they have eigenvalue  $j(j+1)\hbar^2$ :

$$\hat{\mathbf{J}}^2 |j\rangle \equiv j(j+1)\hbar^2 |j\rangle$$

Similarly, we can define the eigenstates of  $\hat{\mathbf{J}}_z$ :

$$\hat{\mathbf{J}}_z |m\rangle = m\hbar |m\rangle$$

Note that  $j$  and  $m$  do not need to be (and rarely are) integers.

We will label shared eigenstates of  $\{\hat{\mathbf{J}}^2, \hat{\mathbf{J}}_z\}$  as  $|kjm\rangle$ , where we include  $k$  in case there's some extra degeneracy for which we need to distinguish states.

Some facts about these eigenstates:

- $-j \leq m \leq j$  Proof:  $0 \leq |\hat{\mathbf{J}}_+ |jm\rangle|^2 = \langle jm | \hat{\mathbf{J}}_- \hat{\mathbf{J}}_+ |jm\rangle = \langle jm | (\hat{\mathbf{J}}^2 - \hat{\mathbf{J}}_z^2 - \hbar \hat{\mathbf{J}}_z) |jm\rangle$ . Next, we can evaluate each of these operators acting on the state:

$$0 \leq (j(j+1) - m^2 - m)\hbar^2$$

so  $m \leq j$ . If we do the same trick starting with  $\hat{\mathbf{J}}_-$  we will find the other half of the inequality.

- $j \geq 0$  ( $\hat{\mathbf{J}}^2 \geq 0$ )
- $m = \pm j$  iff  $\hat{\mathbf{J}}_{\pm} |jm\rangle = 0$ .

$$|\hat{\mathbf{J}}_{\pm} |jm\rangle|^2 = \pm(j(j+1) - m(m+1))\hbar^2 = 0$$

- If  $m \leq -j$  then  $\hat{\mathbf{J}}_z(\hat{\mathbf{J}}_{\pm} |jm\rangle) = (m \pm 1)\hbar(\hat{\mathbf{J}}_{\pm} |jm\rangle)$  and  $\hat{\mathbf{J}}^2(\hat{\mathbf{J}}_{\pm} |jm\rangle) = j(j+1)\hbar^2(\hat{\mathbf{J}}_{\pm} |jm\rangle)$ , so  $\hat{\mathbf{J}}_{\pm}$  acts like a raising/lowering operator for  $m$  but leaves  $j$  unchanged.
- $j \in \mathbb{Z}/2$  (is a half-integer or integer) Proof: Consider lowering the state  $|jm\rangle$   $p$  times using  $\hat{\mathbf{J}}_-$ , we would find that  $-j \leq m-p \leq -j+1$  where  $p$  is an integer. Recall that if  $m = -j$ , lowering it will give us zero.  $m-p-1$  can't be less than  $-j$ . We could also end up exactly at  $-j$ , and if we tried to lower it again we would get 0. Therefore  $\exists p \in \mathbb{Z}$  such that  $m-p = -j$ . We can also say that  $\exists q \in \mathbb{Z}$  such that  $m+q = +j$  using the raising process. We can take these two assertions and subtract them, which would give  $p+q = 2j \in \mathbb{Z}$ .

## 7.1 Particles in Electromagnetic Fields

Suppose we begin with a magnetic field in the  $+z$  direction:

$$\vec{B} = B\hat{e}_z = \vec{\nabla} \times \vec{A}$$

since from electromagnetism, we know that the magnetic field can be described as the curl of a vector potential,  $\vec{A}$ .

**Classical Electrodynamics** We know that Classically, the force on the particle will come from the Lorentz force law:

$$\vec{f} = q\vec{v} \times \vec{B}$$

and it will cause charged particles to move in circular paths (assuming they are already moving with some initial velocity). The radius of these orbits will be proportional to  $\sqrt{E}$ , the square root of the particle's energy, and it will orbit with a frequency

$$\omega_c = -\frac{qB}{m}$$

known as the cyclotron frequency, for a particle with charge  $q < 0$  and mass  $m$ . Note that the frequency is always positive so the negative sign will not be present for positively charged particles.

The Classical Hamiltonian can be written as

$$\mathbf{H} = \frac{1}{2m} [\vec{p} - q\vec{A}]^2$$

since we already know the equations of motion the particle must follow:

$$\dot{\vec{r}} = \frac{\partial H}{\partial \vec{p}} = \frac{\vec{p}}{m}$$

and

$$\dot{\vec{p}} = -\frac{\partial H}{\partial \vec{r}} = q\vec{v} \times \vec{B} = \vec{f}$$

Additionally, we know that the electromagnetic fields are gauge invariant, and particularly we can add any curl-less vector field to the vector potential without changing the resultant fields. In general, we can write a curl-less vector field as  $\vec{\nabla}\chi$  so

$$\vec{A} \rightarrow \vec{A} + \vec{\nabla}\chi$$

is a valid gauge-invariant transformation.

**Quantum Electrodynamics** In the quantum case, we simply promote everything in the Classical Hamiltonian to operators, including the previously discussed gauge invariance:

$$\hat{\mathbf{H}} \rightarrow \hat{\mathbf{H}}' = \frac{1}{2m} [\vec{P} - q\vec{A} - q\vec{\nabla}\chi]^2$$

such that

$$\hat{\mathbf{H}} |\psi\rangle = E |\psi\rangle$$

and

$$\hat{\mathbf{H}}' |\psi'\rangle = E |\psi'\rangle$$

where  $|\psi'\rangle = e^{iq\chi/\hbar} |\psi\rangle$  since the momentum operator acting on this wave function will bring down the necessary derivative of  $\chi$  to cancel the gradient introduced in the gauge invariance condition.

We will examine this system under two different but equivalent gauges and then interpret the results. Most importantly, we want to find a complete set of commuting observables (CSO) which can describe this system and tell us how the degeneracies in quantum states scale as we look at different size scales.

### 7.1.1 The Coulomb Gauge

This gauge is defined from the condition that  $\vec{\nabla} \cdot \vec{A} = 0$ . Using this, we can see that the appropriate vector potential is

$$\vec{A} = -\frac{1}{2}\vec{r} \times \vec{B} = \frac{1}{2}B(x\hat{e}_y - y\hat{e}_x)$$

so that the Hamiltonian is now

$$\hat{H} = \frac{\hat{P}_x^2 + \hat{P}_y^2}{2m} - \underbrace{\frac{qB}{2m}(\hat{X}\hat{P}_y - \hat{Y}\hat{P}_x)}_{\frac{\omega_c}{2}\hat{L}_z} + \underbrace{\frac{q^2B^2}{8m}}_{\frac{1}{2}m\left(\frac{\omega_c}{2}\right)^2} (\hat{X}^2 + \hat{Y}^2)$$

Here, we ignore any  $z$ -dependence because of the symmetry present in the system, and if we included it, we would just find that the particle behaves like a free particle in that direction.

We can now conveniently write out the Hamiltonian using the circularized ladder operators which we discussed in the previous lecture:

$$\hat{H} = \left(\hat{N}_d + \hat{N}_g + 1\right)\hbar\frac{\omega_c}{2} + \left(\hat{N}_d - \hat{N}_g\right)\hbar\frac{\omega_c}{2} = \left(\hat{N}_d + \frac{1}{2}\right)\hbar\omega_c$$

Interestingly, our solution resembles a Quantum Harmonic Oscillator with the cyclotron frequency, but only the right-directed number of quantized turns has any effect on the energy level. If we write our wave function:

$$|\psi_{n_d n_g}\rangle = \frac{1}{\sqrt{n_d! n_g!}} (\hat{a}_d^\dagger)^{n_d} (\hat{a}_g^\dagger)^{n_g} |00\rangle$$

where

$$\langle \vec{r}|00\rangle = \frac{\kappa}{\sqrt{\pi}} e^{-\frac{\kappa^2(x^2+y^2)}{2}}, \quad \kappa^2 = \frac{qB}{2\hbar}$$

we can see that there is a clear degeneracy in energy states for any wave function since the energy is independent of the second quantum number,  $n_g$ . This means  $n_g$  is not a “good” quantum number. Before we complete this set of observables (to create a good set of quantum numbers), it is important to note that the energy levels are

$$E_{n_d n_g} = \left(n_d + \frac{1}{2}\right)\hbar\omega_c$$

and the  $\kappa$  factor used in the wave function can be thought of as a length scale

$$\frac{1}{\kappa} = \sqrt{\frac{2\hbar}{qB}}$$

which we refer to as the “magnetic length”.  $\kappa^2$  is proportional to the area occupied by each orbit, and this is the starting point for the derivation of the Landau Levels.

To complete our set of commuting observables, note that the angular momentum in the  $\hat{z}$ -direction commutes with the Hamiltonian, so our CSCO is  $\{\hat{H}, \hat{L}_z\}$ . To quantify the degeneracy, we can imagine that each orbit of a particular energy level occupies some area, and a box with side length  $\mathcal{L}_x$  and  $\mathcal{L}_y$  can contain a specific number of states of a particular energy. In fact, the degeneracy should be proportional to the area of this box. To better understand why this is true, we will look at another gauge, known as the Landau Gauge:

### 7.1.2 The Landau Gauge

In this gauge, we define  $\vec{A} = Bx\hat{y}$ . Note that we maintain translation invariance in the  $\hat{y}$ -direction:

$$\psi(x, y) = e^{iky} \varphi(x)$$

We can write out the Hamiltonian to see how it looks in this gauge:

$$\hat{\mathbf{H}}\psi(x) = e^{i\vec{k}\cdot\vec{y}} \frac{1}{2m} \left\{ \hat{\mathbf{P}}_x^2 + \hbar k - qB\hat{\mathbf{X}} \right\} \varphi(x) = E\psi = Ee^{i\vec{k}\cdot\vec{y}}\varphi(x)$$

so

$$\hat{\mathbf{H}}_x\varphi(x) = E\varphi(x)$$

where

$$\hat{\mathbf{H}}_x = \frac{1}{2m} \hat{\mathbf{P}}_x^2 + \frac{1}{2} m\omega_c^2 \left( \hat{\mathbf{X}} - \underbrace{\frac{\hbar k}{m\omega_c}}_{X^0} \right)^2$$

This is simply a 1D Quantum Harmonic Oscillator centered at  $X^0$ . Now, instead of circles, our states are plane waves in the  $\hat{\mathbf{y}}$ -direction. If we suppose that, for the box described above, we must have waves which match a periodic boundary condition, we find that the allowed values of  $k$  are quantized:

$$k = \frac{2\pi}{\mathcal{L}_y} N$$

We also want to limit the position of the QHO to be inside the box, so  $0 \leq X_k^0 \leq \mathcal{L}_x$ . Therefore,  $0 \leq N \leq \frac{m\omega_c}{2\pi\hbar} \mathcal{L}_x \mathcal{L}_y$ , where  $N$  is the degeneracy of the state. We see here that

$$N \propto \frac{qB}{h} \times \mathcal{A}$$

where  $\mathcal{A}$  is the area of the box, so the degeneracy is proportional to the magnetic flux,  $\Phi = B\mathcal{A} \times \Phi_0$  where  $\Phi_0 = \frac{\hbar}{q}$  is called the flux quantum.

### Note

There is a relationship between the wave functions in these gauges:

$$\psi_{n_d n_g}(x, y) = \int dk e^{-\frac{k^2}{2\kappa^2}} \psi_{kn_x}(x, y)$$

## LECTURE 42: ROTATIONS OF QUANTUM STATES

Friday, November 22, 2019

## 7.2 Rotations of Quantum States

Let's denote a rotation as a vector  $\vec{\alpha} = \alpha\hat{\mathbf{u}}$ . We think of this rotation as an action  $\mathcal{R}_{\hat{\mathbf{u}}}(\alpha) : \vec{\mathbf{v}} \rightarrow \vec{\mathbf{v}}' = \mathcal{R}\vec{\mathbf{v}}$ . This is what we call an active rotation; The coordinate system is fixed and there is a vector which is being actively transformed. We can combine rotations, and the order of operation doesn't matter as long as we rotate around the same axis:

$$\mathcal{R}_u(\alpha)\mathcal{R}_u(\alpha') = \mathcal{R}_u(\alpha')\mathcal{R}_u(\alpha)$$

However, this is generally not true for rotations by different axes:

$$\mathcal{R}_u(\alpha)\mathcal{R}_{u'}(\alpha') \neq \mathcal{R}_{u'}(\alpha')\mathcal{R}_u(\alpha)$$

How do rotations transform quantum states? First, let's consider a spinless particle. Suppose  $\psi(\vec{\mathbf{r}}) = \langle \vec{\mathbf{r}} | \psi \rangle$ . Let's define a rotation operator  $\mathcal{R} : \vec{\mathbf{r}} \rightarrow \vec{\mathbf{r}}' = \mathcal{R}\vec{\mathbf{r}}$ . We are looking for a state such that  $\psi'(\vec{\mathbf{r}}') = \langle \vec{\mathbf{r}}' | \psi' \rangle = \psi(\vec{\mathbf{r}})$ .

$$\psi'(\mathcal{R}\vec{\mathbf{r}}) = \psi(\vec{\mathbf{r}}) \implies \psi'(\vec{\mathbf{r}}) = \psi(\mathcal{R}^{-1}\vec{\mathbf{r}})$$

by replacing  $\mathcal{R}\vec{r} \equiv \vec{s}$  and then  $\vec{s} \rightarrow \vec{r}$ . These are dummy variables,  $\vec{r}$  can take any value since the coordinate system is standing still. What does the rotation do to the ket vector?

$$\mathcal{R}: |\psi\rangle \rightarrow |\psi'\rangle = \hat{\mathbf{R}} |\psi\rangle$$

Therefore

$$\langle \vec{r} | (\hat{\mathbf{R}} |\psi\rangle) = \langle \mathcal{R}^{-1} \vec{r} | \psi \rangle$$

This is a unitary operator, it is intended to maintain orthogonality of Classical vectors, but we can see it also preserves orthogonality of ket vectors.

How do we connect these operators with angular momentum? Let's think of an infinitesimal rotation,  $\mathcal{R}_{\hat{\mathbf{u}}}(\mathrm{d}\alpha): \vec{r} \rightarrow \vec{r}' \approx \vec{r} + \mathrm{d}\alpha \hat{\mathbf{u}} \times \vec{r} + \dots$ . We can also look at what happens to the wave function:

$$\psi \rightarrow \psi'(\vec{r}) = \psi(\vec{r} - \mathrm{d}\alpha \hat{\mathbf{u}} \times \vec{r})$$

For example, lets take  $\hat{\mathbf{u}} = \hat{\mathbf{e}}_2$ :

$$\begin{aligned} \psi'(x, y, z) &= \psi(x + y \mathrm{d}\alpha, y - x \mathrm{d}\alpha, z) = \psi(x, y, z) + \mathrm{d}\alpha [y \partial_x \psi - x \partial_y \psi] \\ &= \left\{ \left( 1 - \frac{i}{\hbar} \mathrm{d}\alpha \hat{\mathbf{L}}_z \right) \psi \right\} (x, y, z) \\ &= \psi'(x, y, z) \end{aligned}$$

so

$$\hat{\mathbf{R}}_{\hat{\mathbf{u}}}(\mathrm{d}\alpha) = \hat{\mathbf{I}} - \frac{i}{\hbar} \mathrm{d}\alpha \hat{\mathbf{u}} \cdot \hat{\mathbf{L}}$$

We can divide by  $\mathrm{d}\alpha$  (Leibnitz hates this):

$$\frac{\mathrm{d}\hat{\mathbf{R}}_{\hat{\mathbf{u}}}(\alpha)}{\mathrm{d}\alpha} = -\frac{i}{\hbar} \hat{\mathbf{u}} \cdot \hat{\mathbf{L}}$$

so

$$\hat{\mathbf{R}}_{\hat{\mathbf{u}}}(\alpha) = e^{-\frac{i}{\hbar} \alpha \hat{\mathbf{u}} \cdot \hat{\mathbf{L}}}$$

What if we weren't working with a spinless particle? In this case, we are talking about a spinor, a tensor product with the spin state. For spin-1/2,  $\vec{S} = \frac{\hbar}{2} \vec{\sigma}$ , in terms of the Pauli matrices.

Define  $\hat{\mathbf{R}}_{\hat{\mathbf{u}}}(\theta) = e^{-\frac{i}{\hbar} \theta \hat{\mathbf{u}} \cdot \hat{\mathbf{S}}}$ . Therefore

$$\hat{\mathbf{R}}_{\hat{\mathbf{u}}}(\theta) = \cos\left(\frac{\theta}{2}\right) \hat{\mathbf{I}} - i \hat{\mathbf{u}} \cdot \vec{\sigma} \sin\left(\frac{\theta}{2}\right)$$

What does this operator do to a spinor  $|\chi\rangle$ ?

$$|\chi'\rangle \equiv \hat{\mathbf{R}}_{\hat{\mathbf{u}}}(\theta) |\chi\rangle$$

where  $|\chi\rangle$  could be  $|+\rangle_z$ , for example.

Suppose we want to rotate this spinor into the x/y-plane. For such a rotation, the end-state will be defined by the angle  $\varphi$  in the plane, so  $\hat{\mathbf{u}} = (\cos(\varphi + \frac{\pi}{2}), \sin(\varphi + \frac{\pi}{2}), 0)$ , so

$$\hat{\mathbf{R}} = \cos\left(\frac{\theta}{2}\right) \hat{\mathbf{I}} + \frac{1}{2} (\sigma_+ e^{-i\varphi} - \sigma_- e^{i\varphi}) \sin\left(\frac{\theta}{2}\right)$$

so

$$\hat{\mathbf{R}} |\chi\rangle = \cos\left(\frac{\theta}{2}\right) |+\rangle_z + e^{i\varphi} \sin\left(\frac{\theta}{2}\right) |-\rangle_z$$

Homework 3 told us how to interpret such a state: The end state has the property  $\vec{S} = +\frac{\hbar}{2}$  in the direction  $\vec{v}'$ .

Let's now look at the total angular momentum,  $\vec{J} = \vec{L} + \vec{S}$  which acts in the Hilbert space  $\mathcal{H}_{\vec{r}} \otimes \mathcal{H}_S$ . We now want introduce a rotation operator which is a combination of the spatial operator (from the spinless example) and the spin operator:  $\hat{\mathbf{R}} = \hat{\mathbf{R}}^{(r)} \otimes \hat{\mathbf{R}}^{(s)}$ , so

$$\hat{\mathbf{R}} = e^{-\frac{i}{\hbar}\theta \hat{\mathbf{u}} \cdot \vec{J}}$$

One application of this is that if we have a angularly-invariant potential, the total angular momentum is conserved, since

$$\hat{\mathbf{H}} = \frac{\hat{\mathbf{P}}^2}{2m} + \hat{\mathbf{V}}(|\vec{\mathbf{R}}|)$$

is scalar so

$$[\vec{J} \cdot \hat{\mathbf{u}}, \hat{\mathbf{H}}] = 0 \implies \frac{\partial}{\partial t} \langle \vec{J} \rangle = 0$$

Also, because  $[\hat{\mathbf{J}}_{\pm}, \hat{\mathbf{H}}] = 0$ , if  $|kjm\rangle$  is an eigenstate of  $\hat{\mathbf{H}}$ ,

$$\hat{\mathbf{J}}_{\pm}(\hat{\mathbf{H}}|kjm\rangle = E_{kjm}|kjm\rangle) \implies \hat{\mathbf{H}}(\hat{\mathbf{J}}_{\pm}|kjm\rangle) = E_{kjm}(\hat{\mathbf{J}}_{\pm}|kjm\rangle)$$

so

$$E_{kjm} = E_{kj}$$

so there is a degeneracy in  $2j+1$ .

Finally, for some scalar observable  $\hat{\mathbf{A}}$ ,

$$\langle k'j'm'|\hat{\mathbf{A}}|kjm\rangle = \langle k'_{jj}|\hat{\mathbf{A}}|k_{jj}\rangle \delta_{jj'}\delta_{mm'}$$

is independent of  $m$ .

### LECTURE 43: ROTATION OF OBSERVABLES

Friday, November 22, 2019

Let's imagine we have some observable  $\hat{\mathbf{A}}$  with eigenstates  $\hat{\mathbf{A}}|u_n\rangle = a_n|u_n\rangle$ . We first define the rotated eigenvector:  $|u'_n\rangle = \hat{\mathbf{R}}|u_n\rangle$ , and next, we define  $\hat{\mathbf{A}}'|u'_n\rangle = a_n|u'_n\rangle$ . Therefore

$$\hat{\mathbf{A}}'\hat{\mathbf{R}}|u_n\rangle = a_n\hat{\mathbf{R}}|u_n\rangle \quad \forall |u_n\rangle$$

so

$$\hat{\mathbf{A}}' = \hat{\mathbf{R}}\hat{\mathbf{A}}\hat{\mathbf{R}}^{-1}$$

We've discussed some types of observables. Scalar observables commute with all components of angular momentum:  $[\vec{J}, \hat{\mathbf{A}}] = 0$ . For example,  $\hat{\mathbf{H}}$ ,  $|\vec{\mathbf{R}}|^2$ ,  $|\vec{\mathbf{P}}|^2$ ,  $\vec{\mathbf{R}} \cdot \vec{\mathbf{P}}$ , etc.

Additionally, we can have vector observables:  $\vec{\mathbf{A}} = (\hat{\mathbf{A}}_x, \hat{\mathbf{A}}_y, \hat{\mathbf{A}}_z)$ .

$$\mathcal{R}_{\hat{\mathbf{x}}}(\mathrm{d}\alpha) \implies \begin{cases} \hat{\mathbf{x}} \rightarrow \hat{\mathbf{x}}' = \hat{\mathbf{x}} \\ \hat{\mathbf{A}}_x \rightarrow \hat{\mathbf{A}}'_x = \hat{\mathbf{x}}' \cdot \vec{\mathbf{A}} = \hat{\mathbf{A}}_x \\ [\hat{\mathbf{J}}_x, \hat{\mathbf{A}}_x] = 0 \end{cases}$$

However,

$$\mathcal{R}_{\hat{\mathbf{y}}}(\mathrm{d}\alpha) \implies \begin{cases} \hat{\mathbf{x}} \rightarrow \hat{\mathbf{x}}' = \hat{\mathbf{x}} + \mathrm{d}\alpha \hat{\mathbf{y}} \times \hat{\mathbf{x}} = \hat{\mathbf{x}} - \mathrm{d}\alpha \hat{\mathbf{z}} \\ \hat{\mathbf{A}}_x \rightarrow \hat{\mathbf{A}}'_x = \hat{\mathbf{A}}_x - \mathrm{d}\alpha \hat{\mathbf{A}}_z \\ [\hat{\mathbf{J}}_y, \hat{\mathbf{A}}_x] = -i\hbar \hat{\mathbf{A}}_z \end{cases}$$

and similarly

$$[\hat{\mathbf{J}}_z, \hat{\mathbf{A}}_x] = i\hbar \hat{\mathbf{A}}_y$$

Since  $\hat{\mathbf{R}} = e^{-\frac{i}{\hbar} d\alpha \vec{\mathbf{J}} \cdot \hat{\mathbf{u}}} \approx 1 - \frac{i}{\hbar} d\alpha \vec{\mathbf{J}} \cdot \hat{\mathbf{u}}$  so  $\hat{\mathbf{A}}' = \hat{\mathbf{A}} - \frac{i}{\hbar} d\alpha [\vec{\mathbf{J}} \cdot \hat{\mathbf{u}}, \hat{\mathbf{A}}]$ .

We can see that vector observables are things that commute with angular momentum in a way similar to angular momentum's commutation relations:  $\vec{\mathbf{J}}, \vec{\mathbf{L}}, \vec{\mathbf{S}}, \vec{\mathbf{R}}, \vec{\mathbf{P}}$ , etc.

**Example.** 2-D Harmonic Oscillator:  $\hat{\mathbf{V}}(x, y) = \frac{1}{2}m\omega^2(x^2 + y^2)$ , and  $\hat{\mathbf{H}} = \frac{|\vec{\mathbf{P}}|^2}{2m} + \frac{1}{2}m\omega^2|\vec{\mathbf{R}}|^2 = \hat{\mathbf{H}}_x + \hat{\mathbf{H}}_y$ . We can write the eigenstates as

$$|n_x n_y\rangle = |n_x\rangle \otimes |n_y\rangle = (\hat{\mathbf{a}}_x^\dagger)^{n_x} (\hat{\mathbf{a}}_y^\dagger)^{n_y} |00\rangle$$

Note that we can write the Hamiltonian as  $\hat{\mathbf{H}} = (\hat{\mathbf{N}}_x + \hat{\mathbf{N}}_y + 1)\hbar\omega$ , so

$$E_{n_x n_y} = (n_x + n_y + 1)\hbar\omega$$

Therefore,  $E_{00}$  is the ground state,  $E_{10} = E_{01}$  are degenerate first excited states, and  $E_{20} = E_{11} = E_{02}$  are degenerate second excited states. Because of this degeneracy, we know there must be another observable to add to our complete set of commuting observables (CSOCO) to get all the “good” quantum numbers to sufficiently distinguish the states of the system. The angular momentum operator  $\hat{\mathbf{L}}_z = \hat{\mathbf{X}}\hat{\mathbf{P}}_y - \hat{\mathbf{Y}}\hat{\mathbf{P}}_x = i\hbar(\hat{\mathbf{a}}_x\hat{\mathbf{a}}_y^\dagger - \hat{\mathbf{a}}_x^\dagger\hat{\mathbf{a}}_y)$  commutes with the Hamiltonian. Our number states are not eigenstates of the angular momentum, but we can define some new raising and lowering operators (with French suffixes, of course):

$$\hat{\mathbf{a}}_d = \frac{1}{\sqrt{2}}(\hat{\mathbf{a}}_x - i\hat{\mathbf{a}}_y)$$

(droite/right)

$$\hat{\mathbf{a}}_g = \frac{1}{\sqrt{2}}(\hat{\mathbf{a}}_x + i\hat{\mathbf{a}}_y)$$

(gauche/left)

$$[\hat{\mathbf{a}}_{(d,g)}, \hat{\mathbf{a}}_{(d,g)}^\dagger] = 1$$

We can also see that

$$\hat{\mathbf{a}}_d |n_x n_y\rangle = (\dots) |n_x - 1, n_y\rangle + (\dots) |n_x, n_y - 1\rangle$$

$\hat{\mathbf{a}}_d$  and  $\hat{\mathbf{a}}_g$  are lowering operators which take us between linear combinations of energy states. Our previous operators  $\hat{\mathbf{a}}_{(x,y)}$  act on linearly polarized states which are only in the  $x$  or  $y$  direction. However, these operators act on linear combinations of linearly polarized states (which give us circularly or elliptically polarized states), the “droite” operator acting on right-polarized states and “gauche” acting on left-polarized states.

This allows us to express the Hamiltonian as

$$\hat{\mathbf{H}} = \left( \hat{\mathbf{a}}_d^\dagger \hat{\mathbf{a}}_d + \hat{\mathbf{a}}_g^\dagger \hat{\mathbf{a}}_g + 1 \right) \hbar\omega = (\hat{\mathbf{N}}_d + \hat{\mathbf{N}}_g + 1)\hbar\omega$$

Additionally,

$$(\hat{\mathbf{N}}_d - \hat{\mathbf{N}}_g)\hbar = \hat{\mathbf{L}}_z$$

We can now create simultaneous eigenstates of these number operators:

$$|n_d n_g\rangle = \frac{1}{\sqrt{n_d! n_g!}} (\hat{\mathbf{a}}_d^\dagger)^{n_d} (\hat{\mathbf{a}}_g^\dagger)^{n_g} |00\rangle$$

so

$$\hat{\mathbf{H}} |n_d n_g\rangle = (n_d + n_g + 1)\hbar\omega |n_d n_g\rangle$$

and

$$\hat{\mathbf{L}}_z |n_d n_g\rangle = (n_d - n_g)\hbar |n_d n_g\rangle$$

Therefore, we now have a similar ladder of degenerate energy states: One ground state  $\chi_{00} \sim e^{-r^2/2}$ , two first-excited states,  $\chi_{01} \sim r e^{-r^2/2} e^{-i\varphi}$ ,  $\chi_{10} \sim r e^{-r^2/2} e^{i\varphi}$ , and three second-excited states,  $\chi_{02} \sim r^2 e^{-r^2/2} e^{-2i\varphi}$ ,  $\chi_{11} \sim (r^2 - 1) e^{-r^2/2}$ , and  $\chi_{20} \sim r^2 e^{-r^2/2} e^{2i\varphi}$ .  $\diamond$

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## LECTURE 44: THE HYDROGEN ATOM

Friday, December 06, 2019

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If  $\hat{\mathbf{V}}(|\vec{\mathbf{R}}|)$ ,

$$\hat{\mathbf{H}} = \frac{\hat{\mathbf{P}}^2}{2m} + \hat{\mathbf{V}} = \frac{\hat{\mathbf{P}}_r^2}{2m} + \underbrace{\frac{\hat{\mathbf{L}}^2}{2mr^2} + \hat{\mathbf{V}}(r)}_{V_{\text{eff}}(r)}$$

For energy eigenstates,  $\hat{\mathbf{L}}^2\varphi = l(l+1)\hbar^2\varphi$  and  $\hat{\mathbf{L}}_z\varphi = m\hbar\varphi$ . We can separate such eigenstates into a radial part and a spherical part:

$$\varphi(\vec{\mathbf{r}}) = R_{kl}(r)Y_{lm}(\Omega)$$

When we apply our Hamiltonian to this state, we find that

$$\left\{ -\frac{\hbar^2}{2m} \frac{1}{r} \frac{d^2}{dr^2} r + \frac{l(l+1)\hbar^2}{2mr^2} + V(r) \right\} R_{kl}(r) = E_{kl} R_{kl}(r)$$

Let's assume that the radial solution is some power law,

$$R_{kl}(r) \sim Cr^s$$

When we plug this into our radial Schrödinger equation, taking  $r \rightarrow 0$  to neglect the potential, we find that

$$-s(s+1) + l(l+1) = 0$$

such that  $s = l$  or  $s = -(l+1)$ . The second solution would cause the solution to diverge at the origin, so this solution is not viable. Therefore, we would find that the radial function goes like  $R_{kl}(r) \sim r^l$ . This is about as far as we can get before we specify a specific form for the potential. Let's now choose a particular central potential.

### 7.3 Coulomb Potential

$$V(r) = -\frac{e^2}{r}$$

#### Note

The Hamiltonian above is for a single particle. Now consider the mass to be the reduced mass in the center of mass frame of two particles (a proton and electron in the case of the Hydrogen atom).

It's now useful to introduce some dimensionless coordinates. We will scale  $r \rightarrow \frac{r}{a_0}$  and  $E \rightarrow \frac{E}{E_I}$ , where  $a_0 = \frac{\hbar^2}{me^2} = 0.529\text{\AA}$  is the Bohr radius, known as the "Bohr" and  $E_I = \frac{me^4}{2\hbar^2} = 13.6\text{eV}$  and is called the "Rydberg". This is the energy it takes to remove the electron from the Hydrogen atom. Let's also call the radial function

$$u_{kl}(r) = rR_{kl}(r)$$

so that the Schrödinger equation becomes

$$\left\{ \frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + \frac{2}{r} + E_{kl} \right\} u_{kl}(r) = 0$$

If we call  $E_{kl} = -\lambda_{kl}^2$  and take the limit of  $r \rightarrow \infty$ , we find

$$u'' - \lambda^2 u = 0$$

so  $u \sim e^{-\lambda r}$  as  $r \rightarrow \infty$ . We previously found the solution for small  $r$ , so now we want to combine those solutions. We will introduce a function  $y(r)$  in order to solve the equation in between these limits.

$$u(r) = r^{l+1} e^{-\lambda r} y(r)$$

The only thing we currently know about  $y(r)$  is that  $y(0) = 1$ . If we plug in this solution to the Schrödinger equation, we would discover that  $y(r) \sim e^{2\lambda r}$ . This solution will vanish unless  $\lambda = \frac{1}{k+l}$  where  $k \in \mathbb{Z}$  and  $k \geq 1$ . Previously we had assumed there was some additional quantum number,  $k$  which would be necessary to fully define a wave function. This is that quantum number. The specifications on  $k$  are special cases where the wave function will be normalizable, and under this condition,  $y(r)$  is a “Laguerre Polynomial”.

Remember that  $\lambda^2 = -E_{kl}$  so the energy depends on  $k$  and  $l$ . Let  $n \equiv k + l \in \mathbb{Z}$ ,  $n \geq 1$ . Therefore,  $E_{kl} = -\frac{1}{n^2}$ , or, reintroducing the units,  $E = -\frac{13.6\text{eV}}{n^2}$ .

There is now an extra degeneracy in these states because the energy depends on both  $k$  and  $l$ . We have at least  $(2l+1)$ -fold degeneracy, since  $-l \leq m \leq l$  and the energy doesn't depend on  $m$ . For a given  $n$ , only certain values of  $l$  will be valid. Since  $n, k \geq 1$ , we could have  $l = 0, 1, 2, \dots, n-1$ . All of these values of  $l$  can be paired with a value of  $k$  to yield the same energy, so the total degeneracy will be given by

$$g_n = \sum_{l=0}^{n-1} (2l+1) = n^2 = 1, 4, 9, \dots$$

What do these wave functions look like? We know that the angular parts will just be spherical harmonics.

$$\begin{aligned} R_{k=1,l=0}(r) &\sim e^{-\frac{r}{a_0}} \quad 1S \text{ from } n = 1, l = 0 \rightarrow S \\ R_{k=2,l=0} &\sim \left(1 - \frac{r}{a_0}\right) e^{-\frac{r}{2a_0}} \quad 2S \\ R_{k=1,l=1} &\sim \frac{r}{a_0} e^{-\frac{r}{2a_0}} \quad 2P \text{ from } l = 1 \end{aligned}$$

In general,  $R_n \sim e^{-\frac{r}{na_0}}$ .

## 7.4 Origin of the Accidental Coulomb Degeneracy

Imagine a planet orbiting a star in an elliptical path. The point of closest approach, the perihelion, sits at a certain position relative to the star. Let's call this  $\vec{\mathbf{A}}$ . After each orbit, the planet returns to this position with the same momentum. This means that the perihelion is a conserved vector. This conservation is due to the fact that the gravitational potential is  $\sim \frac{1}{r}$ . We can write down the perihelion vector:

$$\vec{\mathbf{A}} = me^2 \hat{\mathbf{r}} - \vec{\mathbf{p}} \times \vec{\mathcal{L}}$$

which is also called the Laplace-Runge-Lenz vector. There is a quantum version of this:

$$\vec{\mathbf{A}} = me^2 \hat{\mathbf{R}} - \frac{1}{2} (\vec{\mathbf{P}} \times \vec{\mathbf{L}} - \vec{\mathbf{L}} \times \vec{\mathbf{P}})$$

with

$$[\hat{\mathbf{A}}_i, \hat{\mathbf{A}}_j] \sim \epsilon_{ijk} \hat{\mathbf{L}}_k$$

and

$$[\hat{\mathbf{L}}_i, \hat{\mathbf{A}}_j] \sim \epsilon_{ijk} \hat{\mathbf{A}}_k$$

and

$$[\vec{\mathbf{A}}, \hat{\mathbf{H}}] = 0$$

This last property tells us that  $\vec{\mathbf{A}}$  is conserved (which we knew) but also that its eigenvalues distinguish degenerate energies. Notice that  $[\hat{\mathbf{A}}_x, \hat{\mathbf{H}}] = 0$  and  $[\hat{\mathbf{A}}_x, \hat{\mathbf{L}}_z] \neq 0$ .

$$\hat{\mathbf{H}}\hat{\mathbf{A}}_x\psi_{klm} = \hat{\mathbf{A}}_x\hat{\mathbf{H}}\psi_{klm} = E_{kl}\psi_{klm}$$

so

$$\hat{\mathbf{A}}_x\psi_{klm}$$

is an eigenstate of  $\hat{\mathbf{H}}$  with energy  $E_{kl}$ . On the other hand, we know that

$$\hat{\mathbf{A}}_x\psi_{klm} \neq c\psi_{klm}$$

since this vector does not commute with the angular momentum operator. Therefore, these shared eigenstates of  $\hat{\mathbf{H}}$  and  $\hat{\mathbf{A}}_x$  are different than the eigenstates we saw from the angular momentum operator, so there is still some degeneracy in these states which we cannot remove by introducing this new observable.

## LECTURE 45: HYBRID ORBITALS

Friday, December 06, 2019

## 7.5 Hybrid Orbitals

This morning, we learned about the Coulomb degeneracy and discovered that

$$E_{kl} = \frac{-E_I}{(k+l)^2}$$

Due to this dependency, we replaced the set of quantum numbers  $\{k, l, m\}$  with  $\{n, l, m\}$  where  $n = k + l \geq 1$ , and  $l = 0, 1, \dots, n - 1$ . In Hydrogen, this means

$$E_{2S} = E_{2P}$$

Because these states are degenerate, the eigenstates of the Hamiltonian can be linear combinations of these states. This turns out to be critical for bonding models. For example,

$$\begin{aligned} \varphi_{n,1,\pm 1} &= \mp \sqrt{\frac{3}{8\pi}} R_{n1}(r) \sin(\theta) e^{\pm i\varphi} \\ \varphi_{n10} &= \sqrt{\frac{3}{4\pi}} R_{n1}(r) \cos(\theta) \end{aligned}$$

We can make linear combinations

$$\begin{aligned} \varphi_{nP_x} &= -\frac{1}{\sqrt{2}} [\varphi_{n,1,+1} - \varphi_{n,1,-1}] = \sqrt{\frac{3}{4\pi}} R_{n1}(r) \frac{x}{r} \\ \varphi_{nP_y} &= \frac{i}{\sqrt{2}} [\varphi_{n,1,+1} + \varphi_{n,1,-1}] = \sqrt{\frac{3}{4\pi}} R_{n1}(r) \frac{y}{r} \end{aligned}$$

and

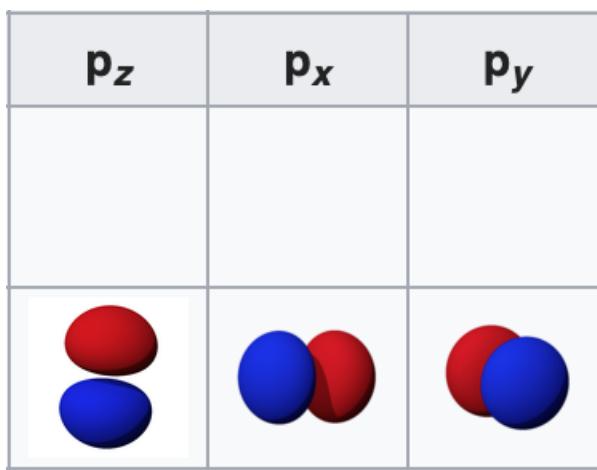
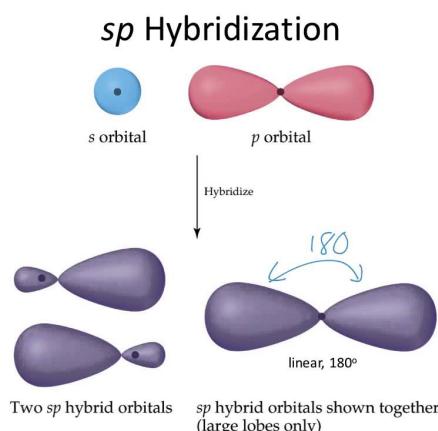
$$\varphi_{nP_z} = \sqrt{\frac{3}{4\pi}} R_{n1}(r) \frac{z}{r}$$

Suppose we constructed a linear combination of the  $\varphi_{P_z}$  and  $\varphi_S$  wave functions. We call the resulting functions “hybrid orbitals”.

We can use these hybrid orbitals to understand interatomic bonding in real atoms and real molecules.

**Example.** Acetylene ( $C_2H_2$ )

The carbon atoms will have the following electron configuration:  $[1s^2]2s2p^3$  where the innermost electron is tightly bound and does not interact. On the other hand, hydrogen has the configuration  $1s$ . If we call  $\varphi_{\pm} = \varphi_{P_z} \pm \varphi_S$ , then we see that the overlapping wave functions between the carbon atoms is an  $s$ -like

**Figure 7.5.1:** Plots of the wave functions  $\varphi_{nP_{x/y/z}}$ **Figure 7.5.2:** *sp* hybrid orbitals

bond which we call a  $\sigma$  bond. Similar bonds will exist between the carbon and hydrogen atoms. Each of these bonds will contain one spin-up and one spin-down electron. Additionally, the  $P_x$  and  $P_y$  orbitals from the carbon atoms can hybridize in planes to form  $\Pi_x$  and  $\Pi_y$  orbitals, which are *p*-like orbitals since rotation around the  $z$ -axis will result in a change in the sign of the wave function.

In conclusion, the  $C - H$  bonds are single bonds, whereas the bonds between the carbon atoms are triple bonds ( $C \equiv C$ ), made up of two  $\Pi$  bonds and a  $\sigma$  bond.

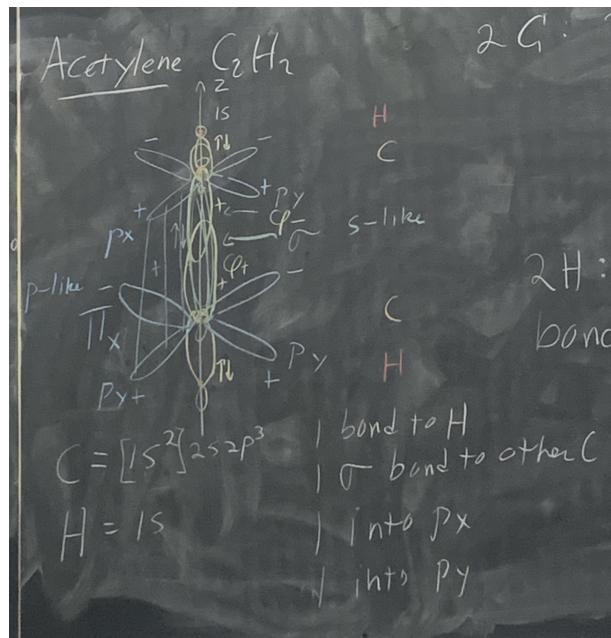
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The  $sp^2$ -hybrids can be described by the wave functions

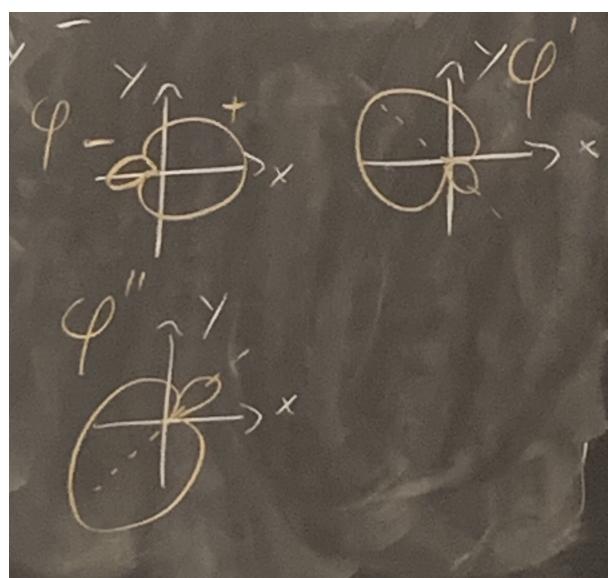
$$\begin{aligned}\varphi_{SP_xP_y} &= \frac{1}{\sqrt{3}}\varphi_S + \sqrt{\frac{2}{3}}\varphi_{P_x} \\ \varphi''_{SP_xP_y} &= \frac{1}{\sqrt{3}}\varphi_S + \frac{1}{\sqrt{6}}\varphi_{P_x} + \frac{1}{\sqrt{2}}\varphi_{P_y} \\ \varphi'''_{SP_xP_y} &= \frac{1}{\sqrt{3}}\varphi_S + \frac{1}{\sqrt{6}}\varphi_{P_x} - \frac{1}{\sqrt{2}}\varphi_{P_y}\end{aligned}$$

**Example.** Ethylene ( $C_2H_4$ ) has  $SP^2$  hybrid orbitals which bond to the hydrogen atoms (the primed orbitals) and to each other (the unprimed orbital). There will also be a  $P_z$  orbital which can bond in a  $\Pi$  bond, creating the double bond between the carbon atoms.

◊



**Figure 7.5.3:** The bonding structure of Acetylene



**Figure 7.5.4:** The  $SP^2$  Hybrids