PHY356F lecture notes.

Originally appeared at:
`http://sites.google.com/site/peeterjoot/math2010/PHY356F.pdf`

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Dec 7, 2010 PHY356F.tex

Contents

1. Disclaimer.

These are personal lecture notes for the Fall 2010, University of Toronto Quantum mechanics I course, taught by Prof. Vatche Deyirmenjian. Typos, if any, are probably mine (Peeter), and no claim nor attempt of spelling or grammar correctness will be made. The first four lectures I had chosen not to take notes for since they followed the text [1] very closely.

PHY356F : Quantum Physics I Fall 2010

Lecture 5 — Review — October 12, 2010

Prof. Vatche Deyirmenjian *Scribe: Peeter Joot*

2. Lecture 5 — Review — October 12, 2010

Review. What have we learned?

2.1. *Chapter 1.*

Information about systems comes from vectors and operators. Express the vector $|\phi\rangle$ describing the system in terms of eigenvectors $|a_n\rangle$. $n \in 1, 2, 3, \cdots$.

of some operator A. What are the coefficients c_n? Act on both sides by $\langle a_m|$ to find

$$\begin{aligned}\langle a_m|\phi\rangle &= \sum_n c_n \underbrace{\langle a_m|a_n\rangle}_{\text{Kronicker delta}} \\ &= \sum c_n \delta_{mn} \\ &= c_m\end{aligned}$$

$$c_m = \langle a_m | \phi \rangle$$

Analogy

$$\mathbf{v} = \sum_i v_i \mathbf{e}_i$$

$$\mathbf{e}_1 \cdot \mathbf{v} = \sum_i v_i \mathbf{e}_1 \cdot \mathbf{e}_i = v_1$$

Physical information comes from the probability for obtaining a measurement of the physical entity associated with operator A. The probability of obtaining outcome a_m, an eigenvalue of A, is $|c_m|^2$

2.2. *Chapter 2.*

Deal with operators that have continuous eigenvalues and eigenvectors.
We now express

$$|\phi\rangle = \int dk \underbrace{f(k)}_{\text{coefficients analogous to } c_n} |k\rangle$$

Now if we project onto k'

$$\begin{aligned} \langle k' | \phi \rangle &= \int dk f(k) \underbrace{\langle k' | k \rangle}_{\text{Dirac delta}} \\ &= \int dk f(k) \delta(k' - k) \\ &= f(k') \end{aligned}$$

Unlike the discrete case, this is not a probability. Probability density for obtaining outcome k' is $|f(k')|^2$.
Example 2.

$$|\phi\rangle = \int dk f(k) |k\rangle$$

Now if we project x onto both sides

$$\langle x | \phi \rangle = \int dk f(k) \langle x | k \rangle$$

With $\langle x | k \rangle = u_k(x)$

$$\begin{aligned}\phi(x) &\equiv \langle x|\phi\rangle \\ &= \int dk f(k) u_k(x) \\ &= \int dk f(k) \frac{1}{\sqrt{L}} e^{ikx}\end{aligned}$$

This is with periodic boundary value conditions for the normalization. The infinite normalization is also possible.

$$\phi(x) = \frac{1}{\sqrt{L}} \int dk f(k) e^{ikx}$$

Multiply both sides by $e^{-ik'x}/\sqrt{L}$ and integrate. This is analogous to multiplying $|\phi\rangle = \int f(k)|k\rangle dk$ by $\langle k'|$. We get

$$\begin{aligned}\int \phi(x) \frac{1}{\sqrt{L}} e^{-ik'x} dx &= \frac{1}{L} \iint dk f(k) e^{i(k-k')x} dx \\ &= \int dk f(k) \Big(\frac{1}{L} \int e^{i(k-k')x} \Big) \\ &= \int dk f(k) \delta(k-k') \\ &= f(k')\end{aligned}$$

$$f(k') = \int \phi(x) \frac{1}{\sqrt{L}} e^{-ik'x} dx$$

We can talk about the state vector in terms of its position basis $\phi(x)$ or in the momentum space via Fourier transformation. This is the equivalent thing, but just expressed different. The question of interpretation in terms of probabilities works out the same. Either way we look at the probability density.

The quantity

$$|\phi\rangle = \int dk f(k)|k\rangle$$

is also called a wave packet state since it involves a superposition of many stats $|k\rangle$. Example: See Fig 4.1 (Gaussian wave packet, with $|\phi|^2$ as the height). This wave packet is a snapshot of the wave function amplitude at one specific time instant. The evolution of this wave packet is governed by the Hamiltonian, which brings us to chapter 3.

2.3. ***Chapter 3.***

For

$$|\phi\rangle = \int dk f(k)|k\rangle$$

How do we find $|\phi(t)\rangle$, the time evolved state? Here we have the option of choosing which of the pictures (Schrödinger, Heisenberg, interaction) we deal with. Since the Heisenberg picture deals with time evolved operators, and the interaction picture with evolving Hamiltonian's, neither of these is required to answer this question. Consider the Schrödinger picture which gives

$$|\phi(t)\rangle = \int dk f(k)|k\rangle e^{-iE_k t/\hbar}$$

where E_k is the eigenvalue of the Hamiltonian operator H.

STRONG SEEMING HINT: If looking for additional problems and homework, consider in detail the time evolution of the Gaussian wave packet state.

2.4. ***Chapter 4.***

For three dimensions with $V(x,y,z) = 0$

$$H = \frac{1}{2m}\mathbf{p}^2$$
$$\mathbf{p} = \sum_i p_i \mathbf{e}_i$$

In the position representation, where

$$p_i = -i\hbar\frac{d}{dx_i}$$

the Sch equation is

$$Hu(x,y,z) = Eu(x,y,z)$$
$$H = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2$$
$$= -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)$$

Separation of variables assumes it is possible to let

$$u(x,y,z) = X(x)Y(y)Z(z)$$

(these capital letters are functions, not operators).

$$-\frac{\hbar^2}{2m}\left(YZ\frac{\partial^2 X}{\partial x^2}+XZ\frac{\partial^2 Y}{\partial y^2}+YZ\frac{\partial^2 Z}{\partial z^2}\right)=EXYZ$$

Dividing as usual by XYZ we have

$$-\frac{\hbar^2}{2m}\left(\frac{1}{X}\frac{\partial^2 X}{\partial x^2}+\frac{1}{Y}\frac{\partial^2 Y}{\partial y^2}+\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2}\right)=E$$

The curious thing is that we have these three derivatives, which is supposed to be related to an Energy, which is independent of any x, y, z, so it must be that each of these is separately constant. We can separate these into three individual equations

$$\begin{aligned}-\frac{\hbar^2}{2m}\frac{1}{X}\frac{\partial^2 X}{\partial x^2}&=E_1\\ -\frac{\hbar^2}{2m}\frac{1}{Y}\frac{\partial^2 Y}{\partial x^2}&=E_2\\ -\frac{\hbar^2}{2m}\frac{1}{Z}\frac{\partial^2 Z}{\partial x^2}&=E_3\end{aligned}$$

or

$$\begin{aligned}\frac{\partial^2 X}{\partial x^2}&=\left(-\frac{2mE_1}{\hbar^2}\right)X\\ \frac{\partial^2 Y}{\partial x^2}&=\left(-\frac{2mE_2}{\hbar^2}\right)Y\\ \frac{\partial^2 Z}{\partial x^2}&=\left(-\frac{2mE_3}{\hbar^2}\right)Z\end{aligned}$$

We have then

$$X(x)=C_1e^{ikx}$$

with

$$\begin{aligned}E_1&=\frac{\hbar^2k_1^2}{2m}=\frac{p_1^2}{2m}\\ E_2&=\frac{\hbar^2k_2^2}{2m}=\frac{p_2^2}{2m}\\ E_3&=\frac{\hbar^2k_3^2}{2m}=\frac{p_3^2}{2m}\end{aligned}$$

We are free to use any sort of normalization procedure we wish (periodic boundary conditions, infinite Dirac, ...)

*2.5. **Angular momentum.***

HOMEWORK: go through the steps to understand how to formulate $\boldsymbol{\nabla}^2$ in spherical polar coordinates. This is a lot of work, but is good practice and background for dealing with the Hydrogen atom, something with spherical symmetry that is most naturally analyzed in the spherical polar coordinates.

In spherical coordinates (We won't go through this here, but it is good practice) with

$$\begin{aligned} x &= r\sin\theta\cos\phi \\ y &= r\sin\theta\sin\phi \\ z &= r\cos\theta \end{aligned}$$

we have with $u = u(r,\theta,\phi)$

$$-\frac{\hbar^2}{2m}\left(\frac{1}{r}\partial_{rr}(ru) + \frac{1}{r^2\sin\theta}\partial_\theta(\sin\theta\partial_\theta u) + \frac{1}{r^2\sin^2\theta}\partial_{\phi\phi}u\right) = Eu$$

We see the start of a separation of variables attack with $u = R(r)Y(\theta,\phi)$. We end up with

$$-\frac{\hbar^2}{2m}\left(\frac{r}{R}(rR')' + \frac{1}{Y\sin\theta}\partial_\theta(\sin\theta\partial_\theta Y) + \frac{1}{Y\sin^2\theta}\partial_{\phi\phi}Y\right)$$

$$r(rR')' + \left(\frac{2mE}{\hbar^2}r^2 - \lambda\right)R = 0$$

$$\frac{1}{Y\sin\theta}\partial_\theta(\sin\theta\partial_\theta Y) + \frac{1}{Y\sin^2\theta}\partial_{\phi\phi}Y = -\lambda$$

Application of separation of variables again, with $Y = P(\theta)Q(\phi)$ gives us

$$\frac{1}{P\sin\theta}\partial_\theta(\sin\theta\partial_\theta P) + \frac{1}{Q\sin^2\theta}\partial_{\phi\phi}Q = -\lambda$$

$$\frac{\sin\theta}{P}\partial_\theta(\sin\theta\partial_\theta P) + \lambda\sin^2\theta + \frac{1}{Q}\partial_{\phi\phi}Q = 0$$

$$\frac{\sin\theta}{P}\partial_\theta(\sin\theta\partial_\theta P) + \lambda\sin^2\theta - \mu = 0\frac{1}{Q}\partial_{\phi\phi}Q = -\mu$$

or

$$\frac{1}{P\sin\theta}\partial_\theta(\sin\theta\partial_\theta P) + \lambda - \frac{\mu}{\sin^2\theta} = 0 \tag{1}$$

$$\partial_{\phi\phi} Q = -\mu Q \tag{2}$$

The equation for P can be solved using the Legendre function $P_l^m(\cos\theta)$ where $\lambda = l(l+1)$ and l is an integer

Replacing μ with m^2, where m is an integer

$$\frac{d^2Q}{d\phi^2} = -m^2 Q$$

Imposing a periodic boundary condition $Q(\phi) = Q(\phi + 2\pi)$, where $(m = 0, \pm 1, \pm 2, \cdots)$ we have

$$Q = \frac{1}{\sqrt{2\pi}} e^{im\phi}$$

There is the overall solution $r(r, \theta, \phi) = R(r)Y(\theta, \phi)$ for a free particle. The functions $Y(\theta, \phi)$ are

$$Y_{lm}(\theta, \phi) = N \left(\frac{1}{\sqrt{2\pi}} e^{im\phi} \right) \underbrace{P_l^m(\cos\theta)}_{-l \leq m \leq l}$$

where N is a normalization constant, and $m = 0, \pm 1, \pm 2, \cdots$. Y_{lm} is an eigenstate of the $\mathbf{L}^2$ operator and L_z (two for the price of one). There's no specific reason for the direction z, but it is the direction picked out of convention.

Angular momentum is given by

$$\mathbf{L} = \mathbf{r} \times \mathbf{p}$$

where

$$\mathbf{R} = x\hat{\mathbf{x}} + y\hat{\mathbf{y}} + z\hat{\mathbf{z}}$$

and

$$\mathbf{p} = p_x\hat{\mathbf{x}} + p_y\hat{\mathbf{y}} + p_z\hat{\mathbf{z}}$$

The important thing to remember is that the aim of following all the math is to show that

$$\mathbf{L}^2 Y_{lm} = \hbar^2 l(l+1) Y_{lm}$$

and simultaneously

$$\mathbf{L}_z Y_{lm} = \hbar m Y_{lm}$$

Part of the solution involves working with $[L_z, L_+]$, and $[L_z, L_-]$, where

$$L_+ = L_x + iL_y$$
$$L_- = L_x - iL_y$$

An exercise (not in the book) is to evaluate

$$[L_z, L_+] = L_z L_x + iL_z L_y - L_x L_z - iL_y L_z \tag{3}$$

where

$$\left[L_x, L_y\right] = i\hbar L_z \tag{4}$$
$$\left[L_y, L_z\right] = i\hbar L_x \tag{5}$$
$$\left[L_z, L_x\right] = i\hbar L_y \tag{6}$$

Substitution back in 3 we have

$$\begin{aligned}[L_z, L_+] &= [L_z, L_x] + i\left[L_z, L_y\right] \\ &= i\hbar(L_y - iL_x) \\ &= \hbar(iL_y + L_x) \\ &= \hbar L_+\end{aligned}$$

PHY356F : Quantum Physics I Fall 2010

Lecture 6 — Orbital and Intrinsic Momentum — October 19, 2010

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3. Lecture 6 — Orbital and Intrinsic Momentum — October 19, 2010

Last time, we started thinking about angular momentum. This time, we will examine orbital and intrinsic angular momentum.

Orbital angular momentum in classical physics and quantum physics is expressed as

$$\mathbf{L} = \mathbf{r} \times \mathbf{p}, \tag{7}$$

and

$$\mathbf{L} = \mathbf{R} \times \mathbf{P}, \tag{8}$$

where $\mathbf{R}$ and $\mathbf{P}$ are quantum mechanical operators corresponding to position and momentum

$$\mathbf{R} = X\hat{\mathbf{x}} + Y\hat{\mathbf{y}} + Z\hat{\mathbf{z}} \tag{9}$$
$$\mathbf{P} = P_x\hat{\mathbf{x}} + P_y\hat{\mathbf{y}} + P_z\hat{\mathbf{z}} \tag{10}$$
$$\mathbf{L} = L_x\hat{\mathbf{x}} + L_y\hat{\mathbf{y}} + L_z\hat{\mathbf{z}} \tag{11}$$

Practice problems:

- a) Determine the commutators $\left[L_x, L_y\right]$, $\left[L_y, L_z\right]$, $\left[L_z, L_x\right]$ and

$$\begin{aligned}\left[L_x, L_y\right] &= (r_y p_z - r_z p_y)(r_z p_x - r_x p_z) - (r_z p_x - r_x p_z)(r_y p_z - r_z p_y) \\ &= r_y p_z (r_z p_x - r_x p_z) - r_z p_y (r_z p_x - r_x p_z) - r_z p_x (r_y p_z - r_z p_y) + r_x p_z (r_y p_z - r_z p_y) \\ &= r_y p_z r_z p_x - r_y p_z r_x p_z - r_z p_y r_z p_x + r_z p_y r_x p_z - r_z p_x r_y p_z + r_z p_x r_z p_y + r_x p_z r_y p_z - r_x p_z r_z p_y\end{aligned}$$

  With $p_i r_j = r_j p_i - i\hbar\delta_{ij}$, we have

$$\begin{aligned}\left[L_x, L_y\right] &= r_y r_z p_z p_x - r_y r_z p_x p_z - r_z r_y p_z p_x + r_z r_y p_x p_z - r_z r_x p_y p_z + r_z r_x p_z p_y + r_x r_z p_y p_z - r_x r_z p_z p_y \\ &+ -i\hbar\left(r_y p_x - r_x p_y\right)\end{aligned}$$

  Since the $p_i p_j$ operators commute, all the first terms cancel, leaving just

$$\left[L_x, L_y\right] = i\hbar L_z$$

- b) L_z in spherical coordinates.

  The answer is

$$L_z \leftrightarrow -i\hbar\frac{\partial}{\partial\phi} \tag{12}$$

  Work through this.

Part of the task in this intro QM treatment is to carefully determine the eigenfunctions for these operators.

The spherical harmonics are given by $Y_{lm}(\theta, \phi)$ such that

$$Y_{lm}(\theta, \phi) \propto e^{im\phi} \tag{13}$$

$$\begin{aligned}L_z Y_{lm}(\theta, \phi) &= -i\hbar\frac{\partial}{\partial\phi} Y_{lm}(\theta, \phi) \\ &= -i\hbar\frac{\partial}{\partial\phi}\text{constants}(e^{im\phi}) \\ &= \hbar m\text{constants}e^{im\phi} \\ &= \hbar m Y_{lm}(\theta, \phi)\end{aligned}$$

The z-component is quantized since, m is an integer $m = 0, \pm 1, \pm 2, ...$ The total angular momentum

$$\mathbf{L}^2 = \mathbf{L} \cdot \mathbf{L} = L_x^2 + L_y^2 + L_z^2 \tag{14}$$

is also quantized (details in the book).

The eigenvalue properties here represent very important physical features. This is also important in the hydrogen atom problem. In the hydrogen atom problem, the particle is effectively free in the angular components, having only r dependence. This allows us to apply the work for the free particle to our subsequent potential bounded solution.

Note that for the above, we also have the alternate, abstract ket notation, method of writing the eigenvalue behavior.

$$L_z|lm\rangle = \hbar m|lm\rangle \tag{15}$$

Just like

$$X|x\rangle = x|x\rangle \tag{16}$$
$$P|p\rangle = p|p\rangle \tag{17}$$

For the total angular momentum our spherical harmonic eigenfunctions have the property

$$\mathbf{L}^2|lm\rangle = \hbar^2 l(l+1)|lm\rangle \tag{18}$$

with $l = 0, 1, 2, \cdots$.

Alternately in plain old non-abstract notation we can write this as

$$\mathbf{L}^2 Y_{lm}(\theta, \phi) = \hbar^2 l(l+1) Y_{lm}(\theta, \phi) \tag{19}$$

Now we can introduce the Raising and Lowering Operators, which are

$$L_+ = L_x + iL_y \tag{20}$$
$$L_- = L_x - iL_y, \tag{21}$$

respectively. These are abstract quantities, but also physically important since they relate quantum levels of the angular momentum. How do we show this?

Last time, we saw that

$$[L_z, L_+] = +\hbar L_+ \tag{22}$$
$$[L_z, L_-] = -\hbar L_- \tag{23}$$

Note that it is implied that we are operating on ket vectors

$$L_z(L_-|lm\rangle)$$

with

$$|lm\rangle \leftrightarrow Y_{lm}(\theta, \phi) \tag{24}$$

Question: What is $L_-|lm\rangle$?
Substitute

$$\begin{aligned} L_z L_- - L_- L_z &= -\hbar L_- \\ &\Longrightarrow \\ L_z L_- &= L_- L_z - \hbar L_- \end{aligned}$$

$$\begin{aligned} L_z\left(L_-|lm\rangle\right) &= L_- L_z|lm\rangle - \hbar L_-|lm\rangle \\ &= L_- m\hbar|lm\rangle - L_-|lm\rangle \\ &= \hbar\left(mL_-|lm\rangle - L_-|lm\rangle\right) \\ &= \hbar(m-1)\left(L_-|lm\rangle\right) \end{aligned}$$

So $L_-|lm\rangle = |\psi\rangle$ is another spherical harmonic, and we have

$$L_z|\psi\rangle = \hbar(m-1)|\psi\rangle \tag{25}$$

This lowering operator quantity causes a physical change in the state of the system, lowering the observable state (ie: the eigenvalue) by $\hbar$.
Now we want to normalize $|\psi\rangle = L_-|lm\rangle$, via $\langle\psi|\psi\rangle = 1$.

$$\begin{aligned} 1 &= \langle\psi|\psi\rangle \\ &= \langle lm|L_-^\dagger L_-|\psi\rangle \\ &= \langle lm|L_+ L_-|\psi\rangle \end{aligned}$$

We can use

$$L_+ L_- = \mathbf{L}^2 - L_z^2 + \hbar L_z, \tag{26}$$

So, knowing (how exactly?) that

$$L_-|lm\rangle = C|l, m-1\rangle \tag{27}$$

we have from 26

$$\begin{aligned} |C|^2 &= \langle lm|(\mathbf{L}^2 - L_z^2 + \hbar L_z)|\psi\rangle \\ &= \underbrace{\langle lm|lm\rangle}_{=1}\left(\hbar^2 l(l+1) - (\hbar m)^2 + \hbar^2 m\right) \\ &= \hbar^2\left(l(l+1) - m^2 + m\right). \end{aligned}$$

we have

$$|C|^2 \underbrace{\langle l, m-1|l, m-1\rangle}_{=1} = \hbar^2\left(l(l+1) - m^2 + m\right). \tag{28}$$

and can normalize the functions $|\psi\rangle$ as

$$L_-|lm\rangle = \hbar\left(l(l+1) - m^2 + m\right)^{1/2}|l, m-1\rangle \tag{29}$$

Abstract notation side note:

$$\langle\theta,\phi|lm\rangle = Y_{lm}(\theta,\phi) \tag{30}$$

3.1. *Generalizing orbital angular momentum.*

To explain the results of the Stern-Gerlach experiment, assume that there is an intrinsic angular momentum **S** that has most of the same properties as **L**. But **S** has no classical counterpart such as $\mathbf{r} \times \mathbf{p}$.

This experiment is the classic QM experiment because the silver atoms not only have the orbital angular momentum, but also have an additional observed intrinsic spin in the outermost electron. In turns out that if you combine relativity and QM, you can get out something that looks like the the **S** operator. That marriage produces the Dirac electron theory.

We assume the commutation relations

$$\left[S_x, S_y\right] = i\hbar S_z \tag{31}$$
$$\left[S_y, S_z\right] = i\hbar S_x \tag{32}$$
$$\left[S_z, S_x\right] = i\hbar S_y \tag{33}$$

Where we have the analogous eigenproperties

$$\mathbf{S}^2|sm\rangle = \hbar^2 s(s+1)|sm\rangle \tag{34}$$
$$S_z|sm\rangle = \hbar m|sm\rangle \tag{35}$$

with $s = 0, 1/2, 1, 3/2, ...$

Electrons and protons are examples of particles that have spin one half.

Note that there is no position representation of $|sm\rangle$. We cannot project these states.

This basic quantum mechanics end up applying to quantum computing and cryptography as well, when we apply the mathematics we are learning here to explain the Stern-Gerlach experiment to photon spin states.

(DRAWS Stern-Gerlach picture with spin up and down labeled $|z+\rangle$, and $|z-\rangle$ with the magnetic field oriented in along the z axis.)

Silver atoms have $s = 1/2$ and $m = \pm 1/2$, where m is the quantum number associated with the z-direction intrinsic angular momentum. The angular momentum that is being acted on in the Stern-Gerlach experiment is primarily due to the outermost electron.

$$S_z|z+\rangle = \frac{\hbar}{2}|z+\rangle \tag{36}$$
$$S_z|z-\rangle = -\frac{\hbar}{2}|z-\rangle \tag{37}$$
$$\mathbf{S}^2|z\pm\rangle = \frac{1}{2}\left(\frac{1}{2}+1\right)\hbar^2|z\pm\rangle \tag{38}$$

where

$$|z+\rangle = |\frac{1}{2}\frac{1}{2}\rangle \tag{39}$$

$$|z-\rangle = |\frac{1}{2}-\frac{1}{2}\rangle \tag{40}$$

What about S_x? We can leave the detector in the x, z plane, but rotate the magnet so that it lies in the x direction.

We have the correspondence

$$S_z \leftrightarrow \frac{\hbar}{2}\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}, \tag{41}$$

but this is perhaps more properly viewed as the matrix representation of the less specific form

$$S_z = \frac{\hbar}{2}\left(|z+\rangle\langle z+| - |z-\rangle\langle z-|\right). \tag{42}$$

Where the translation to the form of 41 is via the matrix elements

$$\langle z+|S_z|z+\rangle \tag{43}$$

$$\langle z+|S_z|z-\rangle \tag{44}$$

$$\langle z-|S_z|z+\rangle \tag{45}$$

$$\langle z-|S_z|z-\rangle. \tag{46}$$

We can work out the same for S_x using S_+ and S_-, or equivalently for σ_x using σ_+ and σ_-, where

$$S_x = \frac{\hbar}{2}\sigma_x \tag{47}$$

$$S_y = \frac{\hbar}{2}\sigma_y \tag{48}$$

$$S_z = \frac{\hbar}{2}\sigma_z \tag{49}$$

The operators $\sigma_x, \sigma_y, \sigma_z$ are the Pauli operators, and avoid the pesky $\hbar/2$ factors.

We find

$$\sigma_x = \begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix} \tag{50}$$

$$\sigma_y = \begin{bmatrix}0 & -i\\ i & 0\end{bmatrix} \tag{51}$$

$$\sigma_z = \begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix} \tag{52}$$

And from $|\sigma_x - \lambda I| = (-\lambda)^2 - 1$, we have eigenvalues $\lambda = \pm 1$ for the σ_x operator. The corresponding eigenkets in column matrix notation are found

$$\begin{aligned}\begin{bmatrix} \mp 1 & 1 \\ 1 & \mp 1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} &= 0 \\ \implies \mp a_1 + a_2 &= 0 \\ \implies a_2 &= \pm a_1\end{aligned}$$

Or

$$|x\pm\rangle \propto \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = a_1 \begin{bmatrix} 1 \\ \pm 1 \end{bmatrix}$$

which can be normalized as

$$|x\pm\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ \pm 1 \end{bmatrix} \tag{53}$$

We see that this is different from

$$|z+\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \tag{54}$$

We will still end up with two spots, but there has been a projection of spin in a different fashion? Does this mean the measurement will be different. There's still a lot more to learn before understanding exactly how to relate the spin operators to a real physical system.

PHY356F : Quantum Physics I Fall 2010

Lecture 7 — Stern Gerlach — October 26, 2010

Prof. Vatche Deyirmenjian *Scribe: Peeter Joot*

4. Lecture 7 — Stern Gerlach — October 26, 2010

Short class today since 43 minutes was wasted since the feedback given the Prof was so harsh that he wants to cancel the mid-term because students have said they aren't prepared. How ironic that this wastes more time that could be getting us prepared!

4.1. Chapter I

Why do this (Dirac notation) math? Because of the Stern-Gerlach Experiment. Explaining the Stern-Gerlach experiment is just not possible with wave functions and the "old style" Sch equation that operates on wave functions

$$-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\Psi(\mathbf{x}, t) + V(\mathbf{x})\Psi(\mathbf{x}, t) = i\hbar\frac{\partial\Psi(\mathbf{x}, t)}{\partial t}. \tag{55}$$

Review all of Chapter I so that you understand the idea of a Hermitian operator and its associated eigenvalues and eigenvectors.

Hermitian operation A is associated with a measurable quantity.

Example. S_z is associated with the measurement of "spin-up" $|z+\rangle$ or "spin-down" $|z-\rangle$ states in silver atoms in the Stern-Gerlach experiment.

Each operator has associated with it a set of eigenvalues, and those eigenvalues are the outcomes of possible measurements.

S_z can be represented as

$$S_z = \frac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \tag{56}$$

or

$$S_z = \frac{\hbar}{2}\left(|z+\rangle\langle z+| - |z-\rangle|z-\rangle\right). \tag{57}$$

Find the eigenvalues of S_z in order to establish the possible outcomes of measurements of the z-component of the intrinsic angular momentum.

This is the point of the course. It is to find the possible outcomes. You have to appreciate that the measurement in the Stern-Gerlach experiment are trying to find the possible outcomes of the z-component measurement. The eigenvalues of this operator give us those possible outcomes.

4.1.1 Example problem. What if you put a brick in the experiment?

In the Stern-Gerlach experiment the "spin down" along the z-direction are atoms are blocked. Diagram: silver going through a hole, with a brick between the detector and the spin-down location on the screen:

FIXME: scan it. Oct 26, Fig 1.

What is the probability of measuring an outcome of $+\hbar/2$ along the x-direction?

Recall from Chapter I

$$|\phi\rangle = \sum_n c_n |a_n\rangle \tag{58}$$

We can express an arbitrary state $|\phi\rangle$ in terms of basis vectors (could be eigenstates of an operator A, but could be for example the eigenstates of the operator B, say.) Note that here in physics we will only work with orthonormal basis sets. The generality . To calculate the $c_n's$ we take inner products

$$\langle a_m|\phi\rangle = \sum_n \langle a_m|a_n\rangle = \sum_n c_n \delta_{mn} = c_m \tag{59}$$

The probability for measured outcome a_m is

$$|c_m|^2 = |\langle a_m|\phi\rangle|^2 \tag{60}$$

In the end we have to appreciate that part of QM is figuring out what the possible outcomes are and the probabilities of those outcomes.

Appreciate that $|\phi\rangle = |z+\rangle$ in this case. This is a superposition of eigenstates of S_z. Why is it a superposition? Because one of the coefficients is 1, and the other is 0.

$$|\phi\rangle = c_1|z+\rangle + c_2|z-\rangle = c_1|z+\rangle + 0|z-\rangle \tag{61}$$

So

$$c_1 = 1 \tag{62}$$

recall that

$$S_z = \frac{\hbar}{2}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix} \tag{63}$$

$$|z+\rangle \leftrightarrow \begin{bmatrix}1\\ 0\end{bmatrix} \tag{64}$$

$$|z+\rangle \leftrightarrow \begin{bmatrix}0\\ 1\end{bmatrix} \tag{65}$$

Also recall that

$$S_x = \frac{\hbar}{2}\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix} \tag{66}$$

$$|x+\rangle \leftrightarrow \frac{1}{\sqrt{2}}\begin{bmatrix}1\\ 1\end{bmatrix} \tag{67}$$

$$|x-\rangle \leftrightarrow \frac{1}{\sqrt{2}}\begin{bmatrix}1\\ -1\end{bmatrix} \tag{68}$$

(with eigenvalues $\pm\hbar/2$).

These eigenvectors are expressed in terms of $|z+\rangle$ and $|z-\rangle$, so that

$$|x+\rangle = \frac{1}{\sqrt{2}}\left(|z+\rangle + |z-\rangle\right) \tag{69}$$

$$|x-\rangle = \frac{1}{\sqrt{2}}\left(|z+\rangle - |z-\rangle\right). \tag{70}$$

Outcome $+\hbar/2$ along the x-direction has an associated state $|x+\rangle$. That probability is

$$\begin{aligned}
|\langle x+|\phi\rangle|^2 &= \left|\frac{1}{\sqrt{2}}\left(\langle z+| + \langle z-|\right)|\phi\rangle\right|^2\\
&= \frac{1}{2}|\langle z+|\phi\rangle + \langle z-|\phi\rangle|^2\\
&= \frac{1}{2}|\langle z+|z+\rangle + \langle z-|z+\rangle|^2\\
&= \frac{1}{2}|1+0|^2\\
&= \frac{1}{2}
\end{aligned}$$

4.1.2 Example problem variation. With a third splitter (SGZ)

The probability for outcome $+\hbar/2$ along z after the second SGZ magnets is

$$\begin{aligned}\left|\langle z+|\phi'\rangle\right|^2 &= |\langle z+|x+\rangle|^2 \\ &= \left|\langle z+|\frac{1}{\sqrt{2}}\left(|z+\rangle + |z-\rangle\right)\right|^2 \\ &= \frac{1}{2}|\langle z+|z+\rangle + \langle z+|z-\rangle|^2 \\ &= \frac{1}{2}\end{aligned}$$

My question: what's the point of the brick when the second splitter is already only being fed by the "spin up" stream. Answer: just to ensure that the states are prepared in the expected way. If the beams are two close together, without the brick perhaps we end up with some spin up in the upper stream. Note that the beam separation here is on the order of centimeters. ie: imagine that it is hard to redirect just one of the beams to the next stage splitter without blocking one of the beams or else the next splitter inevitably gets fed with some of both. Might be nice to see a real picture of the Stern-Gerlach apparatus complete with scale.

Why silver? Silver has 47 electrons, all of which but one are in spin pairs. Only the "outermost" electron is free to have independent spin.

Aside: Note that we have the term "Collapse" to describe the now-known state after measurement. There's some debate about the applicability of this term, and the interpretation that this imposes. Will not be discussed here.

4.2. On section 5.11, the complete wavefunction.

Aside: section 5.12 (Pauli exclusion principle and Fermi energy) excluded.

The complete wavefunction

$$\begin{aligned}|\phi\rangle &= \text{the complete state of an atomic in the Stern-Gerlach experiment} \\ &= |u\rangle \otimes |\chi\rangle\end{aligned}$$

We also write

$$|u\rangle \otimes |\chi\rangle = |u\rangle|\chi\rangle \tag{71}$$

where $|u\rangle$ is associate with translation, and $|\chi\rangle$ is associated with spin. This is a product state where the $\otimes$ is a symbol for states in two or more different spaces.

5. Lecture 8 — Making Sense of Quantum Mechanics — November 2, 2010

5.1. Discussion

Desai: "Quantum Theory is a linear theory ..."

We can discuss SHM without using sines and cosines or complex exponentials, say, only using polynomials, but it would be HARD to do so, and much more work. We want the framework of Hilbert space, linear operators and all the rest to make our life easier.

Dirac: "All the same the Mathematics is only a tool and one should learn to hold the physical ideas on one's mind without reference to the mathematical form"

You have to be able to understand the concepts and apply the concepts as well as the mathematics.

Deyirmenjian: "Think before you compute."

Joke: With his name included it is the 3Ds. There's a lot of information included in the question, so read it carefully.

Q: The equation $A|a_n\rangle = a_n|a_n\rangle$ for operator A, eigenvalue a_n, $n = 1, 2$ and eigenvector $|a_n\rangle$ that is identified by the eigenvalue a_n says that

- (a) measuring the physical quantity associated with A gives result a_n
- (b) A acting on the state $|a_n\rangle$ gives outcome a_n
- (c) the possible outcomes of measuring the physical quantity associated with A are the eigenvalues a_n
- (d) Quantum mechanics is hard.

$|a_n\rangle$ is a vector in a vector space or Hilbert space identified by some quantum number $a_n, n \in 1, 2, \cdots$.

The a_n values could be expressions. Example, Angular momentum is describe by states $|lm\rangle, l = 0, 1, 2, \cdots$ and $m = 0, \pm 1, \pm 2$

Recall that the problem is

$$\mathbf{L}^2|lm\rangle = l(l+1)\hbar^2|lm\rangle \tag{72}$$

$$L_z|lm\rangle = m\hbar|lm\rangle \tag{73}$$

We have respectively eigenvalues $l(l+1)\hbar^2$, and $m\hbar$.

A: Answer is (c). a_n isn't a measurement itself. These represent possibilities. Contrast this to classical mechanics where time evolution is given without probabilities

$$\mathbf{F}_{\text{net}} = m\mathbf{a} \tag{74}$$

$$\mathbf{x}(0), \mathbf{x}'(0) \implies \mathbf{x}(t), \mathbf{x}'(t) \tag{75}$$

The eigenvalues are the possible outcomes, but we only know statistically that these are the possibilities.

(a),(b) are incorrect because we do not know what the initial state is, nor what the final outcome is. We also can't say "gives result a_n". That statement is too strong!

Q: We wouldn't say that A acts on pure state $|a_n\rangle$, instead. If the state of the system is $|\psi\rangle = |a_5\rangle$, the probability of measuring outcome a_5 is

- (a) a_5
- (b) a_5^2
- (c) $\langle a_5|\psi\rangle = \langle a_5|a_5\rangle = 1$.
- (d) $|\langle a_5|\psi\rangle|^2 = |\langle a_5|a_5\rangle|^2 = |1|^2 = 1$.

A: (d) The eigenformula equation doesn't say anything about any specific outcome. We want to talk about probability amplitudes. When the system is prepared in a particular pure eigenstate, then we have a guarantee that the probability of measuring that state is unity. We wouldn't say (c) because the probability amplitudes are the absolute square of the complex number $\langle a_n|a_n\rangle$.

The probability of outcome a_n, given initial state $|\Psi\rangle$ is $|\langle a_n|\Psi\rangle|^2$.

Wave function collapse: When you make a measurement of the physical quantity associated with A, then the state of the system will be the value $|a_5\rangle$. The state is not the number (eigenvalue) a_5.

Example: SGZ. With a "spin-up" measurement in the z-direction, the state of the system is $|z+\rangle$. The state before the measurement, by the magnet, was $|\Psi\rangle$. After the measurement, the state describing the system is $|\phi\rangle = |z+\rangle$. The measurement outcome is $+\frac{\hbar}{2}$ for the spin angular momentum along the z-direction.

FIXME: SGZ picture here.

There is an interaction between the magnet and the silver atoms coming out of the oven. Before that interaction we have a state described by $|\Psi\rangle$. After the measurement, we have a new state $|\phi\rangle$. We call this the collapse of the wave function. In a future course (QM interpretations) the language used and interpretations associated with this language can be discussed.

Q: Express Hermitian operator A in terms of its eigenvectors.

Q: The above question is vague because

- (a) The eigenvectors may form a discrete set.
- (b) The eigenvectors may form a continuous set.
- (c) The eigenvectors may not form a complete set.
- (d) The eigenvectors are not given.

A: None of the above. A Hermitian operator is guaranteed to have a complete set of eigenvectors. The operator may also be both discrete and continuous (example: the complete spin wave function).

discrete:

$$\begin{aligned} A &= A\mathbf{1} \\ &= A\left(\sum_n |a_n\rangle\langle a_n|\right) \\ &= \sum_n (A|a_n\rangle)\langle a_n| \\ &= \sum_n (a_n|a_n\rangle)\langle a_n| \\ &= \sum_n a_n|a_n\rangle\langle a_n| \end{aligned}$$

continuous:

$$\begin{aligned} A &= A\mathbf{1} \\ &= A\left(\int d\alpha|\alpha\rangle\langle\alpha|\right) \\ &= \int d\alpha(A|\alpha\rangle)\langle\alpha| \\ &= \int d\alpha(\alpha|\alpha\rangle)\langle\alpha| \\ &= \int d\alpha\alpha|\alpha\rangle\langle\alpha| \end{aligned}$$

An example is the position eigenstate $|x\rangle$, eigenstate of the Hermitian operator X. α is a label indicating the summation.

general case with both discrete and continuous:

$$\begin{aligned} A &= A\mathbf{1} \\ &= A\left(\sum_n |a_n\rangle\langle a_n| + \int d\alpha|\alpha\rangle\langle\alpha|\right) \\ &= \sum_n (A|a_n\rangle)\langle a_n| + \int d\alpha\,(A|\alpha\rangle)\langle\alpha| \\ &= \sum_n (a_n|a_n\rangle)\langle a_n| + \int d\alpha\,(\alpha|\alpha\rangle)\langle\alpha| \\ &= \sum_n a_n|a_n\rangle\langle a_n| + \int d\alpha\alpha|\alpha\rangle\langle\alpha| \end{aligned}$$

Problem Solving

- MODEL – Quantum, linear vector space
- VISUALIZE – Operators can have discrete, continuous or both discrete and continuous eigenvectors.
- SOLVE – Use the identity operator.
- CHECK – Does the above expression give $A|a_n\rangle = a_n|a_n\rangle$.

Check

$$\begin{aligned} A|a_m\rangle &= \sum_n a_n|a_n\rangle \langle a_n|a_m\rangle + \int d\alpha\alpha|\alpha\rangle \langle\alpha|a_n\rangle \\ &= \sum_n a_n|a_n\rangle\delta_{nm} \\ &= a_m|a_m\rangle \end{aligned}$$

What remains to be shown, used above, is that the continuous and discrete eigenvectors are orthonormal. He has an example vector space, not yet discussed.

Q: what is $\langle\Psi_1|A|\Psi_1\rangle$, where A is a Hermitian operator, and $|\Psi_1\rangle$ is a general state.

A: $\langle\Psi_1|A|\Psi_1\rangle$ = average outcome for many measurements of the physical quantity associated with A such that the system is prepared in state $|\Psi_1\rangle$ prior to each measurement.

Q: What if the preparation is $|\Psi_2\rangle$. This isn't necessarily an eigenstate of A, it is some linear combination of eigenstates. It is a general state.

A: $\langle\Psi_2|A|\Psi_2\rangle$ = average of the physical quantity associated with A, but the preparation is $|\Psi_2\rangle$, not $|\Psi_1\rangle$.

Q: What if our initial state is a little bit of $|\Psi_1\rangle$, and a little bit of $|\Psi_2\rangle$, and a little bit of $|\Psi_N\rangle$. ie: how to describe what comes out of the oven in the Stern-Gerlach experiment. That spin is a statistical mixture. We could understand this as only a statistical mix. This is a physical relevant problem.

A: To describe that statistical situation we have the following.

$$\langle A\rangle_{\text{average}} = \sum_j w_j\langle\Psi_j|A|\Psi_j\rangle \tag{76}$$

We sum up all the expectation values modified by statistical weighting factors. These w_j's are statistical weighting factors for a preparation associated with $|\Psi_j\rangle$, real numbers (that sum to unity). Note that these states $|\Psi_j\rangle$ are not necessarily orthonormal.

With insertion of the identity operator we have

$$\begin{aligned}
\langle A\rangle_{\text{average}} &= \sum_j w_j \langle \Psi_j | \mathbf{1} A | \Psi_j \rangle \\
&= \sum_j w_j \langle \Psi_j | \left(\sum_n |a_n\rangle\langle a_n| \right) A | \Psi_j \rangle \\
&= \sum_j \sum_n w_j \left\langle \Psi_j | a_n \right\rangle \langle a_n | A | \Psi_j \rangle \\
&= \sum_j \sum_n w_j \langle a_n | A | \Psi_j \rangle \left\langle \Psi_j | a_n \right\rangle \\
&= \sum_n \langle a_n | A \left(\sum_j w_j |\Psi_j\rangle\langle\Psi_j| \right) |a_n\rangle
\end{aligned}$$

This inner bit is called the density operator ρ

$$\rho \equiv \sum_j w_j |\Psi_j\rangle\langle\Psi_j| \tag{77}$$

Returning to the average we have

$$\langle A\rangle_{\text{average}} = \sum_n \langle a_n | A\rho | a_n\rangle \equiv \text{Tr}(A\rho) \tag{78}$$

The trace of an operator A is

$$\text{Tr}(A) = \sum_j \langle a_j | A | a_j \rangle = \sum_j A_{jj} \tag{79}$$

5.2. *Section 5.9, Projection operator.*

Returning to the last lecture. From chapter 1, we have

$$P_n = |a_n\rangle\langle a_n| \tag{80}$$

is called the projection operator. This is physically relevant. This takes a general state and gives you the component of that state associated with that eigenvector. Observe

$$P_n |\phi\rangle = |a_n\rangle \langle a_n | \phi\rangle = \underbrace{\langle a_n | \phi\rangle}_{\text{coefficient}} |a_n\rangle \tag{81}$$

Example: Projection operator for the $|z+\rangle$ state

$$P_{z+} = |z+\rangle\langle z+| \tag{82}$$

We see that the density operator

$$\rho \equiv \sum_j w_j |\Psi_j\rangle\langle\Psi_j|, \tag{83}$$

can be written in terms of the Projection operators

$$|\Psi_j\rangle\langle\Psi_j| = \text{Projection operator for state} |\Psi_j\rangle$$

The projection operator is like a dot product, determining the quantity of a state that lines in the direction of another state.

Q: What is the projection operator for spin-up along the z-direction.

A:

$$P_{z+} = |z+\rangle\langle z+| \tag{84}$$

Or in matrix form with

$$\langle z+| = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \tag{85}$$

$$\langle z-| = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \tag{86}$$

so

$$P_{z+} = |z+\rangle\langle z+| = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \tag{87}$$

Q: A harder problem. What is P_χ, where

$$|\chi\rangle = \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} \tag{88}$$

Note: We want normalized states, with $\langle\chi|\chi\rangle = |c_1|^2 + |c_2|^2 = 1$.

A:

$$P_\chi = |\chi\rangle\langle\chi| = \begin{bmatrix} c_1^* \\ c_2^* \end{bmatrix} \begin{bmatrix} c_1 & c_2 \end{bmatrix} = \begin{bmatrix} c_1^* c_1 & c_1^* c_2 \\ c_2^* c_1 & c_2^* c_2 \end{bmatrix} \tag{89}$$

Observe that this has the proper form of a projection operator is that the square is itself

$$\begin{aligned} (|\chi\rangle\langle\chi|)(|\chi\rangle\langle\chi|) &= |\chi\rangle(\langle\chi|\chi\rangle)\langle\chi| \\ &= |\chi\rangle\langle\chi| \end{aligned}$$

Q: Show that $P_\chi = a_0\mathbf{1} + \mathbf{a}\cdot\sigma$, where $\mathbf{a} = (a_x, a_y, a_z)$ and $\sigma = (\sigma_x, \sigma_y, \sigma_z)$.

A: See Section 5.9. Note the following about computing $(\sigma\cdot\mathbf{a})^2$.

$$\begin{aligned}(\sigma\cdot\mathbf{a})^2 &= (a_x\sigma_x + a_y\sigma_y + a_z\sigma_z)(a_x\sigma_x + a_y\sigma_y + a_z\sigma_z)\\ &= a_xa_x\sigma_x\sigma_x + a_xa_y\sigma_x\sigma_y + a_xa_z\sigma_x\sigma_z + a_ya_x\sigma_y\sigma_x + a_ya_y\sigma_y\sigma_y + a_ya_z\sigma_y\sigma_z + a_za_x\sigma_z\sigma_x + a_za_y\sigma_z\sigma_y + a_za_z\sigma_z\sigma_z\\ &= (a_x^2 + a_y^2 + a_z^2)I + a_xa_y(\sigma_x\sigma_y + \sigma_y\sigma_x) + a_ya_z(\sigma_y\sigma_z + \sigma_z\sigma_y) + a_za_x(\sigma_z\sigma_x + \sigma_x\sigma_z)\\ &= |\mathbf{x}|^2 I\end{aligned}$$

So we have

$$(\sigma\cdot\mathbf{a})^2 = (\mathbf{a}\cdot\mathbf{a})\mathbf{1} \equiv \mathbf{a}^2 \tag{90}$$

Where the matrix representations

$$\sigma_x \leftrightarrow \begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix} \tag{91}$$

$$\sigma_y \leftrightarrow \begin{bmatrix}0 & -i\\ i & 0\end{bmatrix} \tag{92}$$

$$\sigma_z \leftrightarrow \begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}, \tag{93}$$

would be used to show that

$$\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = I \tag{94}$$

and

$$\sigma_x\sigma_y = -\sigma_y\sigma_x \tag{95}$$

$$\sigma_y\sigma_z = -\sigma_z\sigma_y \tag{96}$$

$$\sigma_z\sigma_x = -\sigma_x\sigma_z \tag{97}$$

PHY356F : Quantum Physics I Fall 2010

Lecture 9 — Bound-state problems. — November 16, 2010

Prof. Vatche Deyirmenjian *Scribe: Peeter Joot*

6. Lecture 9 — Bound-state problems. — November 16, 2010

Motivation. Motivation for today's physics is Solar Cell technology and quantum dots.

6.1. ***Problem:***

What are the eigenvalues and eigenvectors for an electron trapped in a 1D potential well?

6.1.1 MODEL.

Quantum state $|\Psi\rangle$ describes the particle. What $V(X)$ should we choose? Try a quantum well with infinite barriers first.

These spherical quantum dots are like quantum wells. When you trap electrons in this scale you'll get energy quantization.

6.1.2 VISUALIZE.

Draw a picture for $V(X)$ with infinite spikes at $\pm a$. (ie: figure 8.1 in the text).

6.1.3 SOLVE.

First task is to solve the time independent Schrödinger equation.

$$H|\Psi\rangle = E|\Psi\rangle \tag{98}$$

derivable from

$$H|\Psi\rangle = i\hbar\frac{\partial}{\partial t}|\Psi\rangle \tag{99}$$

In the position representation, we project $\langle x|$ onto $H|\Psi\rangle$ and solve for $\langle x|\Psi\rangle = \Psi(x)$. For the problems in Chapter 8,

$$H = \frac{\mathbf{P}^2}{2m} + V(X, Y, Z), \tag{100}$$

where

$$\begin{aligned} P &= \text{momentum operator} \\ X &= \text{position operator} \\ m &= \text{electron mass} \end{aligned}$$

We should be careful to be strict about the notation, and not interchange the operators and their specific representations (ie: not interchanging "little-x" and "big-x") as we see in the text in this chapter.

Here the potential energy operator $V(X, Y, Z)$ is time independent.

If $i\hbar\frac{d|\Psi\rangle}{dt} = H|\Psi\rangle$ and H is time independent then $|\Psi\rangle = |u\rangle e^{-iEt/\hbar}$ implies

$$i\hbar\frac{-iE}{\hbar}|u\rangle e^{-iEt/\hbar} = H|u\rangle e^{-iEt/\hbar}$$

or

$$E|u\rangle = H|u\rangle \tag{101}$$

Here E is the energy eigenvalue, and $|u\rangle$ is the energy eigenstate. Our differential equation now becomes

$$-\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2} + V(x)u(x) = Eu(x) \tag{102}$$

where $V(x) = 0$ for $|x| < a$. We won't find anything like this for real, but this is our first approximation to the quantum dot.

Our differential equation in the well is now

$$-\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2} = Eu(x) \tag{103}$$

or with $\alpha = \sqrt{2mE/\hbar^2}$

$$\frac{d^2u(x)}{dx^2}u(x) = -\frac{2mE}{\hbar^2}u(x) = -\alpha^2 u(x) \tag{104}$$

Our solution for $|x| < a$ is then

$$u(x) = A\cos\alpha x + B\sin\alpha x \tag{105}$$

and for $|x| > a$ we have $u(x) = 0$ since $V(x) = \infty$.

Setting $u(a) = u(-a) = 0$ we have

$$A\cos\alpha a + B\sin\alpha a = 0$$
$$A\cos\alpha a - B\sin\alpha a = 0$$

6.1.4 Type I.

$B = 0$, $A\cos\alpha a = 0$. For $A \neq 0$ we must have

$$\cos\alpha a = 0$$

or $\alpha a = n\frac{\pi}{2}$, where $n = 1, 3, 5, ...$, so our solution is

$$u(x) = A\cos\left(\frac{n\pi}{2a}x\right) \tag{106}$$

6.1.5 Type II.

$A = 0$, $B\sin\alpha a = 0$. For $B \neq 0$ we must have

$$\sin\alpha a = 0$$

or $\alpha a = n\frac{\pi}{2}$, where $n = 1, 2, 4, ...$, so our solution is

$$u(x) = B\sin\left(\frac{n\pi}{2a}x\right) \tag{107}$$

6.1.6 Via determinant

We could also write

$$\begin{bmatrix} \cos \alpha a & \sin \alpha a \\ \cos \alpha a & -\sin \alpha a \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} = 0$$

and then must have zero determinant, or

$$-2 \sin \alpha a \cos \alpha a = -\sin 2\alpha a \tag{108}$$

so we must have

$$2\alpha a = n\pi$$

or

$$\alpha = \frac{n\pi}{2a}$$

regardless of A and B. We can then determine the solutions 106, and 107 simply by noting that this value for α kills off either the sine or cosine terms of 105 depending on whether n is even or odd.

6.2. ***CHECK.***

$$u_n(x) = A \cos\left(\frac{n\pi}{2a} x\right)$$
$$u_n(x) = B \sin\left(\frac{n\pi}{2a} x\right)$$

satisfy the time independent Schrödinger equation, and the corresponding eigenvalues from from

$$\alpha = \sqrt{\frac{2mE}{\hbar^2}},$$

or

$$E = \frac{\hbar^2 \alpha^2}{2m} = \frac{\hbar^2}{2m} \left(\frac{n\pi}{2a}\right)^2$$

for $n = 1, 2, 3, \cdots$.

6.3. *On the derivative of u at the boundaries*

Integrating

$$-\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2}u(x) + V(x)u(x) = Eu(x), \tag{109}$$

over $[a-\epsilon, a+\epsilon]$ we have

$$-\frac{\hbar^2}{2m}\int_{a-\epsilon}^{a-\epsilon}\frac{d^2u(x)}{dx^2}dx + \int_{a-\epsilon}^{a-\epsilon}V(x)u(x)dx = \int_{a-\epsilon}^{a-\epsilon}Eu(x)dx \tag{110}$$

$$-\frac{\hbar^2}{2m}\left(\frac{du}{dx}\Big|_{a-\epsilon}^{a+\epsilon} + 0 = 0\right) \tag{111}$$

which gives us

$$\frac{du}{dx}\Big|_{a+\epsilon} - \frac{du}{dx}\Big|_{a-\epsilon} = 0 \tag{112}$$

or

$$\frac{du}{dx}\Big|_{a+\epsilon} = \frac{du}{dx}\Big|_{a-\epsilon} \tag{113}$$

We can infer how the derivative behaves over the potential discontinuity, so in the limit where $\epsilon \to 0$ we must have wave function continuity at despite the potential discontinuity.

This sort of analysis, which is potential dependent, we see that for this infinite well potential, our derivative must be continuous at the boundary.

6.4. *Problem:*

non-infinite step well potential.

Given a zero potential in the well $|x| < a$

$$-\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2}u(x) + 0 = Eu(x), \tag{114}$$

and outside of the well $|x| > a$

$$-\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2}u(x) + V_0u(x) = Eu(x) \tag{115}$$

Inside of the well, we have the solution worked previously, with $\alpha = \sqrt{2mE/\hbar^2}$

$$u(x) = A\cos\alpha x + B\sin\alpha x \tag{116}$$

Then we have outside of the well the same form

$$-\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2}u(x) = (E - V_0)u(x) \tag{117}$$

With $\beta = \sqrt{2m(V_0 - E)/\hbar^2}$, this is

$$\frac{d^2u(x)}{dx^2}u(x) = \beta^2 u(x) \tag{118}$$

If $V_0 - E > 0$, we have $V_0 > E$, and the states are "bound" or "localized" in the well.
Our solutions for this $V_0 > E$ case are then

$$u(x) = De^{\beta x} \tag{119}$$
$$u(x) = Ce^{-\beta x} \tag{120}$$

for $x \leq a$, and $x \geq a$ respectively.

Question: Why can we not have

$$u(x) = De^{\beta x} + Ce^{-\beta x} \tag{121}$$

for $x \leq -a$?

Answer: As $x \to -\infty$ we would then have

$$u(x) \to Ce^{\beta\infty} \to \infty$$

This is a non-physical solution, and we discard it based on our normalization requirement.
Our total solution, in regions $x < -a$, $|x| \leq a$, and $x > a$ respectively

$$u_1(x) = De^{\beta x}$$
$$u_2(x) = A\cos\alpha x + B\sin\alpha x$$
$$u_3(x) = Ce^{-\beta x}$$

To find the coefficients, set $u_1(-a) = u_2(-a)$, $u_2(a) = u_3(a)$ $u_1'(-a) = u_2'(-a)$, $u_2'(a) = u_3'(a)$, and NORMALIZE $u(x)$.

Now, how about in region 2 ($x < -a$), $V_0 < E$ implies that our equation is

$$\frac{d^2u(x)}{dx^2}u(x) = -\frac{2m}{\hbar^2}(E - V_0)u(x) = -k^2u(x) \tag{122}$$

We no longer have quantized energy for such a solution. These correspond to the "unbound" or "continuum" states. Even though we do not have quantized energy we still have quantum effects. Our solution becomes

$$u_1(x) = C_2 e^{ikx} + D_2 e^{-ikx}$$
$$u_2(x) = A e^{i\alpha x} + B e^{-i\alpha x}$$
$$u_3(x) = C_3 e^{ikx}$$

Question. Why no $D_2 e^{-ikx}$, in the $u_3(x)$ term?

Answer. We can, but this is not physically relevant. Why is because we associate e^{ikx} with an incoming wave, with reflection in the $x < -a$ interval, and both $e^{\pm i\alpha x}$ in the $|x| < a$ interval, but just an outgoing wave e^{ikx} in the $x > a$ region.

FIXME: scan picture: 9.1 in my notebook.

Observe that this is not normalizable as is. We require "delta-function" normalization. What we can do is ask about current densities. How much passes through the barrier, and so forth.

Note to self. We probably really we want to consider a wave packet of states, something like:

$$\Psi_1(x) = \int dk f_1(k) e^{ikx}$$
$$\Psi_2(x) = \int d\alpha f_2(\alpha) e^{i\alpha x}$$
$$\Psi_3(x) = \int dk f_3(k) e^{ikx}$$

Then we'd have something that we can normalize. Play with this later.

PHY356F : Quantum Physics I Fall 2010

Lecture 10 — Hydrogen atom. — November 23, 2010

Prof. Vatche Deyirmenjian *Scribe: Peeter Joot*

7. Lecture 10 — Hydrogen atom. — November 23, 2010

7.1. *Introduce the center of mass coordinates.*

We'll want to solve this using the formalism we've discussed. The general problem is a proton, positively charged, with a nearby negative charge (the electron).

Our equation to solve is

$$\left(-\frac{\hbar^2}{2m_1}\boldsymbol{\nabla}_1^2 - \frac{\hbar^2}{2m_2}\boldsymbol{\nabla}_2^2 \right) \bar{u}(\mathbf{r}_1, \mathbf{r}_2) + V(\mathbf{r}_1, \mathbf{r}_2)\bar{u}(\mathbf{r}_1, \mathbf{r}_2) = E\bar{u}(\mathbf{r}_1, \mathbf{r}_2). \tag{123}$$

Here $\left(-\frac{\hbar^2}{2m_1}\boldsymbol{\nabla}_1^2 - \frac{\hbar^2}{2m_2}\boldsymbol{\nabla}_2^2 \right)$ is the total kinetic energy term. For hydrogen we can consider the potential to be the Coulomb potential energy function that depends only on $\mathbf{r}_1 - \mathbf{r}_2$. We can transform this using a center of mass transformation. Introduce the center of mass coordinate and relative coordinate vectors

$$\mathbf{R} = \frac{m_1\mathbf{r}_1 + m_2\mathbf{r}_2}{m_1 + m_2} \tag{124}$$

$$\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2. \tag{125}$$

The notation $\boldsymbol{\nabla}_k^2$ represents the Laplacian for the positions of the k'th particle, so that if $\mathbf{r}_1 = (x_1, x_2, x_3)$ is the position of the first particle, the Laplacian for this is:

$$\boldsymbol{\nabla}_1^2 = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial y_1^2} + \frac{\partial^2}{\partial z_1^2} \tag{126}$$

Here $\mathbf{R}$ is the center of mass coordinate, and $\mathbf{r}$ is the relative coordinate. With this transformation we can reduce the problem to a single coordinate PDE.

We set $\bar{u}(\mathbf{r}_1, \mathbf{r}_2) = u(\mathbf{r})U(\mathbf{R})$ and $E = E_{rel} + E_{cm}$, and get

$$-\frac{\hbar^2}{2\mu}\boldsymbol{\nabla}_{\mathbf{r}}{}^2 u(\mathbf{r}) + V(\mathbf{r})u(\mathbf{r}) = E_{rel}u(\mathbf{r}) \tag{127}$$

and

$$-\frac{\hbar^2}{2M}\boldsymbol{\nabla}_{\mathbf{R}}{}^2 U(\mathbf{R}) = E_{cm}U(\mathbf{R}) \tag{128}$$

where $M = m_1 + m_2$ is the total mass, and $\mu = m_1 m_2 / M$ is the reduced mass.

Aside: WHY do we care (slide of Hydrogen line spectrum shown)? This all started because when people looked at the spectrum for the hydrogen atom, a continuous spectrum was not found. Instead what was found was quantized frequencies. All this abstract Hilbert space notation with its bras and kets is a way of representing observable phenomena.

Also note that we have the same sort of problems in electrodynamics and mechanics, so we are able to recycle this sort of work, either applying it in those problems later, or using those techniques here.

In Electromagnetism these are the problems involving the solution to

$$\boldsymbol{\nabla} \cdot \mathbf{E} = 0 \tag{129}$$

or for

$$\mathbf{E} = -\boldsymbol{\nabla}\Phi \tag{130}$$

$$\boldsymbol{\nabla}^2\Phi = 0, \tag{131}$$

where $\mathbf{E}$ is the electric field and Φ is the electric potential.

We need sol solve 127 for $u(\mathbf{r})$. In spherical coordinates

$$-\frac{\hbar^2}{2m}\frac{1}{r}\frac{d^2}{dr^2}(rR_l) + \left(V(\mathbf{r}) + \frac{\hbar^2}{2m}l(l+1)\right)R_l = ER_l \tag{132}$$

where

$$u(\mathbf{r}) = R_l(\mathbf{r})Y_{lm}(\theta, \phi) \tag{133}$$

This all follows by the separation of variables technique that we'll use here, in E and M, in PDEs, and so forth.

FIXME: picture drawn. Theta measured down from $\mathbf{e}_3$ axis to the position $\mathbf{r}$ and ϕ measured in the x, y plane measured in the $\mathbf{e}_1$ to $\mathbf{e}_2$ orientation.

For the hydrogen atom, we have

$$V(\mathbf{r}) = -\frac{Ze^2}{r} \tag{134}$$

Here is what this looks like.

We introduce

$$\rho = \alpha r \tag{135}$$

$$\alpha = \sqrt{\frac{-8mE}{\hbar^2}} \tag{136}$$

$$\lambda = \frac{2mZe^2}{\hbar^2\alpha} \tag{137}$$

$$\frac{2m(-E)}{\hbar^2\alpha^2} = \frac{1}{4} \tag{138}$$

and write

$$\frac{d^2R_l}{d\rho^2} + \frac{2}{\rho}\frac{dR_l}{d\rho} + \left(\frac{\lambda}{\rho} - \frac{l(l+1)}{\rho^2} - \frac{1}{4}\right) R_l = 0 \tag{139}$$

7.2. *Large ρ limit.*

For $\rho \to \infty$, 139 becomes

$$\frac{d^2R_l}{d\rho^2} - \frac{1}{4}R_l = 0 \tag{140}$$

which implies solutions of the form

$$R_l(\rho) = e^{\pm\rho/2} \tag{141}$$

but keep $R_l(\rho) = e^{-\rho/2}$ and note that $R_l(\rho) = F(\rho)e^{-\rho/2}$ is also a solution in the limit of $\rho \to \infty$, where $F(\rho)$ is a polynomial.

Let $F(\rho) = \rho^s L(\rho)$ where $L(\rho) = a_0 + a_1\rho + \cdots a_\nu\rho^\nu + \cdots$.

7.3. *Small ρ limit.*

We also want to consider the small ρ limit, and piece together the information that we find. Think about the following. The small $\rho \to 0$ or $r \to 0$ limit gives

$$\frac{d^2R_l}{d\rho^2} - \frac{l(l+1)}{\rho^2}R_l = 0 \tag{142}$$

Question: Is this correct?

Not always. Also: we will also think about the $l = 0$ case later (where λ/ρ would probably need to be retained.)

We need:

$$\frac{d^2R_l}{d\rho^2} + \frac{2}{\rho}\frac{dR_l}{d\rho} - \frac{l(l+1)}{\rho^2}R_l = 0 \tag{143}$$

Instead of using 142 as in the text, we must substitute $R_l = \rho^s$ into the above to find

$$s(s-1)\rho^{s-2} + 2s\rho^{s-2} - l(l+1)\rho^{s-2} = 0 \tag{144}$$

$$\left(s(s-1) + 2s - l(l+1)\right)\rho^{s-2} = \tag{145}$$

for this equality for all ρ we need

$$s(s-1) + 2s - l(l+1) = 0 \tag{146}$$

Solutions $s = l$ and $s = -(l+1)$ can be found to this, and we need s positive for normalizability, which implies

$$R_l(\rho) = \rho^l L(\rho) e^{-\rho/2}. \tag{147}$$

Now we need to find what restrictions we must have on $L(\rho)$. Recall that we have $L(\rho) = \sum a_\nu \rho^\nu$. Substitution into 142 gives

$$\rho\frac{d^2L}{d\rho} + \left(2(l+1) - \rho\right)\frac{dL}{d\rho} + (\lambda - l - 1)L = 0 \tag{148}$$

We get

$$A_0 + A_1\rho + \cdots A_\nu\rho^\nu + \cdots = 0 \tag{149}$$

For this to be valid for all ρ,

$$a_{\nu+1}\left((\nu+1)(\nu+2l+2)\right) - a_\nu\left(\nu - \lambda + l + 1\right) = 0 \tag{150}$$

or

$$\frac{a_{\nu+1}}{a_\nu} = \frac{\nu - \lambda + l + 1}{(\nu+1)(\nu+2l+2)} \tag{151}$$

For large ν we have

$$\frac{a_{\nu+1}}{a_\nu} = \frac{1}{\nu+1} \to \frac{1}{\nu} \tag{152}$$

Recall that for the exponential Taylor series we have

$$e^\rho = 1 + \rho + \frac{\rho^2}{2!} + \cdots \tag{153}$$

for which we have

$$\frac{a_{\nu+1}}{a_\nu} \to \frac{1}{\nu} \tag{154}$$

$L(\rho)$ is behaving like e^ρ, and if we had that

$$R_l(\rho) = \rho^l L(\rho) e^{-\rho/2} \to \rho^l e^{\rho} e^{-\rho/2} = \rho^l e^{\rho/2} \tag{155}$$

This is divergent, so for normalizable solutions we require $L(\rho)$ to be a polynomial of a finite number of terms.

The polynomial $L(\rho)$ must stop at $\nu = n'$, and we must have

$$a_{\nu+1} = a_{n'+1} = 0 \tag{156}$$

$$a_{n'} \neq 0 \tag{157}$$

From 150 we have

$$a_{n'} \left(n' - \lambda + l + 1 \right) = 0 \tag{158}$$

so we require

$$n' = \lambda - l - 1 \tag{159}$$

Let $\lambda = n$, an integer and $n' = 0, 1, 2, \cdots$ so that $n' + l + 1 = n$ says for $n = 1, 2, \cdots$

$$l \leq n - 1 \tag{160}$$

If

$$\lambda = n = \frac{2mZe^2}{\hbar^2 \alpha} \tag{161}$$

we have

$$E = E_n = -\frac{Z^2 e^2}{2a_0} \frac{1}{n^2} \tag{162}$$

where $a_0 = \hbar^2/me^2$ is the Bohr radius, and $\alpha = \sqrt{-8mE/\hbar^2}$. In the lecture m was originally used for the reduced mass. I've switched to μ earlier so that this cannot be mixed up with this use of m for the azimuthal quantum number associated with $L_z Y_{lm} = m\hbar Y_{lm}$.

PICTURE ON BOARD. Energy level transitions on $1/n^2$ graph with differences between $n = 2$ to $n = 1$ shown, and photon emitted as a result of the $n = 2$ to $n = 1$ transition.

From Chapter 4 and the story of the spherical harmonics, for a given l, the quantum number m varies between $-l$ and l in integer steps. The radial part of the solution of this separation of variables problem becomes

$$R_l = \rho^l L(\rho) e^{-\rho/2} \tag{163}$$

where the functions $L(\rho)$ are the Laguerre polynomials, and our complete wavefunction is

$$u_{nlm}(r, \theta, \phi) = R_l(\rho) Y_{lm}(\theta, \phi) \tag{164}$$

$$n = 1, 2, \cdots \tag{165}$$

$$l = 0, 1, 2, \cdots, n - 1 \tag{166}$$

$$m = -l, -l + 1, \cdots 0, 1, 2, \cdots, l - 1, l \tag{167}$$

Note that for $n = 1, l = 0$, $R_{10} \propto e^{-r/a_0}$, as graphed here.

PHY356F : Quantum Physics I Fall 2010

Lecture 11 — Harmonic oscillator. — November 30, 2010

Prof. Vatche Deyirmenjian *Scribe: Peeter Joot*

8. Lecture 11 — Harmonic oscillator. — November 30, 2010

9. Setup.

Why study this problem?

It is relevant to describing the oscillation of molecules, quantum states of light, vibrations of the lattice structure of a solid, and so on.

FIXME: projected picture of masses on springs, with a ladle shaped well, approximately Harmonic about the minimum of the bucket.

The problem to solve is the one dimensional Hamiltonian

$$V(X) = \frac{1}{2}KX^2 \tag{168}$$

$$K = m\omega^2 \tag{169}$$

$$H = \frac{P^2}{2m} + V(X) \tag{170}$$

where m is the mass, ω is the frequency, X is the position operator, and P is the momentum operator. Of these quantities, ω and m are classical quantities.

This problem can be used to illustrate some of the reasons why we study the different pictures (Heisenberg, Interaction and Schrödinger). This is a problem well suited to all of these (FIXME: lookup an example of this with the interaction picture. The book covers H and S methods.

We attack this with a non-intuitive, but cool technique. Introduce the raising $a^\dagger$ and lowering a operators:

$$a = \sqrt{\frac{m\omega}{2\hbar}}\left(X + i\frac{P}{m\omega}\right) \tag{171}$$

$$a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(X - i\frac{P}{m\omega}\right) \tag{172}$$

Question: are we using the dagger for more than Hermitian conjugation in this case.

Answer: No, this is precisely the Hermitian conjugation operation.

Solving for X and P in terms of a and $a^\dagger$, we have

$$a + a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}2X$$

$$a - a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}2i\frac{P}{m\omega}$$

or

$$X = \sqrt{\frac{\hbar}{2m\omega}}(a^\dagger + a) \tag{173}$$

$$P = i\sqrt{\frac{\hbar m\omega}{2}}(a^\dagger - a) \tag{174}$$

Express H in terms of a and $a^\dagger$

$$\begin{aligned} H &= \frac{P^2}{2m} + \frac{1}{2}KX^2 \\ &= \frac{1}{2m}\left(i\sqrt{\frac{\hbar m\omega}{2}}(a^\dagger - a)\right)^2 + \frac{1}{2}m\omega^2\left(\sqrt{\frac{\hbar}{2m\omega}}(a^\dagger + a)\right)^2 \\ &= \frac{-\hbar\omega}{4}\left(a^\dagger a^\dagger + a^2 - aa^\dagger - a^\dagger a\right) + \frac{\hbar\omega}{4}\left(a^\dagger a^\dagger + a^2 + aa^\dagger + a^\dagger a\right) \end{aligned}$$

$$H = \frac{\hbar\omega}{2}\left(aa^\dagger + a^\dagger a\right) = \frac{\hbar\omega}{2}\left(2a^\dagger a + \left[a, a^\dagger\right]\right) \tag{175}$$

Since $[X, P] = i\hbar\mathbf{1}$ then we can show that $\left[a, a^\dagger\right] = \mathbf{1}$. Solve for $\left[a, a^\dagger\right]$ as follows

$$\begin{aligned} i\hbar &= [X, P] \\ &= \left[\sqrt{\frac{\hbar}{2m\omega}}(a^\dagger + a), i\sqrt{\frac{\hbar m\omega}{2}}(a^\dagger - a)\right] \\ &= \sqrt{\frac{\hbar}{2m\omega}}i\sqrt{\frac{\hbar m\omega}{2}}\left[a^\dagger + a, a^\dagger - a\right] \\ &= \frac{i\hbar}{2}\left(\left[a^\dagger, a^\dagger\right] - \left[a^\dagger, a\right] + \left[a, a^\dagger\right] - [a, a]\right) \\ &= \frac{i\hbar}{2}\left(0 + 2\left[a, a^\dagger\right] - 0\right) \end{aligned}$$

Comparing LHS and RHS we have as stated

$$\left[a, a^\dagger\right] = \mathbf{1} \tag{176}$$

and thus from 175 we have

$$H = \hbar\omega\left(a^\dagger a + \frac{\mathbf{1}}{2}\right) \tag{177}$$

Let $|n\rangle$ be the eigenstate of H so that $H|n\rangle = E_n|n\rangle$. From 177 we have

$$H|n\rangle = \hbar\omega\left(a^\dagger a + \frac{\mathbf{1}}{2}\right)|n\rangle \tag{178}$$

or

$$a^\dagger a|n\rangle + \frac{|n\rangle}{2} = \frac{E_n}{\hbar\omega}|n\rangle \tag{179}$$

$$a^\dagger a|n\rangle = \left(\frac{E_n}{\hbar\omega} - \frac{1}{2}\right)|n\rangle = \lambda_n|n\rangle \tag{180}$$

We wish now to find the eigenstates of the "Number" operator $a^\dagger a$, which are simultaneously eigenstates of the Hamiltonian operator.

Observe that we have

$$\begin{aligned} a^\dagger a(a^\dagger|n\rangle) &= a^\dagger(aa^\dagger|n\rangle) \\ &= a^\dagger(\mathbf{1} + a^\dagger a)|n\rangle \end{aligned}$$

where we used $\left[a, a^\dagger\right] = aa^\dagger - a^\dagger a = \mathbf{1}$.

$$\begin{aligned} a^\dagger a(a^\dagger|n\rangle) &= a^\dagger\left(\mathbf{1} + \frac{E_n}{\hbar\omega} - \frac{\mathbf{1}}{2}\right)|n\rangle \\ &= a^\dagger\left(\frac{E_n}{\hbar\omega} + \frac{\mathbf{1}}{2}\right)|n\rangle, \end{aligned}$$

or

$$a^\dagger a(a^\dagger|n\rangle) = (\lambda_n + 1)(a^\dagger|n\rangle) \tag{181}$$

The new state $a^\dagger|n\rangle$ is presumed to lie in the same space, expressible as a linear combination of the basis states in this space. We can see the effect of the operator $aa^\dagger$ on this new state, we find that the energy is changed, but the state is otherwise unchanged. Any state $a^\dagger|n\rangle$ is an eigenstate of $a^\dagger a$, and therefore also an eigenstate of the Hamiltonian.

Play the same game and win big by discovering that

$$a^\dagger a(a|n\rangle) = (\lambda_n - 1)(a|n\rangle) \tag{182}$$

There will be some state $|0\rangle$ such that

$$a|0\rangle = 0|0\rangle \tag{183}$$

which implies

$$a^\dagger(a|0\rangle) = (a^\dagger a)|0\rangle = 0 \tag{184}$$

so from 180 we have

$$\lambda_0 = 0 \tag{185}$$

Observe that we can identify $\lambda_n = n$ for

$$\lambda_n = \left(\frac{E_n}{\hbar\omega} - \frac{1}{2}\right) = n, \tag{186}$$

or

$$\frac{E_n}{\hbar\omega} = n + \frac{1}{2} \tag{187}$$

or

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right) \tag{188}$$

where $n = 0, 1, 2, \cdots$.
We can write

$$\begin{aligned}\hbar\omega\left(a^\dagger a + \frac{1}{2}\mathbf{1}\right)|n\rangle &= E_n|n\rangle \\ a^\dagger a|n\rangle + \frac{1}{2}|n\rangle &= \frac{E_n}{\hbar\omega}|n\rangle\end{aligned}$$

or

$$a^\dagger a|n\rangle = \left(\frac{E_n}{\hbar\omega} - \frac{1}{2}\right)|n\rangle = \lambda_n|n\rangle = n|n\rangle \tag{189}$$

We call this operator $a^\dagger a = N$, the number operator, so that

$$N|n\rangle = n|n\rangle \tag{190}$$

10. **Relating states.**

Recall the calculation we performed for

$$L_+|lm\rangle = C_+|l, m+1\rangle \tag{191}$$
$$L_-|lm\rangle = C_+|l, m-1\rangle \tag{192}$$

Where C_+, and C_+ are constants. The next game we are going to play is to work out C_n for the lowering operation

$$a|n\rangle = C_n|n-1\rangle \tag{193}$$

and the raising operation

$$a^\dagger|n\rangle = B_n|n+1\rangle. \tag{194}$$

For the Hermitian conjugate of $a|n\rangle$ we have

$$(a|n\rangle)^\dagger = (C_n|n-1\rangle)^\dagger = C_n^*|n-1\rangle \tag{195}$$

So

$$(\langle n|a^\dagger)(a|n\rangle) = C_n C_n^* \langle n-1|n-1\rangle = |C_n|^2 \tag{196}$$

Expanding the LHS we have

$$\begin{aligned}|C_n|^2 &= \langle n|a^\dagger a|n\rangle \\ &= \langle n|n|n\rangle \\ &= n\langle n|n\rangle \\ &= n\end{aligned}$$

For

$$C_n = \sqrt{n} \tag{197}$$

Similarly

$$(\langle n|a^\dagger)(a|n\rangle) = B_n B_n^* \langle n+1|n+1\rangle = |B_n|^2 \tag{198}$$

and

$$\begin{aligned} |B_n|^2 &= \langle n| \underbrace{aa^\dagger}_{aa^\dagger - a^\dagger a = \mathbf{1}} |n\rangle \\ &= \langle n| \left(\mathbf{1} + a^\dagger a\right) |n\rangle \\ &= (1+n) \langle n|n\rangle \\ &= 1+n \end{aligned}$$

for

$$B_n = \sqrt{n+1} \tag{199}$$

11. **Heisenberg picture.**

How does the lowering operator a evolve in time?

A: Recall that for a general operator A, we have for the time evolution of that operator

$$i\hbar \frac{dA}{dt} = [A, H] \tag{200}$$

Let's solve this one.

$$\begin{aligned} i\hbar \frac{da}{dt} &= [a, H] \\ &= \left[a, \hbar\omega(a^\dagger a + \mathbf{1}/2)\right] \\ &= \hbar\omega \left[a, (a^\dagger a + \mathbf{1}/2)\right] \\ &= \hbar\omega \left[a, a^\dagger a\right] \\ &= \hbar\omega \left(aa^\dagger a - a^\dagger aa\right) \\ &= \hbar\omega \left((aa^\dagger)a - a^\dagger aa\right) \\ &= \hbar\omega \left((a^\dagger a + \mathbf{1})a - a^\dagger aa\right) \\ &= \hbar\omega a \end{aligned}$$

Even though a is an operator, it can undergo a time evolution and we can think of it as a function, and we can solve for a in the differential equation

$$\frac{da}{dt} = -i\omega a \tag{201}$$

This has the solution

$$a = a(0)e^{-i\omega t} \tag{202}$$

here $a(0)$ is an operator, the value of that operator at $t = 0$. The exponential here is just a scalar (not effected by the operator so we can put it on either side of the operator as desired).

CHECK:

$$a' = a(0)\frac{d}{dt}e^{-i\omega t} = a(0)(-i\omega)e^{-i\omega t} = -i\omega a \tag{203}$$

12. **A couple comments on the Schrödinger picture.**

We don't do this in class, but it is very similar to the approach of the hydrogen atom. See the text for full details.

In the Schrödinger picture,

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dx^2} + \frac{1}{2}m\omega^2x^2u = Eu \tag{204}$$

This does directly to the wave function representation, but we can relate these by noting that we get this as a consequence of the identification $u = u(x) = \langle x|u\rangle$.

In 204, we can switch to dimensionless quantities with

$$\xi = \text{“xi (z)”} = \alpha x \tag{205}$$

with

$$\alpha = \sqrt{\frac{m\omega}{\hbar}} \tag{206}$$

This gives, with $\lambda = 2E/\hbar\omega$,

$$\frac{d^2u}{d\xi^2} + (\lambda - \xi^2)u = 0 \tag{207}$$

We can use polynomial series expansion methods to solve this, and find that we require a terminating expression, and write this in terms of the Hermite polynomials (courtesy of the clever French once again).

When all is said and done we will get the energy eigenvalues once again

$$E = E_n = \hbar\omega\left(n + \frac{1}{2}\right) \tag{208}$$

13. **Back to the Heisenberg picture.**

Let us express

$$\langle x|n\rangle = u_n(x) \tag{209}$$

With

$$a|0\rangle = 0, \tag{210}$$

we have

$$0 = \left(X + i\frac{P}{m\omega}\right)|0\rangle, \tag{211}$$

and

$$\begin{aligned} 0 &= \langle x| \left(X + i\frac{P}{m\omega} \right) |0\rangle \\ &= \langle x|X|0\rangle + i\frac{1}{m\omega}\langle x|P|0\rangle \\ &= x\langle x|0\rangle + i\frac{1}{m\omega}\langle x|P|0\rangle \end{aligned}$$

Recall that our matrix operator is

$$\langle x'|P|x\rangle = \delta(x - x')\left(-i\hbar\frac{d}{dx}\right) \tag{212}$$

$$\begin{aligned} \langle x|P|0\rangle &= \langle x|P \underbrace{\int |x'\rangle\langle x'|dx'}_{=\mathbf{1}}|0\rangle \\ &= \int \langle x|P|x'\rangle \langle x'|0\rangle \, dx' \\ &= \int \delta(x - x')\left(-i\hbar\frac{d}{dx}\right)\langle x'|0\rangle \, dx' \\ &= \left(-i\hbar\frac{d}{dx}\right)\langle x|0\rangle \end{aligned}$$

We have then

$$0 = xu_0(x) + \frac{\hbar}{m\omega}\frac{du_0(x)}{dx} \tag{213}$$

NOTE: picture of the solution to this LDE on slide.... but I didn't look closely enough.

PHY356F : Quantum Physics I Fall 2010

Lecture 12 — Rotations, Angular Momentum. — December 6, 2010

Prof. Vatche Deyirmenjian *Scribe: Peeter Joot*

14. Lecture 12 — Rotations, Angular Momentum. — December 6, 2010

Last time. The Harmonic Oscillator

14.1. This time. Rotations (chapter 26).

Why are we doing the math? Because it applies to physical systems. Slides of IBM's SEM quantum coral and others shown and discussed.

PICTURE: Standard right handed coordinate system with point (x, y, z). We'd like to discuss how to represent this point in other coordinate systems, such as one with the x, y axes rotated to x', y' through an angle ϕ.

Our problem is to find in the rotated coordinate system from (x, y, z) to (x', y', z').

There's clearly a relationship between the representations. That relationship between x', y', z' and x, y, z for a counter-clockwise rotation about the z axis is

$$x' = x\cos\phi - y\sin\phi \tag{214}$$
$$y' = x\sin\phi + y\cos\phi \tag{215}$$
$$z' = z \tag{216}$$

Treat (x, y, z) and (x', y', z') like vectors and write

$$\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} \tag{217}$$

Or

$$\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = R_z(\phi) \begin{bmatrix} x \\ y \\ z \end{bmatrix} \tag{218}$$

Q: Is $R_z(\phi)$ a unitary operator? Definition U is unitary if $U^\dagger U = \mathbf{1}$, where $\mathbf{1}$ is the identity operator. We take Hermitian conjugates, which in this case is just the transpose since all elements of the matrix are real, and multiply

$$\begin{aligned}
(R_z(\phi))^\dagger R_z(\phi) &= \begin{bmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix} \\
&= \begin{bmatrix} \cos^2\phi + \sin^2\phi & -\sin\phi\cos\phi + \sin\phi\cos\phi & 0 \\ -\cos\phi\sin\phi + \cos\phi\sin\phi & \cos^2\phi + \sin^2\phi & 0 \\ 0 & 0 & 1 \end{bmatrix} \\
&= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \\
&= \mathbf{1}
\end{aligned}$$

Apply the above to a vector $\mathbf{v} = (v_x, v_y, v_z)$ and write $\mathbf{v}' = (v_x', v_y', v_z')$. These are related as

$$\mathbf{v} = R_z(\phi)\mathbf{v} \tag{219}$$

Now we want to consider the infinitesimal case where we allow the rotation angle to get arbitrarily small. Consider this specific z axis rotation case, and assume that ϕ is very small. Let $\phi = \epsilon$ and write

$$\mathbf{v}' = \begin{bmatrix} v_x' \\ v_y' \\ v_z' \end{bmatrix} = R_z(\phi) \begin{bmatrix} v_x \\ v_y \\ v_z \end{bmatrix} = \begin{bmatrix} \cos\epsilon & -\sin\epsilon & 0 \\ \sin\epsilon & \cos\epsilon & 0 \\ 0 & 0 & 1 \end{bmatrix} \mathbf{v} \tag{220}$$

$$\approx \begin{bmatrix} 1 & -\epsilon & 0 \\ \epsilon & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \mathbf{v} = \left(\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} + \begin{bmatrix} 0 & -\epsilon & 0 \\ \epsilon & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \right) \mathbf{v} \tag{221}$$

Define

$$S_z = i\hbar \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{222}$$

which is the generator of infinitesimal rotations about the z axis.
Our rotated coordinate vector becomes

$$\begin{aligned} \mathbf{v}' &= \left(\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} + \frac{i\hbar\epsilon}{i\hbar} \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \right) \mathbf{v} \\ &= \left(\mathbf{1} + \frac{\epsilon}{i\hbar} S_z \right) \mathbf{v} \end{aligned}$$

Or

$$\mathbf{v}' = \left(\mathbf{1} - \frac{i\epsilon}{\hbar} S_z \right) \mathbf{v} \tag{223}$$

Many infinitesimal rotations can be combined to create a finite rotation via

$$\lim_{N\to\infty} \left(1 + \frac{\alpha}{N} \right)^N = e^{\alpha} \tag{224}$$

$$\alpha = -i\phi S_z/\hbar \tag{225}$$

For a finite rotation

$$\mathbf{v}' = e^{-i\frac{\phi S_z}{\hbar}} \mathbf{v} \tag{226}$$

Now think about transforming $g(x, y, z)$, an arbitrary function. Take ϵ is very small so that

$$x' = x\cos\phi - y\sin\phi = x\cos\epsilon - y\sin\epsilon \approx x - y\epsilon \tag{227}$$

$$y' = x\sin\phi + y\cos\phi = x\sin\epsilon + y\cos\epsilon \approx x\epsilon + y \tag{228}$$

$$z' = z \tag{229}$$

Question: Why can we assume that ϵ is small.

Answer: We declare it to be small because it is simpler, and eventually build up to the general case where it is larger. We want to master the easy task before moving on to the more difficult ones. Our function is now transformed

$$\begin{aligned} g(x', y', z') \approx g(x - y\epsilon, y + x\epsilon, z) & \\ &= g(x, y, z) - \epsilon y \frac{\partial g}{\partial x} + \epsilon x \frac{\partial g}{\partial y} + \cdots \\ &= \left(\mathbf{1} - \epsilon y \frac{\partial}{\partial x} + \epsilon x \frac{\partial}{\partial y} \right) g(x, y, z) \end{aligned}$$

Recall that the coordinate definition of the angular momentum operator is

$$L_z = -i\hbar \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) = x p_y - y p_x \tag{230}$$

We can now write

$$\begin{aligned} g(x', y', z') &= \left(\mathbf{1} + \frac{-i\hbar\epsilon}{-i\hbar} \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) \right) g(x, y, z) \\ &= \left(\mathbf{1} + \frac{i\epsilon}{\hbar} L_z \right) g(x, y, z) \end{aligned}$$

For a finite rotation with angle ϕ we have

$$g(x', y', z') = e^{i \frac{\phi L_z}{\hbar}} g(x, y, z) \tag{231}$$

Question: somebody says that the rotation is clockwise not counterclockwise. I didn't follow the reasoning briefly mentioned on the board since it looks right to me. Perhaps this is the age old mixup between rotating the coordinates and the basis vectors. Review what's in the text carefully. Can also check by

If you rotate a ket, and examine how the state representation of that ket changes under rotation, we have

$$|x', y', z'\rangle = |x - \epsilon y, y + \epsilon x, z\rangle \tag{232}$$

Or

$$\begin{aligned} \langle \Psi | x', y', z' \rangle &= \Psi^*(x', y', z') \\ &= \Psi^*(x - \epsilon y, y + \epsilon x, z) \\ &= \Psi^*(x, y, z) - \epsilon \frac{\partial \Psi^*}{\partial y} + \epsilon \frac{\partial \Psi^*}{\partial x} \\ &= \left(\mathbf{1} + \frac{i\epsilon}{\hbar} L_z \right) \Psi^*(x, y, z) \end{aligned}$$

Taking the complex conjugate we have

$$\Psi(x', y', z') \left(\mathbf{1} - \frac{i\epsilon}{\hbar} L_z \right) \Psi(x, y, z) \tag{233}$$

For infinitesimal rotations about the z axis we have for functions

$$\Psi(x', y', z') = e^{-\frac{i\epsilon}{\hbar}L_z}\Psi(x, y, z) \tag{234}$$

For finite rotations of a vector about the z axis we have

$$\mathbf{v}' = e^{-\frac{i\phi S_z}{\hbar}}\Psi(x, y, z)\mathbf{v} \tag{235}$$

and for functions

$$\Psi(x', y', z') = e^{-\frac{i\phi L_z}{\hbar}}\Psi(x, y, z) \tag{236}$$

Vatche has mentioned some devices being researched right now where there is an attempt to isolate the spin orientation so that, say, only spin up or spin down electrons are allowed to flow. There are some possible interesting applications here to Quantum computation. Can we actually make a quantum computing device that is actually usable? We can make NAND devices as mentioned in the article above. Can this be scaled? We don't know how to do this yet.

Recall that one description of a "particle" that has both a position and spin representation is

$$|\Psi\rangle = |u\rangle \otimes |sm\rangle \tag{237}$$

where we have a tensor product of kets. One usually just writes the simpler

$$|u\rangle \otimes |sm\rangle \equiv |u\rangle|sm\rangle \tag{238}$$

An example of the above is

$$\begin{bmatrix} u_1(\mathbf{r}) \\ u_2(\mathbf{r}) \\ u_3(\mathbf{r}) \end{bmatrix} = \Big(\langle \mathbf{r}|\langle sm|\Big)|\Psi\rangle \tag{239}$$

where u_1 is spin component one. For $s = 1$ this would be $m = -1, 0, 1$.

Here we have also used

$$\begin{aligned} |\mathbf{r}\rangle = |x\rangle \otimes |y\rangle \otimes |z\rangle & \\ &= |x\rangle|y\rangle|z\rangle \\ &= |xyz\rangle \end{aligned}$$

We can now ask the question of how this thing transforms. We transform each component of this as a vector. The transformation of

$$\begin{bmatrix} u_1(\mathbf{r}) \\ u_2(\mathbf{r}) \\ u_3(\mathbf{r}) \end{bmatrix}$$

results in

$$\begin{bmatrix} u_1(\mathbf{r}) \\ u_2(\mathbf{r}) \\ u_3(\mathbf{r}) \end{bmatrix}' = e^{-i\phi(S_z+L_z)/\hbar} \begin{bmatrix} u_1(\mathbf{r}) \\ u_2(\mathbf{r}) \\ u_3(\mathbf{r}) \end{bmatrix} \tag{240}$$

Or with $J_z = S_z + L_z$

$$|\Psi'\rangle = e^{-i\phi J_z/\hbar}|\Psi\rangle \tag{241}$$

Observe that this separates out nicely with the S_z operation acting on the vector parts, and the L_z operator acting on the functional dependence.

References

[1] BR Desai. *Quantum mechanics with basic field theory*. Cambridge University Press, 2009. 1