Physics 143a - Quantum Mechanics I

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This course was taught by Matthew Reece, at TTh 10-11:30 in Jefferson 356. The textbook was *A Modern Approach to Quantum Mechanics* by John Townsend. There were 34 undergraduates and 1 graduate student enrolled and the grading was based on weekly problem sets, two in-class midterm, and a three-hour final exam. The teaching fellow was Mobolaji Williams.

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1 January 24, 2017

There will be weekly problem sets due Tuesdays. There will be two in-class midterms, on Feb 16 and Mar 28. Our textbook is Townsend, *A Modern Approach to Quantum Mechanics*, 2nd edition. The main prerequisite will be linear algebra. You don't necessarily have to take Physics 15c to take this course.

1.1 Introduction

Quantum mechanics is more of a principle that underlies many theories, e.g., classical mechanics. There are many forms of classical mechanics. The underlying principle of Newtonian mechanics is $\vec{F} = m\vec{a}$, the principle in Lagrangian mechanics is $\partial L/\partial q - (d/dt)\partial L/\partial \dot{q} = 0$. The universal law in Hamiltonian mechanics is $\dot{q} = \partial H/\partial p$ and $\dot{p} = -\partial H/\partial q$.

Once you have the universal principle, you can study different theories by applying that law to different situations. Let me list a few of these theories.

- hydrogen atom: its energy levels and transitions (Ch. 10)
- quantum electrodynamics: relativistic theory of EM field (photons), electrons, positrons, ...
- BCS superconductivity: Cooper pairs, ...
- theory of nuclear matter
- cosmology: inflation and destiny perturbations
- standard model
- string theory

Most of the things here are things we won't see in the course, but I wanted to give a sense of where you can go with quantum mechanics.

The logic of quantum mechanics is very weird, in the sense that it is different from the classical world. Classical physics emerges from quantum mechanics of large numbers of particles. This emergence is largely due to entanglement and decoherence. We will get a glipse by the end of the semester, but the real world is quantum mechanical.

1.2 Linear superpositions

Consider the wave equation

$$\frac{\partial^2}{\partial t^2} f(x,t) - \frac{\partial^2}{\partial x^2} f(x,t) = 0.$$

If $f_1(x,t)$ and $f_2(x,t)$ are solutions, then $c_1 f_1(x,t) + c_2 f_2(x,t)$ is also a solution for any constants c_1, c_2. However, the equation

$$\frac{\partial^2}{\partial t^2} f(x,t) - \frac{\partial^2}{\partial x^2} f(x,t) = \epsilon f(x,t)^2$$

does not have this property.

Quantum mechanics postulates that linear superpositions of physical states are physical states. So linearity is built into quantum mechanics in a fundamental way. This is a postulate that we assume because it matches experiment.

Example 1.1. Let us look at a "qubit", a quantum bit. The classical bit takes values in 0 or 1. What happens in quantum mechanics is that the bit can take any linear combination:

$$|\psi\rangle = c_0|0\rangle + c_1|1\rangle$$

These $|0\rangle$ and $|1\rangle$ are quantum states corresponding to the classical state, and c_0 and c_1 are complex numbers. This notation is something like the vector notation $\vec{v} = v_1\vec{e}_1 + v_2\vec{e}_2$ in mathematics. Sometimes we might change the notation, e.g., $|\uparrow\rangle$ and $|\downarrow\rangle$ if it represents a spin, or $|L\rangle$ and $|R\rangle$ if it represents light polarization.

When we work with vectors, we take the dot product as

$$\vec{w} \cdot \vec{v} = w_1v_1 + w_2v_2 + w_3v_3 = w^T v.$$

We are going to do something similar with quantum states. Assume we have an orthonormal basis,

$$\langle 0|1\rangle = 1, \quad \langle 1|1\rangle = 1, \quad \langle 0|1\rangle = 0, \quad \langle 1|0\rangle = 0.$$

I've introduced some funny notation here. For two quantum states $|\psi\rangle$ and $|\chi\rangle$, we write the inner product as $\langle\chi|\psi\rangle$. Suppose $|\psi\rangle = c_0|0\rangle + c_1|1\rangle$ and $|\chi\rangle = d_0|0\rangle + d_1|1\rangle$. Then their inner product is

$$\langle\chi|\psi\rangle = d_0^* c_0 + d_1^* c_1.$$

If we were taking the inner product in the other way, we would get

$$\langle\psi|\chi\rangle = c_0^* d_0 + c_1^* d_1 = (\langle\chi|\psi\rangle)^*.$$

We will choose to work with normal states, i.e., $\langle\psi|\psi\rangle = 1$. Note that if I define $|\psi'\rangle = e^{i\theta}|\psi\rangle$ by rephasing it, then $\langle\psi'|\psi'\rangle = \langle\psi|\psi\rangle = 1$. Physics doesn't really care about phase change, and so we can say that quantum states is a complex vector space modulo scaling and phase change.

The reason we flipped the angle on the right is because the angle on the left has a meaning of its own:

$$\text{if } |\psi\rangle = c_0|0\rangle + c_1|1\rangle \text{ then } \langle\psi| = c_0^*\langle 0| + c_1^*\langle 1|.$$

This is called the **Dirac notation**. The $|\psi\rangle$ is called a **ket** and $\langle\psi|$ is called a **bra** so that the inner product becomes a bracket. We can represent $|\psi\rangle$ as column vectors and $\langle\psi|$ as row vectors. In this context, the inner product is like $w^\dagger v$, where $\dagger$ is Hermitian conjugation.

2 January 26, 2017

2.1 The Stern–Gerlach experiment

An electron has an intrinsic spin $\vec{S}$, and a non-uniform magnetic field exerts a force. The force is given by

$$\vec{F} \propto \vec{S} \cdot \hat{n}.$$

When (non-polarized) particles pass though a Stern–Gerlach device, it turns out that there are discrete outcomes observed, not a continuous pattern. Let us write the Stern–Gerlach device that checks the $\vec{S} \cdot \hat{n}$ by $SG\hat{n}$. You can do the experiment with multiple devices like letting the particles pass tough $SG\hat{z}$, choose one of the beams, and then let us pass though $SG\hat{x}$. The result is that the particles split into two deflection patterns, with 50% chance each.

At the early state of quantum mechanics, there were many confusing experiments like this. There is a mathematical formalism that matches the result. Let us write $|+n\rangle$ the quantum state that is definitely deflected up and $|-n\rangle$ the quantum state that is definitely deflected down. Then we can write any quantum state as

$$|\psi\rangle = c_+|+n\rangle + c_-|-n\rangle,$$

where $|c_+|^2 + |c_-|^2 = 1$.

Now we make the following assumptions:

- If $|\psi\rangle$ goes through an $SG\hat{n}$ device, and the outgoing particle is detected, we see $|+n\rangle$ with probability $|c_+|^2$ and $|-n\rangle$ with probability $|c_-|^2$.
- After measuring, the state is *is* $|+n\rangle$ or $|-n\rangle$.

It turns out that the state space for an electron's spin is really 2-dimensional. So we can choose a basis and write $|\psi\rangle = c_+|+z\rangle + c_-|-z|$. There should be states $|+x\rangle$ and $|-x\rangle$ and so there must be presentations

$$|+x\rangle = c_+|+z\rangle + c_-|-z\rangle, \quad |-x\rangle = d_+|+z\rangle + d_-|-z\rangle,$$

with $|c_+|^2 = |c_-|^2 = |d_+|^2 = |d_-|^2 = 1/2$ and $d_+^* c_+ + d_-^* c_- = 0$. There will also be states in the y direction. If you solve the equation, you can choose the states

$$|+x\rangle = \frac{1}{\sqrt{2}}|+z\rangle + \frac{1}{\sqrt{2}}|-z\rangle, \quad |-x\rangle = \frac{1}{\sqrt{2}}|+z\rangle - \frac{1}{\sqrt{2}}|-z\rangle$$

work. If you solve the equations, you see that

$$|+y\rangle = \frac{1}{\sqrt{2}}|+z\rangle + \frac{i}{\sqrt{2}}|-z\rangle, \quad |-y\rangle = \frac{1}{\sqrt{2}}|+z\rangle - \frac{i}{\sqrt{2}}|-z\rangle$$

work.

2.2 Unitary transformations

For a vector $|\psi\rangle + c_+|+z\rangle + c_-|-z\rangle$, we associate a vector $(c_+\ c_-)^T$. If we have the same vector in another bases, say $|\psi\rangle = c'_+|+x\rangle + c'_-|-x\rangle$, then

$$\begin{pmatrix} c'_+ \\ c'_- \end{pmatrix} = \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & -1/\sqrt{2} \end{pmatrix} \begin{pmatrix} c_+ \\ c_- \end{pmatrix}.$$

If we note $|+z\rangle = (\langle +x| + z\rangle)|+x\rangle + (\langle -x| + z\rangle)|-x\rangle$, we can abstractly write

$$\begin{pmatrix} \langle +x|\psi\rangle \\ \langle -x|\psi\rangle \end{pmatrix} = \begin{pmatrix} \langle +x| + z\rangle & \langle +x| - z\rangle \\ \langle -x| + z\rangle & \langle -x| - z\rangle \end{pmatrix} \begin{pmatrix} \langle +z|\psi\rangle \\ \langle -z|\psi\rangle \end{pmatrix}.$$

This matrix is **unitary**, i.e., $U^\dagger U = UU^\dagger = 1$. This is because

$$U = \begin{pmatrix} \langle +x| + z\rangle & \langle +x| - z\rangle \\ \langle -x| + z\rangle & \langle -x| - z\rangle \end{pmatrix}, \quad U^\dagger = \begin{pmatrix} \langle +z| + x\rangle & \langle +z| - x\rangle \\ \langle -z| + x\rangle & \langle -z| - x\rangle \end{pmatrix}.$$

Note that the $U^\dagger$ is then going from the x-basis to the z-basis. This shows that $U^\dagger U = 1$.

3 January 31, 2017

One remark I would like to make is that when we measure the spin $\vec{S}$, its magnitude is

$$|S| = \frac{\hbar}{2}, \qquad \hbar \approx 6.6 \times 10^{-16}\text{eV} \cdot \text{sec} \approx 1.1 \times 10^{-34}\text{J} \cdot \text{s}.$$

Because this is a fundamental constant in nature, this allows us to write time as inverse energy, or distance as inverse momentum. The reason why particle physicists like to see what happens when particles collide with large momentum is because they want to know things in small length scale.

One other thing is, if you have a device that is a like $SG\hat{z}$ plus $SG(-\hat{z})$ so that the result is always the same, then you get $|\psi\rangle$ again. This is because we don't measure the state of the particle. A **measurement** is any physical process that "strongly" depends on the result. When you measure something in a lab, you usually have something like when an electron comes in then some material absorb it and emits lots of photons. This kind of transports the information from the electron to the material. In short, the laws of quantum mechanics applies to everything including measuring devices and there is nothing too special about measuring. It is just that the device has a complex structure and it is hard to follow all the details in the device.

Finally, in the homework you found out that

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

Now this has two parameters θ and ϕ and so it is a 2-dimensional state. A general quantum state is of the form $\alpha|+\hat{z}\rangle + \beta|-\hat{z}\rangle$ and so there are 4 degrees of freedom. In quantum mechanics we normalize our states and so that leaves 3. But we also don't care about phase so that leaves 2. So there are 2 important real degrees of freedom, parameterized by

$$\mathbb{CP}^1 = \{(z_1, z_2) \in \mathbb{C}^2 : (z_1, z_2) \sim \lambda(z_1, z_2)\}.$$

So problem 1.3 can be thought as giving a link $S^2 \cong \mathbb{CP}^1$.

3.1 Linear operators

Given a matrix M, its entries can be read of as $M_{ij} = e_i^T M e_j^T$. So in quantum mechanics, given basis states $|1\rangle, |2\rangle, \ldots, |n\rangle$, we have

$$\langle m|n\rangle = \delta_{mn} = \begin{cases} 1 & m = n \\ 0 & m \neq n, \end{cases} \qquad M_{ij} = \langle i|M|j\rangle.$$

We normalize states $|\psi\rangle$ to compute probabilities. But in general we do not normalize $M|\psi\rangle$.

The states $|+z\rangle$ and $|-z\rangle$ are orthonormal, and $SG\hat{z}$ will output either $\hbar/2$ or $-\hbar/2$. Now define a matrix

$$S_z = \begin{pmatrix} +\hbar/2 & 0 \\ 0 & -\hbar/2 \end{pmatrix}.$$

We observe that $|+z\rangle$ and $|-z\rangle$ are eigenstates of S_z with eigenvalues $+\hbar/2$ and $-\hbar/2$. This is a very general thing we can do. When we have a measurable quantity, we can represent it with a linear operator whose eigenstates have definite measurement outcomes given by the eigenvalues. This doesn't mean anything, because it's just a construction.

But this is a useful notion because we can compute things nicely. Given a quantum state $|\psi\rangle = c_+|+z\rangle + c_-|-z\rangle$, we can compute its expectation value as

$$\langle S_z\rangle = p_+\Big(\frac{\hbar}{2}\Big) + p_-\Big(-\frac{\hbar}{2}\Big) = (|c_+|^2 - |c_-|^2)\frac{\hbar}{2}.$$

We also have

$$\langle\psi|S_z|\psi\rangle = \begin{pmatrix} c_+^* & c_-^* \end{pmatrix}\begin{pmatrix} \hbar/2 & 0 \\ 0 & -\hbar/2 \end{pmatrix}\begin{pmatrix} c_+ \\ c_- \end{pmatrix} = \frac{\hbar}{2}(|c_+|^2 - |c_-|^2).$$

This is going to be true in general, because we made the states into eigenvectors with suitable eigenvalues. But the second definition is more useful, because we don't need to use the eigenstate basis.

3.2 Rotation matrices

Suppose we have the 90° rotation along the y-axis that takes $+z$ to $+x$. For classical vectors this is easy. But we need to know how this acts on 2-dimensional quantum states.

This linear operator should map

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \mapsto \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}, \quad \begin{pmatrix} 0 \\ 1 \end{pmatrix} \mapsto e^{i\varphi}\begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix}, \quad \begin{pmatrix} 1/\sqrt{2} \\ i/\sqrt{2} \end{pmatrix} \mapsto e^{i\varphi'}\begin{pmatrix} 1/\sqrt{2} \\ i\sqrt{2} \end{pmatrix}.$$

This is satisfied by the unitary operator

$$\hat{R}\Big(\frac{\pi}{2}\hat{j}\Big) = \begin{pmatrix} 1/\sqrt{2} & -1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{pmatrix} \qquad \text{in the } z\text{-basis.}$$

This matches our answers up to a phase, but we don't mind.

Now we would like to build a general rotation that acts on the vectors in a nice way. We want to define rotations around the z-axis. $\hat{R}(\phi\hat{k})$ should obey:

- $\hat{R}((\phi_1+\phi_2)\hat{k}) = R(\phi_1\hat{k})R(\phi_2\hat{k}) = R(\phi_2\hat{k})R(\phi_1\hat{k})$
- $\hat{R}(\phi\hat{k}) = 1 + (\cdots)d\phi$.

4 February 2, 2017

We want a family of rotations given by $\hat{R}(\theta, \hat{n})$. It is reasonable to ask that if we do a rotation by θ_1 then do a rotation by θ_2 the result is a rotation by $\theta_1 + \theta_2$. Another thing we would like to require is that rotation by a small angle is almost the identity. This can be written as $\hat{R}(d\phi\hat{k}) = 1 + \hat{M}d\phi + O(d\phi^2)$. We are going to write $\hat{M} = -i/\hbar \hat{J}_z$ for reasons that will become clear later.

We can write

$$\hat{R}(Nd\phi\hat{k}) = \hat{R}(d\phi\hat{k})^N = \Big(1 - \frac{i}{\hbar}\hat{J}_z d\phi + O(d\phi^2)\Big)^N,$$

where $\phi = Nd\phi$. Thus

$$\hat{R}(\phi\hat{k}) = \lim_{N\to\infty}\Big(1 - \frac{i}{\hbar}\hat{J}_z\frac{\phi}{N}\Big)^N = \exp\Big(-\frac{i}{\hbar}\hat{J}_z\phi\Big),$$

where $\exp(M) = 1 + M + M^2/2 + M^3/6 + \cdots$. This may seem intimidating to compute, but there is a nice trick. If M is a diagonal matrix with diagonal entries $m_1, \ldots, m_n$, then

$$\exp(M) = 1 + \begin{pmatrix} m_1 & & 0 \\ & \ddots & \\ 0 & & m_n \end{pmatrix} + \frac{1}{2}\begin{pmatrix} m_1^2 & & 0 \\ & \ddots & \\ 0 & & m_n^2 \end{pmatrix} + \cdots = \begin{pmatrix} e^{m_1} & & 0 \\ & \ddots & \\ 0 & & e^{m_n} \end{pmatrix}.$$

For general matrices, we can diagonalize it and apply this formula. If $M = UDU^{-1}$ then

$$\exp(M) = \exp(UDU^{-1}) = \sum_{n=0}^{\infty}\frac{1}{n!}UD^nU^{-1} = U\exp(D)U^{-1}.$$

Because the rotation matrices must not change the probability and inner products, we need $\hat{R}(\phi\hat{k})$ to be unitary. If we take ϕ to be a very small angle, we have

$$\hat{R} \approx 1 - \frac{i}{\hbar}\hat{J}_z d\phi, \quad \hat{R}^{-1} \approx 1 + \frac{i}{\hbar}\hat{J}_z d\phi, \quad \hat{R}^{+} \approx 1 + \frac{i}{\hbar}\hat{J}_z^{+} d\phi.$$

So unitarity of $\hat{R}$ implies $\hat{J}_z = \hat{J}_z^{+}$. That is, $\hat{J}_z$ is **hermitian**.

We also want $\hat{R}(\phi\hat{k})|+\hat{z}\rangle$ to be equal to $|+\hat{z}\rangle$ possibly up to some phase change. So we we want $\hat{R}(\phi\hat{k})$ and $\hat{J}_z$ to be diagonal matrices. We would also want $\hat{R}(\pi/2\hat{k})$ to send $|+\hat{x}\rangle$ to $|+\hat{y}\rangle$ up to some phase. If you work these out and make some choices, you can see that

$$\hat{J}_z = \begin{pmatrix} \hbar/2 & 0 \\ 0 & -\hbar/2 \end{pmatrix}$$

works.

Recall that

$$\hat{S}_z = \begin{pmatrix} \hbar/2 & 0 \\ 0 & -\hbar/2 \end{pmatrix}, \quad \langle\psi|\hat{S}_z|\psi\rangle = \text{expectation.}$$

This is not a coincidence. There is a very general correspondence

$$\text{observables} \quad \longleftrightarrow \quad \begin{array}{c}\text{hermitian operators whose} \\ \text{eigenvalues are the result,}\end{array}$$

with states of definite measurements corresponding to eigenvectors. These are some of the examples:

$$\begin{array}{ll} \text{rotate through angle } \phi\text{:} & \exp\Big(-\frac{i}{\hbar}\hat{J}_z\phi\Big) \\ \text{evolve a state through time } t\text{:} & \exp\Big(-\frac{i}{\hbar}\hat{H}t\Big) \\ \text{evolve a state through space } x\text{:} & \exp\Big(-\frac{i}{\hbar}\hat{p}x\Big) \end{array}$$

4.1 Projection operators

Take a matrix

$$\begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix}$$

in the z-basis. This matrix can also be written as

$$m_{11}|+z\rangle\langle+z| + m_{12}|+z\rangle\langle-z| + m_{21}|-z\rangle\langle+z| + m_{22}|-z\rangle\langle-z|.$$

A **projection operator** is an operator P such that $P^2 = P$. For example, let $P_+ = |+z\rangle\langle+z|$. Then

$$P_+|\psi\rangle = c_+|+z\rangle = P_+^2|+z\rangle.$$

Likewise we have $P_- = |-z\rangle\langle-z|$ is a projection operator, and we have $P_+ + P_- = 1$.

5 February 7, 2017

This is going to be a midterm on Thursday, February 16. You will be given a formula sheet, which will be posted online soon. The reason we are having an exam early is that I want some feedback before the add-drop deadline.

We had these operators $\hat{J}_x, \hat{J}_y, \hat{J}_z$, which are hermitian and have eigenvalues and eigenvectors corresponding to measurement outcomes and states. We also had these rotations $\hat{R}(\phi\hat{k}) = \exp(-i/\hbar \hat{J}_z \phi)$, which are unitary. These rotations are generated by $\hat{J}$.

5.1 Commutator of rotations

The rotations don't commute in general; rotation by 90° around the x-axis and around the z-axis do not commute. So although we have

$$\hat{R}((\phi_1 + \phi_2)\hat{k}) = \hat{R}(\phi_1\hat{k})\hat{R}(\phi_2\hat{k}),$$

we don't have $\hat{R}(\phi\hat{k})\hat{R}(\theta\hat{j}) \neq \hat{R}(\theta\hat{j})\hat{R}(\phi\hat{k})$. One way to measure the failure of this is to introduce the **commutator**

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}.$$

Let us see what the commutator looks like. Consider the case of rotations in 3-dimensional space. A rotation around the z-axis and the x-axis by a small angle ϕ is given by the matrix

$$R_x = \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad R_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\phi' & -\sin\phi' \\ 0 & \sin\phi' & \cos\phi' \end{pmatrix}.$$

Then the commutator up to second order can be computed as

$$\begin{aligned}[R_z, R_x] &= \begin{pmatrix} 1 - \frac{\phi^2}{2} & -\phi & \phi\phi' \\ \phi & 1 - \frac{\phi^2}{2} - \frac{\phi'^2}{2} & -\phi' \\ 0 & \phi' & 1 - \frac{\phi'^2}{2} \end{pmatrix} - \begin{pmatrix} 1 - \frac{\phi^2}{2} & -\phi & 0 \\ \phi & 1 - \frac{\phi^2}{2} - \frac{\phi'^2}{2} & -\phi' \\ \phi\phi' & \phi' & 1 - \frac{\phi'^2}{2} \end{pmatrix} \\ &= \begin{pmatrix} 0 & 0 & \phi\phi' \\ 0 & 0 & 0 \\ -\phi\phi' & 0 & 0 \end{pmatrix}.\end{aligned}$$

This looks very like

$$R_y(\phi'') - 1 = \begin{pmatrix} -\frac{\phi''^2}{2} & 0 & -\phi'' \\ 0 & 0 & 0 \\ \phi'' & 0 & -\frac{\phi''^2}{2} \end{pmatrix}.$$

So rotating around the x-axis and then rotating around the z-axis is almost the same as rotating around the z-axis and then rotating around the x-axis, but the difference looks like rotation around the y-axis.

We can also see this by looking at the generating matrices. We have $\hat{R}(\phi\hat{k}) \approx 1 - i/\hbar \hat{J}_z \phi$. So

$$\begin{aligned}[\hat{R}_z(\phi), \hat{R}_x(\phi')] &\approx [-i/\hbar \hat{J}_z \phi, -i/\hbar \hat{J}_x \phi'] = (-i/\hbar)^2 \phi\phi' [\hat{J}_z, \hat{J}_x] \\ &\approx -i/\hbar \hat{J}_y (\phi\phi').\end{aligned}$$

So we get

$$[\hat{J}_z, \hat{J}_x] = i\hbar \hat{J}_y,$$

and similarly

$$[\hat{J}_x, \hat{J}_y] = i\hbar \hat{J}_z, \quad [\hat{J}_y, \hat{J}_z] = i\hbar \hat{J}_x.$$

5.2 Non-commuting observables and uncertainty

Let us first look at commuting observables. It is a fact that

$$\vec{J}^2 = \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2$$

commutes with $\hat{J}_x, \hat{J}_y, \hat{J}_z$. Suppose we have a Stern-Gerlach device that can measure $\hat{J}_z$, and suppose we have another device that measures $\vec{J}^2$.

Suppose we measure a particle using a $SG\hat{z}$ device. Take the particles that give $|+z\rangle$, measure its $\hat{J}^2$, and then again measure using $SG\hat{z}$. In this case the first outcome is always $3/4\hbar^2$ and the second outcome is always $|+z\rangle$.

On the other hand, if you replace $\hat{J}^2$ with a $SG\hat{x}$ device, we know that the results will split in the first outcome, and even if we use only the $|+x\rangle$ we again get a split result.

The first experiment is related to the fact that $[\vec{J}^2, \hat{J}_z] = 0$ but $[\hat{J}_x, \hat{J}_z] \neq 0$. That is, commuting observables can be measured without changing each other's values, while non-commuting observables cannot be measured without affecting each other.

Define the **uncertainty** ΔA of a hermitian operator $\hat{A}$ of a state $|\psi\rangle$ to be

$$(\Delta A)^2 = \langle (A - \langle A \rangle)^2 \rangle = \langle \psi | \hat{A}^2 | \psi \rangle - \langle \psi | \hat{A} | \psi \rangle^2.$$

This ΔA measure the uncertainty about measure outcomes. Suppose $\hat{A}$ has eigenvalues $\lambda_1, \ldots, \lambda_n$. Then $\Delta A = 0$ if and only if $P(\lambda_i) = 1$ for some i and $P(\lambda_j) = 0$ for $j \neq i$.

Theorem 5.1 (The uncertainty principle)**.** *Given $\hat{A}, \hat{B}$ observables (hermitian operators) and a state $|\psi\rangle$,*

$$\Delta A \cdot \Delta B \geq \frac{1}{2} \big| \langle \psi | [\hat{\tilde{A}}, \hat{\tilde{B}}] | \psi \rangle \big|,$$

where $\hat{\tilde{A}} = \hat{A} - \langle A \rangle$ and $\hat{\tilde{B}} = \hat{B} - \langle B \rangle$.

Proof. Define two kets (not necessarily normalized)

$$|x\rangle = \hat{\tilde{A}}|\psi\rangle = (\hat{A} - \langle A\rangle)|\psi\rangle,$$
$$|y\rangle = i\hat{\tilde{B}}|\psi\rangle = i(\hat{B} - \langle B\rangle)|\psi\rangle.$$

These states are constructed so that

$$\langle x|x\rangle = \langle\psi|(\hat{A} - \langle A\rangle)^2|\psi\rangle = (\Delta A)^2.$$

Similarly $\langle y|y\rangle = (\Delta B)^2$. By the Cauchy–Schwartz inequality,

$$\langle x|x\rangle\langle y|y\rangle \geq \frac{1}{4}\big|\langle x|y\rangle + \langle y|x\rangle\big|^2.$$

Now

$$\langle x|y\rangle = i\langle\psi|\hat{\tilde{A}}\hat{\tilde{B}}|\psi\rangle, \quad \langle y|x\rangle = -i\langle\psi|\hat{\tilde{B}}\hat{\tilde{A}}|\psi\rangle.$$

So we get the inequality. □

6 February 9, 2017

6.1 Representations of $\mathfrak{su}(2)$ (1)

Last time we say that $[\hat{J}_x, \hat{J}_y] = i\hbar\hat{J}_z$ ad that $\vec{\hat{J}}^2 = \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2$ commute with $\hat{J}_x$, $\hat{J}_y$, and $\hat{J}_z$.

These are what mathematicians call **Lie algberas**. They are collections of objects with addition and the commutator $[x, y]$ satisfying the Jacobi identity

$$[[x, y], z] + [[y, z], x] + [[z, x], y] = 0.$$

The physical interpretation is that these things correspond to some symmetries. In this class we are not going to see the general theory. This specific algebra of $\hat{J}_x, \hat{J}_y, \hat{J}_z$ is $\mathfrak{su}(2)$. We can write rotations as 3×3 matrices and also as 2×2 complex matrices. These two are different **representations** of $\mathfrak{su}(2)$.

For $\hat{\vec{J}}^2 = \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z$, we claim that $[\hat{\vec{J}}^2, \hat{J}_x] = 0$. This is because

$$\begin{aligned}
[\hat{\vec{J}}^2, \hat{J}_x] &= [\hat{J}_x^2, \hat{J}_x] + [\hat{J}_y^2, \hat{J}_x] + [\hat{J}_z^2, \hat{J}_x] \\
&= 0 + \hat{J}_y[\hat{J}_y, \hat{J}_x] + [\hat{J}_y, \hat{J}_x]\hat{J} + \hat{J}_z[\hat{J}_z, \hat{J}_x] + [\hat{J}_z, \hat{J}_x]\hat{J}_z \\
&= -i\hbar\hat{J}_y\hat{J}_z - i\hbar\hat{J}_z\hat{J}_y + i\hbar\hat{J}_z\hat{J}_y + i\hbar\hat{J}_y\hat{J}_z = 0.
\end{aligned}$$

Similarly $[\vec{\hat{J}}^2, \hat{J}_y] = [\vec{\hat{J}}^2, \hat{J}_z] = 0$. Also $\vec{\hat{J}}^2$ is hermitian. Note that all the states of a spin-1/2 particle is an eigenvector with eigenvalue $3/4\hbar^2$.

Here are some examples satisfying the commutation relations. First we take the matrices

$$\hat{J}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{J}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \hat{J}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

or alternatively, $\hat{J}_i = \hbar/2\sigma_i$ where σ_i are the Pauli matrices. Then $\vec{\hat{J}}^2 = \frac{3\hbar^2}{4}$. We can also take

$$\hat{J}_x = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \hat{J}_y = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad \hat{J}_z = \hbar\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

These also satisfies the relations $[\hat{J}_x, \hat{J}_y] = i\hbar\hat{J}_z$ mathematically, but it has $\vec{\hat{J}}^2 = 2\hbar^2$. So different choices of matrices may give different $\vec{\hat{J}}^2$.

There is a systematic way to find all such representations. Because $[\vec{\hat{J}}^2, \hat{J}_z] = 0$, they share the same eigenstates. Suppose I have a state $|\lambda, m\rangle$ such that

$$\vec{\hat{J}}^2|\lambda, m\rangle = \hbar^2\lambda|\lambda, m\rangle, \quad \hat{J}_z|\lambda, m\rangle = \hbar m|\lambda, m\rangle.$$

We have $\langle\lambda, m|\vec{\hat{J}}^2|\lambda, m\rangle = \lambda\hbar^2$ because our states are normalized. On the other hand,

$$\langle\lambda, m|\vec{\hat{J}}^2|\lambda, m\rangle = \langle\lambda, m|\hat{J}_x^2|\lambda, m\rangle + \langle\lambda, m|\hat{J}_y^2|\lambda, m\rangle + \hbar^2 m^2 \geq \hbar^2 m^2.$$

This shows that $\lambda \geq m^2 \geq 0$.

The next step relies on a very clever trick. Introduce

$$\hat{J}_\pm = \hat{J}_x \pm i\hat{J}_y.$$

These are not hermitian, and $\hat{J}_+^\dagger = \hat{J}_-$. Consider the identity

$$[\hat{J}_z, \hat{J}_+] = [\hat{J}_z, \hat{J}_x] + i[\hat{J}_z, \hat{J}_y] = i\hbar\hat{J}_y + \hbar\hat{J}_x = \hbar\hat{J}_+,$$
$$[\hat{J}_z, \hat{J}_-] = [\hat{J}_z, \hat{J}_x] - i[\hat{J}_z, \hat{J}_y] = i\hbar\hat{J}_y - \hbar\hat{J}_x = -\hbar\hat{J}_+.$$

These are almost eigenvalue equations.

Using this, we see

$$\vec{J}^2\hat{J}_+|\lambda, m\rangle = \hat{J}_z\vec{J}^2|\lambda, m\rangle = \lambda\hbar^2\hat{J}_+|\lambda, m\rangle,$$
$$\hat{J}_z\hat{J}_+|\lambda, m\rangle = [\hat{J}_z, \hat{J}_+]|\lambda, m\rangle + \hat{J}_+\hat{J}_z|\lambda, m\rangle = (m+1)\hbar\hat{J}_+|\lambda, m\rangle.$$

To summarize, $\hat{J}_+|\lambda, m\rangle$ is an eigenstate of $\vec{J}^2$ with eigenvalue $\lambda\hbar^2$ and an eigenstate of $\hat{J}_z$ with eigenvalue $(m+1)\hbar$. Likewise $\hat{J}_-|\lambda, m\rangle$ is an eigenstate of $\vec{J}^2$ with eigenvalue $\lambda\hbar^2$ and of $\hat{J}_z$ with eigenvalue $(m-1)\hbar$.

Now we have some kind of a puzzle. It seems that we can start with some λ and m and change m by ± 1 if we wanted to. But it has to always satisfy $\lambda \leq m^2$! This is because $\hat{J}_+|\lambda, m\rangle$ may be zero.

7 February 14, 2017

We had the commutation relation $[\hat{J}_x, \hat{J}_y] = i\hbar\hat{J}_z$ and $[\vec{\hat{J}}^2, \hat{J}_x] = 0$. We define $\hat{J}_\pm = \hat{J}_x \pm i\hat{J}_y$ and showed that

$$[\hat{J}_z, \hat{J}_\pm] = \pm\hbar\hat{J}_\pm,$$

which resembles the eigenvalue equation. For a eigenstate $|\lambda, m\rangle$ with

$$\vec{\hat{J}}^2|\lambda, m\rangle = \lambda\hbar^2|\lambda, m\rangle, \quad \hat{J}_z|\lambda, m\rangle = m\hbar|\lambda, m\rangle,$$

we showed that $\lambda \geq m^2$ and that $\hat{J}_\pm$ is proportional to $|\lambda, m \pm 1\rangle$. This is the reason we introduced $\hat{J}_\pm$: the relation $[\hat{J}_z, \hat{J}_\pm] = \pm\hbar\hat{J}_\pm$ means that $\hat{J}_\pm$ add or subtract $\hbar$ from the $\hat{J}_z$-eigenvalue.

So this means that we can act by $\hat{J}_+$ or $\hat{J}_-$ to increase or decrease m by 1. This means that given $|\lambda, m\rangle$, the procedure has to stop somewhere.

7.1 Representations of $\mathfrak{su}(2)$ (2)

For a fixed λ, label the largest m that makes sense as j. In other words, there is a state $|\lambda, j|$ with $\hat{J}_+|\lambda, j\rangle = 0$. Additional we cam assume that no $|\lambda, j+1|$ exists. We know that $\hat{J}_-\hat{J}_+|\lambda, j\rangle = 0$. Let us expand this out. We get

$$\begin{aligned} 0 &= (\hat{J}_x - i\hat{J}_y)(\hat{J}_x + i\hat{J}_y)|\lambda, j\rangle = (\hat{J}_x^2 + \hat{J}_y^2 + i[\hat{J}_x, \hat{J}_y])|\lambda, j\rangle \\ &= (\vec{\hat{J}}^2 - \hat{J}_z^2 - \hbar\hat{J}_z)|\lambda, j\rangle = \hbar^2(\lambda - j^2 - j)|\lambda, j\rangle. \end{aligned}$$

This implies that $\lambda = j(j+1)$. We check that for a spin-1/2 particle, $\lambda = (1/2)(3/2) = 3/4$. This agrees with what we know.

We now learned the relationship between λ (the eigenvalue of $\vec{\hat{J}}^2$) and the largest eigenvalue of $\hat{J}_z$ in the ladder, which is given by $\lambda = j(j+1)$. We can do this in the other direction. Consider the most negative eigenvalue $\tilde{j}$ so that $J_-|\lambda, \tilde{j}\rangle = 0$. Then we would get $\lambda = \tilde{j}(\tilde{j} - 1)$.

Because

$$\lambda = j(j+1) = \tilde{j}(\tilde{j} - 1),$$

we have either $\tilde{j} = -j$ or $\tilde{j} = j + 1$. But the latter doesn't make sense because $\tilde{j}$ is the minimum. So we get $\tilde{j} = -j$.

Now we derived that $J_-|\lambda, m\rangle = 0$ only if $m = -j$. So if we want $J_-^k|\lambda, j\rangle = 0$ for some large enough k, then we need $-j$ to be j minus an integer. Thus j is an half-integer.

Now because j is nicer than λ, we introduce this new notation

$$\vec{\hat{J}}^2|j, m\rangle = j(j+1)\hbar^2|j, m\rangle, \quad \hat{J}_z|j, m\rangle = m\hbar|j, m\rangle.$$

A **spin-j representation** of angular momentum algebra has a basis $|j, m\rangle$ for $m = -j, -j+1, \ldots, j-1, j$. So a spin-0 representation has basis $|0, 0\rangle$, a spin-1/2 representation has basis $|1/2, 1/2\rangle = |+z\rangle$ and $|1/2, -1/2\rangle = |-z\rangle$.

There are some problems though. Photons are spin-1 particles, but the number of independent states is 2. Gravitons are spin-2 particles but the number of independent polarizations is 2. These are special massless particles, and they always move at speed c. The resolution of this puzzle is gauge invariance. We won't talk about this, but it is something worth being aware of.

For a spin-j representation suppose we want $\hat{J}_x, \hat{J}_y, \hat{J}_z$ as matrices, in basis $|j, m\rangle$. Then

$$\hat{J}_z = \begin{pmatrix} j\hbar & & & \\ & (j-1)\hbar & & \\ & & \ddots & \\ & & & -j\hbar \end{pmatrix}.$$

To compute $\hat{J}_x$ and $\hat{J}_y$, we compute $\langle j, m|\hat{J}_-\hat{J}_+|j, m\rangle$. We can let

$$\hat{J}_+|j, m\rangle = \sqrt{j(j+1) - m(m+1)}\hbar|j, m+1\rangle,$$
$$\hat{J}_-|j, m\rangle = \sqrt{j(j+1) - m(m-1)}\hbar|j, m-1\rangle.$$

Then $\hat{J}_+$ and $\hat{J}_-$ are matrices with entries on the off-diagonal.

7.2 The uncertainty principle

We stated the uncertainty principle as

$$\Delta A \cdot \Delta B \geq \frac{1}{2}|\langle\psi|[\hat{A}, \hat{B}]|\psi\rangle|.$$

For example, take $A = \hat{J}_x$ and $B = \hat{J}_y$. Then we get

$$\Delta J_x \cdot \Delta J_y \geq \frac{1}{2}\hbar|\langle J_z\rangle|.$$

We know that $\Delta J_x = 0$ in the state $|+x\rangle$. So the uncertainty principle implies that $\langle J_z\rangle = 0$ in the state $|+x\rangle$, which is true. In the other direction, we know that $\langle J_z\rangle = \hbar/2$ in the state $|+z\rangle$. So the uncertainty principle tells us that $\Delta J_x \cdot \Delta J_y \geq \hbar^2/4$. This tells us that the outcomes of the x and y measurements are necessarily certain.

8 February 21, 2017

If you want to compute the exponential of a matrix, you should first diagonalize it.

In Chapter 4, we are going to learn time evolution and the Hamiltonian. In Chapter 6, we are going to deal with continuous systems, position, momentum. Then we would need to solve differential equation. In Chapter 7, we are going to look at the example of a quantum harmonic oscillator.

8.1 Classical story to the Hamiltonian

In classical mechanics we study the "phase space" given by positions x_i and momenta p_i. The key function is the Hamiltonian H, which is a function of the x_is and p_is. We interpret this as the total energy of the system.

Example 8.1. For a non-relativistic particle with mass m in a potential V, we have

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

The equations of motion in Hamiltonian mechanics is given by

$$\dot{x}_i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial x_i}.$$

So in the case of a non-relativistic particle, we recover

$$\frac{\partial H}{\partial p} = \frac{p}{m} = \dot{x}, \quad \dot{p} = -\frac{\partial H}{\partial x} = -\frac{\partial V}{\partial x} = F.$$

This is precisely Newton's laws.

Given a function $f(x_i, p_i, t)$, we have

$$\begin{aligned}\frac{df}{dt} &= \frac{\partial f}{\partial t} + \sum_i \Big[\frac{\partial f}{\partial x_i}\frac{dx_i}{dt} + \frac{\partial f}{\partial p_i}\frac{dp_i}{dt}\Big] = \frac{\partial f}{\partial t} + \sum_i \Big[\frac{\partial f}{\partial x_i}\frac{\partial H}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial H}{\partial x_i}\Big] \\ &= \frac{\partial f}{\partial t} + \{f, H\},\end{aligned}$$

where $\{f, g\}$ is the Poisson bracket. This Poisson bracket is some complicated object that is not intuitive at all, in classical mechanics. In quantum mechanics, these become simply commutators of Hermitian operators.

8.2 Time evolution

The problem we want to solve is, given a quantum state $|\psi(0)\rangle$, what is $|\psi(t)\rangle$? We expect it to look like $|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle$. We like to keep our state normalized, so we want $\hat{U}(t)$ to be unitary. We also expect that if dt is small, then $\hat{U}(dt) = 1 + O(dt)$. It is reasonable to also assume

$$\hat{U}(t_1 + t_2) = \hat{U}(t_1)\hat{U}(t_2) = \hat{U}(t_2)\hat{U}(t_1).$$

Mathematically this identical to what we did with rotations. Then

$$\hat{U}(t) = \lim_{N\to\infty}\Big[1 - \frac{i}{\hbar}\hat{H}\Big(\frac{t}{N}\Big)\Big]^N = \exp\Big(-\frac{i}{\hbar}t\hat{H}\Big).$$

Since $\hat{U}$ is unitary, $\hat{H}$ is hermitian. This operator $\hat{H}$ is called the **Hamiltonian** an it is the generator of time evolution. We will later see that this actually corresponds to the classical notion of Hamiltonian. We saw that the eigenvalues of $\hat{J}_z$ corresponded to angular momentum, and so the eigenvalues of $\hat{H}$ will be energies.

We can take the derivative and then write

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

This is called the **time-dependent Schrödinger equation**. Note that we could have written the rotation as

$$i\hbar\frac{d}{d\theta}|\psi(\theta)\rangle = \hat{J}_z|\psi(\theta)\rangle.$$

So there is not too much mathematical content in writing in the differential equation form.

If $\hat{H}|\psi(t)\rangle = E|\psi(t)\rangle$, then we call $|\psi(t)\rangle$ and energy eigenstate, and write it as $|E\rangle$. In this case, we get $\hat{H}|E\rangle = E|E\rangle$. This is called the **time-independent Schrödinger equation**. If $|\psi(0)\rangle = |E\rangle$, then

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar}|E\rangle = \Big(1 - \frac{i\hat{H}t}{\hbar} + \frac{1}{2}\Big(\frac{i\hat{H}t}{\hbar}\Big)^2 - \cdots\Big)|E\rangle = e^{-iEt/\hbar}|E\rangle.$$

So time-evolution of energy eigenstates simply oscillates by a phase and oscillates at frequency proportional to E. We sometimes write $\omega = E/\hbar$. For this reason, energy eigenstates are sometimes called **stationary states**. Measurements on energy eigenstates have time-independent probabilities.

Here is a general procedure to solve the time-dependent Schrödinger equation. First, write

$$|\psi(0)\rangle = \sum_i c_i|E_i\rangle.$$

You can do this by finding all the eigenstates $|E_i\rangle$ and then letting $c_i = \langle E_i|\psi(0)\rangle$. From this finding time evolution is straightforward. We have

$$|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle = \hat{U}(t)\sum_i c_i|E_i\rangle = \sum_i c_i e^{-iE_it/\hbar}|E_i\rangle.$$

For a general state, probabilities of measurement outcomes are time-dependent. This is important, because otherwise the world would be a boring place.

Given a hermitian operator A, we have

$$\begin{aligned}\frac{d}{dt}\langle A\rangle(t) &= \frac{d}{dt}\langle\psi(t)|\hat{A}(t)|\psi(t)\rangle \\ &= \Big(\frac{d}{dt}\langle\psi(t)|\Big)\hat{A}(t)|\psi(t)\rangle + \langle\psi(t)|\Big(\frac{\partial}{\partial t}\hat{A}(t)\Big)|\psi(t)\rangle + \langle\psi(t)|\hat{A}(t)\Big(\frac{d}{dt}|\psi(t)\rangle\Big) \\ &= \langle\psi(t)|\frac{\partial}{\partial t}\hat{A}|\psi(t)\rangle + \frac{i}{\hbar}\langle\psi(t)|[\hat{H},\hat{A}(t)]|\psi(t)\rangle.\end{aligned}$$

So

$$\frac{d\langle A\rangle}{dt} = \Big\langle\frac{\partial A}{\partial t}\Big\rangle + \frac{i}{\hbar}\langle[H,A]\rangle.$$

This is the quantum analogue of the formula $df/dt = \partial f/\partial t - \{H, f\}$.

9 February 23, 2017

We saw that

$$\frac{d}{dt}\langle \hat{A} \rangle = \left\langle \frac{\partial \hat{A}}{dt} \right\rangle + \frac{i}{\hbar}\langle [\hat{H}, \hat{A}] \rangle.$$

If $\hat{A}$ has no time dependence, then $d\langle A \rangle/dt = 0$ for all states if and only if $[\hat{H}, \hat{A}] = 0$. So conserved quantities correspond to operators that commute with the Hamiltonian. In particular, $[\hat{H}, \hat{H}] = 0$ so H is a conserved quantity.

Recall that the uncertainty principle says that

$$(\Delta A)(\Delta H) \geq \frac{1}{2}|\langle \psi | [\hat{A}, \hat{H}] | \psi \rangle| = \frac{\hbar}{2}\left|\frac{d\langle \hat{A} \rangle}{dt}\right|,$$

assuming that $\hat{A}$ has not time dependence. We can define from this equation a characteristic time scale associated with $\hat{A}$:

$$\Delta t_A = \frac{\Delta A}{|d\langle \hat{A} \rangle/dt|}.$$

We can then rewrite our equation as

$$(\Delta E)\Delta t_A \geq \frac{\hbar}{2}.$$

This is sometimes called the **energy-time uncertainty relation**. So the energy of a rapidly changing state cannot be measured precisely. You can also interpret this as "if you want to energy precisely then you need to do it over a long time."

9.1 Spin particle in a magnetic field

Take a spin particle. Then the Hamiltonian in a magnetic field is given by $\hat{H} = -\hat{\vec{\mu}} \cdot \vec{B}$, where the magnetic moment is given by

$$\vec{\mu} = \frac{gq}{2mc}\vec{S}.$$

Let us choose $\vec{B} = B_z \hat{z}$. Then we get

$$\hat{H} = \omega_0 \hat{S}_z$$

for some constant ω_0.

Suppose we have a spin-1/2 particle. The eigenstates of $\hat{H}$ are $|+z\rangle$ and $|-z\rangle$ with eigenvalues $\hbar\omega_0/2$ and $-\hbar\omega_0/2$. Then we have

$$\hat{U}(t) = e^{-\hat{H}t/\hbar} = e^{-i\omega_0 \hat{J}_z t/\hbar} = \hat{R}(\omega_0 t \hat{k}).$$

So, for instance, if $|\psi(0)\rangle = |+x\rangle$ we get

$$|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle = |+\cos(\omega_0 t)x + \sin(\omega_0 t)y\rangle$$

up to a phase.

Now let us take a magnetic field

$$\vec{B} = B_0\hat{k} + B_1\cos(\omega t)\hat{i}.$$

Then our Hamiltonian is $\hat{H} = \omega_0\hat{S}_z + \omega_1\cos(\omega t)\hat{S}_x$. The equation we have to solve is

$$\frac{\hbar}{2}\begin{pmatrix}\omega_0 & \omega_1\cos\omega t\\ \omega_1\cos\omega t & -\omega_0\end{pmatrix}\begin{pmatrix}a(t)\\ b(t)\end{pmatrix} = i\hbar\begin{pmatrix}da/dt\\ db/dt\end{pmatrix}.$$

We solve in the special case when $\omega_1 \ll \omega_0$. The strategy we are going to exploit is to write

$$\begin{pmatrix}a(t)\\ b(t)\end{pmatrix} = \begin{pmatrix}c(t)e^{-i\omega_0 t/2}\\ d(t)e^{i\omega_0 t/2}\end{pmatrix}.$$

If $\omega_1 = 0$ then $c(t)$ and $d(t)$ are constants. If you just plug in the equation, we get

$$i\begin{pmatrix}dc/dt\\ dd/dd\end{pmatrix} = \frac{\omega_1}{2}\cos\omega t\begin{pmatrix}d(t)e^{i\omega_0 t}\\ c(t)e^{-i\omega_0 t}\end{pmatrix} = \frac{\omega_1}{4}\begin{pmatrix}(e^{i(\omega_0-\omega)t} + e^{i(\omega_0+\omega)t})d(t)\\ (e^{-i(\omega_0-\omega)t} + e^{-i(\omega_0+\omega)t})c(t)\end{pmatrix}.$$

If $\omega_0 = \omega$, then $e^{i(\omega_0+\omega)t}$ average to zero. So then we get the smeared equation

$$i\begin{pmatrix}dc/dt\\ dd/dt\end{pmatrix} = \frac{\omega_1}{4}\begin{pmatrix}d\\ c\end{pmatrix}.$$

This gives the approximate solution that are linear combinations of $e^{\pm i\omega_1 t/4}$.

10 February 28, 2017

We are now going to look at continuous space. This is Chapter 6 of Townsend.

10.1 Position

Suppose there is a particle with discrete position so that particles can only be at positions $x_1, \dots, x_n$. Then the quantum state can be written as

$$|\psi\rangle = \sum_{i=1}^{n} c_i |x_i\rangle.$$

This is very much like what we have been doing so far. We would have $\langle x_i | x_j \rangle = \delta_{ij}$. For instance, you might have some laboratory experiment where there are finitely many potential wells. But more commonly we are used to continuous space.

We generalize this to a continuous quantity. We have position x, which is a continuous quantity. Our state is going to be parametrized by a continuous function $\psi(x)$, often called the **wave function** of the state.

In this case, the probability of the particle being at exactly position 0 is going to be zero. But we have this probability density

$$\psi(x) = \langle x | \psi \rangle.$$

Then the probability of the particle being found at $x_0 \le x \le x_1$ is

$$\int_{x_0}^{x_1} dx |\psi(x)|^2 = \int_{x_0}^{x_1} dx |\langle x|\psi\rangle|^2.$$

We also note that we can also write

$$|\psi\rangle = \int_{-\infty}^{\infty} (\langle x|\psi\rangle)|x\rangle = \int_{-\infty}^{\infty} dx \psi(x)|x\rangle.$$

We note that we are only looking at position now, and we are going to ignore spin. You can look at particles that have both spin and position, but we are going to ignore these to make things simpler.

Analogously to the discrete case, we are going to define the inner product as

$$\langle \chi, \psi \rangle = \int dx \chi^*(x)\psi(x).$$

A normalized state satisfies

$$\langle \psi | \psi \rangle = \int dx \psi^*(x)\psi(x) = \int dx |\psi(x)|^2 = 1.$$

We want $|\psi\rangle$ to have no units, because they are normalized. This implies that $\psi(x)$ has units of length$^{-1/2}$ and so $|x\rangle$ also has units of length$^{-1/2}$. The

position eigenstate $|x\rangle$ is not really a state, and in particular, $\langle x|x\rangle \neq 1$. Our position eigenstates of the inner product

$$\langle x|x'\rangle = \delta(x - x'),$$

where δ is the **Dirac delta**. This is the closest we can get to orthonormality.

10.2 Position and momentum operators

Given a wave function $\psi(x)$, we can translate it to get a new wave function $\psi'(x) = \psi(x - a)$. You can see that this is a linear operation. So we have an operator $\hat{T}(a)$ such that

$$\hat{T}(a)|x\rangle = |x + a\rangle,$$

and make $\langle x|\hat{T}(a)|\psi\rangle = \langle x - a|\psi\rangle$.

This is analogous to the rotation $\hat{R}(\theta\hat{k})$. We are going to have something like

$$\hat{T}(da) \approx 1 - \frac{i}{\hbar}\hat{p}_x da,$$

where $\hat{p}_x$ is the hermitian generator of translations. It has units of momentum, and we call it the **momentum operator**. We can also define the **position operator**

$$\hat{x}|x\rangle = x|x\rangle,$$

so that

$$\hat{x}|\psi\rangle = \int dx\, \psi(x)\hat{x}|x\rangle = \int dx\, x\psi(x)|x\rangle.$$

Let us compute the commutator of the position and momentum operators. We have

$$\hat{x}\hat{T}(a)|\psi\rangle = \hat{x}\int_{dx} dx\, \psi(x - a)|x\rangle = \int dx\, x\psi(x - a)|x\rangle,$$
$$\hat{T}(a)\hat{x}|\psi\rangle = \hat{T}(a)\int dx\, x\psi(x)|x\rangle = \int dx\, (x - a)\psi(x - a)|x\rangle.$$

So the operations don't commute and we get

$$(\hat{x}\hat{T}(a) - \hat{T}(a)\hat{x})|\psi\rangle = a\int dx\, \psi(x - a)|x\rangle \approx a|\psi\rangle + a^2\int dx\, \psi'(x)|x\rangle + \cdots.$$

Using the fact that $\hat{p}_x$ is the generator, we get

$$[\hat{x}, \hat{p}_x] = i\hbar.$$

The uncertainty principle implies that

$$(\Delta x)(\Delta p_x) \geq \frac{\hbar}{2},$$

which is called **Heisenberg's uncertainty principle**.

Still we haven't talked about what the momentum operator actually does. This can be computed as

$$\hat{T}(\Delta x)|\psi\rangle = \Big(1 - \frac{i}{\hbar}\hat{p}_x \Delta x\Big)|\psi\rangle = \int dx\, \psi(x - \Delta x)|x\rangle \approx |\psi\rangle - \Delta x \int dx \psi'(x)|x\rangle.$$

So we get

$$\hat{p}_x|\psi\rangle = -i\hbar \int dx \frac{d\psi(x)}{dx}|x\rangle.$$

That is, momentum operators act by taking derivatives.

Let us find eigenstates of momentum. We have $-i\hbar(d\psi/dx) = p\psi(x)$, and so $\psi(x) = e^{ipx/\hbar}$. These are called **plane waves**. These are not normalizable just like the position eigenstates $|x\rangle$. However we still have

$$\langle p|p'\rangle = \delta(p - p'), \quad \langle x|p\rangle = \psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}.$$

For a nontrivial particle, the Hamiltonian is given by

$$\hat{H} = \frac{1}{2m}\hat{p}_x^2 + V(\hat{x}).$$

Then $|\psi(t)\rangle$ obeys the Schrödinger equation. Since this does not have explicit time dependence,

$$\frac{d}{dt}\langle x\rangle = \frac{i}{\hbar}\langle\psi|[\hat{H}, \hat{x}]|\psi\rangle = \frac{1}{m}\langle\hat{p}_x\rangle.$$

11 March 2, 2017

We defined the momentum and position operators, each with eigenstates $|p\rangle$ and $|x\rangle$. The relation between them are

$$\langle x|x'\rangle = \delta(x-x'), \quad \langle p|p'\rangle = \delta(p-p'), \quad \langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}.$$

11.1 Base change between position and momentum

We know that $|x\rangle$ states are a basis, and any state can be written as

$$|\psi\rangle = \int dx\, \psi(x)|x\rangle.$$

The states $|p\rangle$ also is a basis, and thus we should be able to always write

$$|\psi\rangle = \int dp\, \tilde{\psi}(p)|p\rangle.$$

To change basis, we have

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

The inverse transform will be given by

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

That is, basis change is given by a **Fourier transform**.

Note that when we look at $|x\rangle$ in the momentum basis, the wave function is given by

$$\tilde{\psi}_x(p) = \frac{1}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar}.$$

So $\hat{x}|p\rangle$ is given by the wave function

$$x\tilde{\psi}_x(p) = i\hbar\frac{\partial}{\partial p}\tilde{\psi}_x(p).$$

That is, $\hat{x}$ looks like $i\hbar(\partial/\partial p)$ in the $|p\rangle$-basis.

11.2 Gaussian wave packet

There is a **Gaussian wave packet** given by the formula

$$\psi(x) = \frac{1}{\pi^{1/4}a^{1/2}} e^{-x^2/2a^2},$$

for some real constant a. This satisfies $\int dx|\psi(x)|^2 = 1$. Given this function, we can compute $\langle x\rangle = 0$ and

$$\langle x^2\rangle = \int dx\, x^2|\psi(x)|^2 = \frac{1}{2}a^2.$$

So $\Delta x = a/\sqrt{2}$. If you look at the same state in momentum space,

$$\begin{aligned}\tilde{\psi}(p) &= \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar} \frac{1}{a^{1/2}\pi^{1/4}} e^{-x^2/2a^2} \\ &= \frac{1}{(2\hbar a)^{1/2}\pi^{3/4}} \int_{-\infty}^{\infty} dx\, e^{-(x-x_0)^2/2a^2} e^{-p^2a^2/2\hbar^2} = \frac{a^{1/2}}{\hbar^{1/2}\pi^{1/4}} e^{-p^2a^2/2\hbar^2}.\end{aligned}$$

This is still a Gaussian form! The width is given by $\hbar/a$. Then we can compute $\langle p_x\rangle = 0$ and $\langle p_x^2\rangle = \hbar^2/2a^2$ and $\Delta p = \hbar/(\sqrt{2}a)$. We can then calculate

$$\Delta x \Delta p = \frac{a}{\sqrt{2}} \frac{\hbar}{\sqrt{2}a} = \frac{\hbar}{2}.$$

So it satisfies the equality for the Heisenberg uncertainty principle. Gaussian wave packets are minimum-uncertainty states, i.e., has the smallest possible value of $\Delta x \Delta p$.

If $\psi(x)$ is a minimum-uncertainty state at $t = 0$, is it still at time $t > 0$? The answer will necessarily depend on the Hamiltonian. Let us consider the case of a free particle, $\hat{H} = \hat{p}_x^2/2m$. Notice that $[\hat{H}, \hat{p}_x] = 0$ and so energy and momentum eigenstates are the same. Then $|p\rangle$ has energy $E_p = p^2/2m$.

Now we can compute the time evolution of a free particle. We want to find $\psi(x,t)$. We have

$$\tilde{\psi}(p,0) = \frac{a^{1/2}}{\hbar^{1/2}\pi^{1/4}} e^{-p^2a^2/2\hbar^2}.$$

So we get

$$\tilde{\psi}(p,t) = \frac{a^{1/2}}{\hbar^{1/2}\pi^{1/4}} e^{-ip^2t/2m\hbar} e^{-p^2a^2/2\hbar^2}.$$

Taking the Fourier transform gives

$$\begin{aligned}\psi(x,t) &= \int dp\, \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar} e^{-ip^2t/2m\hbar} \frac{a^{1/2}}{\hbar^{1/2}\pi^{1/4}} e^{-p^2a^2/2\hbar^2} \\ &\sim \exp\Big(-\frac{x^2}{2a^2(1 - i\hbar t/ma^2)}\Big),\end{aligned}$$

and this has uncertainty

$$\Delta x = \frac{a}{\sqrt{2}}\Big(1 + \frac{\hbar^2t^2}{m^2a^4}\Big)^{1/2}.$$

12 March 7, 2017

For a free particle, the Hamiltonian is given by $\hat{H} = \hat{p}_x^2/2m$. This has kinetic energy but no potential energy. The energy eigenstates are $|p\rangle$ and $\hat{H}|p\rangle = (p^2/2m)|p\rangle$.

12.1 Particle in potential

For a particle in a potential, the Hamiltonian is given by

$$\hat{H} = \frac{1}{2m}\hat{p}_x^2 + V(\hat{x})$$

for a potential function V.

Let us solve an actual problem. Consider the potential well

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

for some $V_0 > 0$ a real number. Then $V(\hat{x})$ as an operator is

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

Clearly position eigenstates are always eigenstates of potential energy and momentum eigenstates are always eigenstates of kinetic energy.

Given $|\psi(0)\rangle$ we want to know $|\psi(t)\rangle$. In the position basis, the time-dependent Schrödinger equation becomes

$$\Big[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\Big]\psi(x,t) = i\hbar\frac{\partial}{\partial t}\psi(x,t).$$

To actually solve it, we look at the time-independent Schrödinger equation. We are then trying to solve

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

There are two regions:

$$\begin{cases} \frac{d^2}{dx^2}\psi(x) = -\frac{2mE}{\hbar^2}\psi(x), & |x| < a/2, \\ \frac{d^2}{dx^2}\psi(x) = -\frac{2m(E-V_0)}{\hbar^2}\psi(x), & |x| > a/2. \end{cases}$$

The solutions to these equations depend on the signs of the constants.

Consider first the range $0 < E < V_0$. Then in $|x| < a/2$ the solution is going to be oscillating and in $|x| > a/2$ it is going to be exponential.[1] Then

$$\psi(x) = \begin{cases} A\sin kx + B\cos kx, & |x| < a/2, \\ Ce^{qx} + De^{-qx}, & x > q/2, \\ Fe^{qx} + Ge^{-qx}, & x < -q/2, \end{cases} \qquad k = \sqrt{\frac{2mE}{\hbar^2}}, \quad q = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}.$$

Here, the wavefunction must not blow up as $|x| \to \infty$. This shows that $C = G = 0$.

There are also some boundary conditions at $x = \pm a/2$. We want to require $\psi(x)$ to be continuous. Because we need to be able to take the derivative. Then

$$\begin{aligned} A\sin(ka/2) + B\cos(ka/2) &= De^{-qa/2}, \\ -A\sin(ka/2) + B\cos(ka/2) &= Fe^{-qa/2}. \end{aligned}$$

In this case, we can also impose that $d\psi/dx$ is continuous, because $d^2\psi/dx^2$ is locally bounded by the equation we are trying to solve. So we get two more equations. There is also a normalization constraint. That is, we won't find a solution for all E and get a discrete spectrum.

You can solve the equation, but we are going to simplify it by sending $V_0 \to \infty$. Then $q \to \infty$ and so $\psi(x) \to 0$ for all $|x| > a/2$. The equations become

$$\begin{aligned} A\sin(ka/2) + B\cos(ka/2) &= 0, \\ -A\sin(ka/2) + B\cos(ka/2) &= 0. \end{aligned}$$

Because I don't want $A = B = 0$, either $\sin(ka/2) = 0$ or $\cos(ka/2) = 0$. That means $k = 0, \pi/a, 2\pi/a, 3\pi/a, \ldots$. Then

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{2ma^2}.$$

The solutions are given by

$$\begin{aligned} k_1 &= \frac{\pi}{a}, & \psi_1(x) &= \sqrt{\frac{2}{a}}\cos\Big(\frac{\pi x}{a}\Big), \\ k_2 &= \frac{2\pi}{a}, & \psi_2(x) &= \sqrt{\frac{2}{a}}\sin\Big(\frac{2\pi x}{a}\Big), \ldots. \end{aligned}$$

For unbound particles, the eigenstates are going to be joined oscillating functions. They are not normalizable and have a continuous spectrum. But you can add (integrate) them together to get normalizable states, like the free particle in Gaussian state.

[1] A general rule is that if $E > V(x)$ the wave function will be locally oscillating and if $E < V(x)$ the wave function will be locally exponential. In classical mechanics, $E < V(x)$ doesn't make sense, and this is usually reflected in quantum mechanics by exponential decay.

13 March 9, 2017

For the time-independent Schrödinger equation, $E < V$ gives an oscillating solution and $E > V$ gives an exponentially growing or decreasing solution. The bound solutions are going to have discrete energy, and the oscillating solutions are going to be a continuum.

13.1 Physical interpretation of oscillating solutions

Although the oscillating states are not normalizable, there is some physics we can extract from these solutions. Consider a potential given by

$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & x \geq 0. \end{cases}$$

Let us look at the solutions for $0 < E < V_0$, i.e., solutions that exponentially decay on the right and oscillates on the left. They are going to look like

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{ikx} & x < 0, \\ Ce^{-qx} & x > 0, \end{cases} \quad k = \sqrt{\frac{2mE}{\hbar^2}}, \quad q = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}.$$

The conditions ψ begin continuous and differentiable at $x = 0$ give $A+B = C$ and $ikA - ikB = -qC$. Then $C = (2k/(k + iq))A = (2k/(k - iq))B$. From this we see that $|A| = |B|$.

You can solve the similar problem for $E > V_0$ and the answer is going to have a slightly different form:

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x < 0, \\ Ce^{ik'x} + De^{-ik'x} & x > 0, \end{cases} \quad k = \sqrt{\frac{2mE}{\hbar^2}}, \quad k' = \sqrt{\frac{2m(E - V_0)}{\hbar^2}}.$$

Let us just look at the solutions with $D = 0$. Then continuity of ψ and ψ' again gives $C = (2k/(k + k'))A = (2k/(k - k'))B$. Here we observe $|A| \neq |B|$.

The time evolution of the energy eigenstates are given by

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

Then e^{ikx} becomes $e^{i(kx-\omega t)}$ where $\omega = E/\hbar$. This is a right moving wave, and likewise e^{-ikx} is a left moving wave.

In the case of $E < V_0$, the interpretation is that there is stream of particles going in the left direction and another stream of particles with same intensity going in the right direction, on the $x < 0$ region. From the classical perspective, you can think of these particle bouncing back from the potential wall.

Now what is happening for $E > V_0$? We can think of A as particles that are moving to the right. Then B are the particles that bounces back, and C are the particles that get through.

There is a conservation law related to the conservation of the particles in the interpretation. We define the **probability current** as

$$j_x = \frac{\hbar}{2\pi i}\Big(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}\Big).$$

If we write the probability density $\rho = \psi^* \psi$, then there is the conservation law

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} j_x = 0.$$

In the case of $\psi = Ae^{i(kx-\omega t)} + Be^{i(-kx-\omega t)}$, the current is given by

$$j_x = \frac{\hbar k}{m}\big(|A|^2 - |B|^2\big).$$

This $\hbar k/m$ can be thought of as velocity and $|A|^2$ can be thought of as right-moving flux and $|B|^2$ as left-moving flux.

This let us define **reflection/transmission coefficients**. In the case of $E < V_0$, we have

$$j_x = \begin{cases} \frac{\hbar k}{m}(|A|^2 - |B|^2) = 0 & x < 0, \\ 0 & x > 0. \end{cases}$$

The reflection coefficient is given by

$$R = \frac{|B|^2}{|A|^2} = 1.$$

For the $E > V_0$ case, the currents are

$$j_{\text{trans}} = \frac{\hbar k'}{m}|C|^2, \quad j_{\text{inc}} = \frac{\hbar k}{m}|A|^2, \quad j_{\text{ref}} = \frac{\hbar k}{m}|B|^2.$$

Then the reflection and transmission coefficients are

$$R = \frac{j_{\text{ref}}}{j_{\text{inc}}} = \Big(\frac{k-k'}{k+k'}\Big)^2, \quad T = \frac{j_{\text{trans}}}{j_{\text{inc}}} = \frac{4kk'}{(k+k')^2}, \quad R + T = 1.$$

Consider potential that looks like

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

If we send things from the left, there is something coming out from the right, unlike the classical case. This is called **tunneling**. I will not compute this, but the result is

$$T = \frac{j_{\text{trans}}}{j_{\text{inc}}} = \frac{1}{1 + \frac{k^2+q^2}{2kq}\sinh^2(qa)} \approx \Big(\frac{4kq}{k^2+q^2}\Big)e^{-2qa}.$$

The price you pay for tunneling is the exponential factor e^{-2qa}.

13.2 Ladder operators

The Hamiltonian for the harmonic oscillator is given by

$$\hat{H} = \frac{\hat{p}_x^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2.$$

We have a useful fact that $[\hat{x}, \hat{p}_x] = i\hbar$. In the case of $\hat{J}$, we used the trick of defining $\hat{J}_\pm = \hat{J}_x \pm i\hat{J}_y$ and showed that $[\hat{J}_z, \hat{J}_\pm] = \pm\hbar\hat{J}_\pm$.

We are going to use a similar trick and find **ladder operators** $\hat{a}$ and $\hat{a}^\dagger$ such that

$$[\hat{H}, \hat{a}] = -\hbar\omega\hat{a}, \quad [\hat{H}, \hat{a}^\dagger] = \hbar\omega\hat{a}^\dagger.$$

Note that $[\hat{x}^2, \hat{p}_x]$ is proportional to $\hat{x}$ and $[\hat{p}_x^2, \hat{x}]$ is proportional to $\hat{p}_x$. So we can define

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\Big(\hat{x} + \frac{i}{m\omega}\hat{p}_x\Big).$$

Then $[\hat{H}, \hat{a}] = -\hbar\omega\hat{a}$ and $[\hat{a}, \hat{a}^\dagger] = 1$ and $\hat{H} = \hat{a}^\dagger\hat{a} + \frac{1}{2}\hbar\omega$.

14 March 21, 2017

There is a midterm on March 28, which will cover mostly chapters 3, 4, 6, and a little bit of 1, 2, 7.

14.1 The harmonic oscillator

We are now going to look at the **harmonic oscillator** given by the Hamiltonian

$$\hat{H} = \frac{1}{2m}\hat{p}_x^2 + \frac{1}{2}m\omega^2\hat{x}^2.$$

You would expect the wavefunction to be large in the middle and decay. We are going to just guess the ground state as a Gaussian wave function, and it turns out to work. This is a good guess because $\hat{H}$ is roughly symmetric in $\hat{p}_x$ and $\hat{x}$, and the Fourier transform of the Gaussian has exactly the same form.

So let us see what happens when we plug it in. We are looking for energy eigenstates, $\psi(x)$ such that

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

If we guess $\psi(x) = Ce^{-Ax^2}$, we get $A = m\omega/2\hbar$ and $E = \hbar\omega/2$. So we have found an energy eigenstate. I claim, but am not going to prove, that this is the lowest energy eigenstate. That is, it really is the ground state. Let us give this state a name

$$|0\rangle = \int_{-\infty}^{\infty} dx \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/2\hbar}|x\rangle.$$

Last class we talked about the latter operators $\hat{a}, \hat{a}^\dagger$ such that

$$[\hat{H}, \hat{a}^\dagger] = \hbar\omega\hat{a}^\dagger, \quad [\hat{H}, \hat{a}] = -\hbar\omega\hat{a}.$$

These relations come from $[\hat{H}, \hat{x}] = -i\hbar/m\hat{p}_x$ and $[\hat{H}, \hat{p}_x] = i\hbar m\omega^2\hat{x}$. We can set

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\Big(\hat{x} + \frac{i}{m\omega}\hat{p}_x\Big), \quad \hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\Big(\hat{x} - \frac{i}{m\omega}\hat{p}_x\Big).$$

We have normalized the operators so that they satisfy $[\hat{a}, \hat{a}^\dagger] = 1$.

So the claim is, given an energy eigenstate $|E\rangle$ where $\hat{H}|E\rangle = E|E\rangle$, we can find a new state $\hat{a}^\dagger|E\rangle$ such that

$$\hat{H}\hat{a}^\dagger|E\rangle = (E + \hbar\omega)\hat{a}^\dagger|E\rangle.$$

Similarly, we can lower the energy by acting with $\hat{a}$:

$$\hat{H}\hat{a}|E\rangle = (E - \hbar\omega)\hat{a}|E\rangle.$$

We already have an eigenstates $|0\rangle$. We can ask what $\hat{a}|0\rangle$ and $\hat{a}^\dagger|0\rangle$ are. Our guess is that $\hat{a}|0\rangle = 0$ since $E = -\hbar\omega/2$ is awkward for $V(x) \geq 0$. Indeed, we compute

$$\langle x|\hat{a}|0\rangle = \sqrt{\frac{m\omega}{2\hbar}}\Big(xe^{-m\omega x^2/2\hbar} + \frac{i}{m\omega}(-i\hbar)\Big(-\frac{m\omega x}{\hbar}\Big)e^{-m\omega x^2/2\hbar}\Big) = 0.$$

On the other hand, if we act $\hat{a}^\dagger$, we get

$$\langle x|\hat{a}^\dagger|0\rangle = \sqrt{\frac{2m\omega}{\hbar}}x\psi(x).$$

This state should have $E = 3\hbar\omega/2$. We might as well call

$$|1\rangle = \frac{\hat{a}^\dagger|0\rangle}{(\langle 0|\hat{a}\hat{a}^\dagger|0\rangle)^{1/2}}.$$

Then you can define $|2\rangle$ to be the normalization of $\hat{a}^\dagger|1\rangle$, and if you work out the algebra, you should get $\psi_2(x) = (c_1x^2 + c_2)e^{-m\omega x^2/2\hbar}$. In general, if you define $|n\rangle$ to be the normalization of $\hat{a}^\dagger|n-1\rangle$, its wavefunction will be given by

$$\psi_n(x) = \langle x|n\rangle = P_n(x)e^{-m\omega x^2/2\hbar}$$

for some degree n polynomial $P_n(x)$.

It is useful to define the **number operator**

$$\hat{N} = \hat{a}^\dagger\hat{a}.$$

Note that $\hat{N}|0\rangle = 0$. It turns out that $\hat{N}|n\rangle = n|n\rangle$ for all n. This follows from the useful relations

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

You can also check that $\hat{H} = \hbar\omega(\hat{N} + 1/2)$.

15 March 23, 2017

This lecture was taught by Prateek Agrawal. We defined the raising operator

$$\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\Big(\hat{x} - \frac{i}{m\omega}\hat{p}\Big),$$

and applying this operator gives higher eigenstates by $\hat{a}^\dagger = \sqrt{n+1}|n+1\rangle$. The wave functions have the pattern of $\psi_n(-x) = (-1)^n\psi_n(x)$, and

$$\psi_n(x) = P_n(x)e^{-m\omega^2x^2/2\hbar}$$

for some degree n polynomial $P_n(x)$. We can express this using the **parity operator**

$$\hat{\Pi}|n\rangle = (-1)^n|n\rangle.$$

This commutes with the Hamiltonian: $[\hat{H}, \hat{\Pi}] = 0$.

15.1 Coherent states

We want to find eigenfunctions of the lowering operator. Recall that if we set up a Gaussian wave function with a free particle, it spreads out. But for the Harmonic oscillator, this does not happen.

For $n \neq 0$, the states $|n\rangle$ are not minimum uncertainty states. Indeed, Gaussian wave functions are the only minimum uncertainty states. We want our wave function to take the form of a Gaussian wave packet for any given time. That is,

$$\psi(x,t) = Ce^{i\phi(t)}e^{-(x-x_0(t))^2/2a^2(t)}e^{ip_0(t)x/\hbar}.$$

Now we want this wave function to satisfy the Hamiltonian equation. Then it has to satisfy the equations

$$\frac{d\langle p_x\rangle}{dt} = -\Big\langle\frac{\partial V}{\partial x}\Big\rangle = -m\omega^2\langle x\rangle, \quad \frac{d\langle x\rangle}{dt} = \frac{\langle p_x\rangle}{m}.$$

Note that $\langle x\rangle = x_0(t)$ and $\langle p_x\rangle = p_0(t)$. This is then just the classical harmonic oscillator. It can be written as

$$x_0(t) = A\sin(\omega t + \phi).$$

Using this, you can then compute $a(t) = \sqrt{\hbar/m\omega}$ and $\phi(t) = -\omega t/2 - p_0(t)x_0(t)/2\hbar$. If you write out, we get

$$\psi(x,t) = \Big(\frac{m\omega}{\pi\hbar}\Big)^{1/4}e^{-\frac{i}{2}(\omega t + \frac{p_0(t)x_0(t)}{\hbar})}e^{-m\omega(x-x_0(t))^2/2\hbar}e^{ip_0(t)x/\hbar}.$$

These have $\Delta x = a/\sqrt{2}$ and $\Delta x\Delta p = \hbar/2$ at any time.

You can check that

$$\begin{aligned}\langle x|\hat{a}|\psi\rangle &= \sqrt{\frac{m\omega}{2\hbar}}\Big(x + \frac{\hbar}{m\omega}\frac{d}{dx}\Big)\psi(x,t) = \sqrt{\frac{m\omega}{2\hbar}}\Big(x_0(t) + \frac{i}{m\omega}p_0(t)\Big)\psi(x,t)\\ &= \sqrt{\frac{m\omega}{2\hbar}}Ae^{-i\omega t}\psi(x,t).\end{aligned}$$

So

$$\hat{a}|\psi\rangle = \alpha(t)|\psi\rangle, \quad \alpha(t) = \sqrt{\frac{m\omega}{2\hbar}}Ae^{-i\omega_0 t}.$$

You can also define coherent state as eigenstates of $\hat{a}$ and then deduce this.

16 March 30, 2017

Coherent states are eigenstates of the lowering operator:

$$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle.$$

Here $\hat{a}$ is not hermitian and so $|\alpha\rangle$ is not associated with a measurement. I think this is not a good motivation for coherent states.

The other way to characterize them is that they are minimum uncertainty states. The ground state $|0\rangle$ is a Gaussian wave packet and so it is a minimum uncertainty state. But for $|n\rangle$, it is not a minimum uncertainty state. It is a special fact of the harmonic oscillator that there are minimum uncertainty states that remain so under time evolution.

The wavefunctions of coherent states are given by

$$\psi(x,t) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{i}{2}[\omega t + \frac{1}{\hbar}p_0(t)x_0(t)]} e^{-\frac{1}{2\hbar}m\omega(x-x_0(t))^2} e^{\frac{1}{\hbar}ip_0(t)x},$$

where $x_0(t)$ and $p_0(t)$ solve the classical equation of motion.

If we look at $|n\rangle$ for $n \gg 1$, it looks complicated but it stays the same as time evolves, up to a phase. If we take a coherent state, it looks like a Gaussian, but it oscillates as time evolves. So it is more closer to classical physics. This is used in experiments a lot because they have minimum uncertain.

Given a coherent state $|\alpha\rangle$, the probability of finding energy $E_n = \hbar\omega(n+\frac{1}{2})$ is

$$P_n = |\langle n|\alpha\rangle|^2 = \left|e^{-\frac{1}{2}|\alpha|^2}\frac{\alpha^n}{\sqrt{n!}}\right|^2 = e^{-|\alpha|^2}\frac{|\alpha|^{2n}}{n!}.$$

Because $\langle\hat{N}\rangle = \langle\hat{a}^\dagger\hat{a}\rangle = |\alpha|^2$, we can also write

$$P_n = e^{-\langle N\rangle}\frac{|N|^n}{n!}.$$

This is a Poisson distribution. If $\langle N\rangle \gg 1$, then the mean is $\langle N\rangle$ and its standard deviation is $\sqrt{\langle N\rangle}$. This means that states with higher energy are more well explained by classical physics.

16.1 Particles in three dimension

We are now going to look at particles in higher dimension. There are different coordinates we can work with. In the future, we are going to solve the Schrödinger equation for the hydrogen atom. It is natural to work in spherical coordinates there.

In 3-dimension, there are going to be position operators in 3-dimensions: $\hat{x}$, $\hat{y}$, $\hat{z}$. We assume that they commute with each other.

$$[\hat{x},\hat{y}] = [\hat{y},\hat{z}] = [\hat{z},\hat{x}] = 0.$$

This allows us to talk about simultaneous eigenstates $|x,y,z\rangle$ such that

$$\hat{x}|x,y,z\rangle = x|x,y,z\rangle, \quad \hat{y}|x,y,z\rangle = y|x,y,z\rangle, \quad \hat{z}|x,y,z\rangle.$$

Just as we did in the 1-dimensional problem, we can write a general state as

$$|\psi\rangle = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz\, \psi(x,y,z)|x,y,z\rangle = \int d^3r\, \psi(\vec{r})|\vec{r}\rangle.$$

A stated is normalized if

$$\int d^3\vec{r}|\psi(r)|^2 = 1.$$

We also chose

$$\langle x,y,z|x',y',z'\rangle = \delta(x-x')\delta(y-y')\delta(z-z').$$

We are going to write this as

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

Define the (unitary) translation operator as

$$\hat{T}(\vec{a})|\vec{r}\rangle = |\vec{r}+\vec{a}\rangle.$$

Translations in different direction are supposed to commute. For instance, we should have $\hat{T}(a_x\hat{i})\hat{T}(a_y\hat{j}) = \hat{T}(a_y\hat{j})\hat{T}(a_x\hat{i})$.

There are the (hermitian) momentum operators $\hat{p}_x, \hat{p}_y, \hat{p}_z$ that generate the translation operators:

$$\hat{T}(a_x\hat{i}) = e^{-ia_x\hat{p}_x/\hbar}.$$

For a general vector $\hat{a}$, we can also define

$$\hat{T}(\vec{a}) = e^{-i\hat{\vec{p}}\cdot\vec{a}/\hbar}, \quad \hat{\vec{p}} = (\hat{p}_y, \hat{p}_y, \hat{p}_z).$$

This is well-defined because $\hat{p}_x, \hat{p}_y, \hat{p}_z$ pairwise commute.

In the case of 1-dimension, we had

$$[\hat{x}, \hat{p}_x] = i\hbar, \quad [\hat{y}, \hat{p}_y] = i\hbar, \quad [\hat{z}, \hat{p}_z] = i\hbar.$$

We can also ask about commutators with mixed directions. If I translate in the y-direction and then act by $\hat{x}$, this is the same as acting by $\hat{x}$ and then translating. So $\hat{x}$ and $\hat{p}_y$ should commute. So to summarize,

$$[\hat{x}_i, \hat{p}_y] = i\hbar\delta_{ij}.$$

If we act on a wavefunction, the momentum operators are going to look like

$$\hat{p}_x \mapsto -i\hbar\frac{\partial}{\partial x}, \quad \hat{p}_y \mapsto -i\hbar\frac{\partial}{\partial y}, \quad \hat{p}_z \mapsto -i\hbar\frac{\partial}{\partial z}.$$

Also the momentum eigenstates are going to look like

$$\langle \vec{r}|\vec{p}\rangle = \frac{1}{(2\pi\hbar)^{3/2}} e^{i\vec{p}\cdot\vec{r}/\hbar} = \langle x|p_x\rangle\langle y|p_y\rangle\langle z|p_z\rangle.$$

16.2 Multiparticle states

Eventually we want to look at the hydrogen atom, and this is a system of two particles. If we have two particles, the position eigenstates has to contain the data of the position of both particles. So we can write this eigenstate as

$$|\vec{r}_1, \vec{r}_2\rangle = |\vec{r}_1\rangle_1 \otimes |\vec{r}_2\rangle_2 = |\vec{r}_1\rangle_1 |\vec{r}_2\rangle_2.$$

If I have a general vector space V consisting of $|\psi\rangle = \sum_{i=1}^{n} c_i |v_i\rangle$ then its tensor product $V \otimes V$ consists of

$$|\psi\rangle = \sum_{i=1}^{n} \sum_{j=1}^{n} c_{ij} |v_i\rangle_1 |v_j\rangle_2 = \sum_{i=1}^{n} c_{ij} |v_i, v_j\rangle.$$

We will use both notations.

17 April 4, 2017

I want to resume what we are talking last time, which is states of two particles. We can label the position eigenstates as

$$|\vec{r}_1, \vec{r}_2\rangle = |\vec{r}_1\rangle_1 |\vec{r}_2\rangle_2.$$

There are position operators that act as

$$\hat{x}_1|\vec{r}_1, \vec{r}_2\rangle = x_1|\vec{r}_1, \vec{r}_2\rangle, \quad \hat{x}_2|\vec{r}_1, \vec{r}_2\rangle = x_2|\vec{r}_1, \vec{r}_2\rangle, \quad \hat{y}_1|\vec{r}_1, \vec{r}_2\rangle = y_1|\vec{r}_1, \vec{r}_2\rangle, \quad \cdots.$$

There are also translation operators

$$T_1(\vec{a})|\vec{r}_1, \vec{r}_2\rangle = |\vec{r}_1 + \vec{a}, \vec{r}_2\rangle, \quad T_2(\vec{a}) = |\vec{r}_1, \vec{r}_2\rangle = |\vec{r}_1, \vec{r}_2 + \vec{a}\rangle.$$

We can talk about their generators,

$$\hat{T}_1(\vec{a}) = e^{-i\hat{\vec{p}}_1 \cdot \vec{a}/\hbar}, \quad \hat{T}_2(\vec{a}) = e^{-i\hat{\vec{p}}_2 \cdot \vec{a}/\hbar},$$

where $\hat{\vec{p}}_1$ and $\hat{\vec{p}}_2$ are hermitian momentum operator. We can also talk about the total momentum,

$$\hat{\vec{P}} = \hat{\vec{p}}_1 + \hat{\vec{p}}_2, \quad \hat{P}_x = \hat{p}_{1x} + \hat{p}_{2x}, \quad \cdots.$$

Generally, a 2-particle Hamiltonian is going to be given by

$$\hat{H} = \frac{1}{2m_1}\hat{\vec{p}}_1^2 + \frac{1}{2}\hat{\vec{p}}_2^2 + V(\hat{\vec{r}}_1, \hat{\vec{r}}_2).$$

We are interested in the special case of a central potential, given by $V(\vec{r}_1, \vec{r}_2) = V(|\vec{r}_1 - \vec{r}_2|)$. For instance, in the case of the hydrogen atom, the Coulomb potential is given by

$$V(\vec{r}_1, \vec{r}_2) = -e^2/|\vec{r}_1 - \vec{r}_2|.$$

Here $V(\vec{r}_1, \vec{r}_2)$ defines an operator

$$\langle \vec{r}_1', \vec{r}_2'|V(\hat{\vec{r}}_1, \hat{\vec{r}}_2)|\psi\rangle = \psi(\vec{r}_1', \vec{r}_2')V(\vec{r}_1', \vec{r}_2').$$

17.1 Center-of-mass frame

Our goal now is to go to the center-of-mass frame to simplify the problem. We observe that $[\hat{H}, \hat{\vec{p}}_1] \neq 0$ because $[V(\hat{\vec{r}}_1, \hat{\vec{r}}_2), \hat{\vec{p}}_1] \neq 0$ if V has any $\hat{\vec{r}}_1$ dependence. Likewise $[\hat{H}, \hat{\vec{p}}_2] \neq 0$ if V has any $\vec{r}_2$-dependence. However,

$$[\hat{H}, \hat{\vec{P}}] = 0$$

if V is translation invariant, i.e., $V(\vec{r}_1, \vec{r}_2) = V(\vec{r}_1 - \vec{r}_2)$. This is because $\hat{T}(\vec{a})$ commutes with $\hat{H}$. So we can talk about states $|E, \vec{P}\rangle$ because $[\hat{H}, \hat{\vec{P}}] = 0$ just as we have talked about states $|j, m\rangle$.

Let us define the center of mass operator $\hat{\vec{R}}$, relative momentum $\hat{\vec{p}}$, and relative position $\hat{\vec{r}}$ as

$$\hat{\vec{R}} = \frac{m_1\hat{\vec{r}}_1 + m_2\hat{\vec{r}}_2}{m_1+m_2}, \quad \hat{\vec{p}} = \frac{m_2\hat{\vec{p}}_1 - m_1\hat{\vec{p}}_2}{m_1+m_2}, \quad \hat{\vec{r}} = \hat{\vec{r}}_1 - \hat{\vec{r}}_2.$$

We note that $\hat{\vec{R}}, \hat{\vec{P}}$ are associated with overall motion, while $\hat{\vec{r}}, \hat{\vec{p}}$ are associated with relative motion. So

$$[\hat{X}, \hat{P}_x] = i\hbar, \quad [\hat{x}, \hat{p}_x] = i\hbar, \quad [\hat{X}, \hat{p}_x] = 0, \quad [\hat{x}, \hat{P}_x] = 0.$$

That is, $(\hat{X}, \hat{P})$ and $(\hat{x}, \hat{p}_x)$ both behave like one-particle motion and momentum.

Using them, we can write

$$\frac{1}{2m_1}\hat{\vec{p}}_1^2 + \frac{1}{2m_2}\hat{\vec{p}}_2^2 = \frac{1}{2M}\hat{\vec{P}}^2 + \frac{1}{2\mu}\hat{\vec{p}}^2, \quad \text{where } \begin{cases} M = m_1 + m_2 \\ \mu = \frac{m_1 m_2}{m_1+m_2}. \end{cases}$$

Let us look more closely at this reduced mass μ. We have

$$\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2}.$$

So if $m_2 \gg m_1$ then $\mu \approx m_1$. In the case of the hydrogen atom, we have $m_p \approx 2000 m_e$ and so $\mu \approx m_e$. Intuitively, the proton states put and the electron moves.

We can write the entire Hamiltonian as

$$\hat{H} = \hat{H}_{\text{cm}} + \hat{H}_{\text{rel}},$$

where

$$\hat{H}_{\text{cm}} = \frac{1}{2M}\hat{\vec{P}}^2, \quad \hat{H}_{\text{rel}} = \frac{1}{2\mu}\hat{\vec{p}}^2 + V(\vec{r}_1 - \vec{r}_2).$$

18 April 6, 2017

Today we are going to talk about orbital angular momentum and spin.

18.1 Orbital angular momentum

Recall that the angular momentum algebra

$$[\hat{J}_x, \hat{J}_y] = i\hbar \hat{J}_z$$

followed from $R \sim e^{-iJ\theta/\hbar}$ and properties of rotations. We introduce operators for **orbital angular momentum**

$$\hat{\vec{L}} = \hat{\vec{r}} \times \hat{\vec{p}}, \quad \hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y, \quad \hat{L}_y = \hat{z}\hat{p}_x - \hat{x}\hat{p}_z, \quad \hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x.$$

If we compute the commutator between the two angular momentum operators, we get

$$\begin{aligned}[\hat{L}_x, \hat{L}_y] &= [\hat{y}\hat{p}_x - \hat{z}\hat{p}_y, \hat{z}\hat{p}_x - \hat{x}\hat{p}_z] \\ &= [\hat{y}\hat{p}_z, \hat{z}\hat{p}_x] - [\hat{z}\hat{p}_y, \hat{z}\hat{p}_x] - [\hat{y}\hat{p}_z, \hat{x}\hat{p}_z] + [\hat{z}\hat{p}_y, \hat{x}\hat{p}_z] \\ &= \hat{y}\hat{p}_x[\hat{p}_z, \hat{z}] + \hat{x}\hat{p}_y[\hat{z}, \hat{p}_z] = i\hbar \hat{L}_z.\end{aligned}$$

There are also the commutation relations

$$[\hat{L}_x, \hat{y}] = i\hbar\hat{x}, \quad [\hat{L}_x, \hat{x}] = 0, \quad [\hat{L}_x, \hat{p}_y] = i\hbar\hat{p}_z, \quad [\hat{L}_x, \hat{p}_x] = 0.$$

We also have $[\hat{L}_x, \hat{\vec{r}}^2] = 0$ and so

$$[\hat{\vec{L}}, V(\hat{\vec{r}})] = 0$$

when V is a central potential. Likewise, $[\hat{\vec{L}}, \hat{\vec{p}}^2] = 0$. The conclusion is that,

$$[\hat{\vec{L}}, \hat{H}] = 0, \quad \text{if } \hat{H} = \frac{1}{2\mu}\hat{\vec{p}}^2 + V(|\vec{r}|).$$

This is ignoring spin. If there is spin, the conserved quantity is going to be $\hat{\vec{J}} = \hat{\vec{L}} + \hat{\vec{S}}$.

Because $\hat{H}$ and $\hat{\vec{L}}$ commute, we can find a basis of simultaneous eigenstates. If you remember the case the spin system, we also had another commuting operator $\hat{\vec{J}}^2$. The analogue of this is

$$[\hat{\vec{L}}^2, \hat{L}_z] = 0, \quad [\hat{\vec{L}}^2, \hat{H}] = 0.$$

So we can name the simultaneous eigenstates of $\hat{L}^2$ and $\hat{L}_z$ as

$$\hat{\vec{L}}^2|l, m\rangle = l(l+1)\hbar^2|l, m\rangle, \quad \hat{L}_z|l, m\rangle = m\hbar|l, m\rangle,$$

where l and m are integers with $|m| \leq l$.

Because $\hat{H}$ also commute with these, we can search for eigenstates of all three:

$$\hat{H}|E,l,m\rangle = E|E,l,m\rangle, \quad \hat{\vec{L}}^2|E,l,m\rangle = l(l+1)\hbar^2|E,l,m\rangle, \quad \hat{L}_z|E,l,m\rangle = m\hbar|E,l,m\rangle.$$

We also have raising and lowering operators

$$\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y, \quad [\hat{L}_z, \hat{L}_\pm] = \pm\hbar\hat{L}_\pm.$$

Then $\hat{L}_+|l,m\rangle \propto |l,m+1\rangle$.

18.2 Particle in a central potential

But we are not satisfied with this abstract description, because these are actual particles in space. There should be wave functions. To work out the wave function, it is useful to work in polar coordinates:

$$|r,\theta,\phi\rangle = |x,y,z\rangle \text{ where } x = \sin\theta\cos\phi, \quad y = r\sin\theta\sin\phi, \quad z = r\cos\theta.$$

Then $\hat{L}_z$ corresponds to

$$\hat{L}_z \;\leftrightarrow\; -i\hbar\frac{\partial}{\partial\phi}, \text{ i.e., } \langle r,\theta,\phi|\hat{L}_z|\psi\rangle = -i\hbar\frac{\partial}{\partial\phi}(\langle r,\theta,\phi|\psi\rangle).$$

The other operators correspond to

$$\hat{L}_x \;\leftrightarrow\; -i\hbar\Big(\sin\phi\frac{\partial}{\partial\theta} - \cot\theta\cos\phi\frac{\partial}{\partial\phi}\Big), \quad \hat{L}_y \;\leftrightarrow\; -i\hbar\Big(\cos\phi\frac{\partial}{\partial\theta} - \cot\theta\sin\phi\frac{\partial}{\partial\phi}\Big).$$

Note that none of these involve r or $\partial/\partial r$. Because of this, we can separate the variables and guess

$$\psi_{E,l,m}(r,\theta,\phi) = \langle r,\theta,\phi|E,l,m\rangle = R(r)Y_{l,m}(\theta,\phi).$$

It turns out that this works. The functions $Y_{l,m}(\theta,\phi)$ are called **spherical harmonics**. We them to be normalized as

$$\int_0^{2\pi} d\phi \int_{-1}^{1} d(\cos\theta)|Y_{l,m}(\theta,\phi)|^2 = 1.$$

So let us find $Y_{l,m} = \langle\theta,\phi|l,m\rangle$. We have $\langle\theta,\phi|\hat{L}_z|l,m\rangle = m\hbar|l,m\rangle$. We know that $\hat{L}_z$ act as $-i\hbar\partial/\partial\phi$ and so

$$-i\hbar\frac{\partial}{\partial\phi}Y_{l,m}(\theta,\phi) = m\hbar Y_{l,m}(\theta,\phi).$$

So we expect $Y_{l,m}(\theta,\phi) \propto e^{im\phi}$ for the ϕ part. But $\hat{L}^2$ is going to be complicated.

Instead of expanding everything out, we use $\hat{L}_+|l,l\rangle = 0$. We can write

$$\hat{L}_\pm = \hat{L}_z \pm i\hat{L}_y = \pm i\hbar e^{\pm i\phi}\Big(\pm i\frac{\partial}{\partial\phi} - \cot\theta\frac{\partial}{\partial\phi}\Big).$$

Using this, we can write

$$\Big(\frac{\partial}{\partial\theta} - l\cot\theta\Big)Y_{ll}(\theta,\phi) = 0$$

and so $Y_{ll}(\theta,\phi) = c_{ll}(\sin\theta)^l e^{il\phi}$.

19 April 11, 2017

We were studying a particle in a central potential

$$\hat{H} = \frac{\hat{p}^2}{2\mu} + V(|\hat{\vec{r}}|).$$

This gave rotationally invariant operators $\hat{\vec{L}}^2$ and $\hat{L}_z$ that commute with $\hat{H}$. Our strategy is to look for states $|E, \ell, m\rangle$ which are eigenstates of $\hat{H}, \hat{\vec{L}}^2, \hat{L}_z$ simultaneously. We are also going go work in polar coordinates. Because $\hat{p}^2$ decomposes into a radial part and an angular part, we can look for wavefunctions

$$\langle r, \theta, \phi | E, \ell, m\rangle = R_\ell(r) Y_{\ell m}(\theta, \varphi).$$

Here we want

$$\hat{\vec{L}}^2 |\ell, m\rangle = \ell(\ell+1)\hbar^2 |\ell, m\rangle, \quad \hat{L}_z |\ell, m\rangle = m\hbar |\ell, m\rangle.$$

In particular, $Y_{\ell,m}(\theta, \phi)$ are universal for all central potentials but $R_\ell(r)$ depends on $V(|r|)$. So these functions are going useful for any central potentials.

Our goal is to solve this for the Coulomb potential

$$V(r) = -\frac{e^2}{r}, \text{ where } e^2 \approx \frac{1}{137}\hbar c.$$

19.1 Spherical harmonics

Last time we have worked out the operators

$$\hat{L}_z \to -i\hbar \frac{\partial}{\partial \phi}, \quad \hat{L}_\pm \to -i\hbar e^{\pm i\phi}\Big(\pm i \frac{\partial}{\partial \theta} - \cot\theta \frac{\partial}{\partial \phi}\Big).$$

From the first equation, we expect $Y_{\ell,m}(\theta, \phi) \propto e^{im\phi}$. Then we would expect $\hat{L}_+ |\ell, \ell\rangle = 0$ and so $(\partial/\partial\theta - \ell \cot\theta) Y_{\ell,\ell}(\theta, \phi) = 0$. This gives

$$Y_{\ell,\ell}(\theta, \phi) = c_{\ell,\ell} (\sin\theta)^\ell e^{i\ell\phi} = \frac{(-1)^\ell}{2^\ell \ell!} \sqrt{\frac{(2\ell+1)!}{4\pi}} e^{i\ell\phi} (\sin\theta)^\ell.$$

Here, note that if we want $Y_{\ell,m}(\theta, \phi) \propto e^{im\phi}$, then

$$Y_{\ell,m}(\theta, \phi + 2\pi) \propto e^{im(\phi+2\pi)} = \begin{cases} e^{im\phi} & \text{if } m \in \mathbb{Z} \\ -e^{im\phi} & \text{if } m \in \mathbb{Z} + \frac{1}{2}. \end{cases}$$

Then if we want this to be a single-valued wave function, we would need $\ell, m \in \mathbb{Z}$. But for spin particles, we did not require this because spin are not rotations.

Anyways, once we know $|\ell, m\rangle$, we can compute $|\ell, m-1\rangle$ by applying $\hat{L}_-$ and then normalizing it:

$$Y_{\ell,m-1}(\theta, \phi) = \frac{1}{\sqrt{\ell(\ell+1) - m(m-1)}} \frac{1}{\hbar} (-i\hbar e^{-i\phi}) \Big(-i \frac{\partial}{\partial \theta} - \cot\theta \frac{\partial}{\partial \phi}\Big) Y_{\ell,m}(\theta, \phi).$$

The operator $\hat{\vec{L}}^2$ is given by

$$\hat{\vec{L}}^2 = -\hbar^2\Big[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\Big(\sin\theta\frac{\partial\psi}{\partial\theta}\Big) + \frac{1}{\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}\Big].$$

Even though we have not solved the eigenvalue equation for $\hat{\vec{L}}^2$, it is automatically going to be satisfied because we have used the raising and lowering operators $\hat{L}_\pm$. You can explicitly check $\hat{\vec{L}}^2|\ell,m\rangle = \ell(\ell+1)\hbar^2|\ell,m\rangle$ if you want.

19.2 Boundary condition for the radial function

To compute the radial functions, we now actually need to solve the time-independent Schrödinger equation:

$$\Big\langle r,\theta,\phi\Big|\Big(\frac{\hat{p}^2}{2\mu} + V(|r|)\Big)\Big|E,\ell,m\Big\rangle = E\psi_{E,\ell,m}(r,\theta,\phi) = ER_{E,\ell}(r)Y_{\ell,m}(\theta,\phi).$$

Then the equation we want to solve is

$$\Big[-\frac{\hbar^2}{2\mu}\Big(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\Big) + \frac{1}{2\mu r^2}\ell(\ell+1)\hbar^2 + V(r)\Big]R_{E,\ell}(r) = ER_{E,\ell}(r)$$

after canceling out the angular part.

The equation is getting is nicer but it is still ugly to solve. The trick is to convert $(\partial^2/\partial r^2 + (2/r)\partial/\partial r)R$ into a nice factor $(\partial^2/\partial r^2)u$. Note that

$$\frac{\partial^2}{\partial r^2}(rR) = r\Big(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\Big)R.$$

So $u_{E,\ell}(r) = rR_{E,\ell}(r)$ satisfies the equation

$$\Big[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{\ell(\ell+1)\hbar^2}{2\mu r^2} + V(r)\Big]u_{E,\ell}(r) = Eu_{E,\ell}(r).$$

If we can solve this for $u_{E,\ell}(r)$ for $V(r) = -e^2/r$, we will have solved the hydrogen atom. This now just looks like a one-dimensional particle in a potential well, with

$$V_{\text{eff}}(r) = \frac{\ell(\ell+1)\hbar^2}{2\mu r^2} - Z\frac{e^2}{r}.$$

We're looking for bound states with $E < 0$, since plane wave-like solutions exist when $E > 0$. We are going to impose normalizability:

$$\int d^3r|\psi(r)|^2 = 1 = c\int r^2 dr R(r)^2.$$

So we want $r^2R(r)^2$ to not grow too fast. The decay $r^2R^2 \sim r^{-1-\epsilon}$ is enough.

20 April 13, 2017

We are looking for solutions to $\psi_{E,\ell,m}(r,\theta,\phi) = R_{E,\ell}(r)Y_{\ell,m}(\theta,\phi)$. If we define $u_{E,\ell}(r) = rR_{E,\ell}(r)$, then

$$-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}u_{E,\ell}(r) + V_{\text{eff}}(r)u_{E,\ell}(r) = Eu_{E,\ell}(r),$$

where

$$V_{\text{eff}}(r) = -Z\frac{e^2}{r} + \frac{\ell(\ell+1)\hbar^2}{2\mu r^2}.$$

The boundary condition for large r was that $\int dr r^2 |R(r)|^2 < \infty$. For small r, we have (assuming that $\ell > 0$)

$$\left|\frac{\ell(\ell+1)\hbar^2}{2\mu r^2}\right| \gg \left|-Z\frac{e^2}{r}\right|.$$

Then the centrifugal term dominates and the equation looks like

$$-\frac{d^2}{dr^2}u_{E,\ell}(r) + \frac{\ell(\ell+1)}{r^2}u_{E,\ell}(r) \approx E\frac{2\mu}{\hbar^2}u_{E,\ell}(r).$$

If we guess that the leading term is $u_{E,\ell}(r) \propto r^{-\alpha}$, then

$$[-\alpha(\alpha+1)u^{-\alpha-2} + \cdots] + [\ell(\ell+1)r^{-\alpha-2} + \cdots] \approx E\frac{2\mu}{\hbar^2}r^{-\alpha}.$$

So we get $\alpha(\alpha+1) = \ell(\ell+1)$ and so either $\alpha = \ell$ or $\alpha = -(\ell+1)$. But we again have $\int dr r^2|R(r)|^2 = \int dr|u|^2$. This shows that the solution for $\alpha = \ell$ grows too fast and so $\alpha = -(\ell+1)$. So for $\ell \geq 1$, we want $u_{E,\ell}(r) \sim r^{\ell+1}$ as $r \to 0$.

The case $\ell = 0$ is a bit subtle. We only have the Coulomb term and so

$$-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}u(r) - Z\frac{e^2}{r}u(r) = Eu(r).$$

If we assume $u(r) = r^{-\alpha} + \cdots$ then the equation becomes

$$-\frac{\hbar^2}{2\mu}\alpha(\alpha+1)r^{-\alpha-2} + \cdots - Ze^2r^{-\alpha-1} + \cdots = Er^{-\alpha} + \cdots.$$

So $\alpha = 0$ or $\alpha = -1$. Both of $u \sim r^0$ and $u \sim r^1$ satisfies normalizability.

The "correct" choice is to pick $u \sim r^1$ and $R \sim$ const. The textbook gives two reasons for this:

(1) problem 10.1: $\langle p_r \rangle$ is not real if $R \sim r^{-1}$.

(2) Because $\nabla^2 r^{-1} = \delta^3(\vec{r})$, and so the solution with $R \sim r^{-1}$ is really solving the Schrödinger equation with

$$V(r) = -Z\frac{e^2}{r} + b\delta^3(\vec{r}).$$

Really, it is not clear whether the interaction between the proton and the electron is just $-Ze^2/r$ or $-Ze^2/r + b\delta^3(\vec{r})$. This is an empirical fact that in our universe, b is really small. So $R_{E,\ell}(r) = \text{const}$ is a good approximation.

Anyways, in both $\ell = 0$ and $\ell \geq 1$, we have the boundary conditions $R_{E,\ell}(r) \sim r^\ell$ as $r \to 0$.

20.1 Radial function for the Coulomb potential

Now we really need to solve the equation. First choose units of length based on

$$\rho = \kappa_E r, \quad E = -\frac{\hbar^2 \kappa_E^2}{2\mu}.$$

Note that this is possible since $E < 0$. The Schrödinger equation then becomes

$$-\frac{d^2}{d\rho^2} u_{E,\ell}(\rho) + \Big(-\frac{\xi_E}{r} + \frac{\ell(\ell+1)}{\rho^2}\Big) u_{E,\ell}(\rho) = -u_{E,\ell}(\rho),$$

where $\xi_E = 2\mu Ze^2/(\kappa_E \hbar^2)$.

We know that the behavior of $u_{E,\ell}(\rho)$ as $\rho \to 0$ is like $\rho^{\ell+1}$ and the behavior as $\rho \to \infty$ is something like exponential decay. So we make an ansatz

$$u_{E,\ell}(\rho) = \rho^{\ell+1} e^{-\rho} F_{E,\ell}(\rho).$$

This can be expected to go to a constant as $\rho \to 0$, and is somewhat controlled as $\rho \to \infty$.

Plugging this in, we get

$$\frac{d^2 F_{E,\ell}}{d\rho^2} - 2\Big(1 - \frac{\ell+1}{\rho}\Big)\frac{dF_{E,\ell}}{d\rho} + \Big(\frac{\xi_E - 2\ell - 2}{\rho}\Big) F_{E,\ell}(\rho) = 0.$$

If we try a series solution $F(\rho) = \sum_{n=0}^\infty a_n \rho^n$ where $a_0 \neq 0$, we get

$$\sum_{n=0}^\infty [a_n n(n-1)\rho^{n-2} - 2n a_n \rho^{n-1} + 2(\ell+1) n a_n \rho^{n-2} + (\xi_E - 2\ell - 2) a_n \rho^{n-1}] = 0.$$

There are no ρ^{-2} terms, and ρ^{-1} terms give

$$(\xi_E - 2\ell - 2)a_0 + 2(\ell+1)a_1 = 0 \text{ and so } a_2 = \frac{2(\ell+1) - \xi_E}{2(\ell+1)} a_0.$$

Next, ρ^0 terms give

$$2a_2 - 2a_1 + 4(\ell+1)a_2 + (\xi_E - 2\ell - 2)a_1 = 0 \text{ and so } a_2 = \frac{(2\ell + 3 - \xi_E)a_1}{4\ell + 6}.$$

In general, we are going to see

$$a_{n+1} = a_n \frac{(-\xi_E + 2n + 2\ell + 2)}{(n + 2\ell + 2)(n+1)}.$$

Note that for large n, $a_{n+1} \approx (2/n)a_n$. This means that asymptotically, $F(\rho) \sim e^{2\rho}$ for large ρ. But note that $F \sim e^{2\rho}$ is not the solution we want, because then $u_{E,\ell}(\rho)$ would grow too fast. What this tells us is that the power series for F must end at some point.

Recall that

$$\xi_E = \frac{2\mu Z e^2}{\kappa_E \hbar^2} = \frac{2\mu Z e^2}{\sqrt{2\mu|E|/\hbar^2}\hbar^2} = \frac{1}{\hbar} Z e^2 \sqrt{\frac{2\mu}{|E|}}.$$

In order for the power series for F to be finite, one of $-\xi_E + 2n + 2\ell + 2$ must be zero. That means that

$$\xi_E = 2n + 2\ell + 2$$

for some integer $n \geq 0$. Then $k = \mu Z e^2/\kappa_E \hbar^2 = n + \ell + 1$ is a positive integer and

$$E = -\frac{\hbar^2 \kappa_E^2}{2\mu} = -\frac{e^4 \mu Z^2}{2\hbar k^2}.$$

This k is called the **principal quantum number** and is usually denoted n. So if $F_{E,\ell}(\rho)$ is a degree p polynomial, the principal quantum number is $n = p + \ell + 1 \geq \ell + 1$.

This starts to look like chemistry. For $n = 1$, there is only $\ell = 0$, ($1s$ orbital) for $n = 2$ there are $\ell = 0, 1$ ($2s$ and $2p$ orbitals), and for $n = 3$ there are $\ell = 0, 1, 2$ ($3s$, $3p$, $3d$ orbitals).

We define the **Bohr radius** as

$$a_0 = \frac{\hbar^2}{\mu e^2} \approx 0.53 \times 10^{-10}\text{m},$$

and the **Rydberg constant** as

$$E_n = -\frac{\hbar^2}{2\mu a_0^2 n^2} = -13.6\text{eV}\frac{Z^2}{n^2}.$$

Here $m_e c^2 = 511\text{keV}$ and $\alpha = e^2/\hbar c \approx 1/137$ and $\text{Rydberg} = \frac{1}{2}\alpha^2 m_e c^2$.

The radial functions are given by

$$R_{1,0} = 2\Big(\frac{Z}{a_0}\Big)^{3/2} e^{-Zr/a_0}, \quad R_{2,0} = 2\Big(\frac{Z}{2a_0}\Big)^{3/2}\Big(1 - \frac{Zr}{a_0}\Big)e^{-Zr/a_0},$$
$$R_{2,1} = \frac{1}{\sqrt{3}}\Big(\frac{Z}{2a}\Big)^{3/2}\frac{Zr}{a_0}e^{-Zr/a_0}, \ldots.$$

21 April 18, 2017

We found that the energy levels of hydrogen atom are given by $E_n = 13.6\text{eV}/n^2$. There are various transitions of between the eigenstates, by emitting a photon. The Lyman series are the state transitions going down to $n = 1$, which correspond to ultraviolet light, and the Balmer series are the transitions to $n = 2$, and these are in the visible spectrum. This is useful in astronomy, because you can calculate the velocity of a moving source since there is a Doppler shift.

We saw that that there are lots of degeneracy: the number n determine E, and there are $\ell = 0, 1, \dots, n-1$ and $m = -\ell, \dots, \ell$. These all have equal energy. Also, electrons and protons have spin-1/2. There are various small effects, like the spin-orbit coupling $\vec{L} \cdot \vec{S}$, and these split the states. Also only $\vec{J} = \vec{L} + \vec{S}$ is conserved.

21.1 Entangled states

We go back to chapter 5 and two distinct spin-1/2 particles. We are going to label the states like

$$|\uparrow\uparrow\rangle = |\uparrow\rangle_1 \otimes |\uparrow\rangle_2,$$

where $|\uparrow\rangle = |+z\rangle$ and $|\downarrow\rangle = |-z\rangle$. Some states factor like

$$\frac{1}{\sqrt{2}}|\uparrow\uparrow\rangle + \frac{1}{\sqrt{2}}|\downarrow\uparrow\rangle = \frac{1}{2}(|\uparrow\rangle_1 + |\downarrow\rangle_1) \otimes |\uparrow\rangle_2,$$

but other states like

$$\frac{1}{\sqrt{2}}|\uparrow\uparrow\rangle + \frac{1}{\sqrt{2}}|\downarrow\downarrow\rangle$$

do not factor. We call this an **entangled state**. Entanglement can be a useful resource: quantum computing, quantum cryptography, quantum teleportation, etc. These entanglements can happen between particles with different spin.

A rule of thumb is that Hamiltonians $\hat{H} = [\vec{S}_1 \cdot \vec{S}_2]\omega/\hbar$ that couple two particles tend to create entanglements.

We define spin operators for particles 1 and 2:

$$\hat{\vec{S}}_1 = \hat{\vec{S}}_1 \otimes \hat{\mathbf{1}}, \quad \hat{\vec{S}}_2 = \hat{\mathbf{1}} \otimes \hat{\vec{S}}_2, \quad \hat{\vec{S}} = \hat{\vec{S}}_1 + \hat{\vec{S}}_2.$$

For instance,

$$\hat{S}_{1z}|\uparrow\downarrow\rangle = +\frac{\hbar}{2}|\uparrow\downarrow\rangle, \quad \hat{S}_{2z}|\uparrow\downarrow\rangle = -\frac{\hbar}{2}|\uparrow\downarrow\rangle, \quad \hat{S}_z|\uparrow\downarrow\rangle = 0.$$

We have $[\hat{\vec{S}}_1, \hat{\vec{S}}_2] = 0$. You can check that

$$\hat{\vec{S}}_1 \cdot \hat{\vec{S}}_2 = \frac{1}{2}(\hat{S}_{1+}\hat{S}_{2-} + \hat{S}_{1-}\hat{S}_{2+}) + \hat{S}_{1z}\hat{S}_{2z}.$$

Here the lower operator $\hat{S}_- = \hat{S}_{1-} + \hat{S}_{2-}$ acts like

$$\hat{S}_-|\uparrow\downarrow\rangle = \hbar|\downarrow\downarrow\rangle, \quad \hat{S}_-|\downarrow\uparrow\rangle = \hbar|\downarrow\downarrow\rangle, \quad \hat{S}_-|\uparrow\uparrow\rangle = \hbar(|\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle), \quad \hat{S}_-|\downarrow\downarrow\rangle = 0.$$

If you look at this, it looks like a spin-1 particle, with levels

$$m = 1 : |\uparrow\uparrow\rangle, \quad m = 0 : \frac{1}{\sqrt{2}}(|\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle), \quad m = -1 : |\downarrow\downarrow\rangle.$$

You can check that $\hat{\vec{S}}^2|\psi\rangle = 2\hbar^2|\psi\rangle$ for these states. There is a fourth state

$$m = 0 : \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

that becomes 0 when acted on by either $\hat{S}_+$ or $\hat{S}_-$.

So hydrogen can be in a spin-1 multiplet or a spin-0 multiplet. This can be thought of as

$$2 \times 2 = 3 + 1.$$

You can do the same thing for two spin-1 particles:

$$3 \times 3 = 5 + 3 + 1.$$

This is related to the representation theory of SU(2).

The spin-0 hydrogen state

$$\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

is an entangled state. It turns out that this is the state with minimal angular momentum.

21.2 Density operator

How do we know if a state is entangled? We will use the **density operator (matrix)** $\hat{\rho}$. This is supposed to general the projection operator $\hat{P}_\psi = |\psi\rangle\langle\psi|$. This also has the property

$$\langle\hat{A}\rangle = |\psi|\hat{A}|\psi\rangle = \mathrm{tr}(\hat{P}_\psi\hat{A}).$$

The states $|\psi\rangle$ will be called **pure states**, and they have corresponding density operator

$$\hat{\rho} = \hat{P}_\psi.$$

Now a **mixed state** as a classical probability of being a different pure state: probability p_i of being $|\psi_i\rangle$. Note that a mixed state of a particle either being $|\uparrow\rangle$ with probability 3/4 and $|\downarrow\rangle$ with probability 1/4, is not the same as a $\sqrt{3}/2|\uparrow\rangle + 1/2|\downarrow\rangle$.

Now the expectation in a mixed state can be computed as

$$\langle\hat{A}\rangle_{\hat{\rho}} = \sum_i p_i\langle i|\hat{A}|i\rangle = \sum_i p_i \,\mathrm{tr}(\hat{P}_{\psi_i}\hat{A}) = \mathrm{tr}(\hat{\rho}\hat{A}).$$

This is one way $\hat{\rho}$ generalizes $\hat{P}_\psi$.

22 April 20, 2017

We were talking about density operators:

$$\hat{\rho} = \sum_i p_i |\psi_i\rangle\langle\psi_i|,$$

where $\sum_i p_i = 1$ and $0 \le p_i \le 1$. This p_i is the classical probability of being in different quantum states. For example,

$$\hat{\rho} = \frac{3}{4}|\uparrow\rangle\langle\uparrow| + \frac{1}{4}|\downarrow\rangle\langle\downarrow|$$

is a mixed state, different from $|\psi\rangle = \frac{\sqrt{3}}{2}|\uparrow\rangle + \frac{1}{2}|\downarrow\rangle$.

For a pure state, the corresponding density operator $\hat{\rho} = \hat{P}_\psi = |\psi\rangle\langle\psi|$ is a projection, i.e., $\hat{P}_\psi^2 = \hat{P}_\psi$. For a mixed state $\hat{\rho}$, this is not true, i.e., $\hat{\rho}^2 \neq \hat{\rho}$. For example,

$$\left(\frac{3}{4}|\uparrow\rangle\langle\uparrow| + \frac{1}{4}|\downarrow\rangle\langle\downarrow|\right)^2 = \frac{9}{16}|\uparrow\rangle\langle\uparrow| + \frac{1}{16}|\downarrow\rangle\langle\downarrow|.$$

For any $\hat{\rho}$, we have $\mathrm{tr}(\hat{\rho}) = 1$. We also have $0 \le \mathrm{tr}(\hat{\rho}^2) \le 1$ always, with $\mathrm{tr}(\hat{\rho})^2 = 1$ if and only if $\hat{\rho}$ is a pure state.

22.1 Reduced density operator

If a quantum system decomposed into subsystems A and B, we define the **reduced density operator** of the subsystem A as

$$\hat{\rho}_A = \mathrm{tr}_B(\hat{\rho}),$$

where tr_B is the partial trace over the subsystem B.

Example 22.1. Take the pure state $|\psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$. We can work in the basis $|\uparrow\uparrow\rangle$, $|\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$. In this basis,

$$\hat{\rho} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & -\frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

Now we take the trace over the second particle. Take an orthonormal basis of the states of B, $\{|\uparrow\rangle_2, |\downarrow\rangle_2\}$. Then

$$\hat{\rho}_A = \sum_{|j\rangle_B \text{ in orthonormal basis}} {}_B\langle j|\hat{\rho}|j\rangle_B.$$

In our example, we are going to get

$$\hat{\rho}_A = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}.$$

This is a mixed state. Intuitively, this is the state for A you will get after measuring B.

In this example,

$$\hat{\rho}_A^2 = \begin{pmatrix} 1/4 & 0 \\ 0 & 1/4 \end{pmatrix} \neq \hat{\rho}_A$$

so the reduced density matrix is not a projection operator even though the complete 2-state is pure. This is the hallmark of entanglement. Subsystems A and B and entangled if and only if $\hat{\rho}_A = \mathrm{tr}_B\, \hat{\rho}$ is not a projection operator.

22.2 Decoherence and interpretation of quantum physics

These are examples of open quantum systems. We have access to only a subset of the degrees of freedom of the system. This is very important for the emergence of classical physics from the microscopic law of quantum mechanics. There is a tension in the laws of quantum mechanics:

(1) Given $|\psi(0)\rangle$ and $\hat{H}$, you can tell me $|\psi(t)\rangle = e^{-i\hat{H}t/\hbar}|\psi(0)\rangle$.

(2) If you measure a state, you change it to an eigenstate of what you measure, with some probability.

You can consider the whole measuring device as a quantum state, but the first law seems deterministic and the second law seems uncertain and random. There has been a lot of discussion on these among physicists and philosophers, and there is a whole subject on interpretation of quantum physics.

This is related to the decoherence and measurement. Suppose I have a $|+x\rangle$ particle and we feed it to a $+z$ Stern–Gerlach device, with one light turning on if it goes up and another light turning on if it goes down. This whole apparatus is a very complex system:

$$\frac{1}{\sqrt{2}}(|+z\rangle + |-z\rangle) \otimes |\text{measuring device, lights off}\rangle \otimes |\text{air in the room}\rangle \otimes \cdots .$$

If our measuring device worked as we wanted, this is going to be

$$\Big[\frac{1}{\sqrt{2}}\Big|+z, \begin{matrix}\text{upper lights} \\ \text{turned on}\end{matrix}\Big\rangle + \frac{1}{2}\Big|-z, \begin{matrix}\text{lower lights} \\ \text{turned on}\end{matrix}\Big\rangle\Big] \otimes |\text{air in the room}\rangle \otimes \cdots .$$

If more time passes, you are going to get

$$\frac{1}{\sqrt{2}}\Big|+z, \begin{matrix}\text{upper lights} & \text{atoms in air} \\ \text{turned on} & \text{in state (\# 1)}\end{matrix}\Big\rangle + \frac{1}{2}\Big|-z, \begin{matrix}\text{lower lights} & \text{atoms in air} \\ \text{turned on} & \text{in state (\# 2)}\end{matrix}\Big\rangle.$$

So the measuring device correlate a microscopic quantum state with a huge number of other particles. You can never measure the entire air, and What you can access is described by the reduced density density matrix tracing over the air's state. This is effective like the classical probability.

22.3 Bell's inequality

A lot of people tried to make different theories that agree with experimental results, but failed. Bell was one of those people, and in the course, he showed something that need to be true. Bell's inequality is one of them, and I am going to present one version from John Preskill's lecture notes.

Two experimenters, Alice and Bob play a game. Each flip a coin, and they may share some information beforehand. These information has to be classical or an entangled quantum state

$$\frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle).$$

They communicate a bit (classical 0 or 1) and the sefult of their coin flip. They win the game if "the XOR of the bits they send is 0 if and only if both coins show heads".

Here is a classical strategy that winds 75% of the time. Both Alice say 0. Then they lose exactly when the coins are both heads.

It turns out this is the best possible strategy. This follows from the **CHSH (Clauser–Horne–Shimony–Holt) inequality**. For four number $\alpha_H, \alpha_T, \beta_H, \beta_T$, each of which is ± 1, we have

$$C = (\alpha_H + \alpha_T)\beta_T + (\alpha_T - \alpha_H)\beta_H = \pm 2$$

and so

$$|\langle \alpha_T \beta_T \rangle + \langle \alpha_T \beta_H \rangle + \langle \alpha_H \beta_T \rangle - \langle \alpha_H \beta_H \rangle| \leq 2.$$

Let $\alpha_H = 1$ if Alice says 0 if the when she sees H, and $\alpha_H = -1$ if Alice says 1 when she sees T. Then if you work out,

$$|2(p_{TT} + p_{TH} + p_{HT} + p_{HH}) - 4| \leq 2$$

and so the average winning probability is $(1/4)\sum p_{Ij} \leq 3/4$.

23 April 25, 2017

We were talking about Alice and Bob, who can share information in advance. They flip a coin, choose a bit and communicate the results. They win if both coins are heads and the XOR of their bits is true, or one of the coins are tails and the XOR of their bits is false.

There is an easy classical 75% winning strategy: both say false always. It turned out that this is the best possible due to the CHSH inequality, which is similar to the Bell inequality. If α_T is the random variable

$$\alpha_T = \begin{cases} -1 & \text{if Alice says true when she sees tails,} \\ 1 & \text{if Alice says false when she sees tails,} \end{cases}$$

and define other variables $\alpha_H, \beta_H, \beta_T$ analogously, then the CHSH inequality says

$$|\langle \alpha_T \beta_T \rangle + \langle \alpha_T \beta_H \rangle + \langle \alpha_H \beta_T \rangle - \langle \alpha_H \beta_H \rangle| \leq 2.$$

Now our claim is that $\langle \alpha_T \beta_T \rangle$ is $2p_{TT}^{\text{win}} - 1$ where p_{TT}^{win} is the conditional probability of winning when the coins are both tails. Similar interpretations work, and so the overall probability of winning is $\frac{1}{4}\sum_{i,j} p_{ij}^{\text{win}}$. Then the inequality tells us

$$\left| 2 \sum_{i,j} p_{ij}^{\text{win}} - 4 \right| \leq 1.$$

So the probability of wining for any strategy based on classical probability is at most 75%.

23.1 A quantum mechanical strategy

Now suppose that Alice and Bob share an entangled pair of spins

$$\langle \psi \rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle_A \otimes |\uparrow|_B - |\downarrow\rangle_A \otimes |\downarrow\rangle_B).$$

Here is a strategy that wins more that 75% of the time.

- If Alice sees heads, she measures the spin's z-component, and says true if she sees $+\hbar/2$ and false if she sees $-\hbar/2$.
- If Alice sees tails, she first act on her state with the unitary matrix

  $$U = \begin{pmatrix} \cos 3\pi/8 & -\sin 3\pi/8 \\ \sin 3\pi/8 & \cos 3\pi/8 \end{pmatrix}$$

  and then measures the z-component of the spin, and says true if she sees $+\hbar/2$ and false if she sees $-\hbar/2$.
- Bob does the same thing, but gives the opposite answers: false if $+\hbar/2$ and true if $-\hbar/2$.

Now let us calculate the probability of winning.

(1) Alice and Bob both see heads.

The winning condition is that they disagree. Then either they both sees $\uparrow$ or both sees $\downarrow$. So they win 100% of the time.

(2) Alice sees heads, Bob sees tails.

It doesn't matter, but let's assume Alice first does the measurement. Then $1/2$ of the time she sees $\uparrow$ and says T, and $1/2$ of the time she sees $\downarrow$ and says F. If Alice sees $\uparrow$, this measurement effectively collapses Bob's state into $|\uparrow\rangle_B$ and after acting by U, it becomes

$$U\begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}\cos 3\pi/8\\ \sin 3\pi/8\end{pmatrix}.$$

So Bob $\cos^2 3\pi/8$ of the time sees $\uparrow$ and says F, and $\sin^2 3\pi/8$ of the time sees $\downarrow$ and says T.

Alice sees $\downarrow$ for $1/2$ of the time F, and says F. Likewise, Bob says F with probability $\sin^2 3\pi/8$ and T with probability $\cos^2 3\pi/8$. So they win $\sin^2 3\pi/8$ of the time in total.

(3) Alice sees tails, Bob sees heads.

This is going to be the same probability of $\sin^2 3\pi/8$ of winning, because it is basically case (2).

(4) Alice and Bob both see tails.

They win if they say the same thing. Suppose Alice goes first. The state becomes

$$\frac{1}{\sqrt{2}}\Big[\cos\frac{3\pi}{8}|\uparrow\uparrow\rangle + \sin\frac{3\pi}{8}|\downarrow\uparrow\rangle + \sin\frac{3\pi}{8}|\uparrow\downarrow\rangle - \cos\frac{3\pi}{8}|\downarrow\downarrow\rangle\Big].$$

When Alice measures, 50% times of the time she sees $|\uparrow\rangle$ and project Bob onto $\cos 3\pi/8|\uparrow\rangle_B + \sin 3\pi/8|\downarrow\rangle_B$. Now Bob sees tails so acting on U gives

$$U\begin{pmatrix}\cos 3\pi/8\\ \sin 3\pi/8\end{pmatrix} = \begin{pmatrix}\cos 3\pi/4\\ \sin 3\pi/4\end{pmatrix}.$$

Then they in 50% of the time. Same goes for when Alice sees $|\downarrow\rangle$. So overall they win 50% of the time.

So the overall chance of winning is

$$\frac{1}{4}\Big[1 + 2\sin^2\frac{3\pi}{8} + \frac{1}{2}\Big] \approx 0.80 > 0.75.$$

The lesson of all this is that quantum entanglement is distinctly quantum phenomenon; no complicated classical theory can do the same thing.

Another lesson is that quantum entanglement can be a resource. This is the basic premise behind quantum computing, quantum cryptography, ... If you're interested in these kinds of stuff, you can read Preskill's lecture notes on quantum information, Nielson and Chuany's *Quantum Information and Quantum Computing*.

23.2 No-cloning theorem and quantum transportation

This basically says that you can't copy a quantum state. That is, there is no map

$$U : |\psi\rangle \otimes |0\rangle \mapsto |\psi\rangle \otimes |\psi\rangle.$$

This is because of linearity. If we assume $U(|0\rangle \otimes |0\rangle) = |00\rangle$ and $U(|1\rangle \otimes |0\rangle) = |11\rangle$, then for $|\psi\rangle = a|0\rangle + b|1\rangle$,

$$U(|\psi\rangle \otimes |0\rangle) = a|00\rangle + b|11\rangle \neq (a|0\rangle + b|1\rangle) \otimes (a|0\rangle + b|1\rangle).$$

We can't clone information, but could we transmit it?

$$|\psi\rangle \otimes |\chi\rangle \mapsto |\xi\rangle \otimes |\psi\rangle$$

We can do this if we share an entangled state, even without being at the same place.

Here is the idea. Let Alice have the qubit $|\psi\rangle_C = \alpha|0\rangle_C + \beta|1\rangle_C$. She wants to send this to Bob. Suppose Alice and Bob share an entangled state

$$|\Phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle_{AB} + |11\rangle_{AB}).$$

The three particles state can be written as

$$\begin{aligned}
|\psi\rangle_C \otimes |\Phi^+\rangle_{AB} &= \frac{1}{\sqrt{2}}(\alpha|000\rangle_{CAB} + \alpha|011\rangle_{CAB} + \beta|100\rangle_{CAB} + \beta|111\rangle_{CAB}) \\
&= \frac{1}{2}|\Phi^+\rangle_{CA} \otimes (\alpha|0\rangle_B + \beta|1\rangle_B) + \frac{1}{2}|\Phi^-\rangle_{CA} \otimes (\alpha|0\rangle_B - \beta|1\rangle_B) \\
&\quad + \frac{1}{2}|\Psi^+\rangle_{CA} \otimes (\alpha|1\rangle_B + \beta|0\rangle_B) + \frac{1}{2}|\Psi^-\rangle_{CA} \otimes (\alpha|1\rangle - \beta|0\rangle_B),
\end{aligned}$$

where

$$|\Phi^\pm\rangle_{CA} = \frac{1}{\sqrt{2}}(|00\rangle_{CA} \pm |11\rangle_{CA}), \quad |\Psi^\pm\rangle_{CA} = \frac{1}{\sqrt{2}}(|01\rangle_{CA} \pm |10\rangle_{CA}).$$

Now Alice's goal is to project onto one of $|\Phi^\pm\rangle_{CA}$, $|\Psi^\pm\rangle_{CA}$. Note that she has access to the particles C and A. If the outcome is $|\Phi^+\rangle_{CA}$, then she knows that Bob's state would be a copy. If the outcome is $|\Phi^-\rangle_{CA}$, then Alice could call Bob and tell him to act with $\left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$. To project it, Alice can apply the CNOT operation.

You still need to send some classical information. So complete quantum transportation is not possible faster than the speed of light.

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