8.05 Fall 2024

David Lee

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1 Lecture 1 (2024-09-04)

No notes available.

2 Recitation 1 (2024-09-05)

2.1 Variational Principle

We have the Schrödinger equation:

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

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

Normally, we want to find eigenfunctions and eigenstates $E_n\varphi_n = \hat{H}\varphi_n$.

We will now discuss the following theorem:

Theorem 2.1(Variational Principle)

Given $\hat{H}$ with eigenvalues $E_0 \leq E_1 \leq E_2$ and corresponding eigenfunctions φ_0, φ_1, and φ_2, any trial wavefunction ψ provides a bound on the ground state E_0 of the system as follows:

$$F[\psi] = \frac{\int \psi^*(x)\hat{H}\psi(x)\mathrm{d}x}{\int \psi^*\psi\mathrm{d}x} \geq E_0$$

Proof. We can expand any trial wavefunction over our eigenfunctions:

$$\psi(x) = \sum_n a_n\varphi(x)$$

Remember that these eigenfunctions are orthonormal, i.e.

$$\int \mathrm{d}x\varphi_n^*(x)\varphi_m(x) = \delta_{mn}$$

where δ is the kronecker delta function.

Expanding,

$$F[\psi] = \frac{\int \mathrm{d}x \sum_n a_n^*\varphi_n(x)^*\hat{H}\sum_m a_m\varphi_m(x)}{\int \mathrm{d}x \sum_n a_n^*\varphi_n^*(x)\sum_m a_m\varphi_m(x)}$$

The integral in the denominator becomes

$$\sum_n\sum_m \int \mathrm{d}x\varphi_n^*\varphi_m = \sum_n a_n^*a_n$$

Similarly, the numerator becomes

$$\int \mathrm{d}x \sum_n a_n^* \phi_n^* \sum_m a_m E_m \phi_m = \sum_n a_n^* a_n E_n$$

Therefore,

$$F[\psi] = \frac{\sum_n |a_n^2| E_n}{\sum_n |a_n|^2}$$

Since all energies are at least the ground state,

$$F[\psi] \geq \frac{\sum_n |a_n|^2 E_0}{\sum_n |a_n|^2} = E_0$$

□

For example, let's consider the harmonic oscillator, $V = \frac{1}{2}m\omega^2 x^2$. What trial functions can we use?

In physics, there are only two functions, polynomials and exponents. The ground state should be even, and it should vanish as $|x|$ gets large. With this in mind, let's guess the following trial wavefunction:

$$\psi_1(x) = \begin{cases} \frac{N}{a^{9/2}}(x-a)^2(x+a)^2 & |x| \leq a \\ 0 & |x| > a \end{cases}$$

Now,

$$\langle F \rangle = \langle \hat{H} \rangle_{\psi_1} = \int_{-a}^{a} \mathrm{d}x \psi_1^* \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2 \right) \psi_1$$

We can split this into two integrals (the complex conjugations disappear because ψ is real):

$$-\frac{\hbar^2}{2m}\int_{-a}^{a} \mathrm{d}x \psi_1 \psi'' = \frac{\hbar^2}{2m}\int_{-a}^{a} \mathrm{d}x (\psi_1')^2 = \frac{\hbar^2}{2m}\frac{3}{a^2}$$

and

$$\frac{1}{2}m\omega^2 \int_{-a}^{a} x^2 \psi_1^2 \mathrm{d}x = \frac{1}{2}m\omega^2 \frac{a^2}{11}$$

So,

$$\langle H \rangle_{\psi_1} = f(a) = \frac{m\omega^2}{22}a^2 + \frac{3\hbar^2}{2ma^2} \geq \sqrt{\frac{3}{11}}\hbar\omega \approx 0.522\hbar\omega$$

Now, let's try another trial function:

$$\psi_2 = \sqrt{\alpha} e^{-\alpha|x|}$$

We can calculate:

$$\langle F \rangle = \int_{-\infty}^{\infty} \mathrm{d}x \psi_1 \hat{H} \psi_1 = \frac{\hbar^2}{2m}\int_{-\infty}^{\infty} \mathrm{d}x (\psi_1')^2 + \frac{m\omega^2}{2}\int_{-\infty}^{\infty} x^2 \psi_1^2 \mathrm{d}x$$

After calculating this (we ran out of time), we will get $\hbar\omega/\sqrt{2}$.

3 Lecture 2 (2024-09-09)

Last time, we discussed the variational principle and vector spaces. Today, we will talk about linear operators.

3.1 Linear Operators

Definition 3.1(Linear Operator)

A linear operator $\hat{T}$ on a vector space V is a map that takes a vector $v \in V$ to a vector $u \in V$. It must satisfy linearity properties:

1. $$\hat{T}(u+v) = \hat{T}u + \hat{T}v$$

2. $$\hat{T}(av) = a\hat{T}(v)$$

These can be condensed into the following

$$\forall a, b \in \mathbb{F}, \forall u, v \in V, \hat{T}(au+bv) = a\hat{T}u + b\hat{T}v$$

These properties imply $\hat{T} \cdot 0 = 0$. There is also a linear operator $\hat{0}(v) = 0$. So there are three different types of 0 so far.

Let's define $\mathcal{L}(V)$ to be the set of all linear operators on V.

Example 3.1

Let V be a vector space of real polynomials of a real variable x. Are the following operators linear?

1) $$\hat{S}(p) = (3x^2 - 5x + 2)p$$

2) $$\hat{D}(p) = \frac{\mathrm{d}}{\mathrm{d}x}p$$

3) $$\hat{R}(p) = p^3$$

4) $$\hat{Q}(p) = \int_{-1}^{1} p\mathrm{d}x$$

All but the third are linear.

Remark: $\mathcal{L}(V)$ also forms a vector space. We define addition as follows:

$$\forall S, T \in \mathcal{L}(V), (S+T)(v) = S(v) + T(v)$$

For scalar multiplication:

$$\forall a \in \mathbb{F}, T \in \mathcal{L}(v), (aT)v = aTv$$

Remark: There are also some properties, however, that operators have that vector spaces in general do not. For example, operators in $\mathcal{L}(v)$ can be multiplied.

Definition 3.2(Operator multiplication)

$$\forall S, T \in \mathcal{L}(v)$$

we define

$$(ST)v = S(Tv)$$

We can check that ST is linear. Therefore, $ST \in \mathcal{L}(v)$.
This multiplication is associative, but not commutative in general.

Example 3.2

Consider $V = \{(x_1, x_2, x_3, \ldots)\}$, the set of infinite dimensional vectors. Define

$$\hat{L}(x_1, x_2, x_3, \ldots) = (x_2, x_3, x_4, \ldots)$$
$$\hat{R}(x_1, x_2, x_3, \ldots) = (0, x_1, x_2, \ldots)$$

Note that $LR = \not\Vdash$. However,

$$RL(x_1, x_2, \ldots) = (0, x_2, x_3, \ldots)$$

Therefore, we can calculate the *commutator*:

$$[L, R] = LR - RL = P$$

where

$$P(x_1, x_2, \ldots) = (x_1, 0, 0, \ldots)$$

Definition 3.3(Nullspace)

The null space or *kernel* of $T \in \mathcal{L}(V)$ is the subset of V that is mapped to the 0 vector by T.

$$\text{null}(T) = \{v \in V | T(v) = 0\}$$

Note that the null space forms a subspace of V.

Definition 3.4(Range)

The range of $T \in \mathcal{L}(v)$ is the image of V under T.

$$\text{range}(T) = \{Tv, v \in V\}$$

The range also forms a subspace of V.

Definition 3.5(Injectivity)

A map T is injective (1 to 1) if $T(u) = T(v) \iff u = v$.
This injectivity condition is equivalent to saying $\text{null}(T) = \{0\}$.

Definition 3.6(Surjectivity)

A map T is surjective (onto) if the $\text{range}(T) = V$.
Note that $\dim(V) = \dim(\text{null}(T)) + \dim(\text{range}(T))$

Definition 3.7(Inverse)

For $T \in \mathcal{L}(v)$, if $ST = \infty$, then S is a left inverse of T. If $TS' = \infty$, then S' is a right inverse of T.
If both exist, then we must have that $S = S'$ and unique, and it is called the inverse, and T is called invertible, and $S = S' = T^{-1}$.

T is invertible iff T is injective and surjective. The proof will be more clear when we get on to the deeper structure.

3.2 Matrix Representation

Matrix representation is just some choice of basis, so it is not a universal representation. But it can be useful in many cases.

Consider a vector space V and an ordered basis $\{v_1, v_2, \ldots\}$. Given a linear operator T,

$$T(v_1) = T_{11}v_1 + T_{21}v_2 + \ldots$$
$$T(v_2) = T_{12}v_1 + T_{22}v_2 + \ldots$$

More generally,

$$T(v_j) = \sum_i T_{ij}v_i$$

In this way, if we have a finite dimensional vector space, we can construct a finite dimensional matrix $T(\{v\})$. $\{T_{ij}\}$ are called the matrix elements.

In 8.04, we may have equated matrices to operators, but now that we are grown-ups taking 8.05, we understand that these matrix representations are a result of our basis and so they are not unique.

If we define $\text{mat}(\cdot)$ to mean the matrix representation of something, then $\text{mat}(Ta) = \text{mat}(T)\text{mat}(a)$ and $\text{mat}(TS) = \text{mat}(T) \cdot \text{mat}(S)$.

We can also think about changing bases. Given two bases $\{v_1, v_2, \ldots, v_n\}$, and $\{u_1, u_2, \ldots, u_n\}$. Consider $T \in \mathcal{L}(V)$. We want to look at two matrix representations, $T(\{V\})$ and $T(\{u\})$. We claim that

$$T(\{u\}) = A^{-1}T(\{v\})A$$

and

$$T(\{v\}) = AT(\{u\})A^{-1}$$

Proof. Let A be a linear operator such that $Av_i = u_i$. We claim that $A_{ij}(\{v\}) = A_{ij}(\{u\})$. To see this,

$$Au_k = \sum_i A_{ik}(\{u\})u_i$$

but

$$Au_k = AAv_k = A\sum_i A_{ik}(\{v\})v_i = \sum_i A_{ik}(\{v\})u_i$$

Now consider

$$Tu_k = \sum_i T_{ik}(\{u\})u_i = \sum_i T_{ik}(\{u\})Av_i = \sum_{i,l} T_{ik}(\{u\})A_{li}(\{v\})v_l$$

but

$$Tu_k = TAv_k = \sum_{j,l} T_{lj}(\{v\})A_{jk}v_l$$

Therefore,

$$\sum_i A_{li}T_{ik}(\{u\}) = \sum_j T_{lj}(\{v\})A_{jk}$$

and so

$$T(\{u\}) = A^{-1}T(\{v\})A$$

□

Definition 3.8(Trace)

The trace of a matrix is defined as

$$\text{Tr}(M) = \sum_i M_{ii}$$

Note: $\text{Tr}(AB) = \text{Tr}(BA)$. Because of this, we get

$$\text{Tr}(T\{v\}) = \text{Tr}(AT(\{u\})A^{-1}) = \text{Tr}(T(\{u\})) = \text{Tr}(T)$$

Definition 3.9(Determinant)

$$\det(AB) = \det(A)\det(B)$$

Note that this implies

$$\det(T\{v\}) = \det(AT(\{u\})A^{-1}) = \det(T(\{u\})) = \det(T)$$

4 Recitation 2 (2024-09-10)

Last time we discussed the harmonic oscillator. We discussed this powerful principle where we could bound the ground state energy of the harmonic oscillator. In particular, we considered

$$\psi_1(x) = \begin{cases} \frac{N}{a^{9/2}}(x-a)^2(x+a)^2 & |x| \le a \\ 0 & |x| > a \end{cases}$$

which gave us $\hbar\omega\sqrt{\frac{3}{11}}$, and

$$\psi_2(x) = \alpha^{1/2}e^{-\alpha|x|},$$

which gave us $\hbar\omega/\sqrt{2}$.

Let's try to improve our estimate. We'll use the trial function

$$\psi_3 = \left(\frac{2\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2}$$

We can use the same pattern to calculate the integral:

$$I_1 = \frac{\hbar^2}{2m}\int_{-\infty}^{\infty}(\psi')^2\mathrm{d}x = \frac{\hbar^2}{2m}\int_{-\infty}^{\infty}\left(\frac{2\alpha}{\pi}\right)^{1/2}\cdot 4\alpha^2x^2e^{-2\alpha x^2}\mathrm{d}x = \frac{\hbar^2}{2m}\sqrt{\frac{2\alpha}{\pi}}\cdot 4\alpha^2\cdot\frac{\sqrt{\pi}}{2\sqrt{(2\alpha)^3}} = \frac{\hbar^2\alpha}{2m}$$

$$I_2 = \frac{m\omega^2}{2}\int_{-\infty}^{\infty}x^2\psi^2\mathrm{d}x = \frac{m\omega^2}{2}\int_{-\infty}^{\infty}\left(\frac{2\alpha}{\pi}\right)^{1/2}\cdot x^2e^{-2\alpha x^2} = \frac{m\omega^2}{8\alpha}$$

Minimizing

$$I_1 + I_2 = \frac{\hbar^2\alpha}{2m} + \frac{m\omega^2}{8\alpha} \ge \frac{\hbar\omega}{2}$$

gives the exact result. Of course, this is because we have guessed the exact form of the ground state.

Now, can we guess the values of excited states? It turns out we can. Let's guess a trial function of the form

$$\psi_4 = Nxe^{-\alpha x^2}$$

This will give us $\hbar\omega\cdot\frac{3}{2}$. Let's try to find a way to calculate how close we are. Let E be the result of $F[\psi]$ from $\psi = \sum_c a_c\varphi_c$. Define

$$\sigma^2 = \frac{\int\psi^*(\hat{H}-E)^2\psi\mathrm{d}x}{\int|\psi|^2\mathrm{d}x}$$

We claim that there exists at least one energy eigenvalue in $[E-\sigma, E+\sigma]$.

Proof.

$$\sigma^2 = \frac{\sum_c (E_c - E)^2 |a_c|^2}{\sum_c |a_c|^2}$$

Let E_k be the eigenvalue closest to E (the eigenvalue such that $E_k - E$ is the smallest). Then,

$$\sigma^2 \geq \frac{\sum_c (E_k - E)^2 |a_c|^2}{\sum_c |a_c|^2} = (E_k - E)^2$$

Therefore,

$$|E - E_k| \leq \sigma$$

□

So far we've discussed the simple example of the harmonic oscillator, but now let's give an example of an actual problem we cannot solve exactly, but where we can use the variational principle to get an extremely accurate approximate spectrum.

The problem is eigenstates of the Helium atom. A helium atom consists of three things, a nucleus whose charge is $+Ze$, and two electrons. Let's make a coordinate system where the nucleus is at the origin and the positions of the electrons are $\vec{x_1}$ and $\vec{x_2}$. We can write the Hamiltonian as:

$$\hat{H} = \frac{\hat{p_1}^2}{2m} + \frac{\hat{p_2}^2}{2m} - \frac{Ze^2}{r_1} - \frac{Ze^2}{r_2} + \frac{e^2}{|x_1 - x_2|}$$

Without the extra repulsion term, the solution would just be

$$\psi(x_1, x_2) = \psi_{n_1,l_1,m_1}(x_1)\psi_{n_2,l_2,m_2}(x_2)$$

For future reference,

$$\psi_{100} = \left(\frac{Z^3}{\pi a_0^3}\right)^{1/2} \exp\left(-\frac{Zr}{a_0}\right)$$

The ground state would be $E = -Z^2 E_{Ry}\left(\frac{1}{n_1^2} + \frac{1}{n_2^2}\right) = -2Z^2 E_{Ry} = -110\,\text{eV}$. In reality, the observed energy is $E_0 = -79\,\text{eV}$.

Let's try a trial wavefunction of the form

$$\psi_\alpha = \left(\frac{\alpha^3}{\pi a_0^3}\right)^{1/2} e^{-\alpha r/a_0}$$

Let

$$f(\alpha) = F[\psi_\alpha] = \int \mathrm{d}^3x_1 \mathrm{d}^3x_2 \psi_\alpha^*(x_1)\psi_\alpha^*(x_2)\hat{H}\psi_\alpha(x_1)\psi_a lpha(x_2)$$

Let $\hat{H}_\alpha(r,p) = \frac{p^2}{2m} - \frac{\alpha e^2}{r}$. Then,

$$\hat{H} = \hat{H}_\alpha(r_1, p_1) + \hat{H}_\alpha(r_2, p_2) + e^2\left((\alpha - Z)\left(\frac{1}{r_1} + \frac{1}{r_2}\right) + \frac{1}{|x_1 - x_2|}\right)$$

Our ψ_α are already eigenvalues of $\hat{H}_\alpha$. What remains is

$$e^2(\alpha - Z)\int \mathrm{d}^3x_1\mathrm{d}^3x_2|\psi_1|^2|\psi_2^2|\left(\frac{1}{r_1}+\frac{1}{r_2}\right) = 2e^2(\alpha-Z)\int \mathrm{d}^3x_1\frac{|\psi_1|^2}{r_1}$$

and

$$e^2\int \mathrm{d}^3x_1\mathrm{d}^3x_2\frac{|\psi(x_1)|^2|\psi(x_2)|^2}{|x_1-x_2|}$$

The first integral is pretty standard, and will reduce to $2e^2(\alpha-Z)\frac{\alpha}{a_0}$.

For the second integral, let's use spherical coordinates with x_1 as the z axis. Then $|x_1-x_2| = \sqrt{r_1^2+r_2^2-2r_1r_2\cos\theta}$. The integral becomes

$$e^2\int r_1^2\mathrm{d}r_1r_2^2\mathrm{d}r_2\int_{-1}^{+1}\mathrm{d}\cos\theta\frac{1}{\sqrt{r_1^2+r_2^2-2r_1r_2\cos\theta}}$$

The integral with the cosine is pretty easy to do. It will become

$$\int r_1^2\mathrm{d}r_1\int r_2^2\mathrm{d}r_2\frac{|r_1-r_2|-|r_1+r_2|}{2r_1r_2}$$

$$= 2\int_{r_1=r_2}^{\infty} r_1^2\mathrm{d}r_1\int_{r_2}^{\infty}\frac{r_1-r_2-r_1-r_2}{2r_1r_2}$$

At the end we will get $\frac{5}{4}\alpha E_{Ry}$.

Summing everything,

$$f(\alpha = (-2\alpha^2+4(\alpha-Z)\alpha)+\frac{5}{4}\alpha)E_{Ry}$$

Minimizing gives $\alpha_{\min} = Z-\frac{5}{16}$. We

$$E_{\alpha_{\min}} = -2\left(Z-\frac{5}{16}\right)^2 E_{Ry} = -77.5\,\mathrm{eV}$$

This is within 2% of the correct answer!

5 Lecture 3 (2024-09-11)

Today we'll continue with definitions but also talk about some non-trivial properties.

5.1 Eigenvalues and Eigenvectors

We will try to organize a vector space

$$V = U_1\oplus U_2\oplus\ldots\oplus U_m$$

in relation to a linear operator T.

Consider a subspace

$$U = \{au | a \in \mathbb{F}\}$$

If U is invariant under $T \in \mathcal{L}(V)$, (i.e. $Tu \in U$ for all $u \in U$), then we can write

$$T(u) = \lambda u$$

Whenever we see this, λ is called an eigenvalue of this operator and u is an eigenvector of T.

It may be the case that

$$U = \text{span}(u_1, u_2, \ldots, u_n)$$

where

$$Tu_i = \lambda u_i$$

for each i. Then, we say that λ is degenerate with geometric multiplicity equal to $\dim(U)$. We say that U is an *invariant subspace* of V with respect to T with eigenvalue λ.

We can have different subspaces for different eigenvalues, i.e. $\lambda_1 \to U_1$, $\lambda_2 \to U_2$, and so on.

How can we find these eigenvalues? We can write this equation as

$$(T - \lambda I)u = 0$$

If u is non-trivial, i.e. $u \neq 0$, then we must have that $T - \lambda I$ is non invertible (otherwise we could multiply by the inverse to get $u = 0$). This is equivalent to solving $\det(T - \lambda I) = 0$.

We might wonder, does an eigenvalue always exist? The answer turns out to be no for real vector spaces. For example, consider

$$R = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

(note that this is the 90° rotation matrix). But solving $\det(R - \lambda I) = 0 \implies \lambda = \pm i$, so there is no real eigenvalue.

However, the answer is different for complex vector spaces.

Theorem 5.1

Every linear operator in a finite-dimensional complex vector space has at least one eigenvector (and corresponding eigenvalue).

5.2 Inner Product

Let's consider a vector space

$$V = \text{span}(v_1, v_2, v_3)$$

Definition 5.2(Inner product)

An inner product is a map from a pair of vectors to a number in $\mathbb{F}$ satisfying the following properties:

1. $$\langle v, v\rangle \geq 0$$
2. $$\langle v, v\rangle = 0 \iff v = 0$$
3. $$\langle u, av_1 + bv_2\rangle = a\langle u, v_1\rangle + b\langle u, v_2\rangle \quad \forall a, b \in \mathbb{F},\ v_1, v_2, u \in V$$
4. $$\langle u, v\rangle = \langle v, u\rangle^*$$

Definition 5.3(Orthogonality)

Two vectors $u, v \in V$ are orthogonal if $\langle u, v\rangle = 0$.

Definition 5.4(Norm)

The norm of a vector $v \in V$, denoted $|v|$ or $\|v\|$, as

$$|v|^2 = \langle v, v\rangle$$

and $|v| \geq 0$.
If a vector has norm 1 we say that it is normalized.

Ok, let's talk about a little physics today. In 8.04 we learned how to calculate one version of an inner product of two wavefunctions:

$$\langle \psi_1, \psi_2\rangle = \int_{-\infty}^{\infty} \psi_1^* \psi_2 \mathrm{d}x$$

One physical interpretation of the inner product is the distinguishability of the two wavefunction. When the inner product is 0, there is a measurement where you can tell the difference between the two wavefunctions with 100% probability. If it's 1, then there is no way to tell the difference.

Conceptually, the vector space plus our inner product is what we call a Hilbert Space.

Let's also talk about some properties that will be useful later.

Theorem 5.5(Schwartz Inequality)

$$\langle u, v\rangle \leq |u| \cdot |v|$$

We can prove this by taking

$$w = u - \frac{\langle v, u\rangle\, v}{|v|^2}$$

and requiring $|w| > 0$.

Theorem 5.6(Triangle Inequality)

$$|u + v| \leq |u| + |v|$$

Definition 5.7(Orthonormal bases)

We define a set of vectors $\{e_1, e_2, \ldots, e_n\}$ to be orthonormal if $\langle e_i, e_j\rangle = \delta_{ij}$.
If $n = \dim(V)$, then $\{e_1, e_2, \ldots, e_n\}$ forms an orthonormal basis (ONB).
For all $v \in V$, we can write

$$v = \sum_i a_i e_i,$$

and we can easily compute $a_k = \langle v, e_k\rangle$.
This also gives a nice way to calculate the matrix representation of an operator $T \in \mathcal{L}(V)$: $T_{ij} = \langle e_i, Te_j\rangle$.

Theorem 5.8(Gram Schmidt Procedure)

Given a list of vectors $\{v_1, v_2, \ldots, v_n\}$ that are linearly independent, we can produce an orthonormal list of vectors $\{e_1, e_2, \ldots, e_n\}$ as follows:
First, let $e_1 = v_1/|v_1|$. Now, let $\tilde{e_2} = v_2 - \langle e_1, v_2\rangle\, e_1$. Now we can let $e_2 = \tilde{e_2}/|\tilde{e_2}|$.
We can repeat this procedure:

$$\tilde{e_k} = v_k - \sum_{i=1}^{k-1} \langle e_i, v_k\rangle\, e_i$$

$$e_k = \frac{\tilde{e_k}}{|\tilde{e_k}|}$$

Because the vectors are linearly independent, it is trivial to show that $|\tilde{e_k}|$ is never equal to 0.

5.3 Orthogonal subspaces

Let $U \subset V$ be a subspace.

Definition 5.9(Orthogonal Complement)

Define the orthogonal complement

$$U^\perp = \{v \in V | \langle v, u\rangle = 0 \; \forall u \in U\}$$

We claim that

$$U \oplus U^\perp = V$$

Proof. The claim is equivalent to the claim that we can choose unique $u + u_\perp = v$ such that $u \in U$ and $u_\perp \in U^\perp$.

Let $\{e_1, e_2, \ldots, e_n\}$ be an orthonormal basis for U.

$$\forall v \in V \quad v = \sum_i \langle e_i, v\rangle \, e_i + v - \sum_i \langle e_i, v\rangle \, e_i$$

It's trivial to see that

$$\sum_i \langle e_i, v\rangle \, e_i \in U$$

and that

$$v - \sum_i \langle e_i, v\rangle \, e_i \in U^\perp$$

It remains to prove that $U \cap U^\perp = \{0\}$. Let $w \in U \cap U^\perp$. Then, by definition, $\langle w, w\rangle = 0$, which implies $w = 0$. □

Definition 5.10(Orthogonal Projectors)

Define P_U to be a linear map that projects onto U. That is, for every $v = u + u_\perp$, where $u \in U$ and $u_\perp = U^\perp$, then $P_U(v) = u$.
A more explicit way to write this is

$$P_U(v) = \sum_{i=1}^{\dim(U)} \langle e_i, v\rangle \, e_i$$

where $\{e_i\}$ is an orthonormal basis of U.

6 Recitation 3 (2024-09-12)

Today we will deep dive into vector spaces. Consider one example:

$$V = \left\{ \begin{pmatrix} a \\ b \end{pmatrix} \middle| \, a, b \in \mathbb{R}, b > 0 \in \right\}$$

We define addition as

$$\begin{pmatrix} a_1 \\ b_1 \end{pmatrix} + \begin{pmatrix} a_2 \\ b_2 \end{pmatrix} = \begin{pmatrix} a_1 + a_2 \\ b_1 b_2 \end{pmatrix}$$

and scalar multiplication is

$$c \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} ca \\ b^c \end{pmatrix}$$

Let's check if our vector space satisfies the axioms presented in class.

1. Closure
$$\begin{pmatrix} c \\ d \end{pmatrix} = \begin{pmatrix} a_1 \\ b_1 \end{pmatrix} + \begin{pmatrix} a_2 \\ b_2 \end{pmatrix} = \begin{pmatrix} a_1 + a_2 \\ b_1 b_1 \end{pmatrix} \in V$$
2. Commutativity
$$\begin{pmatrix} a_1 \\ b_1 \end{pmatrix} + \begin{pmatrix} a_2 \\ b_2 \end{pmatrix} = \begin{pmatrix} a_2 \\ b_2 \end{pmatrix} + \begin{pmatrix} a_1 \\ b_1 \end{pmatrix}$$
3. Associativity
$$(u + v) + w = u + (v + w)$$
4. Existence of an identity
$$\exists \phi | \phi + \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} a \\ b \end{pmatrix}$$
We see that $\phi = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ works.
5. Existence of additive inverse.
$$\forall u \in V \exists v \in V | u + v = \phi$$
If $u = \begin{pmatrix} a \\ b \end{pmatrix}$, we can just choose $v = \begin{pmatrix} -a \\ 1/b \end{pmatrix}$.
6. Multiplicative identity
$$1 \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} a \\ b \end{pmatrix}$$
7. Distributivity
$$(a + b)v = av + bv \quad \forall a, b \in \mathbb{R}, v \in V$$
We can check that
$$(a + b) \begin{pmatrix} c \\ d \end{pmatrix} = \begin{pmatrix} (a + b)c \\ d^{a+b} \end{pmatrix} = \begin{pmatrix} ac \\ d^a \end{pmatrix} + \begin{pmatrix} bc \\ d^b \end{pmatrix}$$
We should also have
$$r \left(\begin{pmatrix} a \\ b \end{pmatrix} + \begin{pmatrix} c \\ d \end{pmatrix} \right) = r \begin{pmatrix} a + c \\ bd \end{pmatrix} = \begin{pmatrix} r(a + c) \\ b^r d^r \end{pmatrix} = \begin{pmatrix} ra \\ b^r \end{pmatrix} + \begin{pmatrix} rc \\ d^r \end{pmatrix}$$

8. Compatibility

$$(rs)\begin{pmatrix}a\\b\end{pmatrix} = r\left(s\begin{pmatrix}a\\b\end{pmatrix}\right) \quad \forall r, s \in \mathbb{R}$$

Therefore, this vector space is good.

Let's consider another example.

$$V = \{(x, y, z) \in \mathbb{R}^3 | 3x + 4y - 2z = 1\}$$

Define addition and scalar multiplication to be

$$(x_1, y_1, z_1) + (x_2, y_2, z_2) = (x_1 + x_2, y_1 + y_2, z_1 + z_2)$$
$$a(x, y, z) = (ax, ay, az)$$

This does not satisfy the properties of a vector space. So let's try to fix this by redefining our addition and scalar multiplication:

$$(x_1, y_1, z_1) + (x_2, y_2, z_2) = (x_1 + x_2 + r, y_1 + y_2, z_1 + z_2)$$

We see that we should have $r = -1/3$ to satisfy closure. Now for multiplication:

$$a(x, y, z) = (ax + r(a - 1), ay, az)$$

We can easily check associativity and commutativity. Our additive identity is $\phi = (-r, 0, 0)$.

Let's check additive inverse. The additive inverse of (x, y, z) is $(-x - 2r, y, z)$.

Now let's do the last example for today. Let's see why vector spaces are useful. Consider a vector space:

$$V = \{x | x \in \mathbb{Q}, x \in (-1, 1)\}$$

We define

$$x + y = \frac{x + y}{1 + xy}$$

and

$$\alpha x = \frac{(1 + x)^\alpha - (1 - x)^\alpha}{(1 + x)^\alpha + (1 - x)^\alpha}$$

One fun fact we can see is

$$x + y = \tanh(\tanh^{-1}(x) + \tanh^{-1}(y))$$
$$\alpha x = \tanh(\alpha \tanh^{-1}(x))$$

This is just the formula for relativistic velocity addition. It turns out that relativistic velocities form a vector space! We can use this to solve some interesting problems.

Imagine we have a caravan of spaceships in line with the l^{th} spaceship seeing the $(l + 1)^{\text{th}}$ moving at velocity v. The first spaceship moves at velocity v with respect to the lab frame. What is the apparent velocity of the n^{th} spaceship as seen in the lab frame?

With our vector space interpretation, this problem is trivial. The answer is simply

$$n \cdot v = \frac{(1 + v)^n - (1 - v)^n}{(1 + v)^n + (1 - v)^n}$$

One bonus fact:

Theorem 6.1

If we have a function $f:\mathbb{R} \to V$ is a 1-1 mapping, then V with the operations

$$x + y = f(f^{-1}(x) + f^{-1}(y))$$

$$\alpha x = f(\alpha f^{-1}(x))$$

is a vector space.

7 Lecture 4 (2024-09-16)

We are done with 3 lectures on linear algebra, and there are three more. The next three will be more tuned to applications to quantum mechanics.

Where are we going?

Math	QM
Vectors	Quantum states
Hilbert space	Space of all possible states
Inner product	"Distance", distinguishability
Orthonormal basis	A set of all perfectly distinguishable states
Linear operators	Operators
Orthogonal projection	Measurement
Eigenvalues	Label for measurement outcomes

We are being very abstract here. But this is how we can make mathematical discoveries. So let's continue.

7.1 Adjoint

Given $T \in \mathcal{L}(V)$ and an inner product, we can construct the adjoint of T, $T^\dagger$.

Definition 7.1(Linear functional)

A linear functional ϕ is a map $\phi:V \to \mathbb{F}$ such that

$$\phi(av + bw) = a\phi(v) + b\phi(w)$$

Theorem 7.2

For any linear functional ϕ on V, there exists a unique $u \in V$ such that

$$\phi(v) = \langle u, v \rangle \, \forall v \in V$$

We will define **Dirac notation** as $\langle u|v\rangle = \langle u, v\rangle$. The advantage of this is that we can think of $|v\rangle$ as a vector and $\langle u|$ as a linear functional.

Now let's define adjoint.

Definition 7.3(Adjoint)

We define $T^\dagger$ through the following formula:

$$\left\langle T^\dagger u, v\right\rangle = \langle u, Tv\rangle$$

This is also called the Hermitian conjugate.

We can show that $T^\dagger$ is also a linear operator.

Proof. Consider

$$\begin{aligned}&\langle au_1 + bu_2, Tv\rangle\\ &= a^* \langle u_1, Tv\rangle + b^* \langle u_2, Tv\rangle\\ &= \left\langle aT^\dagger u_1, v\right\rangle + \left\langle bT^\dagger u_2, v\right\rangle\end{aligned}$$

□

Note. For $S, T \in \mathcal{L}(V)$,

$$(ST)^\dagger = T^\dagger S^\dagger$$

Also, $(T^\dagger)^\dagger = T$.

Let's talk a bit about matrix representation. Given an orthonormal basis $\{e_1, e_2, \ldots, e_n\}$, and an operator

$$\hat{T} \to T_{ij} = \langle e_i, Te_j\rangle$$

Then, we can write

$$\begin{aligned}\hat{T}^\dagger = (T^\dagger)_{ij} &= \left\langle e_i, T^\dagger e_j\right\rangle\\ &= \langle Te_i, e_j\rangle = \langle e_j, Te_i\rangle^* = T^*_{ji}\end{aligned}$$

7.2 Hermitian Operators

Definition 7.4(Hermitian)

An operator T is Hermitian if $T^\dagger = T$. We also sometimes call this self-adjoint.
We can think of this as the operator equivalent of a real number. As it turns out, being Hermitian is closely related to observables in quantum mechanics.

Theorem 7.5

$\langle v, Tv\rangle$ is real for all $v \in V$ if and only if T is Hermitian.

Proof. First, we can prove that if T is Hermitian, then $\langle v, Tv\rangle$ is real. We can write

$$\langle v, Tv\rangle^* = \left\langle T^\dagger v, v\right\rangle^* = \left\langle v, T^\dagger v\right\rangle = \langle v, Tv\rangle$$

For the other direction, some portion of this will be on the homework. On the homework, we will prove that for a complex vector space V and a linear operator T, if $\langle v, Tv\rangle = 0$ for all $v \in V$, then $T = 0$. Assuming this theorem, let's complete the proof.

Given

$$\langle v, Tv\rangle = \langle v, Tv\rangle^* = \langle Tv, v\rangle = \left\langle v, T^\dagger\right\rangle v$$

Therefore,

$$\left\langle v, (T - T^\dagger)v\right\rangle = 0$$

Therefore, $T - T^\dagger = 0$ and so $T = T^\dagger$. □

Definition 7.6(Anti-Hermitian)

An operator is anti-hermitian if $T^\dagger = -T$.

Note that this leads to the following fact: any operator O can be written as $O = H + iA$ where H and A are hermitian. We can do this by writing $H = \frac{1}{2}(O + O^\dagger)$ and $iA = \frac{1}{2}(O - O^\dagger)$

Note. Any eigenvalue of a Hermitian operator must be real. This is a direct result of the above theorem.

Theorem 7.7

Another interesting result is that if v_1 and v_2 are eigenvalues of a hermitian operator T with different eigenvalues, then we must have that $\langle v_1, v_2\rangle = 0$.

Let's revisit orthogonal projectors. We have the following theorem:

Theorem 7.8

If $P \in \mathcal{L}(V)$ and $P^2 = P$, then $P^\dagger = P$. The proof is a good exercise, below is a sketch: We want to prove that (a) $\forall \omega \in \text{range}(P)$, $P\omega = \omega$, and (b) $\forall v \in V$ $v = v - Pv + Pv$. Then, all we need to show is that for $u \in \text{range}(P)$ and $v \in \text{null}(P)$, $\langle v, Pu\rangle = \langle v, u\rangle$ and $\langle Pv, u\rangle = 0$.

7.3 Unitary Operators

Definition 7.9(Unitary)

The definition of a unitary operator $\hat{U} \in \mathcal{L}(V)$ is an operator that is surjective and does not change the norm.

$$\forall v \in V, \quad |v| = |\hat{U}v|$$

Immediately, we can get that

1. $(\hat{U}) = \{0\}$.
2. $\hat{U}$ is invertible
3. $U^\dagger U = UU^\dagger = 1$
4. $\langle Ua, Ub\rangle = \langle a, b\rangle$

What unitary operators describe are rotations of the basis. Unitary operators will always map an orthonormal basis to another orthonormal basis.

7.4 Functions of Operators

We have seen that given linear operators T or S, we can create linear operator such as $T \cdot S$, $T^2 = T \cdot T$, T^k, and so on.

Let's say we have a function $f(x)$ which has a taylor series

$$f(x) = \sum_{n=0}^{\infty} c_n x^n$$

We can define

$$f(\hat{T}) = \sum_{n=0}^{\infty} c_n \hat{T}^n$$

Therefore, for any function whose power series is well defined, we can also compute the function of a linear operator. One particularly interesting one is

$$f(M) = e^M \in \mathcal{L}(V)$$

Also, if we have $h(x) = f(x)g(x)$, we will have $h(\hat{T}) = f(\hat{T}) \cdot g(\hat{T})$.

One other fact to note is that $f(\hat{M})^\dagger = f(\hat{M}^\dagger)$. So in particular $\left(e^M\right)^\dagger = e^{M^\dagger}$, and $\left(e^{iH}\right)^\dagger = e^{-iH} = \left(e^{iH}\right)^{-1}$. What we have just derived is the fact that for any hermitian operator H, we have e^{iH} is a unitary operator.

8 Recitation 4 (2024-09-17)

Because of the career fair on Friday, we will have no office hours on Friday. Instead, office hours will be Thursday at 1pm.

Today we'll discuss some linear algebra stuff.

8.1 Projection Operators

As a review, for a subspace, we can express

$$V = U \oplus U^{\perp}$$

where $U^{\perp}$ is the orthogonal complement of U. We can define a projection operator P_U that projects onto U.

If we have an orthonormal basis for V, $\{e_1, e_2, \ldots, e_n\}$, then we can write

$$U = \text{span}(e_1, e_2, \ldots, e_k)$$

and consequently $U^{perp} = \text{span}(e_{k+1}, e_{k+2}, \ldots, e_n)$.

With this, we can write

$$P_U v = \sum_{i=1}^{k} \langle e_i, v \rangle \, e_i$$

In our bra-ket notation, we can write

$$P_U = \sum_{i=1}^{k} |e_i\rangle\langle e_i|$$

Let's define for some orthonormal basis $\{e_1, e_2, \ldots, e_n\}$, the projection operator

$$P_j = \sum_{i=1}^{j} |e_i\rangle\langle e_i|$$

One interesting thing to note is that $P_n = \sum_{i=1}^{n} |e_i\rangle \langle e_i|$ that projects onto the entire space is the identity operator.

Also, $P_j^2 = P_j$. We can see this as follows:

$$P_j^2 = \left(\sum_{i=1}^{j} |e_i\rangle \langle e_i| \right) \left(\sum_{i=1}^{j} |e_i\rangle \langle e_i| \right) = \sum_{i_1=1}^{j} \sum_{i_2}^{j} |e_{i_1}\rangle \langle e_{i_1}|e_{i_2}\rangle \langle e_{i_2}|$$

$$= \sum_{i=1}^{j} |e_i\rangle \langle e_i| = P_j$$

Let's do an example of Gram-Schmidt. Consider a vector space V with an inner produce and a subspace $U \subset V$. Given $v \in V$ such that $v \notin U$, what is $u \in U$ for which $|v - u|$ is minimized? It turns out that the answer is $u = P_U v$. We will prove this on the pset.

This can be very useful. For example, let U be the space of polynomials, and let V be the space of nasty functions. In the pset, we will find the projection of $v = \cos \pi x$ onto U. In class, let's do this for the function $v = \sin \frac{\pi}{2} x$.

Let's first find an orthonormal basis for our simple polynomials: $\{1, x, x^2, x^3\}$ with the inner product defined as $\langle f|g\rangle = \int_{-1}^{1} f(x)g(x)\mathrm{d}x$. The first step is to use the Gram-Schmidt procedure to find an orthonormal basis.

The first vector will be $\hat{e_0} = \frac{e_0}{|e_0|}$. We see that $|e_0|^2 = \int_{-1}^{1} 1\mathrm{d}x = 2$. Therefore, $\hat{e_0} = \frac{1}{\sqrt{2}}$.

Now, we get

$$\hat{e_1} = \frac{e_1 - \langle e_1, \hat{e_0}\rangle \hat{e_0}}{|e_1 - \langle e_1, \hat{e_0}\rangle \hat{e_0}|}$$

Calculating,

$$\langle e_1, \hat{e_0}\rangle = \int_{-1}^{1} \mathrm{d}x \frac{x}{\sqrt{2}} = 0 \implies e_1 - \langle e_1, \hat{e_0}\rangle \hat{e_0} = 0$$

Now,

$$|e_1|^2 = \int_{-1}^{1} x^2 \mathrm{d}x = \frac{2}{3}$$

Therefore,

$$\hat{e_1} = \frac{e_1}{|e_1|} = \sqrt{\frac{3}{2}}x$$

Next,

$$\hat{e_2} = \frac{e_2 - \langle e_2, \hat{e_0}\rangle - \langle e_2, \hat{e_1}\rangle \hat{e_1}}{|e_2 - \langle e_2, \hat{e_0}\rangle - \langle e_2, \hat{e_1}\rangle \hat{e_1}|}$$

After calculating, we will get

$$\hat{e_2} = \left(\frac{45}{8}\right)^{1/2} \left(x^2 - \frac{1}{3}\right)$$

and

$$\hat{e_3} = N\left(x^3 - \frac{3}{5}x\right)$$

So now we want to project $\sin\frac{\pi}{2}x$ onto this basis. We can write

$$P_U \sin\frac{\pi}{2}x = \sum_{i=0}^{3} \left\langle e_i, \sin\frac{\pi}{2}x \right\rangle e_i$$

we can easily do that and then compare the answer. The final result should look like

$$P_U \sin\frac{\pi}{2}x = \frac{8}{\pi^2}\left(\frac{3}{2}\right)x + \frac{175}{8}\frac{96(\pi^2 - 10)}{5\pi^4}\left(x^3 - \frac{3}{5}x\right)$$

Note that this is not the same as the Taylor series! In fact, the projection is more accurate for the region $x \in [-1, 1]$. If we use our approximation at $x = 1$, we'll get 0.990963, while the Taylor series will give 0.9248.

Now, let's talk about unitary operators.

8.2 Unitary Operators

In Quantum Mechanics, unitary operators describe the time evolution of a system. There are two definitions:

1. Unitary operators are operators that preserve the norm of a vector.
2. Unitary operators are operators that are invertible and satisfy $U^\dagger U = UU^\dagger = 1$.

One way of thinking about the unitary condition is that forward and backward time evolution are consistent. This is a direct result of the fact that $U^\dagger U = 1$.

Theorem 8.1

Any matrix representation of a unitary operator U has columns that are orthogonal vectors.

Proof. For any orthonormal basis,

$$\delta_{ij} = \langle e_i, e_j \rangle = \langle e_i | I e_j \rangle = \langle e_i | \, U^\dagger U \, | e_j \rangle$$

By the completeness theorem,

$$I = \sum_{i=1}^{n} |e_i\rangle \langle e_i|$$

so

$$\delta_{ij} = \sum_{k=1}^{n} \langle e_i | \, U^\dagger \, | e_k \rangle \langle e_k | \, U \, | e_j \rangle$$

But $\langle e_i | \, U^\dagger \, | e_k \rangle = U^\dagger_{ik} = U^*_{ki}$, so

$$\delta_{ij} = \sum_{k=1}^{n} U^*_{ki} U_{kj}$$

Therefore, the columns of U are orthogonal. □

9 Lecture 5 (2024-09-18)

Let's continue talking about functions of operators.

9.1 Functions of Operators

Last time we talked about for a power series function

$$f(x) = \sum_{n=0}^{\infty} c_n x^n$$

we can extend this to operators by defining

$$f(\hat{T}) = \sum_{n=0}^{\infty} c_n \hat{T}^n$$

Last time, we wrote $f(T)^\dagger = f(T^\dagger)$. But actually, in the most general case where f can have complex coefficients, we should have $f(T)^\dagger = f^*(T^\dagger)$.

Also, recall that if $h(x) = g(x)f(x)$, then $h(T) = g(T)f(T)$.

Example 9.1

If $f(x) = 1$, then $f(\hat{T}) = 1$, the identity operator.
If $f(x) = e^{ix}$, then we can calculate $e^{i\hat{T}}$. We notice that

$$e^{ix}e^{-ix} = 1 \implies e^{i\hat{T}}e^{-i\hat{T}} = 1$$

If T is hermitian, then $(e^{iT})^\dagger = \left(e^{iT^\dagger}\right)^* = e^{-iT} = \left(e^{iT}\right)^{-1}$.
Therefore, for all Hermitian operators T, e^{iT} is unitary.

If we have two operators T_1 and T_2, do we think that it is true that

$$e^{T_1}e^{T_2} = e^{T_1+T_2}?$$

It turns out this is not true in general, which is why we need to be careful when dealing with functions of operators. Going back to definitions,

$$\text{LHS} = \left(\sum_{n=0}^{\infty} \frac{T_1^n}{n!}\right)\left(\sum_{m=0}^{\infty} \frac{T_2^n}{m!}\right)$$

As for the RHS,

$$\text{RHS} = \sum_{k=0}^{\infty} \frac{(T_1+T_2)^k}{k!}$$

If T_1 and T_2 don't commute, these two are not equal. But for now let's assume that $[T_1, T_2] = 0$.

$$\text{RHS} = \sum_{k=0}^{\infty} \frac{1}{k!} \sum_{n=0}^{k} \frac{k!}{n!(k-n)!} T_1^n T_2^{k-n} = \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} \frac{1}{n!}\frac{1}{m!} T_1^n T_2^m$$

so we see that in this case they are equal.

There's an interesting formula called the Baker-Campbell-Hausdorff formula (BCH)

$$\forall A, B \in \mathcal{L}(V), \exists C \in \mathcal{L}(V) | e^A e^B = e^C$$

It turns out we can write

$$C = A + B + \frac{1}{2}[A, B] + \frac{1}{12}[A, [A, B]] - \frac{1}{12}[B, [A, B]] + \dots$$

In some cases, $[A, B]$ is a number, all higher order terms will be gone and $C = A + B + \frac{1}{2}[A, B]$. Thus the BCH formula becomes useful.

9.2 Unitary Operators

We already talked about the definition of Unitary operators. They are norm-preserving, inner-product preserving, and their inverse is their adjoint. Let's talk more about the properties of unitary operators.

Note. All eigenvalues of unitary operators U lie on the unit circle.

Proof. Say $Uv = \lambda v$. Now, we get $|Uv| = |\lambda|^2|v|$. But since by definition $|Uv| = |v|$, we must have that $|\lambda| = 1$. □

Note. If $Uv = \lambda v$, then $U^\dagger v = \lambda^* v$.

Proof. We know

$$U^\dagger U v = U^\dagger \lambda v = \lambda U^\dagger v = v$$
$$\implies U^\dagger v = \frac{1}{\lambda} v = \lambda^* v$$

□

Note. We know that for Hermitian H, e^{iH} is unitary. But for any U, can we find hermitian H such that $U = e^{iH}$. It turns out the answer is yes.

9.3 Normal Operators

Definition 9.1(Normal Operators)

An operator $T \in \mathcal{L}(V)$ is normal if

$$[T, T^\dagger] = 0$$

Note that Hermitian operators are automatically normal. Unitary operators are also normal.

Theorem 9.2

For a normal operator T, say $Tv = \lambda v$. Then, $T^\dagger v = \lambda^* v$.
Note: last time we showed that $T = A + iB$ for Hermitian A and B. Then, $T^\dagger = A - iB$, and so $[T, T^\dagger] = 0 \iff [A, B] = 0$.

Why are we talking about normal operators? It will become clear in 10 minutes.

Let's talk about diagonalization

Definition 9.3(Diagonalization)

A linear operator T is diagonalizable if there exists a bases $\{v_1, v_2, \ldots, v_n\}$ such that the matrix representation $T(\{v\})$ is diagonal:

$$\begin{pmatrix} \lambda_1 & 0 & 0 & \ldots \\ 0 & \lambda_2 & 0 & \ldots \\ \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & \ldots & \lambda_n \end{pmatrix}$$

Note: not all operators are diagonalizable. Let's consider

$$A = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

We can see that it's eigenvalues are both 0. However, if we were to try to diagonalize it, we would end up with all 0.

Assume we have a diagonalizable operator $T \in \mathcal{L}(V)$. There exists a basis $\{u_1, u_2, \ldots, u_n\}$. But we are given $T(\{v\})$, rather than $T(\{U\})$. How can we convert this into diagonal form? Recall $T(\{u\}) = A^{-1}T(\{v\})A$. We can write

$$A(\{v\}) = \begin{pmatrix} u_1 & u_2 & \ldots & u_n \end{pmatrix}$$

where the columns u_i are written in the v basis.

Definition 9.4(Unitarily Diagonalizable)

A linear operator is unitarily diagonalizable if there exists an orthonormal basis $\{e_1, e_2, \ldots, e_n\}$ such that $T(\{e\})$ is diagonal.

Assume T is unitarily diagonalizable, but given in some other orthonormal basis $T(\{e'\})$. We can diagonalize it

$$T(\{e\}) = U^{-1}T(\{e\})U$$

where U will be a unitary operator.

Let's check that U must be unitary. We have

$$U = \begin{pmatrix} e_1 & e_2 & \ldots & e_n \end{pmatrix}$$

$$U^\dagger = \begin{pmatrix} e_1^* \\ e_2^* \\ \ldots \\ e_n^* \end{pmatrix}$$

Then,

$$U^\dagger U = \begin{pmatrix} e_1^* \\ e_2^* \\ \dots \\ e_n^* \end{pmatrix} \begin{pmatrix} e_1 & e_2 & \dots & e_n \end{pmatrix}$$

Question

Are there any operators that are diagonalizable but not unitarily diagonalizable? Let $\{v_1, v_2, \dots, v_n\}$ be a basis that is not orthogonal. Say the operator in this basis is diagonal with all eigenvalues distinct. Then, we see that the diagonalization of this operator is not in an orthonormal basis.

9.4 Spectral Theorem

Ok, 10 minutes have passed so now we can talk about the spectral theorem.

Theorem 9.5(Spectral Theorem)

There exists an orthonormal basis of complex, finite dimensional vector space V that are eigenvectors of a linear operator T iff T is normal.

Proof. We will first prove that if T is unitarily diagonalizable, then we have $[T, T^\dagger] = 0$.

The commutator is basis-independent, so let's just compute it in the diagonal basis. It is trivial to see that $[T, T^\dagger] = 0$.

Now, we need to show the other direction. Even though this is non trivial, it will not be on the homework. Here's a rough sketch.

1. We know $\exists v \neq 0 | Tv = \lambda v$.
2. Find a unitary transformation such that in the new basis the first vector is v.

$$T(\{e\}) \to T(\{v, \dots\}) = U^\dagger T U$$

Now, we know that

$$T = \begin{pmatrix} \lambda_1 & 0 \\ 0 & T' \end{pmatrix}$$

where T' is a matrix one dimension smaller. We can just repeat until we reach a 1×1 matrix, which is already diagonal.

□

Question

Does this theorem hold for real vector spaces?
The answer is no.

Ok, so what we have learned so far is that given a normal $T \in \mathcal{L}(V)$, we can always find an orthonormal basis $\{e_1, e_2, \ldots, e_n\}$ such that $T(\{e\}) = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$. In general, the eigenvalues can be $\lambda_1, \lambda_2, \ldots, \lambda_m$, where each λ_i has multiplicity d_i, with $\sum_{i=0}^{m} d_i = n$.

Trivially,

$$\text{Tr}(T) = \sum_{k=1}^{m} d_k \lambda_k$$

Rename the eigenvectors to $e_1^{(1)}, e_2^{(1)}, \ldots, e_{d_1}^{(1)}, e_1^{(2)}, \ldots, e_{d_m}^{(m)}$. Define a subspace

$$U_k = \text{span}(e_1^{(k)}, e_2^{(k)}, \ldots, e_{d_k}^{(k)})$$

Then,

$$V = U_1 \oplus U_2 \oplus \ldots \oplus U_m$$

We can also write

$$T = \sum_{k} \lambda_k P_k$$

where P_k is a projection operator U_k. This is called the spectral decomposition.

For the remaining time, let's talk about what we skipped earlier. Previously, we claimed that for all unitary $U \in \mathcal{L}(V)$, there exists a hermitian operator H such that $e^{iH} = U$.

Proof. We know there exists an orthonormal basis $\{e_i\}$ such that in this basis,

$$U = \begin{pmatrix} e^{i\theta_1} & 0 & 0 & \ldots \\ 0 & e^{i\theta_2} & 0 & \ldots \\ \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & \ldots & e^{i\theta_n} \end{pmatrix}$$

Then, we simply have

$$H = \begin{pmatrix} \theta_1 & 0 & 0 & \ldots \\ 0 & \theta_2 & 0 & \ldots \\ \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & \ldots & \theta_n \end{pmatrix}$$

□

10 Recitation 5 (2024-09-19)

Today we will talk about the spectral theorem. This is perhaps the single most important statement in quantum mechanics.

Theorem 10.1(Spectral Theorem)

Let $T \in \mathcal{L}(V)$ be a linear operator on a complex vector space V. The eigenvectors of T for an orthonormal basis in V iff T is normal.

Let's prove this today.

Proof. First, let's establish that if the eigenvectors of T form an orthonormal basis in V iff T is unitarily diagonalizable. Then, we will show that T is unitarily diagonalizable iff T is normal.

For the first direction, we will show that if T is unitarily diagonalizable, then T is normal. We can write

$$T = UDU^\dagger$$

for some unitary U and diagonal D. Then, calculating the commutator simply gives

$$[T, T^\dagger] = [UDU^\dagger, (UDU^\dagger)^\dagger] = [UDU^\dagger, UD^\dagger U^\dagger]$$
$$= UDU^\dagger UD^\dagger U - UD^\dagger U^\dagger UDU^\dagger = U(DD^\dagger - D^\dagger D)U^\dagger$$

But since D is diagonal, $DD^\dagger - D^\dagger D = [D, D^\dagger] = 0$. Therefore, T is normal.

Now, we will show that if T is normal, T is unitarily diagonalizable. We will prove this by induction on $\dim(V)$.

For our base case, this is trivially true for the case that $\dim(V) = 1$. Let's assume that it is true for $\dim(V) = n - 1$. We will prove that it is true for $\dim(V) = n$.

Let $T(\{i\})$ be a $n \times n$ matrix representation of T over the orthonormal basis $\{|1\rangle, |2\rangle, \ldots, |n\rangle\}$. We can write down the matrix elements

$$T_{ij}(\{i\}) = \langle i|Tj\rangle$$

Since $[T, T^\dagger] = 0$, if we have an eigenvector $T|x_1\rangle = \lambda_1 |x_1\rangle$, it follows that the eigenvalue of $T^\dagger = \lambda^*$ with the same eigenvector.

Now, we know that there exists a unitary matrix U_1 such that $|x_1\rangle = U_1|1\rangle$. Define $T_1 = U_1^\dagger T U_1$. Then,

$$T_1|1\rangle = U_1^\dagger T U_1|1\rangle = U_1^\dagger T|x_1\rangle = \lambda_1 U_1^\dagger|x_1\rangle = \lambda_1|x_1\rangle$$

So now,

$$\langle j|T_1 1\rangle = \lambda_1\langle k|1\rangle = \lambda_1 \delta 1j$$
$$\langle 1|T_1 j\rangle = (\left\langle j\middle|T_1^\dagger 1\right\rangle)^* = \langle j|\lambda_1^* 1\rangle^* = \lambda_1 \delta_{1j}$$

So this means that

$$T_1(\{i\}) = \begin{pmatrix} \lambda_1 & \mathbf{0} \\ \mathbf{0} & T' \end{pmatrix}$$

where T' is a $(n-1) \times (n-1)$ matrix. By induction, it is unitarily diagonalizable, where $U'T'(U')^\dagger = D'$. Now, we construct

$$U = \begin{pmatrix} 1 & \mathbf{0} \\ \mathbf{0} & U' \end{pmatrix}$$

and we can apply U to T_1:

$$U^\dagger T U = U^\dagger U_1^\dagger T U_1 U = (U_1 U)^\dagger T (U_1 U)$$

Therefore, T is unitarily diagonalizable. □

The cool part of this is that any operator is isomorphic to a diagonal matrix.

For example, if you have a Hamiltonian, you can always expand

$$\hat{H} = \sum_{n=0}^{\infty} E_n |\psi_n\rangle \langle\psi_n|$$

Then we can see that

$$\hat{H}^2 = \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} E_n E_m |\psi_n\rangle \langle\psi_n|\psi_m\rangle \langle\psi_m| = \sum_{n=0}^{\infty}\sum_{m=0} E_n E_m \delta_{mn} = |\psi_n\rangle \langle\psi_m| = \sum_{n=0}^{\infty} E_n^2 |\psi_n\rangle \langle\psi_n|$$

There's another example I want to show. Imagine that you have a matrix, say a spin operator

$$\begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix} = a_1 P_1 + a_2 P_2$$

It has eigenvalues $a_1 = 1$ and $a_2 = -1$. We get $A = P_1 - P_2$. But by the spectral theorem, $I = P_1 + P_2$. Therefore, $P_1 = \frac{I+A}{2}$, and $P_2 = \frac{I-A}{2}$.

Let $|v\rangle$ be some state of electrons. We want to measure their spin. We get

$$\langle\sigma\rangle = \langle v|Av\rangle = \langle v| a_1 P_1 + a_2 P_2 |v\rangle = a_1 |\langle v|a_1\rangle|^2 + a_2 |\langle v|a_2\rangle|^2$$

Therefore, the overlaps with eigenvectors will give you probability amplitudes.

11 Lecture 6 (2024-09-23)

Congratulations everyone, this will be the last math lecture. After this, we will now move on to quantum mechanics.

Recap

Last time, we talked about normal operators. An operator T is normal if $[T, T^\dagger] = 0$. Hermitian and unitary operators are all normal. We established that if $Tv = \lambda v$, then $T^\dagger v = \lambda^* v$. We forgot to prove this last time, so let's prove it now.

Proof. Assume $Tv = \lambda v$. We will show that $|T^\dagger v - \lambda^* v|^2 = 0$. We can write

$$|T^\dagger v - \lambda^* v|^2 = \left\langle T^\dagger v - \lambda^* v, T^\dagger v - \lambda^* v \right\rangle$$

$$= \left\langle T^\dagger v, T^\dagger v \right\rangle - \lambda^* \left\langle T^\dagger v, v \right\rangle - \lambda \left\langle v, T^\dagger v \right\rangle + \lambda\lambda^* \langle v, v \rangle$$

$$= |\lambda|^2 \langle v, v\rangle - |\lambda|^2 \langle v, v\rangle - |\lambda|^2 \langle v, v\rangle + |\lambda|^2 \langle v, v\rangle = 0$$

where we simplified by moving the $T^\dagger$ so that they became T and rearranged the first term by using $TT^\dagger = T^\dagger T$. □

We learned that T is normal iff T is unitarily diagonalizable. This is the spectral theorem. What this means is that there exists an orthonormal basis $\{u_i\}$ such that $T(\{u\}) = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$, and we can decompose V into

$$V = U^{(1)} \oplus U^{(2)} \oplus \ldots \oplus U^{(m)}$$

where $U^{(i)}$ is the eigenspace of the ith distict eigenvalue.
Also note that given a unitary $W^{(k)}$, then we can arbitrarily rotate our orthonormal basis using W. In particular, assuming $d_k = 1$ for all k, $u_i \mapsto e^{i\theta_i} u_i$ is a new orthonormal basis.

11.1 Simultaneous Diagonalization

Definition 11.1(Simultaneous Diagonalization)

Two operators A and B are simultaneously diagonalizable if there exists a basis $\{u_i\}$ where both A and B are diagonal.

Theorem 11.2

If S and T are commuting normal operators ($[S, T] = 0$, $[S, S^\dagger] = 0$, and $[T, T^\dagger] = 0$), then they can be simultaneously unitarily diagonalized.

Proof. There are two cases:

Case 1: one of them has a non-degenerate spectrum.

Case 2: both have degenerate spectrums.

We will prove Case 1 and then use it to prove case 2.

WLOG, $S = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$ in some orthonormal basis $\{u_1, \ldots, u_n\}$, where all of the eigenvalues are distinct.

Consider STu_k. Since S and T commute, we get

$$STu_k = TSu_k = T(\lambda u_k) = \lambda T u_k$$

Therefore, Tu_k is an eigenvector of S with eigenvalue λ_k. But since S does not have any degenerate eigenvalues, it must be a multiple of u_k. Therefore, $Tu_k = \omega u_k$. We conclude that if u_k is an eigenvector of S, it's also an eigenvector of T. But this means that T in this basis is already diagonal!

Now, for case 2. Let $\{u_1^{(1)}, u_2^{(1)}, \ldots, u_{d_m}^{(m)}\}$ be an orthonormal basis of S, where there are m eigenvalues, with eigenvalue i having degeneracy d_i. Let S in this basis be

$$S = \text{diag}(\lambda^{(1)}, \lambda^{(1)}, \ldots, \lambda^{(2)}, \ldots, \lambda^{(m)})$$

We claim that

$$T = \text{diag}(M_1, M_2, \ldots, M_m)$$

where each M_i has dimension d_i.

To see this, chose some arbitrary $u_j^{(k)}$ and repeat our logic above:

$$STu_j^{(k)} = TSu_j^{(k)} = \lambda^{(k)} Tu_j^{(k)}$$

We see that $Tu_j^{(k)}$ is an eigenvector of S with eigenvalue $\lambda^{(k)}$. This means

$$Tu_j^{(k)} \in U^{(k)}$$

Therefore, our matrix representation of T is 0 everywhere outside the kth box.

From here, we can just apply unitary transformations $W^{(i)}$ on each of those boxes. Unitary transformations won't change S, but they will diagonalize T. Therefore, we have simultaneously diagonalized S and T. □

A corrolary of this is that if $\{S_i\}$ is a set of normal operators such that $[S_i, S_j] = 0$, then there exists an orthonormal basis such that all S_i are diagonalized.

11.2 Complete Set of Commuting Observables

Question: How can we physically specify a single quantum state? What if we have two vectors that are orthogonal but cannot be physically distinguished? We will argue that this shouldn't be the case in a more formal way.

We will show that for a non-degenerate observable S, a measurement outcomes λ_k fully specify the quantum state. In general, let $\{S_1, S_2, \ldots, S_l\}$ be a set of mutually commuting observables. Then, we can find an orthonormal basis $\{u_1, \ldots, u_n\}$ where all operators are simultaneously diagonalized.

$$\begin{aligned} S_1 &= \text{diag}(\lambda_1^1, \lambda_2^1, \ldots, \lambda_n^1) \\ S_2 &= \text{diag}(\lambda_1^2, \lambda_2^2, \ldots, \lambda_n^2) \\ &\ldots \\ S_l &= \text{diag}(\lambda_1^l, \lambda_2^l, \ldots, \lambda_n^l) \end{aligned}$$

Let $s_j = (\lambda_j^1, \lambda_j^2, \ldots, \lambda_j^l)$. If $s_j \neq s_k$ if $j \neq k$, then we say $\{S_1, \ldots, S_l\}$ forms a complete set of commuting observables (CSCO).

So later on we'll talk about different ways of forming a complete set of commuting observables. There are several remarks:

- It is physically important to identify a CSCO.
- A CSCO is NOT unique
- Usually $\hat{H}$ will be in our CSCO. If there are degenerate eigenvalues, then we can add operators $O_1, O_2, \ldots$. These operators will usually be some sort of symmetry operator.

Example 11.1

Consider the 1d simple harmonic oscillator, $\hat{H} = \hbar\omega\left(\hat{N} + \frac{1}{2}\right)$. Since energies are not degenerate, $\hat{H}$ forms a CSCO.
Now, if we consider the 2d harmonic oscillator, $\hat{H} = \hbar\omega\left(N_x + \frac{1}{2} + N_y + \frac{1}{2}\right)$ or

$$\hat{H} = \hbar\omega_x\left(N_x + \frac{1}{2}\right) + \hbar\omega_y\left(N_y + \frac{1}{2}\right)$$

in the more general case.
If we only specify $\hat{H}$, we no longer have a complete set of commuting observables. An example of CSCOs are $\{\hat{H}, N_x\}$, or $\{\hat{H}, N_y\}$, or if we want to to be redundant, $\{\hat{H}, N_x, N_y\}$. Notice that $\{N_x, N_y\}$ also works.

Example 11.2

Consider a 2×2 box with squares labelled $|1\rangle, |2\rangle, |3\rangle, |4\rangle$. Let's define a Hamiltonian whichever way we want. Define operator

$$\begin{aligned} R_{ud}|1\rangle &= |3\rangle \\ R_{ud}|3\rangle &= |1\rangle \\ R_{ud}|2\rangle &= |4\rangle \\ R_{ud}|4\rangle &= |2\rangle \end{aligned}$$

Define R_{lr} similarly.
Let's consider Hamiltonians where $\hat{H}$ commutes with R_{ud}. We can also notice that $[R_{lr}, R_{ud}] = 0$, $R_{lr}^2 = I$, and $R_{ud}^2 = 1$. It turns out that R_{lr} will have two eigenstates with eigenvalues +1 and two eigenstates with eigenvalues -1. Similarly for R_{ud}. Additionally, we have pairs of states such that $R_{lr} = \pm 1$ and $R_{ud} = \pm 1$ for all cases.

12 Recitation 6 (2024-09-24)

Today we have a substitute (Hongyin). First of all, are there any questions about the homework?

Let's talk about simultaneous diagonalization. Two operators S and T are simultaneously diagonalizable if there exists a basis $\{B\}$ such that both S and T are diagonal.

In this case, each element of $\{B\}$ is an eigenvector of S and of T.

In lecture, we talked about a theorem where if S and T are hermitian (or in general, normal), and $[S,T]=0$, then they are simultaneously diagonalizable.

So writing this out, what this means explicitly is

a) All non-degenerate eigenstates of one operator are eigenstates of the other.

b) If S has d degenerate eigenstates, they are not necessarily eigenstates of T, however d orthonormal combinations of these eigenstates of S can be found that are eigenstates of T.

So then, let's consider $A, B \in \mathcal{L}(V)$, and are both Hermitian. If all eigenstates of A are eigenstates of B, and vice versa, then you can write $[A,B]=0$.

What does this mean, and why do we care about it? In physics, if we see two observables, and therefore two hermitian operators, if they commute, then we can find simultaneous eigenstates.

Note that not all matrices whose commutator vanishes are simultaneously diagonalizable. For example,

$$A=\begin{pmatrix}\lambda & 1 & 0\\ 0 & \lambda & 1\\ 0 & 0 & \lambda\end{pmatrix}, \quad B=\begin{pmatrix}\sigma & 1 & 0\\ 0 & \sigma & 1\\ 0 & 0 & \sigma\end{pmatrix}$$

We can check that they commute but they are not simultaneously diagonalizable when $\sigma \neq \lambda$. We can check that they are also not normal.

Example 12.1

So I'll go over a quick example of two operators being simultaneously diagonalizable. Say we're working in an infinite dimensional vector space. Let V be the set of normalizable complex functions of real variables. We have two operators, $\hat{H}=-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}+\frac{1}{2}m\omega x^2$, and $\sigma\psi(x)=\psi(-x)$.
So let's check if these operators commute:

$$\hat{H}\sigma\psi(x)=\frac{\mathrm{d}}{\mathrm{d}x^2}\psi(-x)+x^2\psi(-x)$$

$$\sigma\hat{H}\psi(x)=\sigma\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi+x^2\psi(x)\right)=\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi(-x)+(-x)^2\psi(-x)$$

Since these are the same, these operators commute.
Note that $\sigma^2=1$. Therefore, the eigenvalues of σ are ± 1. The eigenfunctions are

$$\begin{cases}\lambda=1 & \{f|f(x)=f(-x)\}\\ \lambda=-1 & \{f|f(x)=-f(-x)\}\end{cases}$$

For the eigenfunctions of $\hat{H}$, they are

$$\psi_n = N_n H_n(y) \exp\left(-\frac{1}{2}y^2\right)$$

where $y = \sqrt{\frac{mw}{\hbar}}x$, H are the hermite polynomials, and N is a normalization constant. Note that the Hamiltonian has no degeneracies. Therefore, all eigenfunctions of $\hat{H}$ are also eigenfunctions of σ. However, it is not necessarily true that eigenfunctions of σ are eigenfunctions of $\hat{H}$.

13 Lecture 7 (2024-09-25)

Let's say one day aliens come and kill all physicists, but not the mathematicians. I, as the sole survivor, want to lay out the axioms of quantum mechanics so that our knowledge is not lost.

13.1 Axioms of Quantum Mechanics

States of quantum systems

A complete description of a quantum system is given by a ray in a Hilbert space $\mathcal{H}$.

By complete, it means that no more info is needed to describe the system, and no more information can be obtained from it.

Second, notice that this is a state of the entire system, not their constituent particles.

Third, given ψ identify all $\alpha\psi$ for $\alpha \in \mathbb{C}$ given $\alpha \neq 0$. These are all the same state. Therefore, without loss of generality, we usually assume $|\psi| = 1$.

Fourth, identifying $\mathcal{H}$ is going to be the same as identifying different degrees of freedom. One way to define a Hilbert space is to identify a basis and take the span.

Observables

Hermitian operators on $\mathcal{H}$ are observables.

Hermitian operators are operators such that $A^\dagger = A$. The spectral theorem tells us that

$$A = \sum_k \lambda_k P_k, \qquad \lambda_k \in \mathbb{R}$$

and in some basis,

$$A = \operatorname{diag}(\lambda_1, \lambda_2, \ldots, \lambda_m)$$

Therefore, our Hilbert space can be decomposed into

$$\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \ldots \oplus \mathcal{H}_m$$

So we can think about hermitian operators as decomposing $\mathcal{H}$ into different subspaces and assigning them with λ_i.

States from $\mathcal{H}_i$ and $\mathcal{H}_j$ are fully distinguishable for $i \neq j$.

Measurement

If a measurement of an observable A is performed, the quantum state ψ is projected into one of the subspaces:

$$\psi \mapsto \hat{P}_k \psi$$

for a certain k with probability

$$p_k = |\hat{P}_k \psi|^2$$

This is called Born's rule.

Note: nowhere here do we mention the eigenvalues λ_i. It turns out, the eigenvalues λ_i are numbers we give the system. Suppose that I measure position, but with an inaccurate ruler. It's ok, as long as we have a 1 to 1 mapping from our measurements to the actual lengths.

Suppose we have two operators A and B with the exact same spectral decomposition, just with different eigenvalues. Measuring with A or B will give us the exact same information.

Another consequence of this is that repeated measurements lead to the same outcome.

Dynamics

Time evolution is unitary; for any (closed) quantum system, there exists aunitary operator $U(t_1; t_0)$ that describes how a quantum state at time t_0 evolves to a state at t_1.

$$\psi(t_1) = U(t_1; t_0)\psi(t_0)$$

What this means is that U contains everything about dynamics. Suppose I have a unitary operator U, and I wrote it down in my diary, say, given any wavefunction, I will be able to determine the state at some later time.

Also, note that this implies linearity. If we find an orthonormal basis $\{e_i\}$ and find out how each of these basis vectors evolve, then we are done.

Third, the dynamics of any system is deterministic. This might be a common misconception for some. But time evolution is always deterministic, only measurements have uncertainty.

Fourth, unitary implies $U = e^{iH}$ for some Hermitian H. This implies time reversibility, with the inverse being e^{-iH}.

Aside

The second law of thermodynamics says that entropy must always increase. How does this fit with quantum mechanics?
In quantum mechanics, knowing a wavefunction implies that we know the exact param-

eters for every single particle of the system, as much as can be determined. So from a human perspective, while entropy seems to be increasing, if we did actually know all of the parameters of the system, we could reverse it.
Also, particles can fall into black holes but never come out. But we believe a similar thing is going on here!

Also, information is preserved. This means that

$$\langle \psi_1, \psi_2 \rangle = 0 \implies \langle \psi_1(t), \psi_2(t) \rangle = 0$$

Also, no information can be copied. This is the fact that led to quantum information theory.

Question

Do we need extra axioms such as homogeneity, etc.
No. Right now we are talking about a framework. If we want to talk about specific laws of physics, then we can bring in these axioms such as energy conservation, etc. But for now, we will not.

Question

"How did people come up with the axioms?" - David Zhang
Honestly, I'm young enough to not know. If you want to read more you can look at chapter 16.6 of Zweibach's book. Also, there are some other axioms related to composite systems, but we will not talk about them right now.

Question

Quantum evolution is unitary but measurement is not. But what if measurements are being performed in our system?
That's a good question. There's a lot of debate about why measurement is treated so specially. One thought is that from an outside observer's point of view, the measurement action will be unitary.

13.2 Dirac Braket Notation

Consider a Hilbert space. In our old notation, we denoted vectors like $v \in V$. Now, we will call them kets, with the notation $|v\rangle \in V$.

Previously, we represented operators acting on v as $Tv \in V$. In our new notation, we will say $|Tv\rangle \in V$. This notation may seem very redundant, but it's also flexible. For example, say $\psi \in \mathcal{H}$, or in our new notation, $|\psi\rangle \in \mathcal{H}$. This can be for example a bit in a quantum computer. We can write the state as $|0\rangle$, which is notably different from the 0 vector. We can even write things such as $|🍎\rangle$, $|🌙\rangle$, or $|🍑\rangle$.

In our old notation, $\{e_i\}$ goes to $\{|e_i\rangle\}$, which can be abbreviated to just $|i\rangle$.

For example, for the simple harmonic oscillator we can name energy eigenstates $|0\rangle, |1\rangle, \ldots, |n\rangle$. Of course, with flexibility also comes ambiguity. We just talked about three different types of $|1\rangle$. When we write abbreviated kets, we should be careful to specify.

Now let's talk about bra vectors and inner products. We denote bra vectors as $\langle \ldots |$ which is defined as a linear functional

$$\begin{aligned} \langle v| \equiv \phi_v, \quad & V \mapsto \mathbb{C} \\ & u \mapsto \langle v, u\rangle \end{aligned}$$

In terms of vectors, bras represent row vectors while kets represent column vectors.

For operators, we can write them acting on a vector as

$$T|v\rangle = |Tv\rangle$$

Adjoint will be the same:

$$\langle u| T |v\rangle = \langle u|Tv\rangle = \left\langle T^\dagger u \middle| v\right\rangle$$

In old notation, we have

$$v = \sum_j \langle e_j, v\rangle e_j$$

In new notation,

$$|v\rangle = \sum_j \langle j|v\rangle |j\rangle = \sum_j |j\rangle \langle j|v\rangle = \left(\sum_j |j\rangle \langle j|\right) |v\rangle$$

Therefore,

$$\sum_j |j\rangle \langle j| = I$$

This is called resolution of identity.

For general operators, say we are given an operator T:

$$T = I \cdot T \cdot I = \sum_i \sum_j |i\rangle \langle i| T |j\rangle \langle j|$$

In fact, we have talked about this. $\langle i| T |j\rangle = T_{ij}$ is the matrix representation of T. Therefore,

$$T = \sum_{i,j} T_{ij} |i\rangle \langle j|$$

Projection operators onto a single eigenvector P_k can be written as $|k\rangle \langle k|$. In general,

$$P_k = \sum_j = |k, j\rangle \langle k, j|$$

14 Recitation 7 (2024-09-26)

Today we will discuss Dirac notation.

As a review, a ket is a representation of a vector in our vector space: $|v\rangle$. A bra $\langle u|$ is a dual vector as something that you need to produce an inner product $\langle u|v\rangle$. $|u\rangle$ is a linear functional acting of v that returns a scalar such that $\langle u|\left(|v\rangle\right) = \langle u, v\rangle$. This notation has the nice property that any operator A that lives in vector space V can be expressed as

$$A = \sum \alpha_{ij} |u_i\rangle \langle u_j|$$

for some pairs on vectors and coefficients. Then,

$$A|v\rangle = \sum \alpha_{ij} |u_i\rangle \langle u_j|v\rangle$$

Given an orthonormal basis $\{e_i\}$,

$$Ae_i = \sum_k A_{ik} e_k$$

and we can expand any vector over the basis

$$v = \sum_k v_k e_k$$

A is our operation that maps a vector to another vector:

$$u = Av = \sum_j v_j Ae_j = \sum_{j,k} v_j A_{jk} = \sum_k u_k e_k$$

In bra-ket notation,

$$A = \sum_{i,j} A_{ij} |e_i\rangle \langle e_j|$$

so

$$|u\rangle = |Av\rangle = A|v\rangle = \sum_{i,j} A_{ij} |e_i\rangle \langle e_j|v\rangle = \sum_{i,j} A_{ij} |e_i\rangle v_j = \sum_{i,j} (A_{ij} v_j) |e_i\rangle$$

Therefore, $\sum_j A_{ij} v_j = u_i$.

Recall we can make projection operators

$$P_v = |v\rangle \langle v|$$

Example 14.1

Consider a Hilbert space with orthonormal basis $\{|1\rangle, |2\rangle, |3\rangle\}$. (This is problem 5 of pset 3). What are $\langle\psi|$, $\langle\phi|$, and $\langle\phi|\psi\rangle$?
(Content ommitted because it is already written in the homework solutions.)

15 Lecture 8 (2024-09-30)

The midterm will cover everything up until Lecture 9.

We'll start by recapping what we learned. We learned about braket notation, ket vectors, where we have $|\text{description}\rangle$ to denote a vector in our Hilbert space. Similarly, bra vectors $\langle\text{description}|$ which are functionals that act on vectors to produce a scalar. Also, operators could be written as

$$T = \sum_{i,j} T_{ij} |e_i\rangle \langle e_j|$$

We learned about projection operators

$$P_k = \sum_j |k_j\rangle \langle k_j|$$

and hermitian operators can be written as

$$H = \sum_k \lambda_k P_k$$

where $\lambda_k \in \mathbb{R}$.

Finally, resolution of identity is

$$I = \sum_j |j\rangle \langle j|$$

15.1 Non-denumerable States

Let's define a Hilbert space as

$$\mathcal{H} = \text{span}\{|x\rangle\}$$

where $x \in \mathbb{R}$ is a continuous variable, and $|x\rangle$ is a state that represents a particle at position x. Note that this is an infinite-dimensional Hilbert space, even though our particle lives in 1D.

Let's define our inner product as follows:

$$\langle x|y\rangle = \delta(x - y)$$

In this example, resolution of identity looks like

$$I = \int_{-\infty}^{\infty} |x\rangle \langle x| \, \mathrm{d}x$$

Ok, let's derive what we call wavefunctions. Given $|\psi\rangle \in \mathcal{H}$,

$$|\psi\rangle = I |\psi\rangle = \int_{-\infty}^{\infty} |x\rangle \langle x|\psi\rangle \, \mathrm{d}x = \int_{-\infty}^{\infty} \psi(x) |x\rangle \, \mathrm{d}x$$

where we define $\psi(x) = \langle x|\psi\rangle$. We see that $\psi(x)$ is what we called the wavefunction in 8.04. But now we see that it is nothing but the sum of scaled basis vectors in the position basis.

Definition 15.1(Wavefunction)

The wavefunction $\psi(x)$ is the amplitude of a quantum state $|\psi\rangle$ in the position basis.

So let's "derive" the inner product we considered in 8.04:

$$\langle\phi|\psi\rangle = \langle\phi| I |\psi\rangle = \int_{-\infty}^{\infty} \mathrm{d}x \langle\phi|x\rangle \langle x|\psi\rangle = \int_{-\infty}^{\infty} \phi^* \psi \mathrm{d}x$$

A corrolary of this is

$$| |\psi\rangle |^2 = \langle\psi|\psi\rangle = \int_{-\infty}^{\infty} \mathrm{d}x |\psi(x)|^2$$

Let's talk about the position operator.

$$\hat{x} = \int_{-\infty}^{\infty} \mathrm{d}\tilde{x}\ \tilde{x} |\tilde{x}\rangle \langle\tilde{x}|$$

or alternatively, we can define $\hat{x}$ by $\hat{x} |\tilde{x}\rangle = \tilde{x} |\tilde{x}\rangle$.

Now let's talk about momentum basis. We define $|p\rangle$ to be a momentum eigenstate with momentum p. We get

$$\langle p|q\rangle = \delta(p-q)$$

We similarly define

$$I = \int \mathrm{d}p |p\rangle \langle p|$$

$$\int \mathrm{d}p\ p |p\rangle \langle p| = p |p\rangle$$

and $\tilde{\psi}(p) = \langle p, \psi\rangle$.

Any wavefunction $|\psi\rangle$ can be written in either of these states.

What is the relation between $|x\rangle$ and $|p\rangle$? We define

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx\hbar}$$

15.2 Generalized Uncertainty Principle

We already learned that $\Delta x \Delta p \geq \hbar/2$. This is true for any quantum wavefunction. We'll discuss this for arbitrary pair of operators.

Recall the expectation of an operator:

$$A = \sum_k \lambda_k P_k$$

$$\langle A\rangle = \sum_k \lambda_k p p_k$$

Now

$$\mathrm{var}(A) = \sum_k (\lambda_k - \langle A\rangle)^2 p_k = \sum_k \lambda_k^2 p_k - 2\lambda_k p_k \langle A\rangle + \langle A\rangle^2 p_k = \langle A^2\rangle - \langle A\rangle^2$$

We define $\Delta A = \sigma_A = \sqrt{\mathrm{var}(A)} = \sqrt{\langle A^2\rangle - \langle A\rangle^2} \geq 0$.

Theorem 15.2(Generalized Uncertainty Principle)

For two observables A and B, then for any ψ,

$$\Delta A \cdot \Delta B \geq \left| \langle\psi| \frac{1}{2i}[A, B] |\psi\rangle \right|$$

Proof. Let $|f_A\rangle = (A - \langle A\rangle I)|\psi\rangle = \delta A|\psi\rangle$. Note that in general, this is not a linear map. Similarly, define $|g_B\rangle = (B - \langle B\rangle I)|\psi\rangle = \delta B|\psi\rangle$.

Using the Cauchy Schwartz inequality,

$$||f_A\rangle|^2 |g_B\rangle|^2 \geq |\langle f_A|g_B\rangle|^2$$

Since $||f_A\rangle|^2 = \Delta A^2$ and $||g_B\rangle|^2 = \Delta B^2$, we already have some preliminary form of the uncertainty principle.

Now,

$$|\langle f_A|g_B\rangle|^2 = \mathrm{Re}(\langle f_A|g_B\rangle)^2 + \mathrm{Im}(\langle f_A|g_B\rangle)^2$$

We can get

$$\mathrm{Re}(\langle f_A|g_B\rangle) = \frac{1}{2}(\langle f_A|g_B\rangle + \langle f_A|g_B\rangle) = \frac{1}{2}(\langle\psi|\delta A\delta B + \delta B\delta A|\psi\rangle) = \frac{1}{2}\langle\psi|\{\delta A, \delta B\}|\psi\rangle$$

where $\{\delta A, \delta B\} = \delta A\delta B + \delta B\delta A$ is called the anti-commutator.

Similarly,

$$\mathrm{Im}(\langle f_A|g_B\rangle) = \frac{1}{2i}(\langle\psi|\delta A\delta B - \delta B\delta A|\psi\rangle) = \frac{1}{2i}\langle\psi|[A, B]|\psi\rangle$$

where we used that $[\delta A, \delta B] = [A, B]$ since δA and δB differ from A and B by constants, which commute with everything.

We get

$$\Delta A^2 \Delta B^2 \geq \left|\langle\psi| \frac{1}{2i}[A, B]|\psi\rangle\right|^2 + \left|\langle\psi| \frac{1}{2}\{\delta A, \delta B\}|\psi\rangle\right|^2$$

Since $||\psi\rangle \frac{1}{2}\{\delta A, \delta B\}\langle\psi|\,|^2 \geq 0$, we recover

$$\Delta A \cdot \Delta B \geq \left|\langle\psi| \frac{1}{2i}[A, B]|\psi\rangle\right|$$

□

Now in the last two minutes let's sketch the idea of when the uncertainty principle can be saturated. When we derived this uncertainty principle, we need two inequalities to be saturated: Cauchy Schwartz, so that $\exists\beta \in \mathbb{C}$ such that $|f\rangle = \beta |g\rangle$. Secondly, $\langle\psi| \delta A\delta B + \delta B\delta A |\psi\rangle = 0$.

Turns out, one way to satisfy this trivially is $|g\rangle = 0$ or $|f\rangle = 0$. The only non-trivial case is when $|g\rangle \neq 0$ and $|f\rangle \neq 0$. In this case, let's set $\beta = i\lambda$, where λ is real. Then,

$$(\hat{A} - i\lambda\hat{B}) |\psi\rangle = (a - i\lambda b) |\psi\rangle$$

(This will be expanded on more during recitation)

16 Recitation 8 (2024-10-01)

Let's talk about uncertainty. Given a Hermitian operator A and a state $|\psi\rangle \neq 0$, the uncertainty ΔA_ψ is given by

$$\Delta A_\psi^2 = \langle\psi| A^2 |\psi\rangle - (\langle\psi| A |\psi\rangle)^2$$

Equivalently, this is equal to

$$\Delta A_\psi^2 = |(A - \langle A\rangle_\psi)\psi|^2$$

from this we see that $\Delta A_\psi \geq 0$. This implies $\langle A^2\rangle \geq \langle A\rangle^2$.

Secondly, if $A |\psi\rangle = a |\psi\rangle$, then $\langle A\rangle^2 = \langle A^2\rangle = a^2$. Therefore, $\Delta A_\psi = 0$.

Third, let's think about a geometric interpretation. Consider

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

which is the projection operator onto the subspace ψ. Then,

$$P_\psi(A |\psi\rangle) = |\psi\rangle \langle\psi| A |\psi\rangle = \langle A\rangle |\psi\rangle$$

Now if we consider a state

$$|\psi_\perp\rangle = (1 - P_\psi)A |\psi\rangle = (A - P_\psi A) |\psi\rangle = (A - \langle A\rangle_\psi) |\psi\rangle$$

Therefore,

$$\Delta A_\psi^2 = \langle\psi_\perp|\psi_\perp\rangle$$

So we can visualize the uncertainty as the magnitude of the orthogonal to the projection of $A |\psi\rangle$ onto $|\psi\rangle$.

Also, physically, the uncertainty of A defines the spread of measurements of quantity A in an ensemble of identically prepared states $|\psi\rangle$. For example, have you guys heard of Schrödinger's cat? Before we open the box, the cat is in a superposition of dead and alive. But when we open the box (i.e. take a measurement), the cat will be dead with some probability and alive with some probability. The uncertainty quantifies the variance of our results.

For example, let A be the operator that measures if the cat is dead or alive. Let

$$|\psi\rangle = \alpha \left|😊\right\rangle + \beta \left|💀\right\rangle$$

where $|\alpha^2| + |\beta^2| = 1$.

We can write,

$$\Delta A_\psi^2 = \left\langle A^2 \right\rangle_\psi - \langle A \rangle_\psi^2 = |\alpha|^2 a_1^2 + |\beta|^2 a_2^2 - (a_1|\alpha|^2 + a_2|\beta|^2)^2$$

$$= a_1^2|\alpha|^2(1-|\alpha|^2) + a_2^2|\beta|^2(1-|\beta|^2) - 2a_1a_2|\alpha|^2|\beta|^2$$

$$= a_1^2|\alpha|^2|\beta|^2 + a_2^2|\beta|^2|\alpha|^2 - 2a_1a_2|\alpha|^2|\beta|^2 = (a_1-a_2)^2|\alpha|^2|\beta|^2$$

Now let's talk about the generalized uncertainty relation. Given Hermitian A and B and a state $|\psi\rangle \neq 0$. Define

$$|f\rangle = (A - \langle A \rangle_\psi)|\psi\rangle$$
$$|g\rangle = (B - \langle B \rangle_\psi)|\psi\rangle$$

Now, the Schwartz inequality gives

$$\langle f|f\rangle \langle g|g\rangle \geq |\langle f|g\rangle|^2$$

This gives

$$\Delta A_\psi^2 \Delta B_\psi^2 \geq \mathrm{Re}(\langle f|g\rangle)^2 + \mathrm{Im}(\langle f|g\rangle)^2$$

We know

$$\mathrm{Re}(\langle f|g\rangle) = \frac{1}{2}(\langle f|g\rangle + \langle g|f\rangle) = \frac{1}{2}\left(\langle\psi|\left(\delta A \delta B + \delta B \delta A\right)|\psi\rangle\right)$$

Similarly,

$$\mathrm{Im}(\langle f|g\rangle) = \frac{1}{2i}(\langle f|g\rangle - \langle g|f\rangle) = \frac{1}{2i}\langle\psi|[A,B]|\psi\rangle$$

Therefore,

$$\Delta A_\psi^2 \Delta B_\psi^2 \geq \frac{1}{4}(\langle\psi|\{\delta A, \delta B\}|\psi\rangle)^2 + \frac{1}{4}|\langle\psi|[A,B]|\psi\rangle|^2$$

We usually just write this as

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

Why do we ignore the other term? It turns out we can normally prepare states such that it is 0. Say we want to achieve saturation of our inequality. We need $|g\rangle = \alpha|f\rangle$, and we need $\mathrm{Re}(\langle f|g\rangle) = 0$. This gives

$$0 = \langle f|g\rangle + \langle g|f\rangle = (\alpha + \alpha^*)\langle f|f\rangle$$

So we must have that $\alpha = i\lambda$. Now,

$$(B - \langle B\rangle_\psi)|\psi\rangle = i\lambda(A - \langle A\rangle_\psi)|\psi\rangle$$

Taking the magnitude of both sides, $\lambda = \frac{\Delta B_\psi}{\Delta A_\psi}$.

17 Lecture 9 (2024-10-02)

17.1 Energy Time Uncertainty Principle

In our formulation of quantum mechanics so far, time is not treated as a normal observable. Nevertheless, there have been several formulations of Energy-Time uncertainty principles.

These formulations tend to be more heuristic and practical. For example, we know

$$E = \hbar\omega = hf$$

Since $f = \frac{1}{T}$, we can estimate $\Delta f \geq \frac{1}{\Delta T}$. Therefore,

$$\Delta E = h\Delta f \geq \frac{h}{\Delta T} \implies \Delta E \Delta T \geq h$$

Let's talk about one form of a precise formulation. We will consider how fast a quantum state can evolve, becoming orthogonal to itself. This is non-trivial and will take some time to prove, so it will be on the homework.

Another version of this is based on observables. How fast can an observable change? Given an observable $\hat{Q}$, we have an expectation $\left\langle \hat{Q} \right\rangle$ and an uncertainty $\Delta\hat{Q}$. We are interested in the minimum time for which the expectation value changes by at least $\Delta\hat{Q}$. Let this be

$$\Delta t_q = \frac{\Delta Q}{\left|\frac{\mathrm{d}}{\mathrm{d}t}\langle Q\rangle\right|}$$

We can show that

$$\Delta\hat{H}\Delta t_q \geq \frac{\hbar}{2}$$

Proof. We know that

$$\Delta H \Delta Q \geq \left|\langle\psi| \frac{1}{2i}[H, Q] |\psi\rangle\right|$$

We want to relate this to

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle Q\rangle = \frac{\mathrm{d}}{\mathrm{d}t}\langle\psi| Q |\psi\rangle = \left\langle \frac{\mathrm{d}\psi}{\mathrm{d}t}\right| Q |\psi\rangle + \langle\psi| Q \left|\frac{\mathrm{d}\psi}{\mathrm{d}t}\right\rangle + \langle\psi| \frac{\mathrm{d}Q}{\mathrm{d}t} |\psi\rangle$$

For now, let's only consider operators that are time-independent. Then, the third term will be 0.

From Schrödinger's equation, we know that

$$\frac{\mathrm{d}}{\mathrm{d}t}|\psi\rangle = -i\frac{H}{\hbar}|\psi\rangle$$

Similarly,

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi| = i\frac{\langle\psi| H}{\hbar}$$

Therefore,

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle Q\rangle = \frac{i}{\hbar}\langle\psi|\left[H,Q\right]|\psi\rangle$$

Plugging this into our uncertainty principle,

$$\Delta H\Delta Q \geq \left|\frac{\hbar}{2}\frac{\mathrm{d}}{\mathrm{d}t}\langle Q\rangle\right|$$

Therefore, we recover

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

□

Question

Why can't we define a time operator just like we defined position operators and momentum operators?
In our current formulation, we treat rays in Hilbert space as states at a given time. So time is a parameter, and not an observable. In other formulations such as quantum field theory, time must be treated on equal footing as position. But we will not discuss this in detail in this class.

17.2 Quantum Dynamics

Let's present a broad overview of quantum dynamics. Let's talk about observables specificly:

$$A = \sum_k \lambda_k P_k$$

where λ_k are the eigenvalues of A and P_k are the projection operators onto the eigenspaces of A. We know

$$p_k = \langle\psi|P_k\psi\rangle$$

The goal is to figure out the time evolution of p_k. There are several different ways we can think about this:

- The Schrödinger picture: The state $|\psi\rangle$ evolves in time, but the operators are time-independent.
- The Heisenberg picture: The state is time-independent, but the operators evolve in time. So $P_k(t)$ and therefore $A(t)$ will evolve over time.
- The final picture is both, where the state and the operators evolve in time. But we can't double count, we need to be careful which part of the evolution we are assigning to the state and which part to the operator. This is called the interaction picture.

Recall the axiom of quantum mechanics that time evolution is unitary. This means that

$$\exists U(t,t_0) \text{ such that } |\psi(t)\rangle = U(t,t_0)\,|\psi(t_0)\rangle$$

Note that

1. $U(t=t_0,t_0)=I$.
2. $U(t,t_0)$ is unique.
3. Decomposition: $U(t,t_0)=U(t,t_1)U(t_1,t_0)$.

17.3 Schrödinger's equation

Now let's derive Schrödinger's equation. We know that

$$|\psi(t)\rangle = U(t,t_0)\,|\psi(t_0)\rangle$$
$$\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = \frac{\mathrm{d}}{\mathrm{d}t}U(t,t_0)\,|\psi(t_0)\rangle$$

But in between, let's insert the identity:

$$\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = \left(\frac{\mathrm{d}}{\mathrm{d}t}U(t,t_0)\right)U^\dagger(t,t_0)U(t,t_0)\,|\psi(t_0)\rangle$$

Therefore,

$$\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = \left(\frac{\mathrm{d}}{\mathrm{d}t}U(t,t_0)\right)U^\dagger(t,t_0)\,|\psi(t)\rangle$$

Let's call $\Lambda(t,t_0)=\left(\frac{\mathrm{d}}{\mathrm{d}t}U(t,t_0)\right)U^\dagger(t,t_0)$.

What is Λ? We know that it has units of inverse time, and that it is anti-hermitian. To see this, note that

$$\Lambda^\dagger = U\frac{\mathrm{d}}{\mathrm{d}t}U^\dagger$$

So

$$\Lambda+\Lambda^\dagger = \frac{\mathrm{d}U}{\mathrm{d}t}U^\dagger + U\frac{\mathrm{d}U^\dagger}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}UU^\dagger = 0$$

Also, $\Lambda(t,t_0)$ should not depend on t_0. To show this, let's start with letting $U(t,t_0) = U(t,t_1)U(t_1,t_0)$. Then,

$$\Lambda(t,t_0) = \frac{\mathrm{d}}{\mathrm{d}t}(U(t,t_1)U(t_1,t_0))(U(t,t_1)U(t_1,t_0))^\dagger$$
$$= \frac{\mathrm{d}U(t,t_1)}{\mathrm{d}t}U(t_1,t_0)U(t_1,t_0)^\dagger U(t,t_1)^\dagger = \Lambda(t,t_1)$$

So now, let's define the Hamiltonian as $\hat{H}(t)\equiv i\hbar\Lambda(t)$. This operator has units of energy and is Hermitian. Expanding it out:

$$-\frac{i}{\hbar}H(t)\,|\psi(t)\rangle = \frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle$$

This operator is the generator of time evolution, and it relates $|\psi(t)\rangle$ to $|\psi(t+\mathrm{d}t)\rangle$.

17.4 Hamiltonian

Given an orthonormal basis $\{|i\rangle\}$, we can write

$$H = \sum_i H_{ii} |i\rangle \langle i| + \sum_{i \neq j} H_{ij} |i\rangle \langle j|$$

The values H_{ii} are called the energies, and the H_{ij} are called the transition amplitudes. These transition amplitudes describe the tendency of the system to move from state i to state j.

For example, consider a system with two states $|L\rangle$ and $|R\rangle$. This is a ball in a box with two different sides. What is the tendency of the ball to move across the box? Let's call this J. Say the left side has energy E_L and the right side has energy E_R. Then,

$$H = \begin{pmatrix} E_L & J \\ J & E_R \end{pmatrix}$$

Let's give a different example. Let's say I want to do some tricky business, and so I write my stuff in a different basis. I write

$$|\text{even}\rangle = \frac{1}{\sqrt{2}}(|L\rangle + |R\rangle)$$

and

$$|\text{odd}\rangle = \frac{1}{\sqrt{2}}(|L\rangle - |R\rangle)$$

Then, my Hamiltonian will be

$$H = \begin{pmatrix} J & \frac{E_L - E_R}{2} \\ \frac{E_R - E_L}{2} & -J \end{pmatrix} + \begin{pmatrix} \frac{E_L + E_R}{2} & 0 \\ 0 & \frac{E_L + E_R}{2} \end{pmatrix}$$

On the problem set to come, I made a fun problem. Do you guys know about the towers of Hanoi? Some transitions are allowed and some aren't. The problem asks you to construct a Hamiltonian for this system.

17.5 General Solution of the Schrödinger Equation

We want to solve

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t} U(t, t_0) = H(t) U(t, t_0)$$

Today, we'll write down explicit solutions for a few cases:

1. The Hamiltonian is time independent.
2. The Hamiltonian commutes with itself at different times, i.e. $[H(t), H(t')] = 0$.
3. The Hamiltonian is an arbitrary function of time.

Let's consider the second case and the first case.

$$U(t,t_0) = \exp\left(-\frac{i}{\hbar}\int_{t_0}^{t} H(t')\mathrm{d}t'\right)$$

So in the case where H is time-independent, we can pull it out of the integral:

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

In practice, we find an orthonormal basis $|E_j\rangle$ such that $H|E_j\rangle = E_j(t)|E_j\rangle$. Then, our solution is

$$\frac{\mathrm{d}}{\mathrm{d}t}|E_j\rangle = -i\frac{E_j(t)}{\hbar}|E_j\rangle$$

So

$$U|E_j\rangle = \exp\left(-\frac{i}{\hbar}\int_{t_0}^{t} E_j(t')\mathrm{d}t'\right)|E_j\rangle$$

Therefore, if $|\psi(t_0)\rangle = \sum_j c_j|E_j\rangle$, then

$$|\psi(t)\rangle = \sum_j c_j \exp\left(-\frac{i}{\hbar}\int_{t_0}^{t} E_j(t')\mathrm{d}t'\right)|E_j\rangle$$

In case 3, we have

$$U(t,t_0) = \mathcal{T}_{\exp}\left(-\frac{i}{\hbar}\int_{t_0}^{t} H(t')\mathrm{d}t'\right)$$

where $\mathcal{T}_{\exp}$ is the time-ordered exponential. This is equal to:

$$U(t,t_0) = \sum_{n=0}^{\infty}\left(-\frac{i}{\hbar}\right)^n \int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\ldots\int_{t_0}^{t_{n-1}}\mathrm{d}t_n H(t_1)H(t_2)\ldots H(t_n)$$

where $t_1 \geq t_2 \geq \ldots \geq t_n$.

18 Recitation 9 (2024-10-03)

Today we'll discuss some applications of the uncertainty relations. We'll see how we can get lower bounds of energies from the uncertainty relation.

Example 18.1

Let's say we have

$$\hat{H} = \frac{p^2}{2m} + \alpha x^4$$

Note: in the following equations, a subscript of 0 will denote that the value pertains to the ground state. We know for the ground state,

$$\left\langle \hat{H} \right\rangle_0 = \frac{1}{2m} \left\langle p^2 \right\rangle_0 + \alpha \left\langle x^4 \right\rangle_0$$

We know that

$$\Delta p_0^2 = \left\langle p^2 \right\rangle_0 - \left\langle p \right\rangle_0^2$$

By symmetry, we know that $\langle p \rangle_0 = 0$. Now, what about $\langle x^4 \rangle$? We know

$$\left\langle x^4 \right\rangle \geq \left\langle x^2 \right\rangle^2$$

Since $\langle x^2 \rangle = \Delta x^2 + \langle x \rangle^2 \geq \Delta x^2$, we get

$$\left\langle x^4 \right\rangle \geq \Delta x^4$$

Putting this together,

$$\langle H \rangle_0 \geq \frac{1}{2m} \Delta p_0^2 + \alpha \Delta x_0^4$$

Since $\Delta p \geq \frac{\hbar}{2\Delta x}$, we get

$$\langle H \rangle_0 \geq \frac{\hbar^2}{8m\Delta x_0^2} + \alpha \Delta x_0^4 = f(\Delta x_0)$$

We notice that this function has a single minimum. The weakest bound is at the minimum, so we can bound the ground state energy to be at least this by minimizing this function. The minimum is when

$$\Delta x_0^2 = \sqrt[3]{\frac{\hbar^2}{16m\alpha}}$$

which gives

$$\langle H \rangle_0 \geq 2^{1/3} \frac{3}{8} \left(\frac{\hbar^2 \sqrt{\alpha}}{m} \right)^{2/3} = 0.47 \left(\frac{\hbar^2 \sqrt{\alpha}}{m} \right)^{2/3}$$

The true value is 0.67, so this is a pretty good estimate.

Example 18.2

Let's consider the Hydrogen atom. We know that

$$\hat{H} = \frac{p^2}{2m} - \frac{e^2}{4\pi\epsilon_0 r} = \frac{p_r^2}{2m} + \frac{L^2}{2mr^2} - \frac{e^2}{4\pi\epsilon_0 r}$$

where $p_r = -i\hbar \left(\frac{\mathrm{d}}{\mathrm{d}r} + \frac{1}{r} \right)$, the radial momentum operator. We know that $\Delta p_r \Delta r \geq \frac{\hbar}{2}$.

For the ground state with $l = 0$, we know that

$$\langle H \rangle_0 = \frac{\langle p_r^2 \rangle_0}{2m} - \frac{e^2}{4\pi\epsilon_0} \left\langle \frac{1}{r} \right\rangle_0$$

Let $I(\xi) = \langle f(\xi) | f(\xi) \rangle$. Then

$$|f(\xi)\rangle = (\xi F - iG) |\psi\rangle$$

$$I(\xi) = \xi^2 \langle \psi | F^2 | \psi \rangle + \langle \psi | G^2 | \psi \rangle - i\xi \langle \psi | [F, G] | \psi \rangle$$

So if we choose $F = p_r$ and $G = \frac{1}{r}$, we get

$$\left[p_r, \frac{1}{r} \right] \phi = \frac{i\hbar}{r^2} \phi$$

so

$$I(\xi) = \xi^2 \langle p_r^2 \rangle + \xi\hbar \left\langle \frac{1}{r^2} \right\rangle + \left\langle \frac{1}{r^2} \right\rangle$$

By the way, on the midterm there might be a lot of trick questions that may try to get you to mix up $\langle p \rangle^2$ and $\langle p^2 \rangle$, or $\langle p \rangle$ and $\langle p^3 \rangle^{1/3}$, so be careful, these are different quantities.

Since $I(\xi) \geq 0$, it can't have any real non-zero solutions. This means that it's discriminant should be non-positive. This gives

$$\left(\hbar \left\langle \frac{1}{r^2} \right\rangle \right)^2 - 4 \langle p_r^2 \rangle \left\langle \frac{1}{r^2} \right\rangle \leq 0$$

Our result is that

$$\langle p_r^2 \rangle \geq \frac{\hbar^2}{4} \left\langle \frac{1}{r^2} \right\rangle$$

If we let $\phi = \frac{1}{r}\psi$, then by the Schwartz inequality we get

$$\langle \phi | \phi \rangle \langle \psi | \psi \rangle \geq | \langle \phi | \psi \rangle |^2$$

which gives

$$\left\langle \frac{1}{r^2} \right\rangle \geq \left\langle \frac{1}{r} \right\rangle^2$$

Combining these, we get

$$\langle p_r^2 \rangle \geq \frac{\hbar^2}{4} \left\langle \frac{1}{r} \right\rangle^2$$

Now, we can plug this back in and get

$$\langle H \rangle \geq \frac{\hbar^2}{8m} \left\langle \frac{1}{r} \right\rangle^2 - \frac{e^2}{4\pi\epsilon_0} \left\langle \frac{1}{r} \right\rangle$$

Notice that this goes negative. This means that bound states probably exist. Minimizing, we get

$$\langle H_0 \rangle \geq -\frac{me^4}{8\pi^2\hbar^2\epsilon_0^2}$$

The actual value is

$$E_0 = -\frac{me^4}{32\pi^2\epsilon_0^2\hbar^2}$$

Ok, now let's continue with time dependent Hamiltonians. Let's talk a little bit about problem 6 in your most recent pset.

We will consider a carbon dioxide molecule. We have an electron that can move easily from C to O but not from O to O. Also, from the C, the electron can jump to a fourth atom. The Hamiltonian would look like

$$\begin{pmatrix} \epsilon & -r & 0 & 0 \\ -r & \epsilon & -r & -r \\ 0 & -r & \epsilon & 0 \\ 0 & -r & 0 & \epsilon \end{pmatrix}$$

where ϵ is the energy of the electron on the C or O atoms, and r is the transition amplitude. Then,

$$|\psi(t)\rangle = e^{\frac{i\hat{H}t}{\hbar}} |\psi(0)\rangle \approx \left(1 + \frac{i\hat{H}t}{\hbar}\right) |\psi(0)\rangle$$

We see immediately how these off diagonal elements will help the electron move around between different states.

19 Lecture 10 (2024-10-07)

Last week we talked about the Schrödinger equation:

$$\frac{\mathrm{d}}{\mathrm{d}t}U(t) = -i\frac{\hat{H}}{\hbar}U(t)$$

Alternatively,

$$\hat{H} = i\hbar\left(\frac{\mathrm{d}}{\mathrm{d}t}U(t)\right)U^\dagger(t)$$

We see that we can think of this as either we have a Hamiltonian and we want to solve for the time evolution operator, or we have the time evolution operator and we want to solve for the Hamiltonian.

19.1 The Heisenberg Picture

Given $\hat{A} = \sum_k \lambda_k P_k$, and $p_k = \langle\psi(t)| P_k |\psi(t)\rangle$. Then,

$$\sum_k \lambda_k p_k = \langle A\rangle = \langle\psi(t)| \hat{A} |\psi(t)\rangle$$

We can think of

$$\langle A\rangle(t) = \langle\psi(0)| U^\dagger(t) A U(t) |\psi(0)\rangle \implies \hat{A}(t) = U^\dagger(t)\hat{A}U(t)$$

Then, we will not need to think about the time evolution of the state, but we will need to think about the time evolution of the operators.

What are some properties of Heisenberg operators?

Let's consider two Schrödinger operators A_S and B_S. We know that

$$A_H(t) = U^\dagger(t) A U(t)$$

$$B_H(t) = U^\dagger(t) B U(t)$$

We can show that if $C_S = A_S B_S$, then $C_H = A_H B_H$. If $A_S = I$, then $A_H(t) = I$. Furthermore, $[A_H(t), B_H(t)] = U^\dagger(t)[A_S, B_S]U(t)$.

Let's consider functions of operators. It can be easily shown that also

$$f(A_H(t)) = U^\dagger(t) f(A_S) U(t)$$

Also, say we have some potential V and a position operator $\hat{x}$. Then, we can write

$$\langle V(\hat{x})\rangle_t = \langle V(\hat{x}_H(t))\rangle_0$$

where $\hat{x}_H(t) = U^\dagger(t)\hat{x}U(t)$.

19.2 Heisenberg Equations of Motion

What about equations of motion in the Heisenberg picture?

$$\frac{\mathrm{d}}{\mathrm{d}t}O_H(t) = \left(\frac{\mathrm{d}}{\mathrm{d}t}U^\dagger(t)\right)O_S U(t) + U^\dagger(t)O_S\left(\frac{\mathrm{d}}{\mathrm{d}t}U(t)\right) + U^\dagger(t)\left(\frac{\partial}{\partial t}O_s(t)\right)U(t)$$

We can plug in the Schrödinger equation to get

$$\frac{\mathrm{d}}{\mathrm{d}t}O_H(t) = iU^\dagger\frac{\hat{H}}{\hbar}O_S(t)U(t) - iU^\dagger(t)O_s(t)\frac{\hat{H}}{\hbar}U(t) + U^\dagger(t)\frac{\partial O_S}{\partial t}U(t)$$

If we want to convert this to the Heisenberg picture:

$$\frac{\mathrm{d}}{\mathrm{d}t}O_H(t) = i\frac{\hat{H}_H}{\hbar}O_H(t) - iO_H(t)\frac{\hat{H}_H}{\hbar} + U^\dagger(t)\frac{\partial O_H}{\partial t}U(t)$$

Therefore, we can write the Heisenberg Equation of Motion

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}O_H(t) = [O_H(t), \hat{H}_H(t)] + i\hbar\left(\frac{\partial}{\partial t}O_S(t)\right)_H$$

For example, let $O_S = \hat{H}$. In this case, $U(t) = e^{-\frac{i\hat{H}t}{\hbar}}$. We will have that O_S commutes with U, so $O_H(t) = \hat{H}$.

Similarly, if $[H_S(t_1), H_S(t_2)] = 0$, then by our solution

$$U(t) = e^{-\frac{i}{\hbar}\int_{t_0}^{t} H(t')\mathrm{d}t'}$$

Then we will get that $H_H(t) = H_S(t)$.

In general, for all operators O such that $[O_S, H_S(t)] = 0$ for all time, then $O_H(t) = O_S$. Furthermore, for all states $|\psi_0\rangle$, this implies

$$\langle O\rangle_t = \langle O\rangle_0$$

we see that this quantity is conserved.

Why do we study the Heisenberg picture? It is useful for studying dynamics without having to specify the initial state. For example, given an operator that commutes with the Hamiltonian, we can immediately say that it is conserved.

19.3 Review of the Simple Harmonic Oscillator

Let's review the simple harmonic oscillator.

The Hamiltonian of the simple harmonic oscillator is

$$\hat{H}_{\text{SHO}} = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{x}^2$$

The first step is to notice that we can factor the Hamiltonian as

$$\hat{H} = \frac{m\omega^2}{2}\left(\hat{x} - \frac{i\hat{p}}{m\omega}\right)\left(\hat{x} + \frac{i\hat{p}}{m\omega}\right) + \frac{1}{2}\hbar\omega$$

where we used that $[\hat{x}, \hat{p}] = i\hbar$.

We will call

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i\hat{p}}{m\omega}\right)$$

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

Furthermore, define the number operator

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

Do these operators have eigenvectors and eigenvalues? It turns out that $\hat{a}$ has an infinite number of eigenvectors. However, $\hat{a}^\dagger$ has no eigenvectors. This will be the topic of next lecture.

We can also write

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

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

With some calculation, we can get $[a, a^\dagger] = aa^\dagger - a^\dagger a = 1$. Let's compute

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

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

Also, since $\hat{H} = \hbar\omega\left(\hat{N} + \frac{1}{2}\right)$, we get

$$[a, H] = \hbar\omega a$$

$$[a^\dagger, H] = -\hbar\omega a^\dagger$$

Also, by repeated use of our commutation relation, we can prove that

$$[a, (a^\dagger)^m a^n] = m(a^\dagger)^{m-1}a^n$$

For energy eigenstates, we effectively want to find eigenstates of the number operator

$$\hat{N}\left|\lambda\right\rangle = \lambda\left|\lambda\right\rangle$$

$$\left\langle\lambda\right|\lambda\left|\lambda\right\rangle = \lambda$$

$$\implies \left\langle\lambda\right|\hat{N}\left|\lambda\right\rangle = \left\langle\lambda\right|a^\dagger a\left|\lambda\right\rangle = \left|a\left|\lambda\right\rangle\right|^2 = \lambda$$

Therefore, the eigenvalues of $\hat{N}$ must be non-negative. In terms of the energy, we know that $E \geq \frac{\hbar\omega}{2}$.

Now, what happens when we compute

$$Na\left|\lambda\right\rangle = (a^\dagger aa)\left|\lambda\right\rangle = (aa^\dagger - 1)a\left|\lambda\right\rangle = aa^\dagger a\left|\lambda\right\rangle - a\left|\lambda\right\rangle = (\lambda - 1)a\left|\lambda\right\rangle$$

Therefore, $a\left|\lambda\right\rangle$ is an eigenvector with eigenvalue $\lambda - 1$ (assuming that $|a\left|\lambda\right\rangle| \neq 0$).

Similarly, we can derive that

$$Na^\dagger\lambda = (\lambda + 1)a^\dagger\left|\lambda\right\rangle$$

Therefore, $a^\dagger\left|\lambda\right\rangle$ is an eigenvector of $\hat{N}$ with eigenvalue $\lambda + 1$.

We see that these two operators form a "ladder" that gives us energy eigenstates. But since we know that the eigenvalues of $\hat{N}$ are non-negative, this ladder should end somewhere. Therefore, we can conclude that there must be a state $\left|\lambda_{\min}\right\rangle$ such that $a\left|\lambda_{\min}\right\rangle = 0$.

Since we know that

$$|a\left|\lambda_{\min}\right\rangle|^2 = 0$$
$$\implies \left\langle\lambda_{\min}\right| a^\dagger a\left|\lambda_{\min}\right\rangle = \lambda_{\min} = 0$$

Therefore, the eigenvalues of $\left|\lambda_{\min}\right\rangle$ is 0, and so the eigenvalues of $\hat{N}$ are simply the non-negative integers.

To summarize, the spectrum of $\hat{N}$ is $\{0, 1, 2, \ldots\}$ with eigenvectors $\left|0\right\rangle, \left|1\right\rangle, \left|2\right\rangle, \ldots$. In terms of the Hamiltonian, its eigenvalues will be $\left\{\frac{\hbar\omega}{2}, \frac{3\hbar\omega}{2}, \ldots\right\}$, with the same eigenvalues.

How do we show that we have found the complete spectrum? We know that we have found all of the eigenvalues, since if there was an eigenvalue that was not an integer, we could repeatedly apply a to get a negative eigenvalue, a contradiction. It just remains to show that there is no degeneracy, i.e. the equation $a\left|\lambda\right\rangle = 0$ has only one unique $\left|\lambda\right\rangle$. We get

$$\int \mathrm{d}x' \left\langle x\right| a\left|x'\right\rangle \left\langle x'|\psi_0\right\rangle = 0$$

$$\left(x + \frac{\hbar}{m\omega}\frac{\mathrm{d}}{\mathrm{d}x}\right)\psi_0(x) = 0$$

Which will give a solution

$$\psi_0 = N_0 \exp\left(-\frac{m\omega}{2\hbar}x^2\right)$$

20 Recitation 10 (2024-10-08)

For the midterm, I recommend that you review the recitation where we talked about the variational principle, and last time's recitation where we talked about the uncertainty principle. It is likely that you will see similar questions on the midterm.

This week we'll have a midterm, so this Thursday's recitation will be discussing problems that may show up on the midterm.

Today, let's talk about time dependence.

20.1 Time Dependence

Example 20.1

Consider a model of an electron in a 4 atom molecule. Assume that the atoms are stationary and there is finite energy cost to move from atom 2 to atoms 1, 3, and 4, but infinite cost to move between atoms 1, 3, and 4. As we discussed last time, we can write the wavefunction as

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar}|\psi(0)\rangle \approx \left(1 - \frac{i\hat{H}t}{\hbar}\right)|\psi(0)\rangle$$

Consider a basis where state $|i\rangle$ means that the electron is at site i. In this basis, the Hamiltonian will look like

$$\hat{H} = \begin{pmatrix} \varepsilon & -\Gamma & 0 & 0 \\ -\Gamma & \varepsilon & -\Gamma & -\Gamma \\ 0 & -\Gamma & \varepsilon & 0 \\ 0 & -\Gamma & 0 & \varepsilon \end{pmatrix}$$

where ε is the energy of the electron at sites 1, 3, and 4, and Γ is the transition amplitude.

The first problem is to find eigenvalues and eigenvectors of this Hamiltonian. Calculating eigenvalues, we must have $\det(\hat{H} - \lambda I) = 0$, which will end up giving us the equation

$$(\lambda - \varepsilon)^2(\lambda - 2\varepsilon\lambda + \varepsilon^2 - 3\Gamma^2) = 0$$

We will get eigenvalues of $\varepsilon, \varepsilon, \varepsilon \pm \sqrt{3}\Gamma$.

Let's consider the ground state, $\varepsilon - \sqrt{3}\Gamma$. We can write

$$\begin{pmatrix} \sqrt{3}\Gamma & -\Gamma & 0 & 0 \\ -\Gamma & \sqrt{3}\Gamma & -\Gamma & -\Gamma \\ 0 & -\Gamma & \sqrt{3}\Gamma & 0 \\ 0 & -\Gamma & 0 & \sqrt{3}\Gamma \end{pmatrix} v_1 = 0$$

We will get

$$v_1 = \frac{1}{\sqrt{6}}\begin{pmatrix} 1 \\ \sqrt{3} \\ 1 \\ 1 \end{pmatrix}$$

If we repeat, we will get that the eigenvector with eigenvalue $\varepsilon + \sqrt{3}\Gamma$ is

$$v_2 = \frac{1}{\sqrt{6}}\begin{pmatrix} 1 \\ -\sqrt{3} \\ 1 \\ 1 \end{pmatrix}$$

For our degenerate states, we can choose a set of orthogonal eigenvectors. For example, we can choose

$$v_3 = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\-1\\0\end{pmatrix}, \quad v_4 = \frac{1}{\sqrt{6}}\begin{pmatrix}1\\0\\1\\-2\end{pmatrix}$$

The second problem is to let $|\psi(0)\rangle = |2\rangle$. What is $|\psi(t)\rangle$? We can write

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar}|\psi(0)\rangle = e^{-i\hat{H}t/\hbar}\sum_{k=1}^{4}|v_k\rangle\langle v_k|2\rangle = \sum_{k=1}^{4}\langle v_k|2\rangle\left(e^{-i\hat{H}t/\hbar}|v_k\rangle\right)$$

We can easily calculate the projections: $\langle v_1|2\rangle = \frac{1}{\sqrt{2}}$, $\langle v_2|2\rangle = -\frac{1}{\sqrt{2}}$, $\langle v_3|2\rangle = 0$, and $\langle v_4|2\rangle = 0$. So let's calculate now the wavefunction at time t:

$$|\psi(t)\rangle = \sum_{k=1}^{4}e^{-iE_kt/\hbar}|v_k\rangle\langle v_k|2\rangle$$

$$= \frac{1}{\sqrt{2}}e^{-i(\varepsilon-\sqrt{3}\Gamma)t/\hbar}|v_1\rangle - \frac{1}{\sqrt{2}}e^{-i(\varepsilon+\sqrt{3}\Gamma)t/\hbar}|v_2\rangle$$

Now, the third question. What is the probability to find our system in state $|1\rangle$? To do this, we simply have

$$p_1(t) = |\langle 1|\psi(t)\rangle|^2 = \left|\frac{e^{-i\varepsilon t/\hbar}}{\sqrt{2}}\left(e^{i\Gamma\sqrt{3}t/\hbar}\langle 1|v_1\rangle - e^{-i\Gamma\sqrt{3}t/\hbar}\langle 1|v_2\rangle\right)\right|^2$$

$$= \frac{1}{\sqrt{3}}\sin^2\left(\frac{\Gamma\sqrt{3}t}{\hbar}\right)$$

Note that by symmetry, $p_3(t) = p_1(t)$ and $p_4(t) = p_2(t)$.

20.2 The Origin of Classical Physics

Now let's talk about something fun, the origin of classical physics.

In the Heisenberg picture, we have

$$\hat{A}_H(t) = U^\dagger(t)\hat{A}_S(t_0)U(t)$$

In lecture we derived that

$$i\hbar\frac{\mathrm{d}\hat{A}_H}{\mathrm{d}t} = [\hat{A}_H(t), \hat{H}_H(t)]$$

assuming that $\hat{A}$ is time independent. Taking the expectation value of both sides,

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\langle A_H(t)\rangle = \left\langle[\hat{A}_H(t), \hat{H}_H(t)]\right\rangle$$

For example, if we let $\hat{A} = \hat{p}$, then we have

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t} \langle p \rangle_t = \left\langle [\hat{p}_H(t), \hat{H}_H(t)] \right\rangle$$

But we know that

$$[\hat{p}_H(t), \hat{H}_H(t)] = \left[\hat{p}, \frac{\hat{p}^2}{2m} + V(x)\right] = -i\hbar \frac{\mathrm{d}V}{\mathrm{d}x}$$

Therefore, plugging this in we recover a classical result:

$$\frac{\mathrm{d}}{\mathrm{d}t} \langle p \rangle = -V'(x)$$

21 Lecture 11 (2024-10-9)

We won't go into the details of quantum electrodynamics, but what we talk about today is used widely in quantum electrodynamics, so if I accidentally say "photon", what I mean is just a quantum of our wavefunction.

21.1 Review of the Simple Harmonic Oscillator

We have shown that there is a number operator with eigenvalues $N |\lambda\rangle = \lambda |\lambda\rangle$. If this is true, then $a |\lambda\rangle$ is an eigenvector with eigenvalue $\lambda - 1$ and $a^\dagger |\lambda\rangle$ is an eigenvector with eigenvalue $\lambda + 1$. Therefore we have the spectrum of N:

$$\{|0\rangle, |1\rangle, |2\rangle, \ldots\}$$

Additionally, $|n\rangle \propto a |n+1\rangle$, so we can write

$$|n\rangle = ca |n+1\rangle$$

If we want to normalize this,

$$1 = \langle n+1| a^\dagger a |n+1\rangle |c|^2 = (n+1)|c|^2$$

Therefore, to normalize, we can choose $c = \frac{1}{\sqrt{n+1}}$.

Therefore, we have the identities

$$a |n+1\rangle = \sqrt{n+1} |n\rangle$$

$$a^\dagger |n-1\rangle = \sqrt{n} |n\rangle$$

Or, written in the more conventional way,

$$a^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle$$

$$a |n\rangle = \sqrt{n} |n-1\rangle$$

Now, let's talk about the Heisenberg picture of the simple harmonic oscillator. We can write

$$a_H(t) = U^\dagger(t) a_s U(t)$$

where

$$U(t) = e^{-i\hat{H}t/\hbar} = e^{-i\left(N+\frac{1}{2}\right)\omega t}$$

Then,

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t} a_H(t) = [a_H(t), \hat{H}_H(t)] = \left[a, \hbar\omega\left(N + \frac{1}{2}\right)\right] = \hbar\omega a_H(t)$$

From this differential equation, we can solve that

$$a_H(t) = a_S e^{-i\omega t}$$

Similarly, we can find that $a_H^\dagger(t) = a_S^\dagger e^{i\omega t}$.

If we think about it, $\hat{x}$ is similar to the "Real part" of a, and $\hat{p}$ is similar to the "Imaginary part" of a. So here, we already see that there should be some oscillatory behavior in the position and momentum operators. Doing the calculations, we will get

$$\hat{x}_H(t) = \hat{x}_S \cos(\omega t) + \frac{\hat{p}_S}{m\omega} \sin(\omega t)$$

$$\hat{p}_H(t) = \hat{p}_S \cos(\omega t) - m\omega \hat{x}_S \sin(\omega t)$$

Now, let's talk about coherent states

21.2 Coherent States

A coherent states are states that behave classically in a certain way we will define. Coherent states are uncertainty saturated. Additionally, the time evolution of the state will trace out a classical trajectory. Furthermore, coherent states are useful for more advanced topics later.

Let's consider an eigenstates $|n\rangle$, where $n \gg 1$. We know that $\left\langle \hat{H} \right\rangle = \hbar\omega\left(n + \frac{1}{2}\right)$. By symmetry, $\langle x \rangle = 0$. How about uncertainty in x?

To calculate $\langle x^2 \rangle$:

$$\langle n | x^2 | n \rangle \propto \langle n | (a + a^\dagger)(a + a^\dagger) | n \rangle$$

The only terms that will not cancel are the ones with one a and one $a^\dagger$. So we have

$$\left\langle x^2 \right\rangle \propto \langle n | (aa^\dagger + a^\dagger a) | n \rangle = \langle n | (2a^\dagger a + 1) | n \rangle = 2n + 1$$

Therefore, $\Delta x = \frac{l_0}{\sqrt{2}}\sqrt{2n+1}$. Similarly, we will get $\Delta p = \frac{\hbar}{\sqrt{2}l_0}\sqrt{2n+1}$ for some characteristic length l_0 that we can calculate. Therefore, the uncertainty is very much not saturated.

For a complex number α let's define a coherent state $|\alpha\rangle$.

Definition 21.1(Definition 1 of Coherent States)

A coherent state $|\alpha\rangle$ is an eigenstate of a with eigenvalue α. In other words, $\hat{a}|\alpha\rangle = \alpha|\alpha\rangle$.

Definition 21.2(Definition 2 of Coherent States)

$$|\alpha\rangle = N(\alpha)\sum_{n=0}^{\infty}\frac{1}{\sqrt{n!}}\alpha^n|n\rangle$$

It turns out that this equivalent to our first definition.

Question

Is the thing on the right a coherent state or an energy eigenstate?
Yes, this is terrible notation, but that's why we use it. In general, we will not purposely choose α to be an integer. But in cases where it gets confusing, we can also explicitly write $|\alpha = \ldots\rangle$.

Ok, now let's prove that Definition 2 implies Definition 1.

Proof. If we apply operator a:

$$a|\alpha\rangle = N(\alpha)\sum_{n=0}^{\infty}\frac{1}{\sqrt{n!}}\alpha^n a|n\rangle = N(\alpha)\sum_{n=1}^{\infty}\frac{1}{\sqrt{(n-1)!}}\alpha^n|n-1\rangle = \alpha|\alpha\rangle$$

□

Now, for the other direction:

Proof. If $a|\alpha\rangle = \alpha|\alpha\rangle$, then,

$$\langle n|a|\alpha\rangle = \alpha\langle n|\alpha\rangle = \alpha c_n(\alpha)$$

But we also know that

$$\langle n|a|\alpha\rangle = \langle\alpha|a^\dagger|n\rangle^* = (\langle\alpha|n+1\rangle\sqrt{n+1})^* = \sqrt{n+1}\langle n+1|\alpha\rangle = \sqrt{n+1}c_{n+1}(\alpha)$$

Notice that $\langle n|\alpha\rangle$ are just the coefficients of $|\alpha\rangle$ in the energy eigenstate basis. We will get

$$c_{n+1}(\alpha) = \frac{\alpha}{\sqrt{n+1}}c_n(\alpha)$$

Therefore, we can recover

$$|\alpha\rangle = N(\alpha)\sum_{n=0}^{\infty}\frac{1}{\sqrt{n!}}\alpha^n|n\rangle$$

□

We can find the normalization constant:

$$\langle\alpha|\alpha\rangle = 1 = \sum_{n,m=0}^{\infty} \langle n| \frac{1}{\sqrt{n!}}(\alpha^*)^n \frac{1}{\sqrt{n!}}\alpha^m |m\rangle = e^{|\alpha|^2}|N(\alpha)|^2$$

Therefore, we can choose

$$N(\alpha) = e^{-\frac{1}{2}|\alpha|^2}$$

Let's also talk about the third definition

If we plot our ground state, it looks like a gaussian. Now let's say we displace it by some position. Then we have a coherent state where α is purely real. Similarly, if we do the same thing in the momentum space, we will get a coherent state with α purely imaginary. We will talk about this more next time.

Now, let's talk about the meaning of the parameter α. Let's calculate

$$\langle\hat{x}\rangle_\alpha = \frac{l_0}{\sqrt{2}} \langle\alpha| a + a^\dagger |\alpha\rangle = \frac{l_0}{\sqrt{2}}(\alpha + \alpha^*) = l_0\sqrt{2}\,\mathrm{Re}(\alpha)$$

Similarly,

$$\langle\hat{p}\rangle_\alpha = \frac{i\hbar}{\sqrt{2}l_0} \langle\alpha| a^\dagger - a |\alpha\rangle = \frac{\hbar}{l_0}\sqrt{2}\,\mathrm{Im}(\alpha)$$

What about the uncertainty,

$$(\Delta x)^2 = \langle\alpha| x^2 |\alpha\rangle - \langle\alpha| x |\alpha\rangle^2 = \frac{l_0^2}{2} \langle\alpha| (a^\dagger + a)(a^\dagger + a) |\alpha\rangle - \langle x\rangle^2$$

$$= \frac{l_0^2}{2} \langle\alpha| (a^\dagger + a)(a^\dagger + a) |\alpha\rangle - \langle x\rangle^2 = \frac{l_0^2}{2}((\alpha^*)^2 + 2\alpha^*\alpha + \alpha^2 + 1) - \frac{l_0^2}{2}(\alpha + \alpha^*)^2$$

Therefore, $\Delta x = \frac{l_0}{\sqrt{2}}$. Similarly, we can get that $\Delta p = \frac{\hbar}{\sqrt{2}l_0}$. Therefore, uncertainty is saturated.

In classical physics, we can plot x and p, and any point on this plot will be valid. For coherent states, the value of x will be the real part of α and the value of p will be the imaginary part. But since there's some uncertainty we can draw them as blobs with a specific width and height. Note that this width and height does not depend on the value of α.

21.3 Time Evolution of Coherent States

Let's see what happens when we evolve a state $|\alpha_0\rangle$. This is pretty easy to solve in the energy eigenbasis:

$$|\psi(t)\rangle = e^{-i\omega t\left(\hat{N}+\frac{1}{2}\right)} \sum_{n=0}^{\infty} \frac{1}{\sqrt{n!}}\alpha_0^n |n\rangle = e^{-i\omega t/2} \sum_{n=0}^{\infty} \frac{1}{\sqrt{n!}} e^{-i\omega t n}\alpha_0^n |n\rangle = e^{-i\omega t/2} \left|\alpha = \alpha_0 e^{-i\omega t}\right\rangle$$

For today, we can ignore this global phase, but in the future, it may become relevant. To summarize:

$$|\alpha_0, t\rangle = \left|\alpha = \alpha_0 e^{-i\omega t}\right\rangle e^{-i\omega t/2}$$

Therefore, we see that

$$\langle x\rangle_t = \langle x\rangle_0 \cos\omega t + \frac{\langle p\rangle_0}{m\omega}\sin\omega t$$
$$\langle p\rangle_t = \langle p\rangle_0 \cos\omega t - \langle x\rangle_0 m\omega \sin\omega t$$

What about probability amplitudes?

$$p_n = |\langle n|\alpha\rangle|^2 = \frac{1}{n!}|\alpha|^{2n}e^{-|\alpha|^2}$$

If we let $\lambda = |\alpha|^2$,

$$p_n = \frac{1}{n!}e^{-\lambda}\lambda^n$$

We see that this is a poisson distribution! The average value $\langle n\rangle = \lambda$, the variance $\text{var}(n) = \lambda$, and the uncertainty is $\Delta n = \sqrt{\lambda}$. We see that the relative uncertainty $\frac{\Delta n}{\lambda} \propto \frac{1}{\sqrt{n}}$, which is why the uncertainty effects disapear in the classical limit.

21.4 Overcomplete Bases

Usually, when we work with bases, we want them to be orthonormal. But if we use coherent states, in general, they will not be orthogonal. For example,

$$\langle\beta|\alpha\rangle = e^{-|\alpha|^2/2}e^{-|\beta|^2/2}\sum_{n,m}\langle n|\frac{(\beta^*)^n}{\sqrt{n!}}\frac{\alpha^m}{\sqrt{m!}}|n\rangle$$

$$= e^{-\frac{1}{2}(|\alpha|^2+|\beta|^2)}\sum_n \frac{(\alpha\beta^*)^n}{n!} = e^{-\frac{1}{2}(|\alpha|^2+|\beta|^2-2\alpha\beta^*)}$$

Therefore,

$$|\langle\beta|\alpha\rangle|^2 = e^{-|\alpha-\beta|^2}$$

So, the overlap between two coherent states decays exponentially with their distance in phase space. Usually, this distance will be very large, so we can have many coherent states that are approximately orthogonal.

It turns out, we can always rewrite

$$|\psi\rangle = \int \mathrm{d}^2\alpha\Phi(\alpha)|\alpha\rangle$$

and in fact, we can show

$$\int \frac{\mathrm{d}^2\alpha}{\pi}|\alpha\rangle\langle\alpha| = I$$

So we have some version of resolution of identity.

22 Recitation 11 (2024-10-10)

Today we will talk about problems from the past midterm. Problems 4 and 5 will be similar to problems you will see on the midterm.

23 Lecture 12 (2024-10-16)

23.1 Overcomplete Bases

Last time we talked about a basis of coherent states. We derived that

$$|\langle\beta|\alpha\rangle|^2 = e^{-|\alpha-\beta|^2}$$

We also noted that

$$\int \frac{\mathrm{d}^2\alpha}{\pi} |\alpha\rangle\langle\alpha| = 1$$

Here's a proof sketch:

Proof. Using the definition

$$|\alpha\rangle = \sum_{n=0}^{\infty} \frac{1}{\sqrt{n!}} \alpha^n |n\rangle e^{-|\alpha|^2/2}$$

We get

$$\sum_{n,m=0}^{\infty} e^{-|\alpha|^2} \int \frac{\mathrm{d}^2\alpha}{\pi} \frac{1}{\sqrt{(n!)(m!)}} (\alpha^*)^n \alpha^m |m\rangle\langle n|$$

It remains to show that the integral

$$e^{-|\alpha|^2} \int \frac{\mathrm{d}^2\alpha}{\pi} \frac{1}{\sqrt{(n!)(m!)}} (\alpha^*)^n \alpha^m = \delta_{mn}$$

□

Now let's talk about time evolution. We derived last time that if

$$|\psi\rangle = \int \mathrm{d}^2\alpha \Phi_0(\alpha) |\alpha\rangle$$

then

$$|\psi(t)\rangle = e^{-i\omega t/2} \int \mathrm{d}^2\alpha \Phi_0(\alpha) \left|\alpha e^{-i\omega t}\right\rangle$$

Therefore, we can write

$$\Phi_t(\alpha) = e^{-i\omega t/2} \Phi_0(\alpha e^{i\omega t})$$

So we see that time evolution just corresponds to rotating our function in the complex plane.

Let's see what happens when we consider an eigenstate $|n\rangle$ in our basis. We have

$$\Phi(\alpha) = \frac{1}{\pi} \sum_{m=0} \frac{1}{\sqrt{m!}} (\alpha^*)^m \langle m|n\rangle e^{-|\alpha|^2/2} = \frac{1}{\pi\sqrt{n!}} (\alpha^*)^n e^{-|\alpha|^2/2}$$

So if we plot this in the complex plane, we will see something that decays exponentially radially, while for a fixed radius we will see the phase oscillate n times as we go around.

Now what happens if we try to decompose a coherent state $|\alpha_0\rangle$ in our basis? Plugging it into our formula,

$$\Phi(\alpha) = \frac{1}{\pi}\langle\alpha|\alpha_0\rangle = \frac{1}{\pi}e^{-\frac{1}{2}|\alpha-\alpha_0|^2}$$

Therefore, we get something centered around α_0, decaying exponentially. The fact that it isn't a delta function is evidence that we are in an overcomplete basis.

Now let's talk a bit more about another definition of coherent states:

Definition 23.1(Coherent States)

We define

$$|\alpha\rangle = D(\alpha)|0\rangle$$

where

$$D(\alpha) = \exp(\alpha\hat{a}^\dagger - \alpha^*\hat{a})$$

is called the displacement operator.
We can also write this as

$$D(\alpha) = \exp\left(-i\overline{x}\frac{\hat{p}}{\hbar} + i\overline{p}\frac{\hat{x}}{\hbar}\right)$$

where

$$\overline{x} = \sqrt{2}l_0\,\mathrm{Re}(\alpha) = \langle\alpha|\,x\,|\alpha\rangle$$

$$\overline{p} = \sqrt{2}\frac{\hbar}{l_0}\,\mathrm{Im}(\alpha) = \langle\alpha|\,p\,|\alpha\rangle$$

23.2 Translation Operators

Let me take a small detour to talk about translation operators. Let's define a translation operator $T(l)$ which maps $\psi(x)$ to $\psi(x-l)$. Let's try taylor expanding:

$$T_\epsilon\psi(x) = \psi(x-\epsilon) = \psi(x) - \frac{\mathrm{d}}{\mathrm{d}x}\psi\epsilon + O(\epsilon^2)$$

$$= \left(1 - i\frac{\epsilon}{\hbar}\left(-i\hbar\frac{\mathrm{d}}{\mathrm{d}x}\right)\right)\psi(x) = \left(1 - i\frac{\epsilon}{\hbar}\hat{p}\right)\psi$$

Now what if l is no longer small? We can write it as a combination of smaller translations:

$$\psi(x-l) = \lim_{\epsilon\to 0}\left(1 - i\frac{\epsilon}{\hbar}\hat{p}\right)^{l/\epsilon}\psi(x) = \exp\left(-i\frac{\hat{p}}{\hbar}l\right)\psi(x)$$

Therefore we can write the translation operator in terms of an exponentiation of the momentum operator. We say that the momentum operator *generates* spatial translation. Let's show this more rigorously in 8.05 notation.

We want to prove that $T_l |x\rangle = |x + l\rangle$. Consider

$$\langle p| T_l |x\rangle = \langle p| e^{-il\hat{p}/\hbar} |x\rangle = e^{-ipl/\hbar} \langle p|x\rangle = \frac{1}{\sqrt{2\pi}} e^{-ip(l+x)/\hbar} = \langle p|x + l\rangle$$

where we used the definition of momentum basis:

$$\langle p|x\rangle = \frac{1}{\sqrt{2\pi}} e^{-ipx}$$

Now what about a momentum translation operator? Let's define

$$T_q = e^{iq\hat{x}/\hbar}$$

It behaves similarly to the translation operator in position space.

So now what about general displacement operators. What are some ways we might do this?

- We can try $T_l \cdot T_q$, shifting first by momentum and then by position.
- We can try $T_q \cdot T_l$. This is different from the first choice, since x and p do not commute.
- We can try $U^\dagger(\theta) T_l U(\theta)$, where $U(\theta) = e^{-i\hat{H}\theta/\omega}$, which has the effect of rotating by θ. This will be the definition we use for today.

Therefore,

$$D(l_x, q_p) = U^\dagger(\theta) \exp\left(-i\frac{l\hat{p}}{\hbar}\right) U(\theta)$$

where

$$\cos\theta = \frac{l_x}{l}$$

and

$$\frac{l}{l_0} = \sqrt{\left(\frac{l_x}{l_0}\right)^2 + \left(\frac{q}{\hbar/l_0}\right)^2}$$

$$D(l_x, q_p) = \exp\left(-i\frac{l}{\hbar}\hat{p}(t)\right) = \exp\left(-i\frac{l_x\hat{p} + iq_p\hat{x}}{\hbar}\right)$$

since we established that

$$\hat{p}(t) = \cos(\omega t)\hat{p} + i\sin(\omega t)\hat{x}$$

Now, let's start with

$$|\alpha\rangle = D(\alpha) |0\rangle = e^{\alpha a^\dagger - \alpha^* a} |0\rangle$$

We can expand this using the BCH formula. Since $[\alpha a^\dagger, -\alpha^* a] = -|\alpha|^2[a^\dagger, a] = |\alpha|^2$,

$$D(\alpha) = e^{\alpha a^\dagger} e^{-\alpha^* a} e^{-\frac{1}{2}|\alpha|^2}$$

We then get

$$D(\alpha) |0\rangle = e^{-\frac{1}{2}|\alpha|^2} \sum_{n=0}^{\infty} \frac{1}{n!} (\alpha a^\dagger)^n |0\rangle = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle$$

23.3 Squeezed States

Let's talk a bit about squeezed states. They are called squeezed because they have $\Delta x = \Delta x_0 e^{-\gamma}$ and $\Delta p = \Delta p_0 e^{\gamma}$.

To generate these squeezed states, let's define a squeeze operator:

$$S(\gamma) = \exp\left(-\frac{1}{2}(\gamma aa - \gamma a^\dagger a^\dagger)\right)$$

This is a unitary operator. Thus we can think of

$$a(\gamma) = S^\dagger(\gamma) a S(\gamma)$$

Squeezed states are special cases of what we call Gaussian states:

$$|\alpha, \theta, \gamma\rangle = D(\alpha)U(\theta)S(\gamma)\,|0\rangle$$

In the last two minutes, let's briefly talk about angular momentum. Consider an operator

$$R(\alpha)f(r,\theta) = f(r, \theta - \alpha)$$

We can easily show that

$$R(\alpha) = \lim_{\epsilon \to 0} (1 - \epsilon \partial_\theta)^{\alpha/t} = e^{-i\alpha(-i\partial_\theta)}$$

Then, we can call $\hat{L} = -i\partial_\theta$ to be the angular momentum operator, which generates rotations. In fact,

$$i\frac{\mathrm{d}}{\mathrm{d}\theta} = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x = \hat{r} \times \hat{p}$$

Therefore, we can see that the Hamiltonian generates time evolution, momentum generates translation, and angular momentum generates rotation.

24 Recitation 12 (2024-10-17)

In recitation, we discussed the solutions to problems on the midterm. Solutions will be posted online soon.

25 Lecture 13 (2024-10-21)

Today, Prof. Ivanov will be lecturing.

25.1 Two Level Systems

A two level system is any quantum system with a Hilbert space of dimension 2. This is the simplest possible non-trivial quantum system. These are also called qubits.

The canonical example is the spin-1/2 particle. For example, electrons, etc.

Another example is a system with two approximately degenerate ground states. For example, the ammonia molecule has two states, one where the N is above the plane of the three Hydrogens, one where it is below.

A third example is a system with a ground state and a first excited state. For example, electronic energy levels in an atom.

Finally, any choice of a pair of relevant quantum states can be thought of as a two level system.

Ok, now let's discuss the quantum states of a qubit. We can write our Hilbert space as

$$\mathcal{H} = \text{span}\{|0\rangle, |1\rangle\}$$

Any state can be written as

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

where $|c_0|^2 + |c_1|^2 = 1$. We can write this as

$$|\psi\rangle = e^{i\phi_0}\left(\cos\frac{\theta}{2}|0\rangle + e^{i\phi}\sin\frac{\theta}{2}|1\rangle\right)$$

For now, we will ignore the global phase $e^{i\phi_0}$. Therefore, we see that any state can be parameterized by two angles θ and ϕ. $\theta \in [0, \pi)$ is the polar angle, and $\phi \in [0, 2\pi)$ is the azimuthal angle. This gives us a visualization, called the Bloch sphere. The north pole is $|0\rangle$, and the south pole is $e^{i\phi}|1\rangle$.

We can also think about this using matrix representations. If we let

$$|0\rangle = \begin{pmatrix}1\\0\end{pmatrix}, \qquad |1\rangle = \begin{pmatrix}0\\1\end{pmatrix}$$

then we can write

$$|\theta, \phi\rangle = \begin{pmatrix}\cos\frac{\theta}{2}\\ \sin\frac{\theta}{2}e^{i\phi}\end{pmatrix}$$

What about operators? For any operator, we can rewrite it in the basis of Pauli matrices:

$$T = \begin{pmatrix}a & b\\ c & d\end{pmatrix} = \frac{a+d}{2}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} + \frac{a-d}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} + \frac{b+c}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} + \frac{b-c}{2}i\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}$$

$$= g_0 I + g_1\sigma_1 + g_2\sigma_2 + g_3\sigma_3$$

where σ_i are the Pauli matrices.

Below are some properties of the Pauli matrices:

- They are Hermitian: $\sigma_i^\dagger = \sigma_i$
- They are unitary: $\sigma_i^\dagger = \sigma_i^{-1}$
- They are traceless: $\operatorname{Tr}\sigma_i = 0$
- They square to the identity: $\sigma_i^2 = I$
- The eigenvalues of the Pauli matrices are ± 1.

In addition to this, we can show that

$$\sigma_1\sigma_2 = i\sigma_3, \quad \sigma_2\sigma_3 = i\sigma_1, \quad \sigma_3\sigma_1 = i\sigma_2$$

$$\sigma_2\sigma_1 = -i\sigma_3, \quad \sigma_3\sigma_2 = -i\sigma_1, \quad \sigma_1\sigma_3 = -i\sigma_2$$

Or, more concisely,

$$\sigma_\alpha\sigma_\beta = i\epsilon_{\alpha\beta\gamma}\sigma_\gamma$$

where ϵ_{ijk} is the Levi-Civita symbol.

A consequence of this is that $\{\sigma_i, \sigma_j\} = 2\delta_{ij}I$.

As we discussed earlier, any operator acting on a qubit can be written as a linear combination of the Pauli matrices. This is a consequence of the fact that the Pauli matrices form a basis for the space of 2x2 matrices. For our Hamiltonian specifically, we can write

$$\hat{H} = g_0 I + g_1\sigma_1 + g_2\sigma_2 + g_3\sigma_3$$

where g_i are real numbers. It can be convenient to write this in terms of

$$\vec{g} = (g_1, g_2, g_3) = g\left(\frac{g_1}{g}, \frac{g_2}{g}, \frac{g_3}{g}\right) = g\hat{n}$$

where $g = |\vec{g}|$ and $\hat{n}$ is a unit vector. Therefore,

$$\hat{H} = g_0 I + g\vec{\sigma}\cdot\hat{n} = \sigma_{\hat{n}}$$

where $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$, and $\sigma_{\hat{n}}$ is the Pauli matrix in the direction of $\hat{n}$, defined as $\sigma_{\hat{n}} = \vec{\sigma}\cdot\hat{n}$.

Now let's try calculating eigenvalues $\lambda_\pm$ of our Hamiltonian. We know

$$\operatorname{Tr}\hat{H} = \lambda_+ + \lambda_- = 2g_0$$

$$\operatorname{Tr}\hat{H}^2 = \lambda_+^2 + \lambda_-^2 = \operatorname{Tr}(g_0^2 + g^2\sigma_{\hat{n}}^2 + 2g_0 g\sigma_{\hat{n}}) = 2g_0^2 + g^2 tr\sigma_{\hat{n}}^2$$

Expanding

$$\sigma_{\hat{n}}^2 = (n_1^2 + n_2^2 + n_3^2)I + n_1n_2\sigma_1\sigma_2 + n_2n_1\sigma_2\sigma_1 + \ldots$$

But since $\{\sigma_i, \sigma_j\} = 0$ for $i \neq j$, we get

$$\sigma_{\hat{n}}^2 = I \implies \operatorname{Tr}\sigma_{\hat{n}}^2 = 2$$

Therefore,

$$\operatorname{Tr} \hat{H}^2 = 2g_0^2 + 2g^2$$

Solving for $\lambda_\pm$, we get $\lambda_\pm = g_0 \pm g$.

Now what about the eigenvectors? We claim that if we write $\pm\hat{n}$ in polar coordinates (θ, ϕ), then we can define $|\hat{n}, \pm\rangle$. Then,

$$\hat{H} |\hat{n}, \pm\rangle = (g_0 \pm g) |\hat{n}, \pm\rangle$$

Proof. First, we can ignore g_0 and the identity operator. WLOG,

$$\hat{H} = g\sigma_{\hat{n}} = g(\sin\theta\cos\phi\sigma_1 + \sin\theta\sin\phi\sigma_2 + \cos\theta\sigma_3)$$

$$= g \begin{pmatrix} \cos\theta & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta \end{pmatrix}$$

Now, if we act on a state

$$\begin{pmatrix} \cos\theta & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta \end{pmatrix} \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} e^{i\phi} \end{pmatrix} = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} e^{i\phi} \end{pmatrix}$$

Therefore, we see that $|\hat{n}, +\rangle$ is an eigenvector of $\hat{H}$ with eigenvalue g. Similarly, we can show that $|\hat{n}, -\rangle$ is an eigenvector of $\hat{H}$ with eigenvalue $-g$. □

Let's talk a bit about time evolution. Our time evolution operator looks like

$$U(t) = e^{-i\hat{H}t/\hbar} = e^{-i\frac{gt}{\hbar}\sigma_{\hat{n}}}$$

But since $\sigma_{\hat{n}}^2 = I$, we can write this as

$$U(t) = \cos\left(\frac{gt}{\hbar}\right) I - i\sin\left(\frac{gt}{\hbar}\right)\sigma_{\hat{n}}$$

This means that for any initial state $|\psi(0)\rangle$, we can write

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle = \cos\left(\frac{gt}{\hbar}\right)|\psi(0)\rangle - i\sin\left(\frac{gt}{\hbar}\right)\sigma_{\hat{n}}|\psi(0)\rangle$$

25.2 Stern Gerlach Experiment

In the setup of the Stern Gerlach Experiment, silver atoms were evaporated and sent through a slit. They were then passed through an uneven magnetic field. What Stern and Gerlach found was that the ions would form two distinct lines. This was because silver has only one unpaired electron. This electron makes the atom behave like a magnetic dipole.

Crucially, it was possible to prepare the silver atoms such that the unpaired electrons all had no orbital angular momentum. However, in this case, there were still two distinct states.

This meant that the silver atoms had quantized, intrinsic angular momentum, which was called spin.

From this, they inferred an extra degree of freedom, which had a Hilbert space of dimension 2.

Assuming that this intrinsic angular momentum behaves similarly to normal angular momentum,

$$[\hat{S}_\alpha, \hat{S}_\beta] = i\hbar \sum_\gamma \epsilon_{\alpha\beta\gamma} \hat{S}_\gamma$$

which leads us to define our spin operators as

$$\hat{S}_i = \frac{\hbar}{2}\hat{\sigma}_i$$

The Hamiltonian of our system can be written as

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

where $\vec{\mu} = \gamma\vec{S}$, where γ is the gyromagnetic ratio. This is one of the most precisely measured constants in physics.

Say $\hat{B} = B\hat{z}$. We can calculate spin precession:

$$U(t) = e^{i\frac{\gamma Bt}{2}\sigma_{\hat{n}}} = \begin{pmatrix} e^{i\gamma Bt/2} & 0 \\ 0 & e^{-i\gamma Bt/2} \end{pmatrix}$$

which will give

$$|\psi\rangle = U(t)\,|\theta, \phi\rangle = e^{i\frac{\gamma Bt}{2}} \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} e^{i(\phi - \gamma Bt)} \end{pmatrix}$$

We get $\omega_L = -\gamma B$, which is known as the Larmor frequency.

26 Recitation 13 (2024-10-22)

Today we're going to continue talking about two level systems, and specifically the ammonia molecule that I introduced yesterday. It is one of the canonical examples of two level systems, and also what is used to produce masers.

The ammonia molecule has two states $|1\rangle$, where the N is up, and $|2\rangle$, where the N is down.

Classically, our molecule is just a bunch of balls, and the two states have the same energy. The potential is a symmetric double well.

Quantum mechanically, there is some probability for the N to tunnel through the barrier. In this case, the degeneracy gets broken, as $\langle 1|\,\hat{H}\,|2\rangle \neq 0$. In the basis of $|1\rangle$ and $|2\rangle$, we will now have

$$\hat{H} = \begin{pmatrix} E_0 & -\Delta \\ -\Delta & E_0 \end{pmatrix}$$

where E_0 is the classical energy of the molecule, and $\Delta \in \mathbb{R}$ is the tunneling amplitude.

We can rewrite this in terms of Pauli matrices:

$$\hat{H} = E_0 I - \Delta\sigma_1$$

We can see that the ground state will have energy $E_0 - \Delta$, and the first excited state will have energy $E_0 + \Delta$. In ammonia, $2\Delta \approx 1 \times 10^{-4}\,\text{eV}$, which corresponds to a wavelength of roughly 1.26 cm, in the microwave range.

Furthermore,

$$|G\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle)$$

$$|E\rangle = \frac{1}{\sqrt{2}}(|1\rangle - |2\rangle)$$

Now, considering time evolution, if $|\psi\rangle(0) = |1\rangle$, then

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar}|1\rangle = e^{-i\hat{t}/\hbar}\frac{1}{\sqrt{2}}(|E\rangle + |G\rangle) = \frac{1}{\sqrt{2}}e^{-iE_0t/\hbar}\left(|E\rangle\, e^{-i\Delta t/\hbar} + e^{i\Delta t/\hbar}|G\rangle\right)$$

$$= e^{-iE_0t/\hbar}\left(\cos\left(\frac{t\Delta}{\hbar}\right)|1\rangle + i\sin\left(\frac{t\Delta}{\hbar}\right)|2\rangle\right)$$

Therefore, we see that the probability of finding the molecule up is $\cos^2\left(\frac{t\Delta}{\hbar}\right)$, and the probability of finding the molecule down is $\sin^2\left(\frac{t\Delta}{\hbar}\right)$.

Now let's talk about how to make a maser. Let's turn on an electric field

$$\vec{E} = \varepsilon\hat{z}$$

Since ammonia is polar, there will be a net dipole moment. In the case of $|1\rangle$, it will be down, and in the case of $|2\rangle$, it will be up. Therefore, there will be an extra energy $-\mu\varepsilon$ in the $|1\rangle$ state, and an extra energy $\mu\varepsilon$ in the $|2\rangle$ state. The Hamiltonian becomes

$$\hat{H} = \begin{pmatrix} E_0 - \mu\varepsilon & -\Delta \\ -\Delta & E_0 + \mu\varepsilon \end{pmatrix}$$

Going through the same steps, we can conclude that

$$E_G = E_0 - \sqrt{\Delta^2 + \mu^2\varepsilon^2}$$

$$E_E = E_0 + \sqrt{\Delta^2 + \mu^2\varepsilon^2}$$

We see that the gap between the ground and excited state will grow.

Now imagine a beam of ammonia travelling an inhomogeneous electric field. This means that the beam will split. Now, we can put the excited atoms in a cavity, where the electric field is dependent on time. This will cause the excited atoms to exit the cavity in the ground state, and the energy will be emitted as a microwave photon.

Let's sketch the calculation. The general idea is simple. We want to adjust our electric field and size of the cavity such that the probability that the atom is in the ground state goes to 1.

First, let's assume $\Delta \gg \mu\varepsilon$. Let's work in the basis of the initial ground and excited states $|E\rangle^{(0)} = \begin{pmatrix}1\\0\end{pmatrix}$ and $|G\rangle^{(0)} = \begin{pmatrix}0\\1\end{pmatrix}$. To the leading order,

$$\langle G|\,\hat{H}\,|G\rangle = E_0 - \Delta$$

$$\langle E|\,\hat{H}\,|E\rangle = E_0 + \Delta$$

We will also have

$$\langle E|\,\hat{H}\,|G\rangle = \frac{1}{2}(\langle 1| - \langle 2|)\hat{H}(|1\rangle + |2\rangle) = \frac{1}{2}(H_{11} - H_{21} + H_{12} - H_{22}) = \mu\varepsilon(t)$$

So in our new basis, we will have

$$\hat{H} = \begin{pmatrix} E_0 + \Delta & \mu\varepsilon(t) \\ \mu\varepsilon(t) & E_0 - \Delta \end{pmatrix}$$

In general,

$$|\psi(t)\rangle = \begin{pmatrix} c_E(t) \\ c_G(t) \end{pmatrix}$$

and the Schrödinger equation will give us

$$i\hbar \begin{pmatrix} \dot{c}_E \\ \dot{c}_G \end{pmatrix} = \begin{pmatrix} E_0 + \Delta & \mu\varepsilon(t) \\ \mu\varepsilon(t) & E_0 - \Delta \end{pmatrix} \begin{pmatrix} c_E \\ c_G \end{pmatrix}$$

We can ignore E_0 and treat $\mu\varepsilon(t)$ as a perturbation. Let

$$c_E(t) = e^{-i\Delta t/\hbar} B_E(t)$$

$$c_G(t) = e^{i\Delta t/\hbar} B_G(t)$$

Then we get

$$i\hbar \begin{pmatrix} \dot{B}_E \\ \dot{B}_G \end{pmatrix} = \begin{pmatrix} 0 & e^{i\omega_0 t}\mu\varepsilon(t) \\ -e^{i\omega_0 t}\mu\varepsilon(t) & 0 \end{pmatrix} \begin{pmatrix} B_E \\ B_G \end{pmatrix}$$

where $\omega_0 = \frac{2\Delta}{\hbar}$ is the frequency of the microwave.

Now, say we choose

$$\varepsilon(t) = 2\varepsilon_0 \cos(\omega_0 t) = \varepsilon_0(e^{i\omega_0 t} + e^{-i\omega_0 t})$$

$$\implies \begin{pmatrix} \dot{B}_E \\ B_G \end{pmatrix} = \left(-\frac{i\mu\varepsilon_0}{\hbar}\right) \begin{pmatrix} 0 & 1 + 2e^{2i\omega_0 t} \\ 1 + 2e^{-2i\omega_0 t} & 0 \end{pmatrix} \begin{pmatrix} B_E \\ B_G \end{pmatrix}$$

Since $2\omega_0$ is very fast, we can average over it and therefore ignore the $e^{\pm 2i\omega_0 t}$ terms. This will give us a solution of $B_E(t) = \cos\left(\frac{\mu\varepsilon_0 t}{\hbar}\right)$ and $B_G = -i\sin\left(\frac{\mu\varepsilon_0 t}{\hbar}\right)$. Now, all we have to do is choose $t = \frac{\pi\hbar}{2\mu\varepsilon_0}$, and we will have $B_G = 1$ and $B_E = 0$. If our cavity is length $L = vt$, then we will have a maser.

27 Lecture 14 (2024-10-23)

Soonwon is still travelling this week, so Prof. Senthil Todadri will be giving this lecture.

27.1 Spin 1/2 Particle in a Magnetic Field

The hamiltonian for our system will be

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

where $\vec{\mu} = \gamma \vec{S}$, and γ is the gyromagnetic ratio.

$$S_i = \frac{\hbar}{2}\sigma_i$$

and the eigenvalues of S_i are $\pm\hbar/2$, with eigenvectors $|i, \pm\rangle$.
We will work in the simpler notation that

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

$$|z, 0\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

In this basis,

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

Let's start by considering a field along the z direction. We can write

$$\hat{H} = -\gamma B S_z = -\gamma B \frac{\hbar}{2}\sigma_z$$

The time evolution operator is

$$U(t) = e^{-itH/\hbar} = e^{i\gamma B t \sigma_z/2} = \begin{pmatrix} e^{i\gamma Bt/2} & 0 \\ 0 & e^{-i\gamma Bt/2} \end{pmatrix}$$

Consider a general initial state (θ_0, ϕ_0). In our basis it will look like

$$|\theta_0, \phi_0\rangle = \begin{pmatrix} \cos\frac{\theta_0}{2} \\ \sin\frac{\theta_0}{2} e^{i\phi_0} \end{pmatrix}$$

Applying our time evolution operator, we should get that

$$|\psi(t)\rangle = U(t)\,|\theta_0,\phi_0\rangle = \begin{pmatrix} e^{i\gamma Bt/2}\cos\frac{\theta_0}{2} \\ e^{-i\gamma Bt/2}\sin\frac{\theta_0}{2}e^{i\phi_0}\end{pmatrix} = e^{i\gamma Bt/2}\begin{pmatrix}\cos\frac{\theta_0}{2} \\ \sin\frac{\theta_0}{2}e^{i(\phi_0-\gamma Bt)}\end{pmatrix}$$

which is the same as $|\theta_0,\phi_0-\gamma Bt\rangle$, up to a phase. This spin precesses about the z axis at the Larmor frequency $\omega_L = -\gamma B$.

Now let's repeat this exercise but in the Heisenberg picture.

$$\left\langle \vec{S}\right\rangle = \hat{x}\,\langle\psi_0|\,U^\dagger(t)S_xU(t)\,|\psi_0\rangle + \hat{y}\,\langle\psi_0|\,U^\dagger(t)S_yU(t)\,|\psi_0\rangle + \hat{z}\,\langle\psi_0|\,U^\dagger(t)S_zU(t)\,|\psi_0\rangle$$

So let's define

$$\hat{S}_{i,H}(t) = U^\dagger(t)S_{i,S}U(t)$$

In the case of S_z, we have

$$\hat{S}_{z,H}(t) = U^\dagger(t)S_zU(t) = S_{z,S}$$

since U commutes with S_z.

In the case of S_x, we have

$$S_x = U^\dagger(t)S_{x,S}U(t) = \frac{\hbar}{2}e^{-\alpha\sigma^z/2}\sigma_x e^{\alpha\sigma_z/2}$$

If we do the calculations, we will find that

$$S_{x,H}(t) = \frac{\hbar}{2}\left(\cos\frac{\alpha}{2}+i\sigma_z\sin\frac{\alpha}{2}\right)\sigma_x\left(\cos\frac{\alpha}{2}-i\sigma_z\sin\frac{\alpha}{2}\right)$$

$$= \frac{\hbar}{2}\left(\cos\frac{\alpha}{2}+i\sigma_z\sin\frac{\alpha}{2}\right)\left(\cos\frac{\alpha}{2}+i\sigma_z\sin\frac{\alpha}{2}\right)\sigma_x = \frac{\hbar}{2}\left(\cos\frac{\alpha}{2}+i\sigma_z\sin\frac{\alpha}{2}\right)^2\sigma_z$$

Therefore,

$$S_{x,H} = \frac{\hbar}{2}\left(e^{i\alpha\sigma_z/2}\right)^2\sigma_x = \frac{\hbar}{2}e^{i\alpha\sigma_z}\sigma_x = \frac{\hbar}{2}\left(\cos\alpha + i\sin\alpha\sigma_z\right)\sigma_x = S_{x,S}\cos\alpha - S_{y,S}\sin\alpha$$

If $S_S = \hbar/2\hat{n}\cdot\vec{\sigma}$, then

$$S_H(t) = \frac{\hbar}{2}(n_z\sigma_z + (n_x\cos\alpha + n_y\sin\alpha)\sigma_x + (n_y\cos\alpha - n_x\sin\alpha)\sigma_y)$$

27.2 Nuclear Magnetic Resonance

The goal is to control/manipulate the spin. We will introduce an additional time dependent field rotating in the (x,y) plane.

$$\vec{B}(t) = B_0\hat{z} + B_1(\cos\omega t\hat{x} + \sin\omega t\hat{y})$$

We'll assume that $B_1 \ll B_0$.

The Hamiltonian will be

$$\hat{H} = -\gamma \vec{S} \cdot \vec{B}(t)$$

, which we can sepate into two parts:

$$\hat{H} = -\gamma B_0 S_z - \gamma B_1(\cos\omega t S_x + \sin\omega t S_y) = H_{\text{static}} + H_{\text{control}}$$

The formal solution will involve the time ordered exponential

$$U(t) = \mathcal{T} \exp\left(-\frac{i}{\hbar}\int_0^t \mathrm{d}t' H(t')\right)$$

But this will not be very helpful here.

Instead, let's try solving this problem in the interaction picture, also known as the rotating frame.

The Schrödinger picture tells us that

$$|\psi(t)\rangle = U(t)\,|\psi(0)\rangle$$

Let's define

$$\left|\tilde{\psi}(t)\right\rangle = (U_0(t))^\dagger U(t)\,|\psi(0)\rangle$$

where $U_0(t) = e^{i\nu t S_z/\hbar}$. Let's try to find an equation of motion for $\left|\tilde{\psi}(t)\right\rangle$.

$$\frac{\mathrm{d}}{\mathrm{d}t}\left|\tilde{\psi}(t)\right\rangle = \frac{\mathrm{d}}{\mathrm{d}t}(U_0(t))^\dagger\,|\psi(t)\rangle + U_0^\dagger(t)\frac{\mathrm{d}}{\mathrm{d}t}\,|\psi(t)\rangle$$

$$= \left(\frac{\mathrm{d}}{\mathrm{d}t}U_0^\dagger(t)\right)U_0(t)U_0^\dagger(t)\,|\psi(t)\rangle - iU_0^\dagger(t)\frac{H(t)}{\hbar}\,|\psi(t)\rangle$$

$$= \frac{i\nu S_z}{\hbar}U_0^\dagger(t)\,|\psi(t)\rangle - iU_0^\dagger(t)H(t)U_0(t)U_0^\dagger(t)\,|\psi(t)\rangle$$

$$= \frac{i\nu S_z}{\hbar}\left|\tilde{\psi}(t)\right\rangle - iU_0^\dagger(t)H(t)U_0(t)\left|\tilde{\psi}(t)\right\rangle$$

So

$$\frac{\mathrm{d}}{\mathrm{d}t}\left|\tilde{\psi}(t)\right\rangle = -\frac{i}{\hbar}H_I(t)\left|\tilde{\psi}(t)\right\rangle$$

where $H_I(t) = U_0^\dagger(t)(H(t) - \nu S_z)U_0(t)$ is the "interaction" Hamiltonian.

In our case,

$$H_I(t) = -U_0^\dagger(\gamma B_0 + \nu)S_z U_0 - \gamma B_1 U_0^\dagger(S_{x_S}\cos\omega t + S_{y,S}\sin\omega t)U_0$$

$$= -(\gamma B_0 + \nu)S_z - \gamma B_1(S_x\cos(\omega-\nu)t + S_y\sin(\omega-\nu)t)$$

To make our lives easy, let's choose $\nu = \omega$. This will give us a static Hamiltonian

$$H_I = -(\gamma B_0 + \omega)S_{z,S} - \gamma B_1(S_{x,S})$$

This problem is most interesting at resonance, when $\omega = \omega_L = -\gamma B_0$. Then, $H_I = -\gamma B_1 S_{x,S}$. Since our original spin was along the z axis, we can see that it will rotate about the x axis with frequency $-\gamma B_1$.

So if the initial $|\psi_0\rangle = |z, +\rangle$, but someone said, "I don't like that direction, can you make it $|z, -\rangle$?", we can just tune our frequency to resonance, and then wait for a time $\pi/\gamma B_1$. This is known as a π-pulse in NMR literature. Similarly, if we want it to point along the y axis, we can apply a $\pi/2$ pulse.

28 Recitation 14 (2024-10-24)

Today we will be discussing NMR. Recall that in NMR we have

$$B(t) = B_0\hat{z} + B_1(\cos\omega t\hat{x} - \sin\omega t\hat{y})$$

The Hamiltonian is

$$\hat{H}_S = -\gamma\vec{B}(t)\cdot\vec{S}$$

The time evolution of this system is pretty nasty, especially because $[H_s(t_1), H_s(t_2)] \neq 0$.

Luckily, we can solve this problem by going into the rotating frame. In our initial frame,

$$\hat{H}_S = -\gamma B_0 S_z - \gamma B_1(\cos\omega t S_x - \sin\omega t S_y)$$

We claim that

$$\hat{H}_S(t) = -\gamma B_0 S_z - \gamma B_1 e^{i\omega t S_z/\hbar} S_x e^{-i\omega t S_z/\hbar}$$

Where we call $e^{-i\omega t S_z/\hbar} = U_R(t)$.

Proof. Note that using $S_i = \frac{\hbar}{2}\sigma_i$, we can write

$$e^{i\omega t\sigma_3/2}\sigma_1 e^{-i\omega t\sigma_3/2}$$

Let

$$f(\theta) = e^{i\theta\sigma_3}\sigma_1 e^{-i\theta\sigma_3}$$

and

$$g(\theta) = e^{i\theta\sigma_3}\sigma_2 e^{-i\theta\sigma_3}$$

Then,

$$\frac{\mathrm{d}f}{\mathrm{d}\theta} = e^{i\theta\sigma_3}(i\sigma_3\sigma 1 - \sigma_1 i\sigma_3)e^{-i\theta\sigma_3} = -2e^{i\theta\sigma_3}\sigma_2 e^{-i\theta\sigma_3} = -2g$$

Similarly, by differentiating again we can show that

$$\frac{\mathrm{d}^2 f}{\mathrm{d}\theta^2} = -4f \implies f = A\cos 2\theta + B\sin 2\theta$$

Given our initial conditions $f(0) = \sigma_1$, $g(0) = \sigma_2$, we can see that

$$f(\theta) = \sigma_1\cos 2\theta - \sigma_2\sin 2\theta$$

So plugging this in,

$$e^{i\omega t\sigma_3/2}\sigma_1 e^{-i\omega t\sigma_3/2} = \sigma_1\cos\omega t - \sigma_2\sin\omega t$$

□

Now consider the intuition: set $B_0 = 0$. Consider a fixed spin state sitting in the B_1 field. Let the state $|\psi\rangle$ precess about the z axis by applying $U_R(t)$. Then it will remain stationary relative to B_1, and it should be similar to what we have solved earlier.

Let's define $|\psi_R(t)\rangle = e^{-i\omega t S_z/\hbar}|\psi(t)\rangle$. Let's plug this into the Schrödinger equation:

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

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}e^{i\omega t S_z/\hbar}|\psi_R(t)\rangle = H(t)e^{i\omega t S_z/\hbar}|\psi_R(t)\rangle$$

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}(U_R^\dagger|\psi_R\rangle) = H(t)U_R^\dagger|\psi_R\rangle$$

Note that

$$H(t) = U_R^\dagger(t)H(0)U_R(t)$$

Therefore,

$$i\hbar\left(\frac{i\omega S_z}{\hbar}U_R^\dagger|\psi_R\rangle + U_R^\dagger\frac{\mathrm{d}}{\mathrm{d}t}|\psi_R\rangle\right) = U_R^\dagger H(0)U_R U_R^\dagger|\psi_R\rangle$$

$$-\omega S_z U_R^\dagger|\psi_R\rangle + U_R^\dagger i\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi_R\rangle = U_R^\dagger(-\gamma B_0 S_z - \gamma B_1 S_x)|\psi_R\rangle$$

Then left multiplying by U_R gives

$$-\omega S_z|\psi_R\rangle + i\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi_R\rangle = -\gamma B_0 S_z|\psi_R\rangle - \gamma B_1 S_x|\psi_R\rangle$$

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi_R\rangle = (\omega - \gamma B_0)S_z|\psi_R\rangle - \gamma B_1 S_x|\psi_R\rangle$$

We get an effective magnetic field

$$B_{eff} = \begin{pmatrix} B_1 \\ 0 \\ B_0 - \gamma\omega \end{pmatrix}$$

So our solution will be

$$|\psi_R(t)\rangle = e^{i\vec{S}\cdot\vec{B_{eff}}t/\hbar}|\psi_R(0)\rangle$$

and

$$|\psi(t)\rangle = e^{i\omega S_z t/\hbar}e^{i\gamma\vec{S}\cdot\vec{B_{eff}}t/\hbar}|\psi(0)\rangle$$

In astronomy, we have tidal forces, and because of this, the Earth's axis of rotation precesses. On top of that, there are wobbles known as nutation. This is a similar phenomenon to what we have discussed today.

Imagine we take $B_0 \gg B_1$ and $|\psi_R(0)\rangle = |z, +\rangle$. We choose $\omega = \gamma B_0$. In this case, we will have precession around the axis x_R, the x axis in the rotating frame. Then, we can choose to apply B_1 long enough to rotate the spin to $|y_R, +\rangle$ and then turn it off. Now, with respect to the lab frame, our state will be rotating in the x-z plane. We will be able to detect this rotating dipole because it creates radiation.

29 Lecture 15 (2024-10-28)

Today we'll talk about how to understand the Hilbert space for a composite system, consisting of more than one degree of freedom.

29.1 Tensor Products

A tensor product is a method to form a new vector space from a pair of given vector spaces.

Definition 29.1(Tensor Product)

Say V and W are vector spaces over a field $\mathbb{F}$. We can write

$$Q = V \otimes W$$

such that

- We define $v \otimes w$ for $v \in V$ and $w \in W$
- For scalar multiplication,

$$\alpha(v \otimes w) = (\alpha v) \otimes w = v \otimes (\alpha w)$$

- We should have linearity of addition:

$$v_1 \otimes w + v_2 \otimes w = (v_1 + v_2) \otimes w$$

$$v \otimes w_1 + v \otimes w_2 = v \otimes (w_1 + w_2)$$

- Then, we can define

$$Q = \text{span}\{v \otimes w\}$$

Let's talk about some properties of the tensor product:

- $$v \otimes w = (v/\alpha) \otimes (\alpha w)$$

  Therefore, this tensor product is not actually the same as the Cartesian product.

- There are different ways to form the notion of 0.

$$0 \times w = v \otimes 0 = 0 = 0 \cdot (v \otimes w)$$

These are all the same 0 element.

- If $\{e_i\}$ is a basis for V and $\{f_j\}$ is a basis for W, then $\{e_i \otimes f_j\}$ is a basis for $V \otimes W$. Note that this implies that $\dim(V \otimes W) = \dim(V)\dim(W)$.

Proof. We know that

$$q = \sum_\alpha v_\alpha \otimes w_\alpha$$

for some $v_\alpha \in V$ and $w_\alpha \in W$. Then,

$$q = \sum_\alpha \left(\sum_i a_i^\alpha e_i \right) \otimes \left(\sum_j b_j^\alpha f_j \right) = \sum_{\alpha,i,j} a_i^\alpha b_j^\alpha (e_i \otimes f_j) = \sum_{i,j} c_{i,j} e_i \otimes f_j$$

for some $c_{i,j}$. Therefore, $\{e_i \otimes f_j\}$ is a basis for $V \otimes W$. □

29.2 Entangled States

Let's think about whether or not we can always write $q \in Q$ as $v \otimes w$, for some $v \in V$ and $w \in W$. The answer is no. For example, consider the state

$$q = e_1 \otimes f_1 + e_2 \otimes f_2$$

where we assume that the e_i and f_i are orthonormal. Assume that $q = v \otimes w$ for some $v \in V$ and $w \in W$. Furthermore, $v = \sum_i c_i e_i$ and $w = \sum_j d_j f_j$. Then,

$$q = \sum_{i,j} c_i d_j (e_i \otimes f_j)$$

We see that $c_1 d_1 = 1$, $c_1 d_2 = 0$, $c_2 d_1 = 0$, and $c_2 d_2 = 1$. This is a contradiction, so q cannot be written as a simple tensor product.

Definition 29.2(Product States)

We call a state $q \in V \otimes W$ a product state if it can be written as $v \otimes w$ for some $v \in V$ and $w \in W$.

Definition 29.3(Non-Product States)

We call a state $q \in V \otimes W$ a non-product state if it cannot be written as $v \otimes w$ for any $v \in V$ and $w \in W$. These are also called entangled states.

29.3 Inner Product of Tensor Products

Let's use braket notation. Let

$$|q\rangle \in Q = \text{span}\{|v\rangle \otimes |w\rangle\}$$

Then, we define the inner product as

- For product states,
$$\langle v_1 \otimes w_1 | v_2 \otimes w_2 \rangle = \langle v_1 | v_2 \rangle \langle w_1 | w_2 \rangle$$
- We should impose linearity:
$$\langle x + y | z \rangle = x \otimes z + y \otimes z$$
$$\langle x | y + z \rangle = x \otimes y + x \otimes z$$
$$\langle \alpha x | y \rangle = \alpha^* x \otimes y$$
$$\langle x | \alpha y \rangle = \alpha x \otimes y$$

Therefore, for

$$|q_1\rangle = \sum_{i,j} q_{ij}^{(1)} |i\rangle \otimes |j\rangle$$
$$|q_2\rangle = \sum_{i,j} q_{ij}^{(2)} |i\rangle \otimes |j\rangle$$

Then,

$$\langle q_1 | q_2 \rangle = \sum_{i,j} \left(q_{ij}^{(1)} \right)^* q_{ij}^{(2)}$$

In some cases, we will write $|v\rangle \otimes |w\rangle = |v, w\rangle = |v\rangle |w\rangle$. These are just different conventions for notation.

Example 29.1

One simple example is two spin-1/2 particles. We can write the basis as

$$\{|z, \pm\rangle \otimes |z, \pm\rangle\}$$

Alternatively, we can write it in many different ways, such as

$$\{|z, \pm\rangle \otimes |x, \pm\rangle\}$$

Let's consider two simple harmonic oscillators. We can write the basis as

$$\{|n_1\rangle \otimes |n_2\rangle\}$$

What about one spin-1/2 particle and one harmonic oscillator? We can write the basis as

$$\{|z, \pm\rangle \otimes |n\rangle\}$$

What about one spin-1/2 particle moving in 1D?

$$\{|z,\pm\rangle \otimes |x\rangle\}$$

29.4 Matrix Representation of Tensor Products

We know that

$$|v\rangle \otimes |w\rangle = \sum_{i,j} v_i w_j \, |i\rangle \otimes |j\rangle$$

with a natural basis $\{|i\rangle \otimes |j\rangle\}$. Let's enumerate this basis in the order

$$\{|1,1\rangle, |1,2\rangle, \ldots, |1,m\rangle, |2,1\rangle, \ldots, |n,m\rangle\}$$

Then, we can write the matrix representation of $|v\rangle \otimes |w\rangle$ as

$$\begin{pmatrix} v_1 w_1 \\ v_1 w_2 \\ \vdots \\ v_1 w_m \\ v_2 w_1 \\ v_2 w_2 \\ \vdots \\ v_n w_m \end{pmatrix}$$

This is called the Kronecker product of the two matrices.

Using this matrix representation, we can figure out which states are entangled or not. Given $|q\rangle \in Q$, find it's matrix representation. Then, reshape it into a matrix. If this matrix is rank 1, then it is a product state. Otherwise, it is an entangled state.

30 Recitation 15 (2024-10-29)

Today we're going to review two particle systems.

Example 30.1

Let's consider a state space of two spin-1/2 particles. Our Hilbert space will look like

$$Q = V_1 \otimes V_2 = \text{span}\{|+_1\rangle |+_2\rangle, |+_1\rangle |-_2\rangle, |-_1\rangle |+_2\rangle, |-_1\rangle |-_2\rangle\}$$

A general state of our 2-particle system is given by a linear combination of these basis states:

$$|\psi\rangle = \alpha_1 |+_1\rangle |+_2\rangle + \alpha_2 |+_1\rangle |-_2\rangle + \alpha_3 |-_1\rangle |+_2\rangle + \alpha_4 |-_1\rangle |-_2\rangle$$

where α_i are 4 complex coefficients. Or, by convention, we can write this as

$$|\psi\rangle = \alpha_1 |+\rangle |+\rangle + \alpha_2 |+\rangle |-\rangle + \alpha_3 |-\rangle |+\rangle + \alpha_4 |-\rangle |-\rangle$$

$$= |+\rangle \otimes (\alpha_1 |+\rangle + \alpha_2 |-\rangle) + |-\rangle \otimes (\alpha_3 |+\rangle + \alpha_4 |-\rangle)$$

Now, what about operators? Let $T \in \mathcal{L}(V)$ and $S \in \mathcal{L}(W)$. Then, we can define $T \otimes S \in \mathcal{L}(V \otimes W)$ as

$$(T \otimes S)(v \otimes w) = (Tv) \otimes (Sw)$$

Note that we can conveniently let

$$T \otimes 1 \in \mathcal{L}(V \otimes W) \implies (T \otimes 1)(v \otimes w) = (Tv) \otimes w$$

In particular, this is useful for writing a non-interacting Hamiltonian:

$$\hat{H} = \hat{H}_1 \otimes 1 + 1 \otimes \hat{H}_2$$

where $\hat{H}_1$ and $\hat{H}_2$ are the Hamiltonians for the two particles.

Example 30.2

Let's calculate the total spin of a state of two spin-1/2 particles along the z direction. The total spin of a state is given by

$$S_z^{tot} = S_z \otimes 1 + 1 \otimes S_z$$

Recall that $S_z |\pm\rangle = \pm\frac{\hbar}{2} |\pm\rangle$.
Let's see how this acts on a general state:

$$(S_z \otimes 1) |\psi\rangle = \alpha_1 S_z |+\rangle |+\rangle + \alpha_2 S_z |+\rangle |-\rangle + \alpha_3 S_z |-\rangle |+\rangle + \alpha_4 S_z |-\rangle |-\rangle$$

$$= \alpha_1 \frac{\hbar}{2} |+\rangle |+\rangle + \alpha_2 \frac{\hbar}{2} |+\rangle |-\rangle - \alpha_3 \frac{\hbar}{2} |-\rangle |+\rangle - \alpha_4 \frac{\hbar}{2} |-\rangle |-\rangle$$

Similarly,

$$(1 \otimes S_z) |\psi\rangle = \alpha_1 \frac{\hbar}{2} |+\rangle |+\rangle - \alpha_2 \frac{\hbar}{2} |-\rangle |+\rangle + \alpha_3 \frac{\hbar}{2} |-\rangle |+\rangle - \alpha_4 \frac{\hbar}{2} |-\rangle |-\rangle$$

Therefore,

$$S_z^{tot} |\psi\rangle = \alpha_1 \hbar |+\rangle |+\rangle - \alpha_4 \hbar |-\rangle |-\rangle$$

We see that a general state with zero total spin in the z direction will look like

$$\psi = \alpha_2 |+\rangle |-\rangle + \alpha_3 |-\rangle |+\rangle$$

Example 30.3

Let's try to use this to find a state with 0 total spin. Recall that $S_x|\pm\rangle = \frac{\hbar}{2}|\mp\rangle$. Let's consider

$$S_x^{tot}|+\rangle|-\rangle = S_x|+\rangle|-\rangle + |+\rangle S_x|-\rangle = \frac{\hbar}{2}(|-\rangle|-\rangle + |+\rangle|+\rangle)$$

Similarly,

$$S_x^{tot}|-\rangle|+\rangle = \frac{\hbar}{2}(|+\rangle|+\rangle + |-\rangle|-\rangle)$$

Combining them,

$$S_x^{tot}(\alpha_2|+\rangle|-\rangle + \alpha_3|-\rangle|+\rangle) = \frac{\hbar}{2}(\alpha_2+\alpha_3)(|+\rangle|+\rangle + |-\rangle|-\rangle)$$

so we must have $\alpha_2 = -\alpha_3$. Our state will now look like $\alpha_2(|+\rangle|-\rangle - |-\rangle|+\rangle)$. We can also check that S_y^{tot} will give us 0 for this state.
Now, let's look at how inner products work so that we can normalize this state. The inner product in Q is defined as

$$\langle v_1 \otimes w_1, v_2 \otimes w_2\rangle = \langle v_1, v_2\rangle \langle w_1, w_2\rangle$$

We can verify that

$$\langle\psi|\psi\rangle = \alpha_2^*(\langle+|\langle-| - \langle-|\langle+|)\alpha_2(|+\rangle|-\rangle - |-\rangle|+\rangle)$$

$$= |\alpha_2|^2(\langle+|+\rangle\langle-|-\rangle + \langle-|-\rangle\langle+|+\rangle) = 2|\alpha_2|^2$$

So $\alpha_2 = \frac{1}{\sqrt{2}}$.

We see that this is the simplest example of an entangled state.

A state is entangled if ψ cannot be written as a product $|v\rangle|w\rangle$. Let's introduce orthonormal bases $\{e_i\}$ and $\{f_j\}$ for V and W respectively. Then, we can write

$$\psi = \sum_{i,j} A_{ij} e_i \otimes f_j$$

We can see that ψ is entangled iff $\det A \neq 0$. In the example we had earlier,

$$A = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & 0 \end{pmatrix}$$

Compare this to the product state

$$A_{11} = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} = \alpha(|+\rangle + |-\rangle) \otimes (|+\rangle + |-\rangle)$$

For entangled states, measuring one particle will give us information about the other particle. For product states, measuring one particle will not give us any information about the other particle.

31 Lecture 16 (2024-10-30)

Let's let Q be a vector space which is the tensor product $V \otimes W$. Recall that

$$|q\rangle = \sum_{i,j} A_{ij} |i\rangle \otimes |j\rangle$$

We learned that $|q\rangle$ is a product state if and only if the matrix A_{ij} can be written as a rank-1 matrix.

We can use singular value decomposition to write A_{ij} as a weighted sum of rank-1 matrices. It may be the case that A_{ij} is dominated by one of these rank-1 matrices, which would make it close to being a product state.

For example, let's consider

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

In the ordered basis $\{|+\rangle |+\rangle, |+\rangle |-\rangle, |-\rangle |+\rangle, |-\rangle |-\rangle\}$, we can write

$$|\psi\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix}$$

When we reshape it,

$$\implies \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

We can see that this is not a rank-1 matrix, so this is an entangled state.

31.1 Operators on Composite Systems

Now, let's talk about operators for composite systems. We know we can have linear operators $T \in \mathcal{L}(V)$ and $S \in \mathcal{L}(W)$. We want to construct $\mathcal{L}(V \otimes W)$ in a consistent way.

One idea is to simply consider $\mathcal{L}(V) \otimes \mathcal{L}(W)$. Not too surprisingly, this will work. Let's talk about some properties of the tensor product of operators.

If an operator $(T \otimes S)$ acts on a state $(v \otimes w)$, then we define

$$(T \otimes S)(v \otimes w) = (Tv) \otimes (Sw)$$

Furthermore, demanding linearity will make this a well-defined operator. In general,

$$R \in \mathcal{L}(V) \otimes \mathcal{L}(W) \implies R = \sum_{\alpha} T_\alpha \otimes S_\alpha$$

How do we define the product of two operators? If $R_1 = T_1 \otimes S_1$ and $R_2 = T_2 \otimes S_2$, then

$$R_1 R_2 = (T_1 \otimes S_1)(T_2 \otimes S_2) = T_1 T_2 \otimes S_1 S_2$$

Since product operators form a basis, by linearity, we can extend this to any operators in $\mathcal{L}(V \otimes W)$.

We can upgrade an operator, defining it on a bigger Hilbert space without changing its action on the original Hilbert space. For example, we can define $T \otimes 1$ on $V \otimes W$. Similarly, we can define $1 \otimes S$ on $V \otimes W$. We also can check that

$$(T \otimes 1)(1 \otimes S) = (T \otimes S)$$

and

$$(1 \otimes S)(T \otimes 1) = (T \otimes S)$$

Notice that these operators commute.

Example 31.1

Consider n spin-1/2 particles, with Hilbert space $\mathcal{H}_{spin-1/2}^{\otimes n}$. Recall

$$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

We can upgrade it in several ways. For example,

$$S_{x,1} = S_x \otimes 1 \otimes \cdots \otimes 1$$

$$S_{x,2} = 1 \otimes S_x \otimes \cdots \otimes 1$$

and so on, up to $S_{x,n}$. For any pair of these operators, they will commute.
Consider $S_{x,k}S_{x,k+1}$, we can write this as

$$1 \otimes \cdots \otimes S_x \otimes S_x \otimes \cdots \otimes 1$$

Also, consider the commutator

$$[S_{x,k}, S_{y,l}] = \begin{cases} 0 & \text{if } k \neq l \\ 2iS_{z,l} & \text{if } k = l \end{cases}$$

These are some interesting combinations of upgraded operators that may appear later.

Example 31.2

Factorizable dynamics: say we have a Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$.
Consider a Hamiltonian of the form

$$\hat{H} = \hat{H}_1 \otimes 1 + 1 \otimes \hat{H}_2$$

Now, for time evolution,

$$U(t) = e^{-i\hat{H}t/\hbar} = e^{-i(\hat{H}_1 \otimes 1 + 1 \otimes \hat{H}_2)t/\hbar} = e^{-i\hat{H}_1 t/\hbar} \otimes e^{-i\hat{H}_2 t/\hbar}$$

This means that for product states, the time evolution will be the product of the time evolutions of the individual states.
Now what if we have an entangled state? Will it ever become a product state? The answer is no. This is because if it did, we could reverse the time evolution and turn a product state into an entangled state. But as we see here, the time evolution of a product state can always be written as another product state.
This will not be true for non-factorizable Hamiltonians.

31.2 Matrix Representation for Composite Systems

Consider a Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$. Let's say $\mathcal{H}_A = \text{span}\{|i\rangle_A\}$ and $\mathcal{H}_B = \text{span}\{|j\rangle_B\}$. We need to order the basis states of $\mathcal{H}$ in a consistent way. We can write

$$\mathcal{H} = \text{span}\{|1\rangle|1\rangle, |1\rangle|2\rangle, \ldots, |1\rangle|m\rangle, |2\rangle|1\rangle, \ldots, |n\rangle|m\rangle\}$$

For operators $A \in \mathcal{L}(\mathcal{H}_A)$ and $B \in \mathcal{L}(\mathcal{H}_B)$, we can write

$$A \otimes B = \begin{pmatrix} A_{11}B & A_{12}B & \cdots & A_{1n}B \\ A_{21}B & A_{22}B & \cdots & A_{2n}B \\ \vdots & \vdots & \ddots & \vdots \\ A_{n1}B & A_{n2}B & \cdots & A_{nn}B \end{pmatrix} = \begin{pmatrix} A_{11}B_{11} & A_{11}B_{12} & A_{11}B_{13} & \ldots \\ \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{pmatrix}$$

For example, let's write out

$$\sigma_x \otimes 1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

or

$$\sigma_y \otimes \sigma_z = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & i \\ i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{pmatrix}$$

or

$$1 \otimes \sigma_z = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

$$\sigma_z \otimes 1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

Therefore,

$$\sigma_{z,1} + \sigma_{z,2} = \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix}$$

Therefore,

$$S_{z,1} + S_{z_2} = S_z^{tot} = \hbar \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

We see that there are only three possible values, even though there are four possible states. Therefore, measuring $S_{z,1}$ and $S_{z,2}$ is a complete set of commuting observables. However, measuring S_z^{tot} is different, and is not a complete set of commuting observables.

Say we have some state

$$\left|\psi^-\right\rangle = \frac{1}{\sqrt{2}}(|+\rangle\,|-\rangle - |-\rangle\,|+\rangle)$$

We know that

$$(S_{z+1} + S_{z,2})\left|\psi^-\right\rangle = 0$$

However, we can also see that looking at

$$S_{x,1} + S_{x,2} = \frac{\hbar}{2}\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} + \frac{\hbar}{2}\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}$$

We can see that

$$(S_{x,1} + S_{x,2})\left|\psi^-\right\rangle = 0$$

Furthermore,

$$S_{y,1} + S_{y,2} = \frac{\hbar}{2}\begin{pmatrix} 0 & -i & -i & 0 \\ i & 0 & 0 & -i \\ i & 0 & 0 & -i \\ 0 & i & i & 0 \end{pmatrix}$$

so

$$(S_{y,1} + S_{y,2})\left|\psi^-\right\rangle = 0$$

We get this very interesting result, that we are in a quantum state where the individual particles have spin, but when we put them together, we can form a state, called a singlet state, where the total spin is 0 in any direction.

Question

What about the state

$$\frac{1}{\sqrt{2}}(|x,+\rangle\,|x,-\rangle - |x,-\rangle\,|x,+\rangle)$$

It turns out that this is equivalent to the singlet state, up to a global phase. This will work in any direction.

One interesting result is that if we have

$$(S_{\mu,1} + S_{\mu,2}) \left|\psi^-\right\rangle = 0$$

then we can see that

$$S_{\mu,1} \left|\psi^-\right\rangle = -S_{\mu,2} \left|\psi^-\right\rangle$$

This is a very interesting result, and it implies that the entanglement is such that applying an operator to one particle is equivalent to applying the negative of that operator to the other particle.

Let's finish lecture by considering four states:

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

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

It turns out that one of these states is a singlet state, and the other three are called triplet states. These states were very important in the development of quantum entanglement.

32 Recitation 16 (2024-10-31)

Today, let's talk about how to generate entangled states.

Let's consider the Hamiltonian

$$\hat{H} = \hbar\omega\sigma_3 \otimes \sigma_3$$

Let the initial state be

$$|x, +\rangle \otimes |x, +\rangle$$

Recall that in the S_z basis, $|x, +\rangle = \frac{|+\rangle + |-\rangle}{\sqrt{2}}$.

Let's write our basis for the two particles:

$$|1\rangle = |+\rangle |+\rangle$$

$$|2\rangle = |+\rangle |-\rangle$$

$$|3\rangle = |-\rangle |+\rangle$$

$$|4\rangle = |-\rangle |-\rangle$$

What about operators in this basis? Let's consider $S_z^{tot} = S_z \otimes 1 + 1 \otimes S_z$. We can write

$$S_z \otimes 1 = \frac{\hbar}{2} \begin{pmatrix} 1\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & 0 \\ 0 & -1\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \end{pmatrix}$$

$$1 \otimes S_z = \frac{\hbar}{2} \begin{pmatrix} 1\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} & 0 \\ 0 & 1\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \end{pmatrix}$$

For a total of

$$S_z^{tot} = \hbar \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

We want to form the state

$$|\psi\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix}$$

Let's start with state

$$|\psi\rangle = \frac{|+\rangle + |-\rangle}{\sqrt{2}} \otimes \frac{|+\rangle + |-\rangle}{\sqrt{2}} = \frac{|1\rangle + |2\rangle + |3\rangle + |4\rangle}{2}$$

Recall

$$S_x^{tot} = \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}$$

Now, back to our original Hamiltonian, we have

$$\hat{H} = \hbar\omega \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Time evolution will look like

$$|\psi'\rangle = e^{-iHt/\hbar} |\psi\rangle = e^{-iHt/\hbar}(|x,+\rangle \otimes |x,+\rangle)$$

We can show that

$$e^{-iHt/\hbar} = \cos(\omega t) - i \sin(\omega t) \frac{H}{\hbar\omega}$$

Therefore,

$$|\psi'\rangle = \left(\cos(\omega t) |\psi\rangle - i \sin(\omega t) \frac{H}{\hbar\omega}\right) |\psi\rangle = \frac{1}{2} \cos\omega t \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} - \frac{i}{2} \sin\omega t \begin{pmatrix} 1 \\ -1 \\ -1 \\ 1 \end{pmatrix}$$

Now, $|\psi'\rangle$ is entangled iff the result read as a matrix is not rank 1. Our matrix is

$$A_{ij} = \frac{1}{2} \begin{pmatrix} \cos\omega t - i \sin\omega t & \cos\omega t + i \sin\omega t \\ \cos\omega t + i \sin\omega t & \cos\omega t - i \sin\omega t \end{pmatrix}$$

$$= \frac{1}{2}\begin{pmatrix} e^{-i\omega t} & e^{i\omega t} \\ e^{i\omega t} & e^{-i\omega t} \end{pmatrix}$$

The determinant of this matrix is

$$\frac{1}{4}(e^{-2i\omega t} - e^{2i\omega t}) = -\frac{i}{2}\sin(2\omega t)$$

Therefore, although while the state starts out as a product state, it will evolve into an entangled state.

I also have some tips for problem 2 (? not sure I heard this correctly) of the pset:

- $e^{k\otimes 1 + 1\otimes k} = e^k \otimes e^k$.
- k should correspond to rotations, and should be proportional to $\frac{i\theta}{2}\vec{n}\cdot\vec{\sigma}$. This will rotate an angle θ around the axis $\vec{n}$.

33 Lecture 17 (2024-11-04)

33.1 Bell States

Let's talk about the Bell basis states. Say we have an entangled state

$$|\Phi_0\rangle = \left|\Phi^+\right\rangle = \frac{1}{\sqrt{2}}(|{+}{+}\rangle + |{-}{-}\rangle)$$

Now, let

$$|\Phi_1\rangle = \left|\Psi^+\right\rangle = (1\otimes\sigma_1)\,|\Phi_0\rangle = \frac{1}{\sqrt{2}}(|{+}{-}\rangle + |{-}{+}\rangle)$$

Similarly,

$$|\Phi_2\rangle = \left|\Psi^-\right\rangle = (1\otimes\sigma_2)\,|\Phi_0\rangle = \frac{i}{\sqrt{2}}(|{+}{-}\rangle - |{-}{+}\rangle)$$

$$|\Phi_3\rangle = \left|\Phi^-\right\rangle = (1\otimes\sigma_3)\,|\Phi_0\rangle = \frac{1}{\sqrt{2}}(|{+}{+}\rangle - |{-}{-}\rangle)$$

Therefore,

$$\left|\Phi^\pm\right\rangle = \frac{1}{\sqrt{2}}(|{+}{+}\rangle \pm |{-}{-}\rangle)$$

$$\left|\Psi^\pm\right\rangle = \frac{1}{\sqrt{2}}(|{+}{-}\rangle \pm |{-}{+}\rangle)$$

up to a global phase. Note that these form an orthonormal basis for the two-particle Hilbert space. Also note that we can form non-entangled states with a combination of these, even though the basis is entirely entangled. For example,

$$|{+}{+}\rangle = \frac{1}{\sqrt{2}}(\left|\Phi^+\right\rangle + \left|\Phi^-\right\rangle)$$

and so on.

Although Halloween is over, the purpose of this lecture is to set up our discussion of spooky action at a distance, which will involve these Bell states.

33.2 Partial Measurements

Let's consider an operator

$$\hat{O} = \sum_{\alpha} \lambda_\alpha P_\alpha$$

where P_α is a projector onto

$$U_\alpha = \text{span}(|\alpha, 1\rangle, |\alpha, 2\rangle, \ldots, |\alpha, d_\alpha\rangle)$$

Recall that we can write

$$P_\alpha = \sum_{i=1}^{d_\alpha} |\alpha, i\rangle \langle \alpha, i|$$

and that

$$p_\alpha = |p_\alpha |\psi\rangle|^2 = \langle\psi| p_\alpha |\psi\rangle$$

Let's talk about the specific case where O is a local observable, as opposed to a global observable. A global observable is an observable that acts on the entire Hilbert space, while a local observable acts on a specific particle.

Consider a Hilbert space $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$. Let's consider operators of the form $O^{(1)} = O \otimes 1$, where O is an operator in $\mathcal{H}_1$, and

$$O = \sum_{\alpha} \lambda_\alpha P_\alpha$$

We can see that

$$O^{(1)} = \sum_{\alpha} \lambda_\alpha P_\alpha \otimes 1$$

When we measure on $O^{(1)}$, we will project onto the eigenspaces of $O^{(1)}$. We can write

$$|\psi\rangle \mapsto (P_\alpha \otimes 1) |\psi\rangle$$

with probability $|(P_\alpha \otimes 1) |\psi\rangle|^2$.

We can also easily extend this to the case with many particles.

Example 33.1

Let's think about what happens when we measure a product state

$$|\psi\rangle = |\phi_1\rangle \otimes |\phi_2\rangle$$

with an operator $O^{(1)} = O \otimes 1$. We see that this is equivalent to measuring O on $|\phi_1\rangle$. Similarly, after the measurement, the first state will collapse but the second state will remain untouched.

Example 33.2

What happens to an entangled state? Consider the operator $\sigma_3 \otimes 1 = \sigma_3^{(1)}$ and the state $|\Phi^+\rangle$. Let

$$\sigma_3 = |+\rangle\langle+| - |-\rangle\langle-| = P_+ - P_-$$

We can see that

$$p_+ = \langle\Phi^+| P_+ |\Phi^+\rangle = \frac{1}{\sqrt{2}}(\langle++| + \langle--|)(|+\rangle\langle+| \otimes 1)\frac{1}{\sqrt{2}}(|++\rangle + |--\rangle)$$

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

We see that when measuring P_+ on $|\Phi^+\rangle$, we will get the state $P_+|\Phi^+\rangle = |++\rangle$ with probability $\frac{1}{2}$. We can easily verify that we will get the state $|--\rangle$ with probability $\frac{1}{2}$. Note that measuring the first state in this case also affects the second state!
We can express this in a table. Say we subsequently measure the second state with $\sigma_3^{(2)}$. We can write

First outcome	Second outcome	Probability
$+$	$+$	$\frac{1}{2}$
$+$	$-$	0
$-$	$+$	0
$-$	$-$	$\frac{1}{2}$

But what if the particles are far apart and we are in a reference frame such that the second measurement comes before the first one? In this case, it doesn't really matter, and we can see that the probabilities are the same. Let's see if this is tru for a second example. Say we instead measure the second state with $\sigma_1^{(2)}$. We can write

First outcome	Second outcome	Probability
$+$	$x, +$	$\frac{1}{4}$
$+$	$x, -$	$\frac{1}{4}$
$-$	$x, +$	$\frac{1}{4}$
$-$	$x, -$	$\frac{1}{4}$

Again, we see that the probabilities are the same.

Say we have two observables $O^{(1)}$ and $O^{(2)}$. We can write

$$O^{(1)} = \sum_a \lambda_a P_a \otimes 1$$

$$O^{(2)} = \sum_b \eta_b 1 \otimes P_b$$

Let's consider the measurement

$$p(a,b) = \langle\psi| P_a \otimes P_b |\psi\rangle$$

If $|\psi\rangle$ is a product state $|\phi_1\rangle \otimes |\phi_2\rangle$, then we can easily see that $p(a,b) = \langle\phi_1| P_a |\phi_1\rangle \langle\phi_2| P_a |\phi_2\rangle = p_1(a)p_2(b)$. What about entangled states? Is it possible to get some sort of correlation? This actually gives us a quantitative measure of entanglement. We can measure entanglement as the maximum possible correlation between the two measurements.

33.3 Singlet State

Again, let's consider the Hilbert space which is the tensor product of two spin-1/2 particles. We can write the singlet state as

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

Also, recall the σ_n operator:

$$\sigma_n = n_x\sigma_x + n_y\sigma_y + n_z\sigma_z$$

We know that $\sigma_n^2 = I$. Therefore, we can write

$$\sigma_n = |n,+\rangle \langle n,+| - |n,-\rangle \langle n,-|$$

We claim that if we measure $\sigma_n^{(1)}$ on the first particle with result a, and then measure $\sigma_n^{(2)}$ on the second particle with result b, then we will get the following results, regardless of n:

First outcome	Second outcome	Probability
$+$	$+$	0
$+$	$-$	$\frac{1}{2}$
$-$	$+$	$\frac{1}{2}$
$-$	$-$	0

Proof.

$$\left|\psi^-\right\rangle = (|n,+\rangle \langle n,+| \otimes 1)\frac{1}{\sqrt{2}}(|+-\rangle - |-+\rangle)$$

Note that

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

Therefore, we can write

$$\begin{aligned}\left|\psi^-\right\rangle &= \frac{|n,+\rangle}{\sqrt{2}}\left(\left(\cos\frac{\theta}{2}\langle+| + \sin\frac{\theta}{2}e^{-i\phi}\langle-|\right)\otimes 1\right)(|+-\rangle - |-+\rangle) \\ &= \frac{|n,+\rangle}{\sqrt{2}} \otimes \left(\cos\frac{\theta}{2}|-\rangle - \sin\frac{\theta}{2}e^{-i\phi}|+\rangle\right) \\ &= \frac{e^{-i\phi}}{\sqrt{2}}|n,+\rangle \otimes \left(\sin\frac{\theta}{2}|+\rangle - \cos\frac{\theta}{2}e^{i\phi}|-\rangle\right)\end{aligned}$$

We see we get the state $(\pi - \theta, \phi + \pi)$, which is the same as the state $|n,-\rangle$.

It seems like we can affect the state of one particle by applying measurements to the other particle. This was why Einstein was not very happy about this. We will talk about the resolution of this in the next lecture. □

34 Recitation 17 (2024-11-05)

If I have some general operator A that is on $V \otimes W$, we can define partial traces

$$\mathrm{Tr}_V(A) = \sum_i (\langle e_i| \otimes 1) A (|e_i\rangle \otimes 1)$$

One interesting property of the partial trace is that

$$\mathrm{Tr}(A) = \mathrm{Tr}_V(\mathrm{Tr}_W(A)) = \mathrm{Tr}_W(\mathrm{Tr}_V(A))$$

Note that this implies that $\mathrm{Tr}(A \otimes B) = \mathrm{Tr}(A)\,\mathrm{Tr}(B)$.
Now let's review Bell states.

$$|\phi_0\rangle = \frac{1}{\sqrt{2}}(|+\rangle\,|+\rangle + |-\rangle\,|-\rangle)$$

$$|\phi_1\rangle = \frac{1}{\sqrt{2}}(|+\rangle\,|-\rangle + |-\rangle\,|+\rangle)$$

$$|\phi_2\rangle = \frac{i}{\sqrt{2}}(|+\rangle\,|-\rangle - |-\rangle\,|+\rangle)$$

$$|\phi_3\rangle = \frac{1}{\sqrt{2}}(|+\rangle\,|+\rangle - |-\rangle\,|-\rangle)$$

Now let's review measurement. We can write our generic state as

$$|\psi\rangle = \sum_{i,j} c_{ij}\,|i\rangle\,|j\rangle$$

Then, for a partial projection operator $M_i = |e_i\rangle\, c_{jk}\, \langle e_i| \otimes 1$,

$$p_i = \sum_{j,k} \langle e_j|\,\langle w_k|\,(|e_i\rangle\,\langle e_i| \otimes 1)\,|e_j\rangle\,|w_k\rangle = \langle w_i|w_i\rangle$$

where $w_i = \sum_j c_{ij}\,|w_j\rangle$. After the measurement, the state will collapse to

$$M_i\,|\psi\rangle = \frac{|e_i\rangle\,|w_i\rangle}{\sqrt{\langle w_i|w_i\rangle}}$$

Let's do another example. Say we have a state

$$|\psi\rangle = |\phi_2\rangle_{AB}$$

where Alice has the first particle and Bob has the second particle. Now, suppose Alice measures here particle using $M_+ = |+\rangle\,\langle +|$. We can see that with probability $\frac{1}{2}$, the state will collapse to $|+\rangle\,|-\rangle$, and with probability $\frac{1}{2}$, the state will collapse to $|-\rangle\,|+\rangle$.

Now, let's talk about quantum teleportation. If we have a state $|\psi_c\rangle = \alpha|+\rangle + \beta|-\rangle$, can we measure α and β? The answer is no, because we can only do measurements, which will just give probabilities. Let's think about how we can move the information in our state to another state.

Note: the following section is incomplete because I was falling asleep.

Say Alice and Bob share a Bell state $|\phi_0\rangle$. The overall state of the system is

$$|\phi_0\rangle_{AB}|\phi_c\rangle = \frac{1}{\sqrt{2}}(\alpha|+_A\rangle|+_C\rangle|+\rangle_B + \beta|-_A\rangle|-_C\rangle|-_B\rangle + \alpha|-_A\rangle|+_C\rangle|-_B\rangle + \beta|-_A\rangle|-_C\rangle|-_B\rangle)$$

$$= \frac{1}{2}|\phi_0\rangle_{AC}(\alpha|+_B\rangle + \beta|-\rangle_B) + \frac{1}{2}|\phi_1\rangle\dots$$

$$= \frac{1}{2}\sum_{i=0}^{3}|\phi_i\rangle_{AC}\sigma_i|\psi_B\rangle$$

Therefore $|\phi_i\rangle_{AC}\sigma_i|\psi_B\rangle$. From here, we can just measure some observables, and communicate information about which σ_is to apply to Bob.

35 Lecture 18 (2024-11-06)

Today let's talk about something fun. I looked up Albert Einstein's google scholar, and the number one cited paper is the content we will talk about today. It's also pretty ironic because it's incorrect.

35.1 EPR Paradox

Imagine there's a magical box that can produce pairs of particles in entangled states. Imagine now sending one particle to Alice one side and another particle to Bob on another side. We separate them over a long distance, so that they are space-like separated. Assume for now that these particles are in a singlet state.

We know that if Alice measures the spin of her particle, she will get a random result, and similar for Bob. However, if Alice measures the spin of her particle, Bob's particle will also collapse into a state. How does this information travel faster than the speed of light?

Let's establish the belief of local realism.

1. The result of a measurement at one point B cannot depend on actions taken at a far away point A at the same time (in any frame).
2. Measurement corresponds to some element of reality. For example, if a measurement of an observable is a value, that value was a property of the state before the measurement.

These two conditions are clearly violated by quantum mechanics. This is the EPR paradox.

One potential resolution is called the hidden variable theory. The theory is that there exists a hidden variable λ that contains a lot of information. This variable is very difficult to extract. All measureable observables are just derived from this hidden variable. This is deterministic, however, because we can't measure λ, our best guess is to estimate probabilities of what we can observe.

As an example, let's try explaining the EPR paradox using the hidden variable theory. Let's make a table

λ	A	B
1	$x = +, z = +$	$x = -, z = -$
2	$x = +, z = -$	$x = -, z = +$
3	$x = -, z = +$	$x = +, z = -$
4	$x = -, z = -$	$x = +, z = +$

and let's just let $p(\lambda) = \frac{1}{4}$. We can easily check that if either Alice or Bob measures in either direction, they will get $+$ or $-$ with probability $\frac{1}{2}$. However, all of these results are strictly anti-correlated. This is a deterministic theory, and it is local.

Interestingly, John Bell showed that there were certain phenomenon that could never be explained by a hidden variable theory.

35.2 Bell and CHSH Inequalities

In quantum mechanics, observables are operators a, b, c, etc. In the hidden variable theory, these observables are functions of λ, $a(\lambda)$, $b(\lambda)$, $c(\lambda)$, etc. For the sake of simplicity, let's consider observables that only take on values ± 1.

First, let's prove some inequality on arbitrary $P(\lambda)$.

$$\sum_{\lambda} P(\lambda)a(\lambda)b(\lambda) \leq \sum_{\lambda} P(\lambda)(a(\lambda)c(\lambda) + c(\lambda)b(\lambda))$$

Next, we can prepare a state such that when we measure a and b, it violates this inequality.

Let operators

$$A_0 = \sigma_1, \qquad A_1 = \sigma_3$$

while Bob chooses operators

$$B_0 = \frac{1}{\sqrt{2}}(\sigma_1 + \sigma_3), \qquad B_1 = \frac{1}{\sqrt{2}}(\sigma_1 - \sigma_3)$$

Now consider

$$Q = a_0 b_0 + a_0 b_1 + a_1 b_0 - a_1 b_1$$

We claim that

$$-2 \leq Q \leq 2$$

In terms of observables,

$$\overline{Q} = \langle\psi| A_0 \otimes (B_0 + B) + A_1 \otimes (B_0 - B_1) |\psi\rangle$$
$$= \langle\psi| \sigma_1 \otimes \sqrt{2}\sigma_1 + \sigma_3 \otimes \sqrt{2}\sigma_3 |\psi\rangle = -2\sqrt{2}$$

Therefore, since $-2\sqrt{2} < -2$, we can see that this inequality is violated.

These results were verified experimentally in 1972 by John Clauser, and in 1982 by Alan Aspect. In 2022, the Nobel Prize in Physics was awarded to John Clauser, Alain Aspect, and Anton Zeilinger for their work on this.

35.3 No Cloning Theorem

Let's think about how we can send information. We can move objects physically, or we can send information digitally. When we send information digitally, we are copying information. It turns out, such a technology cannot be established for quantum mechanics.

Theorem 35.1(No Cloning Theorem)

There is no unitary operator $U \in \mathcal{L}(\mathcal{H} \otimes \mathcal{H})$ that does the following:

$$U |\psi\rangle |\phi\rangle = |\psi\rangle |\psi\rangle$$

for all $|\psi\rangle \in \mathcal{H}$ and for some special choice of $|\phi\rangle \in \mathcal{H}$.

Proof. Let's imagine such an operator exists. Consider two distinct states $|\psi_1\rangle$ and $|\psi_2\rangle$, such that $0 < |\langle\psi_1|\psi_2\rangle| < 1$. We have

$$U |\psi_1\rangle |\phi\rangle = |\psi_1\rangle \otimes |\psi_1\rangle$$

$$U |\psi_2\rangle |\phi\rangle = |\psi_2\rangle \otimes |\psi_2\rangle$$

Before applying U, we have

$$\langle\psi_1| \langle\phi| |\psi_2\rangle |\phi\rangle |\phi\rangle = \langle\phi|\phi\rangle \langle\psi_1|\psi_2\rangle = \langle\psi_1|\psi_2\rangle$$

However, after applying U, we have

$$\langle\psi_1| \langle\phi| U^\dagger U |\psi_1\rangle |\phi\rangle = \langle\psi_1|\psi_2\rangle \langle\psi_1|\psi_2\rangle$$

However, since we assumed $0 < |\langle\psi_1|\psi_2\rangle| < 1$, this is a contradiction, since our operator is not norm-preserving. □

Notice that if $\langle\psi_1|\psi_2\rangle = 0$, then there is no contradiction.

Theorem 35.2

It is possible to find $U \in \mathcal{L}(\mathcal{H} \otimes \mathcal{H})$ such that

$$U |\psi\rangle |\phi\rangle = |\psi\rangle |\psi\rangle$$

for $|\psi\rangle \in \{|\psi_1\rangle, |\psi_2\rangle, \ldots, |\psi_d\rangle\}$, where $d \leq \dim \mathcal{H}$.

Example 35.1

Consider the ordered basis $\{|+\rangle |+\rangle, |+\rangle |-\rangle, |-\rangle |+\rangle, |-\rangle |-\rangle\}$. We can choose $|\phi\rangle = |+\rangle$, and we can write

$$U = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

We see that $U |\psi\rangle |\phi\rangle = |\psi\rangle |\psi\rangle$ for all $|\psi\rangle$.

For the final part of this lecture let's introduce the concept of quantum teleportation.

35.4 Quantum Teleportation

Since we can't clone information, let's talk about how we might send information.

Say Alice has a state $|\psi\rangle$, and Alice and Bob each also have a particle in a Bell state $|\Phi_0\rangle$. Alice will measure both her particles in the Bell basis. It turns out all four outcomes a will occur with equal probability. The new quantum state will look like the following: Alice's particles will be in some Bell state $|\Phi_\alpha\rangle$, and Bob's particle will be in some state $\left|\tilde{\psi}\right\rangle$. It turns out the state $\left|\tilde{\psi}\right\rangle$ will be proportional to $\sigma_a |\psi\rangle$. Luckily, since $\sigma_a^2 = I$, Alice can just send Bob the result of her measurement clasically, and Bob can apply the appropriate operator to his particle to get Alice's original state.

This is also a resolution to the EPR paradox. The information is not actually being sent faster than the speed of light, because the information is still being sent classically.

36 Recitation 18 (2024-11-07)

Today we'll review the EPR paradox and Bell's Inequality.

36.1 EPR Paradox

In the pset, we proved that the singlet state

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

is rotationally invariant, i.e. it can be written as

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

for any direction n, up to a global phase.

Let's talk about $p(a,b)$, for any two arbitrary unit vectors a and b, we want the probability of measuring a and b to be $+1$ in our singlet state. We can write

$$p(a,b) = |(\langle a,+|\langle b,+|)|\psi\rangle|^2$$

After some calculation, we can get

$$p(a,b) = \frac{1}{2}|\langle b,+|a,-\rangle|^2 = \frac{1}{2}\cos^2\left(\frac{\pi-\theta_{ab}}{2}\right) = \frac{1}{2}\sin^2\left(\frac{\theta_{ab}}{2}\right)$$

If $b = -a$, then we can see that $p(a,b)$ reaches its maximum value of $\frac{1}{2}$.

Recall the following assumptions of local realism:

1. The result of a measurement at one point B cannot depend on actions taken at a far away point A at the same time (in any frame).
2. Measurement corresponds to some element of reality. For example, if a measurement of an observable is a value, that value was a property of the state before the measurement.

Now, say we have a set of particles, 50% of them are in the state $|+-\rangle$ and 50% of them are in the state $|-+\rangle$. Bell wrote down an inequality:

Say an observer can measure along any of the three unit vectors a, b, and c. Then, we can write

$$p(a,b) \leq p(a,c) + p(c,b)$$

First, let's check that this is violated by our quantum mechanical model. Imagine c is between a and b, with the angle between c and each of a and b is θ, and the angle between a and b is 2θ. The inequality would become

$$\frac{1}{2}\sin^2 2\theta \leq \sin^2\theta$$

which is clearly violated. One way of seeing this is when $\theta \ll 1$, we would have

$$2\theta^2 \leq \theta^2$$

which is off by a significant factor.

Now, let's talk about how Bell came up with his inequality. Say we have N pairs of particles in a Bell state, and we can measure a, b, and c. In a hidden variable model, there would be 8 possible types of particle pairs, as we are enforcing that the spin of one particle is the opposite of the other in any direction. Note that

$$p(a,b) = p_1(a,-b,c) + p_1(a,-b,-c)$$

Furthermore,

$$p(a,c) = p_1(a,b,-c) + p_1(a,-b,-c)$$
$$p(c,b) = p_1(a,-b,c) + p_1(-a,-b,c)$$

where $p_1(a,b,c)$ is the probability that the first particle is of the type a,b,c. We can now clearly see that

$$p(a,b) \leq p(a,c) + p(c,b)$$

Now, let's talk about the correlation function. For a system in state $|\psi_{AB}\rangle$, we can define the correlation function of operators O_A and O_B as

$$\langle O_A \otimes O_B \rangle = \langle \psi_{AB}| \, O_A \otimes O_B \, |\psi_{AB}\rangle$$

If $|\psi_{AB}\rangle$ is a product state, we can see that $\langle O_A \otimes O_B \rangle = \langle O_A \rangle \langle O_B \rangle$. However, if $|\psi_{AB}\rangle$ is entangled, then we can see that $\langle O_A \otimes O_B \rangle \neq \langle O_A \rangle \langle O_B \rangle$.

37 Lecture 19 (2024-11-13)

37.1 Angular Momentum Recap

In classical physics, we have particles with coordinates $\vec{r} = (x,y,z)$ and $\vec{p} = (p_x, p_y, p_z)$. But we also have angular momentum,

$$\vec{L} = (L_x, L_y, L_z) = \vec{r} \times \vec{p} = \vec{r}_{CM} \times m\vec{v}_{CM} + \sum_i \vec{r}_i \times m\vec{v}_{i,rel}$$

We can decompose $\vec{L}$ into orbital and relative angular momentum.

Alternatively, we can write

$$L_i = \epsilon_{ijk} r_j p_k$$

or for example, expanding, $L_x = yp_z - zp_y$, and similarly for L_y and L_z.

Now let's talk about angular momentum from 8.04. In this case, we can just promote the classical angular momentum to operators. We can write

$$\hat{L}_i = \epsilon_{ijk} \hat{r}_j \hat{p}_k$$

Also, recall that $[r_i, p_j] = i\hbar\delta_{ij}$.

Let's also review some commutator formulas:

$$[L_i, r_j] = i\hbar\epsilon_{ijk} r_k$$

$$[L_i, p_j] = i\hbar\epsilon_{ijk} p_k$$

$$[L_i, L_j] = i\hbar\epsilon_{ijk} L_k$$

Definition 37.1(Operators Under Rotation)

We define a vector operator O_i to be an operator that transforms under rotations as

$$[L_i, O_j] = i\hbar\epsilon_{ijk} O_k$$

Let's also define the total angular momentum operator as

$$L^2 = L_x^2 + L_y^2 + L_z^2$$

We can check that $[L^2, L_i] = 0$. This is why we call L^2 a scalar operator. In fact, for operators A and B, we can show that $\vec{A} \cdot \vec{B}$ is a scalar operator.

Also recall from 8.04 that L^2 and L_z form a CSCO.

$$L^2 Y(\theta, \phi) = \lambda_i Y(\theta, \phi) = \hbar^2 l(l+1) Y(\theta, \phi)$$

Similarly, $L_z Y(\theta, \phi) = \hbar m Y(\theta, \phi)$. We can show that l and m must be integers. In terms of 8.05, we can say $|l, m\rangle$ form an orthonormal basis for the Hilbert space of all states, since $\langle l, m | l', m' \rangle = \delta_{l,l'} \delta_{m,m'}$.

The allowed values of l are $0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$.

Question

Shouldn't the allowed values of l be $0, 1, 2, \ldots$?
Yes, in 8.04 this is what we learned. But today I want to be correct, and we will see that with our extra spin degree of freedom, we can have half-integer values of l.

37.2 Angular Momentum in the Algebraic Approach

Remember that the Hamiltonian generates time evolution, and that momentum generates translations. Therefore, let's consider angular momentum J, which we define such that it generates

$$R(\theta, \hat{n}) = e^{-i\theta \hat{n} \cdot \vec{J}/\hbar}$$

, the rotation operator around the axis $\hat{n}$ by an angle θ. In fact, we can derive everything else from this equation.

First of all, since R must be unitary, each J_i must be Hermitian. Let's write down some other non-trivial properties that rotations must satisfy.

Consider

$$R(-\epsilon,\hat{y})R(-\epsilon,\hat{x})R(\epsilon,\hat{y})R(\epsilon,\hat{x}) = e^{i\epsilon J_y/\hbar}e^{i\epsilon J_x/\hbar}e^{-i\epsilon J_y/\hbar}e^{-i\epsilon J_x/\hbar}$$

Note that we can write this as

$$R(-\epsilon,\tilde{x})R(\epsilon,\hat{x}) = e^{i\epsilon J\cdot\tilde{x}/\hbar}e^{-i\epsilon J_x/\hbar}$$

where $\tilde{x}$ is the x-axis rotated by $-\epsilon$.

In the limit as $\epsilon \to 0$, we can show that this is equivalent to a rotation of $-\epsilon^2$ around the z-axis. Therefore, we can write

$$e^{i\epsilon J_y/\hbar}e^{i\epsilon J_x/\hbar}e^{-i\epsilon J_y/\hbar}e^{-i\epsilon J_x/\hbar} = e^{-i(-\epsilon^2)J_z/\hbar}$$

Comparing both sides, we can find that $[J_x, J_y] = i\hbar J_z$.

Note that for an operator $\vec{O}$,

$$e^{i\epsilon J_i}O_j e^{-i\epsilon J_i} = O_j + i\epsilon[J_i, O_j]$$

which is just a rotation of O_j by an angle ϵ. We get $[J_i, O_j] = i\hbar\epsilon_{ijk}O_k$.

Furthrmore, define J^2 and quantum numbers j and m as usual. Note that the expectation of J^2 is always non-negative.

Now, let's introduce raising and lowering operators:

$$J_\pm = J_x \pm iJ_y$$

We can get that

$$[J^2, J_\pm] = 0$$
$$[J_z, J_\pm] = \pm\hbar J_\pm$$

Now, from this,

$$J^2(J_+ |j,m\rangle) = J_+\hbar^2(j+1)\,|j,k\rangle$$

Therefore, we can see that $J_\pm |j,m\rangle$ is an eigenvector of J^2 with the same eigenvalue. Additionally,

$$J_z(J_+ |j,m\rangle) = J_+J_z\,|j,m\rangle + \hbar J_+\,|i,m\rangle = \hbar(m+1)J_+\,|i,m\rangle$$

Therefore,

$$J_+\,|j,m\rangle \propto |j,m+1\rangle = c_+(j,m)\,|j,m+1\rangle$$

Consider

$$|c_+(j,m)|^2 = \langle j,m|\,J_-J_+\,|j,m\rangle$$

Note that

$$J_-J_+ = J^2 - J_z^2 - \hbar J_z$$

Therefore,

$$|c_+(j,m)|^2 = \hbar^2 j(j+1) - \hbar^2 m(m+1) \implies c_+(j,m) = \hbar\sqrt{j(j+1)-m(m+1)}$$

and we conclude that

$$J_+ |j,m\rangle = \hbar\sqrt{j(j+1) - m(m+1)}\, |j,m+1\rangle$$

Similarly, we can show that

$$J_- |j,m\rangle = \hbar\sqrt{j(j+1) - m(m-1)}\, |j,m-1\rangle$$

These equations actually put some bounds on m. For example, since the norm of a vector should be nonnegative, we must have $m \leq j$. Furthermore, since must terminate at some part, we should have one m for which $c_+(j,m) = 0$, which leads us to conclude that the maximum value of m is j. Similarly, we can show that the minimum value of m is $-j$.

Now, we know that $m_{max} - m_{min} = 2j$ should be an integer. Therefore, j can only take on half integer values.

Question

"Are these raising and lowering operators related to, say, raising or lowering operators of a multi-dimensional harmonic oscillator?" - Justin Chen
Good question! Yes, if we consider a 2d harmonic oscillator, it will have a rotationally invariant Hamiltonian, so it will have some properties that are similar to angular momentum.

38 Recitation 19 (2024-11-14)

Today we covered problems 5 and 6 from the practice midterm.

39 Lecture 20 (2024-11-18)

39.1 Multiplets

Last time we reviewed a generalized angular momentum J and its raising and lowering operators $J_\pm$.

Consider a Hilbert space

$$\mathcal{H}_j = \text{span}(\{|j,m\rangle\})$$

where m ranges from $-j$ to j. The $j = 0$ state is called a singlet, the $j = \frac{1}{2}$ state is called a doublet, the $j = 1$ state is called a triplet, and so on. In general, these are called multiplets.

Let's think about some intuition. Say we have $|805, 805\rangle$. This will have angular momentum completely polarized in the z-direction. Similarly, $|805, -805\rangle$ will have angular momentum completely polarized in the $-z$-direction. However, what will $|805, 804\rangle$ look like? It will look mostly polarized in the z direction, but slightly tilted. But the state must be rotationally invariant, so it will be a superposition of states tilted in all possible directions.

We can also think of a state $|\theta, \phi\rangle_{SC}$. What do we think SC stands for? "Soonwon Choi" - Unknown. No, this actually stands for "spin-coherent". We can get a spin coherent state

$$e^{-i(\hat{n}\cdot\vec{J})\tilde{\theta}} |j, j\rangle$$

will give us a state with angular momentum in the direction $\hat{n}$.

39.2 Matrix Representation of Angular Momentum

Let's think about matrix representations of our angular momentum eigenstates.

The case where $j = 0$ is just a scalar, a 1D Hilbert space. It's trivial, so let's not talk about it.

When $j = 1/2$, we have a 2D Hilbert space. This is just spin-1/2.

Now, what about $j = 1$? This is a 3D Hilbert space. In the basis $\{|1, 1\rangle, |1, 0\rangle, |1, -1\rangle\}$, we can write

$$J_z = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

Also, we must have

$$J_+ |j, m\rangle \hbar\sqrt{j(j+1) - m(m+1)} |j, m+1\rangle$$

Which means

$$J_+ |1, 1\rangle = 0$$
$$J_+ |1, 0\rangle = \hbar\sqrt{1 \cdot 2 - 0 \cdot 1} |1, 1\rangle = \hbar\sqrt{2} |1, 1\rangle$$
$$J_+ |1, -1\rangle = \hbar\sqrt{1 \cdot 2 - (-1) \cdot 0} |1, 0\rangle = \hbar\sqrt{2} |1, 0\rangle$$

Therefore,

$$J_+ = \hbar \begin{pmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{pmatrix}$$

Similarly,

$$J_- = \hbar \begin{pmatrix} 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{pmatrix}$$

From this, we can also recover

$$J_x = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$
$$J_y = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}$$

Notice that different from spin-1/2, it is no longer true that $J_x^2 = J_y^2 = J_z^2 = \frac{\hbar^2}{2} I$. However, it is still true that $J^2 = J_x^2 + J_y^2 + J_z^2 = 2\hbar^2 I$.

39.3 Coordinate Representation of Angular Momentum

So far, we've defined for our normal wavefunctions position and momentum bases, $|x\rangle$ and $|p\rangle$. Now what about in angular momentum?

We can write a function $\psi(\vec{r}) = \psi(r, \theta, \phi)$. Let $R_z(\alpha) = e^{-i\alpha L_z/\hbar}$, then

$$\tilde{\psi}(\theta, \phi) = R_z(\alpha)\psi(\theta, \phi) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(-i\frac{\alpha}{\hbar} L_z\right) |\psi\rangle$$

But this is also

$$\tilde{\psi}(\theta, \phi) = \psi(\theta, \phi - \alpha) = \sum_{n=0}^{\infty} \partial_\phi^n \psi|_{\phi=0} (-\alpha)^n$$

Equating these two expressions, we can see that $L_z = -i\hbar\partial_\phi$. Writing out differential equations, we can solve for spherical harmonic wavefunctions:

$$L^2 Y(\theta, \phi) = \hbar^2 l(l+1) Y(\theta, \phi)$$

$$L_z Y(\theta, \phi) = \hbar m Y(\theta, \phi)$$

Where

$$Y_{l,m}(\theta, \phi) = \langle \theta, \phi | l, m \rangle$$

Note that these spherical harmonics form a complete orthonormal basis for the Hilbert space of angular momentum states.

39.4 Central Potential Problems

For this lecture, let's talk about particles moving in 3d with no spin. So we will only consider orbital angular momentum.

In the central potential problem, we have the Hamiltonian

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

In general, we will talk about attractive potentials, so $V(r) \to 0$ as $r \to \infty$, and $V(r) < 0$ as $r \to 0$.

As a recap, a vector operator O is an operator such that $[L_i, O_j] = i\hbar\epsilon_{ijk} O_k$. A scalar operator is an operator such that $[L_i, O] = 0$. Since we showed that if $O = \vec{A} \cdot \vec{B}$, then O is a scalar operator. Therefore, we can show that $\hat{H}$ is a scalar operator.

Note that L_z, L^2, and H are simultaneously diagonalizable. Therefore, we can find quantum numbers E, l, and m_z that describe our states.

Let's talk a bit about the Heisenberg picture. In the Heisenberg picture,

$$L_i(t) = U^\dagger L_i U(t) = L_i$$

since L_i commutes with H. This means that $\langle L_i(t)\rangle = \langle L_i\rangle$, so we have conservation of angular momentum.

Furthermore, since our Hamiltonian is scalar, we have that it is rotationally invariant.

Ok, so let's suppose we find an eigenstate $H|E\rangle = E|E\rangle$. The Hamiltonian should commute with a rotation operator, so

$$HR_n(\theta)|E\rangle = ER_n(\theta)|E\rangle$$

This means $R_n(\theta)|E\rangle$ is also an eigenstate of H with the same eigenvalue. Therefore, we can see that the degeneracy of the energy levels is at least $2l+1$.

40 Recitation 20 (2024-11-19)

Let's discuss entanglement as it relates to problem 5 on our midterm.

In the vanilla case, we had 2 particles and 2 levels. In this case, we discussed how the state is entangled iff $\det A \neq 0$, for matrix A such that

$$|\psi\rangle = \sum A_{ij}|i\rangle|j\rangle$$

However, in the case of 2 particles and 3 levels, like we had on the midterm, this is no longer the case. Instead, the condition is that the rank of A must be 1 for the state to not be entangled.

Now, let's review angular momentum. Classically, $\vec{L} = \vec{r}\times\vec{p}$, or in index notation, $L_i = \epsilon_{ijk}x_jp_k$. In order for quantum mechanics to be consistent, we then define $\hat{L}_i = \epsilon_{ijk}\hat{x}_j\hat{p}_k$. Now, let's calculate

$$[L_i, x_j] = \epsilon_{ilm}x_lp_mx_j - x_j\epsilon_{ilm}x_lp_m = -\epsilon_{ilm}x_l[x_j,p_m] = -i\hbar\epsilon_{ilm}x_l\delta_{jm} = i\hbar\epsilon_{ijl}x_l$$

And similarly,

$$[L_i, p_j] = i\hbar\epsilon_{ijl}p_l$$
$$[L_i, L_j] = i\hbar\epsilon_{ijl}L_l$$

So we see a pattern here. We can define a vector operator O_i to be any operator that satisfies $[L_i, O_j] = i\hbar\epsilon_{ijk}O_k$. Additionally, we can define a scalar to be any operator that commutes with all L_i.

Let's also define a new operator $J_i = S_i + L_i$, where S_i is the spin-1/2 operator. We can check that $[J_i, J_j] = i\hbar\epsilon_{ijk}J_k$. Furthermore, we can check that the operator $J^2 = J_x^2 + J_y^2 + J_z^2$ is a scalar operator. That means that we can choose two operators J^2 and J_z to form a CSCO, and we can write

$$\mathcal{H} = \text{span}\{|j,m\rangle, -j \leq m \leq j\}$$

and

$$J^2|j,m\rangle = \hbar^2 j(j+1)|j,m\rangle$$
$$J_z|j,m\rangle = \hbar m|j,m\rangle$$

Now, we can define raising and lowering operators $J_\pm = J_x \pm iJ_y$, and we can show that

$$[J_z, J_+] = [J_z, J_x + iJ_y] = i\hbar J_y + i(-i\hbar J_x) = \hbar(J_x + iJ_y) = \hbar J_+$$

Similarly,

$$[J_z, J_-] = \hbar(iJ_y - J_x) = -\hbar J_-$$

and since J^2 commutes with J_i,

$$[J^2, J_\pm] = 0$$

Using these relations, we can show that

$$J^2(J_\pm |j,m\rangle) = j(j+1)(J_\pm |j,m\rangle)$$

$$J_z(J_\pm |j,m\rangle) = \hbar(m \pm 1)(J_\pm |j,m\rangle)$$

With some work, we can show the exact action of $J_\pm$ on $|j,m\rangle$:

$$J_\pm |j,m\rangle = \hbar\sqrt{j(j+1) - m(m\pm 1)}\, |j, m\pm 1\rangle$$

Example 40.1

Let's calculate the multiplet of a spin-1/2 particle. We can write

$$S_+ = S_x + iS_y = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

$$S_- = S_x - iS_y = \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

We know that $|1/2, 1/2\rangle$ should be the state annihilated by S_+, so

$$\hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = 0 \implies |1/2, 1/2\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

We can find the state $|1/2, -1/2\rangle$ by applying the lowering operator:

$$S_- |1/2, 1/2\rangle = \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \hbar \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \hbar\sqrt{\frac{1}{2}\left(\frac{1}{2}+1\right) - \frac{1}{2}\left(\frac{1}{2}-1\right)}\, |1/2, -1/2\rangle$$

$$\implies |1/2, -1/2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Example 40.2

Let's talk about a spin-1 particle. We will get

$$S_x = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

$$S_y = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}$$

We will get that

$$S_+ = S_x + iS_y = \hbar\sqrt{2} \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}$$

$$S_- = S_x - iS_y = \hbar\sqrt{2} \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

We want to find the state $|1,1\rangle$ such that $S_+ |1,1\rangle = 0$. We can see that

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

Now,

$$S_- |1,1\rangle = \hbar\sqrt{2} \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \hbar\sqrt{2} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \hbar\sqrt{1 \cdot 2 - 1 \cdot 0}\, |1,0\rangle$$

$$\implies |1,0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

41 Lecture 21 (2024-11-20)

Let's recap the central potential problem. We have a Hamiltonian

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

We learned from last time that $\frac{\mathrm{d}}{\mathrm{d}t} \langle L_i \rangle = 0$, and also that the Hamiltonian is rotationally invariant, i.e. $R^\dagger H R = H$. These are results of the fact that $[H, L_i] = 0$.

We can think of the Hilbert space as a direct sum of the Hilbert spaces of different l values:

$$H = \bigoplus_{l=0}^{\infty} \mathcal{H}_l$$

where $\mathcal{H}_l$ is the Hilbert space of states with angular momentum l.

41.1 Central Potential Problem

By direct calculation, we can verify that

$$L^2 = r^2 p^2 - (r \cdot p)^2 + i\hbar r \cdot p$$

Therefore, we can write

$$\frac{p^2}{2m} = \frac{1}{2mr^2} L^2 + \frac{1}{2m} \frac{1}{r^2} \left((r \cdot p)^2 - i\hbar r \cdot p \right) = \frac{1}{2mr^2} L^2 - \frac{\hbar^2}{2m} \frac{1}{r} \frac{\partial^2}{\partial r^2} r$$

Therefore,

$$H = -\frac{\hbar^2}{2m} \frac{1}{r} \frac{\partial^2}{\partial r^2} r + \frac{1}{2mr^2} L^2 + V(r)$$

Recall our definition of the wavefunction

$$\psi(r, \theta, \phi) = \langle r, \theta\phi | E, l, m \rangle$$

We can rewrite this as

$$\psi(r, \theta, \phi) = \frac{u(r)}{r} Y_{l,m}(\theta, \phi)$$

where $u(r)$ is the radial wavefunction. Plugging this in, we can obtain the effective Schrödinger equation for $u(r)$:

$$\begin{aligned} -\frac{\hbar^2}{2m} \frac{1}{r} \frac{\mathrm{d}^2}{\mathrm{d}r^2} u(r) + V_{\text{eff}}(r) \frac{u(r)}{r} &= E \frac{u(r)}{r} \\ \implies -\frac{\hbar^2}{2m} \frac{\mathrm{d}^2}{\mathrm{d}r^2} u(r) + V_{\text{eff}}(r) u(r) &= E u(r) \end{aligned}$$

where

$$V_{\text{eff}} = V(r) + \frac{\hbar^2 l(l+1)}{2mr^2}$$

We can also check that

$$\int |\psi|^2 \mathrm{d}^3 r = 1 \iff \int_0^\infty |u(r)|^2 \mathrm{d}r = 1$$

Note that for $l > 0$, the effective potential will be dominated by the centrifugal term at small r. This implies that $u(r) \sim r^{l+1}$ as $r \to 0$. For $l = 0$, we want $u(r)$ to be nonzero at $r = 0$, so we can write $u(r) \sim r$ as $r \to 0$.

41.2 3D Isotropic Simple Harmonic Oscillator

Let't think about the 3D harmonic oscillator. We can write

$$H = \frac{p_x^2}{2m} + \frac{1}{2}m\omega_x^2 x^2 + \frac{p_y^2}{2m} + \frac{1}{2}m\omega_y^2 y^2 + \frac{p_z^2}{2m} + \frac{1}{2}m\omega_z^2 z^2$$

If $\omega_x = \omega_y = \omega_z = \omega$, then we can write

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 r^2$$

where $r^2 = x^2 + y^2 + z^2$. We know the solution to this problem is just $|n_x\rangle |n_y\rangle |n_z\rangle$. But for now, let's pretend we don't know the solution and try to solve it by writing it as a central potential.

We claim that $N = N_x + N_y + N_z$, along with L^2 and L_z form a CSCO. Let's think about how to write the ground state:

$$N = N_x + N_y + N_z = 0$$

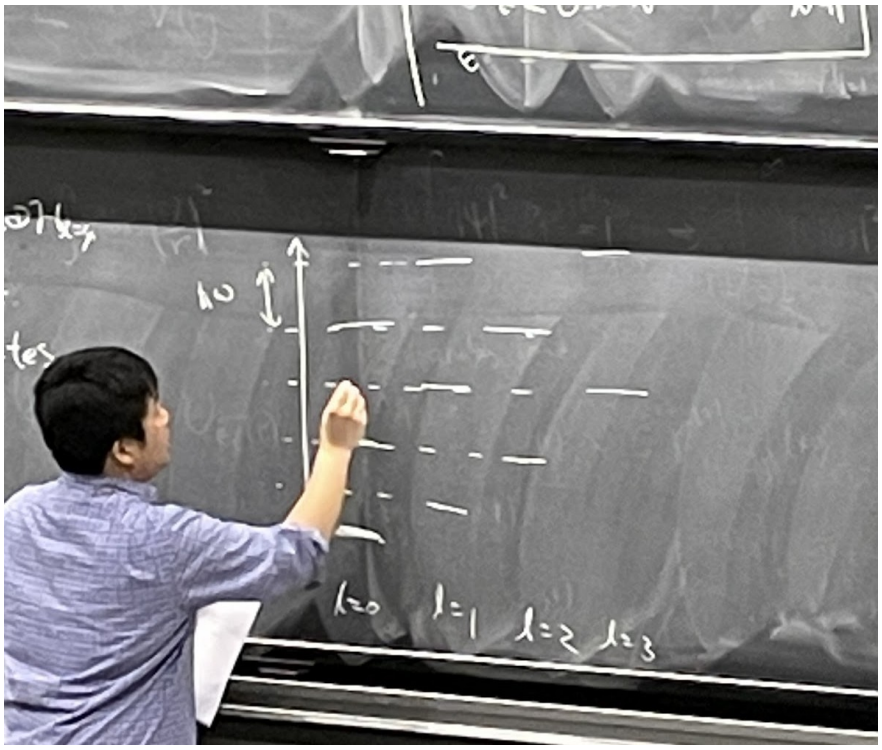
Since the ground state is not degenerate, we should have $l = 0$, and so then $m = 0$. Therefore, the ground state should be $|0, 0, 0\rangle$.

What about the first excited states? There are three states this time, so we should have $l = 1$. We can write the states as $|1, 0, 0\rangle$, $|0, 1, 0\rangle$, and $|0, 0, 1\rangle$ in the number basis. We can also write these states in the angular momentum basis as $|1, 1, 1\rangle$, $|1, 1, 0\rangle$, and $|1, 1, -1\rangle$.

Now what about $N = 2$? We will have 6 states. How can we write this as a combination of multiplets? Since we cannot have two different copies of the same l value, we know that this must be a combination of $l = 0$ and $l = 2$. $\mathcal{H} = \mathcal{H}_{l=0} \oplus \mathcal{H}_{l=2}$. Therefore, we can write a linear combination of our states that will match the 6 angular momentum states.

For $N = 3$, there are 10 states. We can argue that this must be a combination of $l = 1$ and $l = 3$. This is because the ground states of $l = i$ must be monotonically increasing as we increase l, so we cannot see $l = 4$ before we see $l = 3$.

What will happen is we will find a energy level structure that looks like the following:



We can also think about this explicitly by defining operators

$$a_L = \frac{1}{\sqrt{2}}(a_x + ia_y)$$

$$a_R = \frac{1}{\sqrt{2}}(a_x - ia_y)$$

It turns out that if we define $K = a_R^\dagger a_L$ will act as a raising/lowering operator for L_z, since $[L_z, K] = 2\hbar K$.

42 Recitation 21 (2024-11-21)

Last time we discussed a system with spin equal to 1. Today, we will talk about a functional representation, where each state will correspond to a spherical harmonic.

Recall that

$$L = r \times p = -i\hbar r \times \nabla = -i\hbar \left(\hat{e}_\phi \partial_\theta - \frac{\hat{e}_\theta}{\sin\theta} \partial_\phi \right)$$

Then,

$$L_z = -i\hbar \partial_\phi$$

$$L_\pm = \hbar e^{\pm i\phi} \left(\pm \partial_\theta + i \cot\theta \partial_\phi \right)$$

So now, let's build the multiplet. By definition,

$$L_- \left| j, -j \right\rangle = 0$$

$$\implies 0 = \hbar e^{-i\phi} \left(-\partial_\theta + i \cot\theta \partial_\phi\right) Y_{j,-j}(\theta, \phi)$$

We also know that

$$L_z \left|j, -j\right\rangle = -\hbar j \left|j, -j\right\rangle = -i\hbar \partial_\phi Y_{j,-j}$$

Solving this equation tells us that

$$Y_{j,-j}(\theta, \phi) = e^{-ij\phi} f(\theta)$$

Plugging this back into the first equation,

$$0 = \hbar e^{-i\phi} \left(-\partial_\theta f + \cot\theta j f\right)$$

We get

$$\frac{\mathrm{d}f}{\mathrm{d}\theta} = j \frac{\cos\theta}{\sin\theta} f$$

Solving this, we can get that

$$f(\theta) = c \sin^j \theta$$

Therefore, we can write

$$\left|l, -l\right\rangle = c_l e^{-il\phi} \sin^l \theta$$

When we normalize it, we get

$$c_l = \sqrt{\frac{(2l+1)!}{4\pi}} \frac{1}{2^l (l!)}$$

Now, let's try to find other states as well. We know

$$\frac{J_+}{\hbar} \left|l, -l\right\rangle = \sqrt{l(l+1) - l(-l+1)} \left|l, -l+1\right\rangle$$

$$\implies \left|l, -l+1\right\rangle = \frac{J_+ \left|l, -l\right\rangle}{\hbar\sqrt{2l}}$$

Similarly, we can repeat this to get

$$\left|l, -l+2\right\rangle = \frac{J_+^2 \left|l, -l\right\rangle}{\hbar^2 \sqrt{2l(2l-1) \cdot 2}}$$

In general,

$$\left|l, -l+k\right\rangle = \frac{J_+^k \left|l, -l\right\rangle}{\hbar^k} \sqrt{\frac{(2l-k)!}{k!(2l)!}}$$

Plugging this in,

$$\left|l, m\right\rangle = \sqrt{\frac{(l-m)!}{(2l)!(l+m)!}} \left(e^{i\phi}(\partial_\theta + i\cot\theta\partial_\phi)\right)^{l+m} \frac{\sqrt{(2l+1)!}}{\sqrt{4\pi} 2^l l!} e^{-il\phi} \sin^l \theta$$

Now, let's try to understand the action of L_+ on $\left|l, m\right\rangle$.

$$e^{i\phi}(\partial_\theta + i\cot\theta\partial_\phi) \left|l, m\right\rangle = e^{i\phi}(\partial_\theta - m\cot\theta) \left|l, m\right\rangle$$

Now, if we let $x = \cos\theta$, $\partial_\theta = \partial_x \frac{\partial x}{\partial \theta} - \sin\theta \partial_x$. Our expression becomes

$$e^{i\phi}\left(-\sin\theta\partial_x - m\frac{\cos\theta}{\sin\theta}\right)|l,m\rangle = -e^{i\phi}((1-x^2)\partial_x + mx)\,|l,m\rangle$$

Using a trick, we can see that this will actually be equal to

$$-e^{i\phi}(1-x^2)^{1+m/2}\frac{\mathrm{d}}{\mathrm{d}x}\left((1-x^2)^{-m/2}\,|l,m\rangle\right)$$

Therefore,

$$e^{i\phi}\frac{\mathrm{d}}{\mathrm{d}x}\left((1-x^2)^{-m/2}\,|l,m\rangle\right) = -(1-x^2)^{-1-m/2}\sqrt{(l+m+1)(l-m)}\,|l,m+1\rangle$$

But what if we apply this twice?

$$|l,m+1\rangle = \frac{-(1-x^2)^{\frac{m+1}{2}}e^{i\phi}}{\sqrt{(l-m)(l+m+1)}}\frac{\mathrm{d}}{\mathrm{d}x}\left((1-x^2)^{-m/2}\,|l,m\rangle\right)$$

$$= \frac{-(1-x^2)^{\frac{m+1}{2}}e^{i\phi}}{\sqrt{(l-m)(l+m+1)}}\frac{\mathrm{d}}{\mathrm{d}x}\left(-(1-x^2)^{-m/2}\frac{-(1-x^2)^{m/2}e^{i\phi}}{\sqrt{(l-m+1)(l+m)}}\frac{\mathrm{d}}{\mathrm{d}x}\left((1-x^2)^{-\frac{m-1}{2}}\,|l,m-1\rangle\right)\right)$$

$$= \frac{(-1)^2(1-x^2)^{\frac{m+1}{2}}e^{2i\phi}}{\sqrt{(l-m)(l+m+1)(l-m+1)(l+m)}}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\left((1-x^2)^{-\frac{m-1}{2}}\,|l,m-1\rangle\right)$$

We see that in general,

$$|l,m+1\rangle = \frac{(-1)^{l+m+1}}{2^l l!}\sqrt{\frac{(2l+1)(l-m-1)!}{4\pi(l+m+1)!}}e^{i(m+1)\phi}(1-x^2)^{\frac{m+1}{2}}\frac{\mathrm{d}^{l+m+1}}{\mathrm{d}x^{l+m+1}}(1-x^2)^l$$

43 Lecture 22 (2024-11-25)

So far, we have talked about the notion of angular momentum. We talked about decomposing the Hilbert space into different angular momentum subspaces. We also talked about fixing an angular momentum and talking about how m affects the polarization relative to the z direction.

43.1 Addition of Angular Momentum

We start with a simple question: how can we add angular momentum? The simple answer is

$$\vec{J}^{(tot)} = \vec{J}^{(1)} + \vec{J}^{(2)}$$

However, there are some subtleties that we should talk about.

Angular momentum operators should satisfy the commutation relations

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

Since these don't commute, we cannot simultaneously diagonalize all three components of $\vec{J}$. Therefore, we can't exactly treat these as separate degrees of freedom. Additionally, angular momentum is quantized, so we can't have any arbitrary value of J.

Let's start with a simple example. Suppose we have a composite system with Hilbert space $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$. The first Hilbert space has angular momentum operators $J_i^{(1)}$, and the second has $J_i^{(2)}$. Since we are working in a composite system, we will upgrade all of these operators. By definition, $[J_i^{(1)}, J_j^{(1)}] = i\hbar\epsilon_{ijk}J_k^{(1)}$. We can also define $J_i^{(2)}$ such that $[J_i^{(2)}, J_j^{(2)}] = i\hbar\epsilon_{ijk}J_k^{(2)}$. Finally, $[J_i^{(1)}, J_j^{(2)}] = 0$.

We propose $J_i^t = J_i^{(1)} + J_i^{(2)}$. We can check that

$$[J_1^{(t)}, J_2^{(t)}] = i\hbar\epsilon_{ijk}J_k^{(t)}$$

We can also talk about $J^{(t)2} = (J_x^{(t)})^2 + (J_y^{(t)})^2 + (J_z^{(t)})^2$ We can even think about rotations as generated by total angular momentum:

$$e^{-i\theta\hat{n}\cdot\vec{J}} = e^{-i\theta(\hat{n}\cdot\vec{J}^{(1)}+\hat{n}\cdot\vec{J}^{(2)})} = e^{-i\theta\hat{n}\cdot\vec{J}^{(1)}} \otimes e^{-i\theta\hat{n}\cdot\vec{J}^{(2)}}$$

Let's apply this to a pair of spin-1/2 particles: $\mathcal{H}_1 = \mathcal{H}_2 = \text{span}(\{|1/2, 1/2\rangle, |1/2, -1/2\rangle\})$. This Hilbert space has dimension 4. We want to know if it is

- $$(j = 0) \oplus (j = 0) \oplus (j = 0) \oplus (j = 0)$$
- $$(j = 1/2) \oplus (j = 1/2)$$
- $$(j = 1/2) \oplus (j = 0) \oplus (j = 0)$$
- $$(j = 3/2)$$
- $$(j = 1) \oplus (j = 0)$$

How do we know which one it is? We can use the fact that the total angular momentum operator is just the sum of the two individual angular momentum operators. For example, if we apply

$$J_z^{(t)} |1/2, 1/2\rangle \otimes |1/2, 1/2\rangle = \hbar |1/2, 1/2\rangle \otimes |1/2, 1/2\rangle$$

We see that the eigenvalue is $\hbar$. This already rules out all of the options except for the last one. We can think of this decomposition as the equation

$$\frac{1}{2} \otimes \frac{1}{2} = 1 \oplus 0$$

Now, let's think about the state $|1/2, 1/2\rangle \otimes |1/2, 1/2\rangle$. Which subspace does this belong to? Since it's eigenvalue is $\hbar$, it must belong to the triplet ($j = 1$) subspace. Similarly, $|1/2, -1/2\rangle \otimes |1/2, -1/2\rangle$ must also belong to the triplet subspace.

However, the states $|1/2, 1/2\rangle \otimes |1/2, -1/2\rangle$ and $|1/2, -1/2\rangle \otimes |1/2, 1/2\rangle$ must be superpositions of states that belong to the singlet and triplet subspaces, i.e.

$$|\psi\rangle = \alpha \left|\frac{1}{2}, \frac{1}{2}\right\rangle \left|\frac{1}{2}, -\frac{1}{2}\right\rangle + \beta \left|\frac{1}{2}, -\frac{1}{2}\right\rangle \left|\frac{1}{2}, \frac{1}{2}\right\rangle$$

for some $|\psi\rangle$ in the singlet subspace, where we can find α and β by enforcing $J^2 |\psi\rangle = 0$.

Another way of thinking about it is enforcing

$$J_+ |j = 0, m = 0\rangle = 0$$

to get the singlet state. Note that J_+ is the total raising operator,

$$J_+ = J_+^{(1)} + J_+^{(2)} = J_x^{(t)} + J_y^{(t)}$$

Yet another way is to consider

$$J_- |1, 1\rangle = (J_-^{(1)} + J_-^{(2)}) |1, 1\rangle = \hbar\sqrt{1 \cdot (1+1) - 1 \cdot (1-1)}\, |1, 0\rangle$$

Calculating,

$$J_- |1, 1\rangle = (J_-^{(1)} + J_-^{(2)}) \left|\frac{1}{2}, \frac{1}{2}\right\rangle \otimes \left|\frac{1}{2}, \frac{1}{2}\right\rangle$$

$$= \hbar\sqrt{\frac{1}{2}\frac{3}{2} - \frac{1}{2}\left(-\frac{1}{2}\right)} \left|\frac{1}{2}, -\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2}, \frac{1}{2}\right\rangle + \hbar\sqrt{\frac{1}{2}\frac{3}{2} - \frac{1}{2}\left(-\frac{1}{2}\right)} \left|\frac{1}{2}, \frac{1}{2}\right\rangle \otimes \left|\frac{1}{2}, -\frac{1}{2}\right\rangle$$

Therefore, we see that

$$|1, 0\rangle = \frac{1}{\sqrt{2}} (|+-\rangle + |-+\rangle)$$

Similarly, the singlet state is then $\frac{1}{\sqrt{2}} (|+-\rangle - |-+\rangle)$.

Note that

$$J^2 = \sum_i (J_i^{(1)} + J_i^{(2)})^2 = (J^{(1)})^2 + (J^{(2)})^2 + 2 J_i^{(1)} J_i^{(2)}$$

Therefore,

$$J_i^{(1)} J_i^{(2)} = \frac{1}{2}(J^2 - (J^{(1)})^2 - (J^{(2)})^2)$$

Now, let's think about the general case. $\mathcal{H} = \mathcal{H}_{j1} \otimes \mathcal{H}_{j2}$. In the product state basis $|j_1, j_2; m_1, m_2\rangle$,

$$J_z^{(1)} |\psi\rangle = \hbar m_1 |\psi\rangle$$
$$J_z^{(2)} |\psi\rangle = \hbar m_2 |\psi\rangle$$

This is called the uncoupled basis. Note that the dimensionality of our Hilbert space is $(2j_1 + 1)(2j_2 + 1)$.

We can also write this in the coupled basis, where we have a basis $|j_1, j_2; l, m\rangle$. In this basis, we have l is the total angular momentum, and m is the total angular momentum in the z direction.

Since they both form orthonormal bases, there should be a unitary transformation relating them. One way of doing this is using resolution of identity,

$$|j_1, j_2; l, m\rangle = \sum_{m_1, m_2} |j_1, j_2; m_1, m_2\rangle \langle j_1, j_2; m_1, m_2 | j_1, j_2; l, m\rangle$$
$$= \sum_{m_1, m_2} c^{j_1, j_2}_{m_1, m_2, l, m} |j_1, j_2; m_1, m_2\rangle$$

These coefficients are called Clebsch-Gordan coefficients.

These are normally found in tables, but we're at MIT, so let's talk about how to derive them.

Consider the special case when $m_1 = j_1$ and $m_2 = j_2$. That state has the property that $J_z^{(t)} = m_1 + m_2 = j_1 + j_2$. Since this is the maximum possible, we can see that $l = j_1 + j_2$. We can also see that $m = j_1 + j_2$. From here, we can apply the lowering operator $J_-^{(t)}$ multiple times to get all of the states in the multiplet. Doing this, we will find $2l + 1$ states.

Next, consider $m_1 = j_1$ and $m_2 = j_2 - 1$, and also $m_1 = j_1 - 1$ and $m_2 = j_2$. One superposition of these should be $|l, l - 1\rangle$. We can argue that the other superposition should be $|l - 1, l - 1\rangle$. Then, we can continue to repeat this process to find all of the Clebsch-Gordan coefficients.

We will find that

$$j_1 \otimes j_2 = (j_1 + j_2) \oplus (j_1 + j_2 - 1) \oplus \cdots \oplus |j_1 - j_2|$$

44 Recitation 22 (2024-11-26)

"Today, we will learn how to add angular momentum like real men." - Prof. Ivanov

Recall that we have a Hilbert space $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$. We have angular momentum operators $J_i^{(1)}$ and $J_i^{(2)}$, and we define

$$J = J_1 \otimes 1 + 1 \otimes J_2$$

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

We can express our states in the uncoupled basis $|j_1, j_2, m_1, m_2\rangle = |j_1, m_1\rangle \otimes |j_2, m_2\rangle$. We can also express our states in the coupled basis $|j_1, j_2; j, m\rangle$. We can relate these two bases by the Clebsch-Gordan coefficients:

$$|j_1, j_2, j, m\rangle = \sum_{m_1, m_2} |j_1, j_2, m_1, m_2\rangle \langle j_1, j_2, m_1, m_2 | j_1, j_2, j, m\rangle$$

Note that if we calculate

$$J_z |j_1, j_2, j, m\rangle = \hbar m |j_1, j_2, j, m\rangle = \sum_{m_1, m_2} |j_1, j_2, m_1, m_2\rangle \hbar(m_1 + m_2) c_{j_1, j_2, m_1, m_2}$$

In general, we might get something complicated, but for the maximum possible quantum number $j_1 + j_2$, we will get a simple expression.

Let's consider an example, the sum of two spin-1/2 particles. In the uncoupled basis, our states are

$$\left\{ \left|\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right\rangle, \left|\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}\right\rangle, \left|\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, \frac{1}{2}\right\rangle, \left|\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}\right\rangle \right\}$$

In the coupled basis, we have

$$\left\{ \left|\frac{1}{2}, \frac{1}{2}, 1, 1\right\rangle, \left|\frac{1}{2}, \frac{1}{2}, 1, 0\right\rangle, \left|\frac{1}{2}, \frac{1}{2}, 1, -1\right\rangle, \left|\frac{1}{2}, \frac{1}{2}, 0, 0\right\rangle \right\}$$

For the maximum and minimum magnetic quantum numbers, we see that $\left|\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right\rangle = \left|\frac{1}{2}, \frac{1}{2}, 1, 1\right\rangle$ and $\left|\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}\right\rangle = \left|\frac{1}{2}, \frac{1}{2}, 1, -1\right\rangle$. Last time, we derived that

$$\left|\frac{1}{2}, \frac{1}{2}, 0, 0\right\rangle = \frac{1}{\sqrt{2}} \left(\left|\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}\right\rangle - \left|\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, \frac{1}{2}\right\rangle \right)$$

And we also found that

$$J_- \left|\frac{1}{2}, \frac{1}{2}, 1, 1\right\rangle = \hbar\sqrt{2} \left|\frac{1}{2}, \frac{1}{2}, 1, 0\right\rangle = \hbar \left|\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, \frac{1}{2}\right\rangle + \hbar \left|\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}\right\rangle$$

Therefore,

$$\left|\frac{1}{2}, \frac{1}{2}, 1, 0\right\rangle = \frac{1}{\sqrt{2}} \left(\left|\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}\right\rangle + \left|\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, \frac{1}{2}\right\rangle \right)$$

Now, let's understand what's going on with the J^2. We know

$$J^2 |j_1, j_2, j, m\rangle = \hbar^2 j(j+1) |j_1, j_2, j, m\rangle$$

So for example,

$$J^2\left|\frac{1}{2},\frac{1}{2},1,0\right\rangle = 2\hbar^2\left|\frac{1}{2},\frac{1}{2},1,0\right\rangle$$

We should be able to get the same result by applying J^2 to the uncoupled basis.

$$J^2\frac{1}{\sqrt{2}}\left(\left|\frac{1}{2},\frac{1}{2},\frac{1}{2},-\frac{1}{2}\right\rangle + \left|\frac{1}{2},\frac{1}{2},-\frac{1}{2},\frac{1}{2}\right\rangle\right)$$

We can expand

$$J^2 = (J_1+J_2)^2 = J_1^2 + J_2^2 + 2J_1\cdot J_2$$
$$J_1\cdot J_2 = J_{1x}\otimes J_{2x} + J_{1y}\otimes J_{2y} + J_{1z}\otimes J_{2z}$$

We know how to calculate J_z, and we can get J_x and J_y by applying the raising and lowering operators.

$$J_x = \frac{J_+ + J_-}{2}, \qquad J_y = \frac{J_+ + J_-}{2i}$$

Further expanding,

$$J_{1x}\otimes J_{2x} = \frac{J_{1+}+J_{1-}}{2}\otimes\frac{J_{2+}+J_{2-}}{2} = \frac{1}{4}(J_{1+}J_{2+} + J_{1+}J_{2-} + J_{1-}J_{2+} + J_{1-}J_{2-})$$

Similarly,

$$J_{1y}\otimes J_{2y} = -\frac{1}{4}(J_{1+}J_{2+} - J_{1+}J_{2-} - J_{1-}J_{2+} + J_{1-}J_{2-})$$

Therefore,

$$J_{1x}J_{2x} + J_{1y}J_{2y} + J_{1z}J_{2z} = J_{1z}J_{2z} + \frac{1}{2}(J_{1+}J_{2-} + J_{1-}J_{2+})$$

Plugging this in,

$$J^2 = J_1^2 + J_2^2 + 2J_1\cdot J_2 = J_1^2 + J_2^2 + 2J_{1z}J_{2z} + J_{1+}J_{2-} + J_{1-}J_{2+}$$

Now, we can calculate

$$J^2\frac{1}{\sqrt{2}}\left(\left|\frac{1}{2},\frac{1}{2},\frac{1}{2},-\frac{1}{2}\right\rangle + \left|\frac{1}{2},\frac{1}{2},-\frac{1}{2},\frac{1}{2}\right\rangle\right)$$
$$= \frac{1}{\sqrt{2}}\left(\left(\frac{3}{4}\hbar^2+\frac{3}{4}\hbar^2-\frac{1}{2}\hbar^2\right)\left|\frac{1}{2},\frac{1}{2},\frac{1}{2},-\frac{1}{2}\right\rangle + 0 + \hbar^2\left|\frac{1}{2},\frac{1}{2},-\frac{1}{2},\frac{1}{2}\right\rangle\right)$$
$$+\frac{1}{\sqrt{2}}\left(\left(\frac{3}{4}\hbar^2+\frac{3}{4}\hbar^2-\frac{1}{2}\hbar^2\right)\left|\frac{1}{2},\frac{1}{2},-\frac{1}{2},\frac{1}{2}\right\rangle + \hbar^2\left|\frac{1}{2},\frac{1}{2},\frac{1}{2},-\frac{1}{2}\right\rangle + 0\right)$$
$$= 2\hbar^2\left|\frac{1}{2},\frac{1}{2},1,0\right\rangle$$

45 Lecture 23 (2024-11-27)

Last time, we learned a remarkable formula: $\frac{1}{2}\otimes\frac{1}{2} = 1\oplus 0$. Today, we will do general addition, namely $j_1\otimes j_2$. Then, we will talk about perturbation theory.

45.1 General Addition of Angular Momentum

Again, we consider a composite system with two particles, each having angular momentum j_1 and j_2. The Hilbert space will be $\mathcal{H} = \mathcal{H}_{j_1} \otimes \mathcal{H}_{j_2}$. We have learned that we can write the total angular momentum simply by adding upgraded versions of the individual angular momentum operators, and that the total angular momentum operator will satisfy the commutation relations $[J_i, J_j] = i\hbar\epsilon_{ijk}J_k$. This implied that we could write the Hilbert space as a direct sum of the Hilbert spaces of different j values:

$$\mathcal{H} = \mathcal{H}_{j_1} \otimes \mathcal{H}_{j_2} = V_{l_1} \oplus V_{l_2} \oplus \cdots \oplus V_{l_k}$$

On the left hand side, we can write the basis states as $|j_1, j_2, m_1, m_2\rangle$, which is an eigenstate of $(J^2)^{(1)}$, $(J^2)^{(2)}$, $J_z^{(1)}$, and $J_z^{(2)}$. We also learned that we can write the coupled basis, where the basis states are $|j_1, j_2, j, m\rangle$, which is an eigenstate of $(J^2)^{(1)}$, $(J^2)^{(2)}$, J^2, and J_z. Since these bases are orthonormal, they are related to each other by a unitary transformation, known as the Clebsch-Gordan coefficients:

$$c^{j_1,j_2}_{m_1,m_2,j,m} = \langle j_1, j_2, m_1, m_2 | j_1, j_2, j, m\rangle$$

We want to answer two questions:

- What are the allowed values of l?
- How do we find the Clebsch-Gordan coefficients?

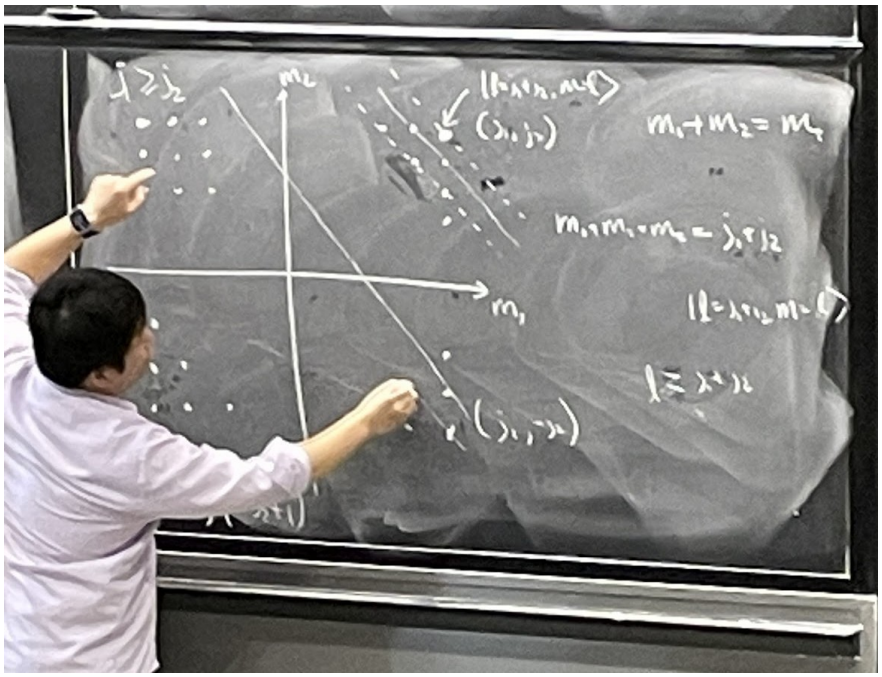
To answer those questions, we will utilize a key insight: we will utilize the fact that $J_z^{(t)} = J_z^{(1)} + J_z^{(2)}$, and the second is counting, and realizing that once we get one state in a multiplet, we get the other $2l$ states along with it.

If we make a plot of the allowed values of m_1 and m_2, we will get a rectangle with width $2j_1 + 1$ and height $2j_2 + 1$. Therefore, we have $(2j_1 + 1)(2j_2 + 1)$ states. If we look in the top right corner, we will see that $m_1 = j_1$ and $m_2 = j_2$. This state will have $m = j_1 + j_2$. Since it is unique and has the maximum m possible, we can conclude that it is the state $|j_1 + j_2, j_1 + j_2\rangle_c$. We can then lower this to get the entire $j_1 + j_2$ multiplet.

Now consider the states with $m_1 + m_2 = j_1 + j_2 - 1$. We see that there are two possibilities. We know that these two states span the subspace where $J_z^{(t)} = j_1 + j_2 - 1$. However, we also know that $\{|j_1 + j_2, j_1 + j_2 - 1\rangle_c, |\phi\rangle\}$ spans this, for some state $|\phi\rangle$. But we can argue that if we raise $|\phi\rangle$, it must get annihilated. This is because otherwise, the eigenstate of $J_z^{(t)} = j_1 + j_2$ would not be unique.

Therefore, we can conclude that $|\phi\rangle = |j_1 + j_2 - 1, j_1 + j_2 - 1\rangle_c$ must be a superposition of $|j_1, j_2, j_1, j_2 - 1\rangle$ and $|j_1, j_2, j_1 - 1, j_2\rangle$ that is orthogonal to $|j_1 + j_2, j_1 + j_2 - 1\rangle_c$. This gives us the Clebsch-Gordan coefficients for the $j_1 + j_2 - 1$ multiplet.

We can then repeat this process to get all of the Clebsch-Gordan coefficients.



Therefore, in general,

$$j_1 \otimes j_2 = (j_1 + j_2) \oplus (j_1 + j_2 - 1) \oplus \cdots \oplus |j_1 - j_2|$$

Now that we know how to add two particles, we can add a third particle. One way of considering this is to consider the sum first two particles, which will be a direct sum of angular momentum subspaces. Now, adding the third one, we can distribute it over the subspaces of the first two particles. This will give us a decomposition of the Hilbert space into a direct sum of angular momentum subspaces.

$$j_1 \otimes j_2 \otimes j_3 = ((j_1 + j_2) \oplus (j_1 + j_2 - 1) \oplus \cdots \oplus |j_1 - j_2|) \otimes j_3$$

$$= ((j_1 + j_2) \otimes j_3) \oplus ((j_1 + j_2 - 1) \otimes j_3) \oplus \cdots \oplus (|j_1 - j_2| \otimes j_3)$$

and we can expand this further to get the direct sum of angular momentum subspaces.

For example, if we have three spin-1/2 particles, we can write

$$\frac{1}{2} \otimes \frac{1}{2} \otimes \frac{1}{2} = (1 \oplus 0) \otimes \frac{1}{2} = \left(\frac{3}{2} \oplus \frac{1}{2}\right) \oplus \frac{1}{2}$$

Note that we can also write this as

$$\frac{1}{2} \otimes \frac{1}{2} \otimes \frac{1}{2} = \frac{1}{2} \otimes (1 \oplus 0) = \frac{1}{2} \oplus \left(\frac{3}{2} \oplus \frac{1}{2}\right)$$

The two $\frac{1}{2}$ multiplets are different in these two cases!

45.2 Perturbation Theory

Let's see how the Hydrogen atom works. The Hamiltonian is

$$H = H_{\text{kinetic}} + H_{\text{coulomb}} + H_{\text{spin-orbit}} + H_{\text{spin-spin}}$$

The third term comes from the fact that the electron is moving in a magnetic field created by the nucleus at relativistic velocities. The fourth term comes from the interaction of the spins of the nucleus and the electron.

In fact, there are more terms that we can add, but these terms will already give us the overall structure of the energy levels. We can let $H_0 = H_{\text{kinetic}} + H_{\text{coulomb}}$ and $\lambda V = H_{\text{spin-orbit}} + H_{\text{spin-spin}}$. We can then write the Hamiltonian as $H = H_0 + \lambda V$, where λ is a small parameter.

The idea behind perturbation theory is the following: suppose we have $H(\lambda) = H_0 + \lambda V$. Assume that H_0 is solvable (i.e. we have a closed form solution $H_0 = \sum_i E_i \left|i\right\rangle \left\langle i\right|$), and assume λ is very small. We expect that the eigenvalues of $H(\lambda)$ will be close to the eigenvalues of H_0.

How do we define small? One case is where the eigenvalues of H_0 are non-degenerate. In this case, we can just enforce that the matrix elements of λV are very small compared to the energy differences of H_0.

In this case, we claim that the eigenvalues of $H(\lambda)$ are given by

$$E_n(\lambda) = E_n^{(0)} + \lambda \left\langle n\right| V \left|n\right\rangle + O(\lambda^2)$$

and the eigenvectors are given by

$$\left|n^\lambda\right\rangle = \frac{1}{\sqrt{1+\lambda^2}}(\left|n^0\right\rangle + \lambda^2 \left|\psi_\perp\right\rangle + O(\lambda^3))$$

where $E_n^{(0)}$ and $\left|n^0\right\rangle$ are the eigenvalues and eigenvectors of H_0.

Now, what about the case where H_0 is degenerate? In this case, for each degenerate subspace, we can ignore all other subspaces. We can treat operator V as if this subspace was the entire Hilbert space, and write

$$V_{a,b}^n = \left\langle n, a\right| V \left|n, b\right\rangle$$

Then, we can diagonalize this matrix and get eigenvalues $\delta E_{n,i}$ with eigenvectors $\left|n, i\right\rangle$. Then, the eigenvalues of $H(\lambda)$ will be

$$E_n^{(\lambda)} = E_n + \lambda \delta E_{n,i}$$

with eigenvectors $\left|n, i\right\rangle$. We will see that the degenerate subspace will be split into multiple closely spaced energy levels.

In the rest of this class, we will see that $H_{\text{spin-orbit}}$ will lead to what we call the fine structure of the Hydrogen atom, and $H_{\text{spin-spin}}$ will lead to the hyperfine structure.

45.3 Hydrogen Atom

Let's be serious about the Hydrogen atom now. First, let's identify the Hilbert space:

$$\mathcal{H} = \mathcal{H}_{\text{e-motion}} \otimes \mathcal{H}_{\text{p-motion}} \otimes \mathcal{H}_{\text{e-spin}} \otimes \mathcal{H}_{\text{p-spin}}$$

The first two terms are affected by H_{kinetic} and H_{coulomb}, and the last two terms are affected by $H_{\text{spin-orbit}}$ and $H_{\text{spin-spin}}$.

We can write

$$H_{\text{kinetic}} + H_{\text{coulomb}} = \frac{p_e^2}{2m_e} + \frac{p_p^2}{2m_p} + V(r)$$

We can introduce $P = p_e + p_p$ and $R = \frac{m_e}{m_e+m_p} r$ to simplify this expression. We will also have to introduce $p = \frac{m_p p_e - m_e p_p}{m_e+m_p}$, which is the relative momentum, and r is the relative position. Then,

$$H_{\text{kinetic}} + H_{\text{coulomb}} = \frac{P^2}{2M} + \frac{p^2}{2\mu} + V(r) = H_0$$

where $M = m_e + m_p$ and $\mu = \frac{m_e m_p}{m_e+m_p}$.

We know how to solve this by considering the center of mass as a free particle and the relative motion as a central potential problem. The energy levels will be

$$E_n = -\frac{E_0}{n^2}$$

where $E_0 = \frac{\mu e^4}{2\hbar^2}$. It turns out that a due to the properties of a $1/r$ potential, the first energy level for $l = 1$ is degenerate with the second energy level for $l = 0$. Similarly, the second energy level for $l = 1$ is degenerate with the third energy level for $l = 0$, and so on. The same also true for higher values of l as well.

46 Recitation 23 (2024-11-28)

Recitation cancelled due to Thanksgiving.

47 Lecture 24 (2024-12-02)

47.1 Overview

Recall we split our Hilbert space into four subspaces: electron motion, proton motion, electron spin, and proton spin. We can write the Hamiltonian as

$$H = H_{\text{kinetic}} + H_{\text{coulomb}} + H_{\text{spin-orbit}} + H_{\text{spin-spin}}$$

We found that only considering the the kinetic and coulomb interactions, the energy levels follow the typical pattern that we learned in chemistry. The energy levels are

$$E_n = -\frac{E_{ry}}{n^2}$$

where

$$E_{ry} = \frac{me^4}{32\pi^2\epsilon_0^2\hbar^2}$$

We can also write this as

$$E_{ry} = \frac{1}{2}\frac{e^2}{3\pi\epsilon_0 a_0}$$

where a_0 is the Bohr radius, $a_0 = \frac{4\pi\epsilon_0\hbar^2}{me^2}$.

Another way we can write this is

$$E_{ry} = \alpha^2 \cdot \frac{1}{2}mc^2$$

where $\alpha = \frac{e^2}{4\pi\epsilon_0\hbar c}$ is the fine structure constant, $\alpha \approx \frac{1}{137.035999177}$. If we define a length scale l, we can think of it as

$$\alpha = \frac{\frac{e^2}{4\pi\epsilon_0 l}}{\hbar c/l}$$

So, in some sense, the fine structure constant defines the ratio between classical electromagnetic energy scale and the quantum mechanical energy scale.

47.2 Fine Structure

We can write the fine structure Hamiltonian as

$$H_{\text{spin-orbit}} = -\vec{mu} \cdot \vec{B_{eff}}$$

, where μ is the magnetic moment $\vec{mu} = \gamma\vec{S}$ and γ is the gyromagnetic ratio $\gamma = \frac{-ge}{2m_e}$. B_{eff} is the effective magnetic field, which is

$$B_{eff} = -\frac{1}{c^2}\vec{v} \times \vec{E}$$

Since $E = \frac{e}{4\pi\epsilon_0}\frac{\hat{r}}{r^2}$,

$$B_{eff} = \frac{1}{4\pi\epsilon_0 c^2}\frac{e}{r^3}\vec{r} \times \vec{v} = \frac{1}{4\pi\epsilon_0}\frac{e}{mc^2r^3}\vec{L}$$

Therefore, what we get is that

$$H_{\text{spin-orbit}} = \frac{ge^2}{8\pi\epsilon_0 m^2c^2}\frac{1}{r^3}\vec{S} \cdot \vec{L}$$

This is the semi-classical picture. However, it is incorrect. The correct formula is

$$H_{\text{spin-orbit}} = \frac{e^2}{8\pi\epsilon_0 m^2c^2}\frac{1}{r^3}\vec{S} \cdot \vec{L}$$

We can introduce $\vec{J} = \vec{L} + \vec{S}$, which is the total angular momentum. We can then write

$$J^2 = L^2 + S^2 + 2\vec{L} \cdot \vec{S}$$

The first result is

$$\vec{L} \cdot \vec{S} = \frac{1}{2}(J^2 - L^2 - S^2)$$

Secondly, this implies that J^2 commutes with the Hamiltonian. This is because L_i and S_j commute in general. We can see that $\{H, J^2, L^2, S^2, J_z\}$ forms a CSCO.

If we want to compute the energy levels, we can find

$$\langle \psi | H_{so} | \psi \rangle = c \langle \psi | \frac{1}{r^3} \vec{S} \cdot \vec{L} | \psi \rangle = c \langle R | \frac{1}{r^3} | R \rangle \langle l, s, j, m_z | \vec{S} \cdot \vec{L} | l, s, j, m_z \rangle$$

We know that

$$\left\langle \vec{S} \cdot \vec{L} \right\rangle = \left\langle \frac{J^2 - L^2 - S^2}{2} \right\rangle = \frac{1}{2}\hbar^2 \left(j(j+1) - l(l+1) - \frac{1}{2}\frac{3}{2} \right)$$

For example, if $l = 1$ and $s = 1/2$, we get that $1 \otimes \frac{1}{2} = \frac{3}{2} \oplus \frac{1}{2}$. Then, the possible values of $\langle S \cdot L \rangle$ are $\frac{1}{2}\hbar^2$ and $-\hbar^2$. This means that the energy levels will split, with one level increased by $\frac{1}{2}\hbar^2$ and the other decreased by $\hbar^2$. If we calculate the energy change associated with this, it will be on the order of

$$\Delta E_{so} \sim \frac{e^2}{8\pi\epsilon_0 m^2 c^2} \frac{1}{r^3}$$

If we substitute $r = a_0$ as an approximation, we will get that

$$\Delta E_{so} \sim \alpha^4 mc^2$$

47.3 Hyperfine Structure

The spin-spin interaction is given by

$$H_{\text{spin-spin}} = -\vec{\mu}_e \cdot \vec{B_e f} f$$

where B_{eff} is the magnetic field created by the proton, which is given as

$$B_p = \frac{\mu_0}{4\pi} \frac{1}{r^3} (3\mu_p \cdot \hat{r}\hat{r} - \mu_p) + \frac{2\mu_0}{3} \mu_p \delta(\vec{r})$$

and $\mu_p = \gamma_p \vec{S}_p = g_p \frac{e}{2m_p} \vec{S}_p$.

For now, let's focus on $n = 1$, $l = 0$. The subspace we are considering is

$$|\psi\rangle = \left| n = 1, l = 0, m_z = 0; s_e = \frac{1}{2}, m_e = \pm\frac{1}{2}; s_p = \frac{1}{2}, m_p = \pm\frac{1}{2} \right\rangle$$

We will abbreviate this as $|m_e, m_p\rangle$. We then use perturbation theory and calculate

$$\langle m_e, m_p | H_{ss} | m_e, m_p \rangle = \int \mathrm{d}r \int \mathrm{d}\Omega R(r) Y_{1,0,0}(\Omega) \langle m_e, m_p | \vec{S}_e \cdot \vec{S}_p | m_e, m_p \rangle$$

It turns out that after much calculation, we will find that the hyperfine splitting energy scale is

$$\Delta E_{hf} = \frac{4}{3} g_p \frac{m_e}{m_p} m_e c^2 \alpha^4$$

and the Hamiltonian simplifies to

$$H_{ss} = \Delta E_{hf} \frac{\vec{S}_e \cdot \vec{S}_p}{\hbar^2}$$

"The physics is very simple" - Soonwon Choi

48 Recitation 24 (2024-12-03)

We discussed in the last few lectures the addition of angular momentum. In some cases, it's convenient to use the coupled basis, and in some cases, it's convenient to use the uncoupled basis. In many cases, we are only able to observe total quantities, and we can't observe individual quantities. We also learned how these bases are related by the Clebsch-Gordan coefficients.

Let's do an example from a past final exam. We need to decompose a system

$$0 \otimes \frac{1}{2} \otimes 1 \otimes \frac{3}{2} \otimes 2$$

Let's do this one by one:

$$0 \otimes \frac{1}{2} = \frac{1}{2}$$

$$\frac{1}{2} \otimes 1 = \frac{3}{2} \oplus \frac{1}{2}$$

$$\left(\frac{3}{2} \oplus \frac{1}{2}\right) \otimes \frac{3}{2} = (3 \oplus 2 \oplus 1 \oplus 0) \oplus (2 \oplus 1)$$

$$\begin{aligned}(3 \oplus 2 \oplus 1 \oplus 0 \oplus 2 \oplus 1) \otimes 2 = {} & (5 \oplus 4 \oplus 3 \oplus 2 \oplus 1 \oplus 0) \oplus (4 \oplus 3 \oplus 2 \oplus 1 \oplus 0) \\ & + (3 \oplus 2 \oplus 1 \oplus 0) \oplus 2 \oplus (4 \oplus 3 \oplus 2 \oplus 1 \oplus 0) \oplus (3 \oplus 2 \oplus 1)\end{aligned}$$

We see that we have 1 multiplet with spin 5, 3 with spin 4, 5 with spin 3, 6 with spin 2, 5 with spin 1, and 2 with spin 0. Counting the number of states, we get

$$11 + 3 \cdot 9 + 5 \cdot 7 + 6 \cdot 5 + 5 \cdot 3 + 2 = 120$$

which matches with what we expect.

49 Lecture 25 (2024-12-04)

So far, we learned that a state of our system is described by a ray in our Hilbert space, and that ray contains all information we could possibly extract. However, there is an intrinsic probabilistic element, where for an observable, we can only predict the probability of measuring a certain value.

But what if we do not know the state completely? This will add an additional element of uncertainty.

49.1 Ensembles of Quantum States

Imagin we have a button. I can press the button, and a machine gives us a quantum state. The state can be different every time, but I know the probability distribution of these states. For each state $|\psi_s\rangle$, we have probability p_s. Let's assume that each $|\psi_s\rangle$ is normalized, but let's not enforce any other constraints on the states for now.

Example 49.1

Say we are considering the spin-1/2 Hilbert space. We have an ensemble

$$\varepsilon = \{(1, |z, +\rangle)\}$$

, meaning that the state is $|z, +\rangle$ with probability 1. Since there is a unique element with $p_s = 1$, we call this a pure state.

Example 49.2

What if we consider the ensemble

$$\varepsilon = \left\{ \left(\frac{1}{2}, |z, +\rangle \right), \left(\frac{1}{2}, |x, +\rangle \right) \right\}$$

This is an example of what we call a mixed state.

Say we want the expectation value of an operator O on the second example. We can simply use

$$\langle O \rangle_\varepsilon = \frac{1}{2} \langle z, + | O | z, + \rangle + \frac{1}{2} \langle x, + | O | x, + \rangle$$

Now, the natural question to ask is, can we always model the behaviour of a mixed state with a certain $|\psi\rangle$ which is in the given Hilbert Space?

The answer is no. Consider the spin-1/2 example, with a $|\phi\rangle \in \mathcal{H}$ $|\phi\rangle = |\theta, \phi\rangle$. Then, consider $S_{\hat{n}}$. The expectation value over this state is $\frac{\hbar}{2}$. However, consider the ensemble $\{(1/2, |x, +\rangle), (1/2, |x, -\rangle)\}$. The expectation value of any spin operator on this ensemble will be 0.

49.2 Density Matrix

Say we want to compute

$$\langle O \rangle_\varepsilon = \sum_\alpha p_\alpha \langle \psi_\alpha | O | \psi_\alpha \rangle = \sum_\alpha p_\alpha \operatorname{Tr}(O |\psi_\alpha\rangle \langle \psi_\alpha|) = \operatorname{Tr}\left(O \sum_\alpha p_\alpha |\psi_\alpha\rangle \langle \psi_\alpha| \right)$$

We call the value

$$\rho_\varepsilon = \sum_\alpha p_\alpha |\psi_\alpha\rangle \langle \psi_\alpha|$$

the density matrix.

Let's talk about some properties of the density matrix. We can easily see that it is Hermitian. It is also positive semi-definite. What this means that for every quantum state, $\langle \phi | \rho | \phi \rangle \geq 0$. Finally, we can see that $\operatorname{Tr}(\rho) = 1$.

It turns out that for any matrix that satisfies these three properties, we can find an ensemble that has that matrix as its density matrix.

Furthermore, the density matrix fully specifies expectation values of an ensemble and is unique. We can prove that if $\forall O \in \mathcal{L}(\mathcal{H})$, $\operatorname{Tr}(O\rho) = \operatorname{Tr}(O\rho')$, then $\rho = \rho'$.

Proof. For all O, $\operatorname{Tr}(O(\rho - \rho')) = 0$. Let $\delta\rho = \rho - \rho'$. Since O can be anything, let's let it be $\delta\rho^\dagger$. Then,

$$\operatorname{Tr}(\delta\rho^\dagger \delta\rho) = 0 \implies \sum_i \langle i | \delta\rho^\dagger \delta\rho | i \rangle = \sum_i |\delta\rho |i\rangle|^2 = 0$$

Since $\delta\rho$ is positive semi definite, we can conclude that $\delta\rho |i\rangle = 0$ for all $|i\rangle$, which means that $\delta\rho$ must be the 0 operator. We can then conclude that $\rho = \delta\rho$. □

Now, let's think about given a ρ, can we construct an ensemble with such a density matrix? We can, and this process is called unravelling. However, this process is not unique, and we can generally construct infinitely many valid ensembles.

Given a ρ, we can unitarily diagonalize it: $U^\dagger \rho U = D$ where D is diagonal. We know that the diagonal entries λ_i are all nonnegative and that they add up to 1.

Let $|\psi_i\rangle = U|i\rangle$. Then, we can actually easily show that ρ is just $\sum_i \lambda_i |\psi_i\rangle \langle \psi_i|$. Additionally, we know that $|\psi_i\rangle$ are all orthonormal. This is called the orthogonal unravelling.

If given a density matrix ρ, can we tell whether it is pure or mixed? We can easily show that if ρ has an eigenvalue of 1, then ρ is pure. Otherwise, it is mixed.

49.3 Purity and Maximally Mixed States

We can define a purity

$$\mathcal{P} = \operatorname{Tr}(\rho^2) = \operatorname{Tr}\left(\sum_\mu \lambda_\mu |\mu\rangle \langle \mu| \sum_\nu |\nu\rangle \langle \nu| \right) = \sum_u \lambda_u^2 \leq 1$$

The purity is 1 if and only if ρ is pure.

Do we think purity is an observable, i.e. can we find an observable Q_p such that $\text{Tr}(Q_p\rho) = \mathcal{P}$? The answer is no, because our definition of $\mathcal{P}$ is not linear.

A maximally mixed state is $\rho_{\max} = \sum_i \frac{1}{d} |i\rangle \langle i| = \frac{1}{d} I$. We can prove that $\text{Tr}(\rho_{\max}^2) = \frac{1}{d}$ is the minimum possible.

50 Recitation 25 (2024-12-05)

Today we will review the density matrix. Recall we learned about ensembles of particles, where each state has some probability of occurring.

Note that different ensembles can be indistinguishable. For example, consider ensembles

$$E_z = \left\{ \left(\frac{1}{2}, |z,+\rangle \right), \left(\frac{1}{2}, |z,-\rangle \right) \right\}$$

$$E_x = \left\{ \left(\frac{1}{2}, |x,+\rangle \right), \left(\frac{1}{2}, |x,-\rangle \right) \right\}$$

For any observable Q,

$$\langle Q \rangle_z = \frac{1}{2} \langle z,+| Q |z,+\rangle + \frac{1}{2} \langle z,-| Q |z,-\rangle$$

$$\langle Q \rangle_x = \frac{1}{2} \langle x,+| Q |x,+\rangle + \frac{1}{2} \langle x,-| Q |x,-\rangle$$

Recall that $|x,\pm\rangle = \frac{1}{\sqrt{2}}(|z,+\rangle \pm |z,-\rangle)$. Therefore, we can see that

$$\langle Q \rangle_x = \frac{1}{2} \cdot \frac{1}{2}(\langle z,+| + \langle z,-|)Q(|z,+\rangle + |z,-\rangle) + \frac{1}{2} \cdot \frac{1}{2}(\langle z,+| - \langle z,-|)Q(|z,+\rangle - |z,-\rangle)$$

$$= \frac{1}{2}(\langle z,+| Q |z,+\rangle + \langle z,-| Q |z,-\rangle) = \langle Q \rangle_z$$

This holds for any observable Q. Therefore, we cannot tell the difference between these two ensembles simply by measuring observables.

For an observable Q,

$$\langle Q \rangle = \sum_a p_a \langle \psi_a| Q |\psi_a\rangle = \sum_a p_a \langle \psi_a| Q \sum_n |n\rangle \langle n|\psi_a\rangle$$

$$= \sum_n \sum_a p_a \langle \psi_a| Q |n\rangle \langle n|\psi_a\rangle$$

$$= \sum_n \langle n| \sum_a p_a |\psi_a\rangle \langle \psi_a| Q |n\rangle$$

$$= \text{Tr}\left(\sum_a p_a |\psi_a\rangle \langle \psi_a| Q \right) = \text{Tr}(\rho Q_p)$$

where $\rho = \sum_a p_a |\psi_a\rangle \langle\psi_a|$ is the density matrix.
Recall that the density matrix satisfies the following properties:

1. ρ_E is Hermitian
2. $\mathrm{Tr}(\rho_E) = 1$. We can easily prove this by using our normalization condition $\langle\psi_a|\psi_a\rangle = 1$.
3. States have a purity $\mathcal{P} = \mathrm{Tr}(\rho^2)$, which is 1 if and only if the state is pure.

Example 50.1

Say we have a pure state where

$$\rho_1 = |\psi\rangle \langle\psi|$$

and a mixed state where

$$\rho_2 = \frac{1}{2} |\psi_1\rangle \langle\psi_1| + \frac{1}{3} |\psi_2\rangle \langle\psi_2| + \frac{1}{6} |\psi_3\rangle \langle\psi_3|$$

This is the difference between a pure and mixed state.
Let's also consider which states maximize mixing (minimize purity). We want to minimize $\sum_a p_a^2$ while we know that $\sum_a p_a = 1$. We can use Lagrange multipliers to solve this problem. We can easily see that this is minimized when all p_a are equal, which gives us the maximally mixed state.

Example 50.2

Let's consider a 2D Hilbert space. Let $|\psi_\pm\rangle = \frac{1}{\sqrt{2}}(|0\rangle \pm |1\rangle)$. We write a density matrix

$$\rho_+ = |\psi_+\rangle \langle\psi_+| = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

This is a pure state, because $\mathrm{Tr}(\rho_+^2) = 1$.
Now, consider instead the density matrix

$$\rho = \frac{1}{2} |1\rangle \langle 1| + \frac{1}{2} |\psi_+\rangle \langle\psi_+| = \frac{1}{4} \begin{pmatrix} 3 & 1 \\ 1 & 1 \end{pmatrix}$$

We can see that this is a mixed state, because $\mathrm{Tr}(\rho^2) < 1$.

51 Lecture 26 (2024-12-09)

Today's lecture will be given by Barton Zwiebach.

51.1 Density Matrix of Spin-1/2

We will talk about density matrices. Last time, we briefly talked about the density matrix for spin 1/2. The matrix must be Hermitian, positive semi-definite, and have a trace of 1. We can write the density matrix as

$$\rho = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \frac{1}{2}\vec{a}\cdot\vec{\sigma}$$

where the first term is determined because the total must have trace 1.

$\vec{a} = (a_1, a_2, a_3)$ is a real vector, and for the density matrix to be positive semi-definite, we can check

$$\rho = \frac{1}{2}I + \frac{1}{2}|a|\sigma_{na}$$

It is then easy to see that $|n_a, \pm\rangle$ are eigenvalues of ρ with eigenvalues $\frac{1}{2}(1 \pm |a|)$. Therefore, the density matrix is positive semi-definite if $|a| \leq 1$.

The pure states are the ones exactly on this boundary, where $|a| = 1$. With some algebra, we can show that $\rho = \frac{1}{2}I + \frac{1}{2}\vec{a}\cdot\vec{\sigma} = |n_a\rangle\langle n_a|$.

When $|a| = 0$, we get the maximally mixed state, where $\rho = \frac{1}{2}I$.

51.2 Measurement

Imagine we have a Hilbert space with dimension N and orthonormal basis $|i\rangle$.

Say we have a density matrix ρ and we want to measure an observable O. In ρ, state $|\psi_i\rangle$ has probability p_i. Let

$$p(i) = \sum_{a=1}^{n} p_a p(|i\rangle \,|\, |\psi_a\rangle) = \sum_{a=1}^{n} p_a |\langle i, \psi_a||\rangle^2 = \langle i| \sum_{a=1}^{n} p_a |\psi_a\rangle\langle\psi_a| |i\rangle$$

Therefore, $p(i) = \langle i|\rho|i\rangle$.

Then, after a measurement, the state will become

$$\tilde{\rho} = \sum_i p(i)|i\rangle\langle i| = \sum_i |i\rangle p(i)\langle i| = \sum_i |i\rangle\langle i|\rho|i\rangle\langle i| = \sum_i M_i \rho M_i$$

where $M_i = |i\rangle\langle i|$.

51.3 Dynamics

If we start with an ensembel $p_a, |\psi_a\rangle$, and we evolve it with a unitary operator U, we get that at time t, $|\psi_a, t\rangle = U(t)|\psi_a\rangle$ and $i\hbar\frac{\mathrm{d}U}{\mathrm{d}t} = HU$. By plugging in our expression for $|\psi_a, t\rangle$, we can see that

$$\rho(t) = U(t)\rho(0)U^\dagger(t)$$

Taking the derivative,

$$\begin{aligned} i\hbar\frac{\mathrm{d}\rho}{\mathrm{d}t} &= i\hbar\frac{\mathrm{d}U}{\mathrm{d}t}\rho(0)U^\dagger + U\rho(0)i\hbar\frac{\mathrm{d}U^\dagger}{\mathrm{d}t} \\ &= HU\rho(0)U^\dagger - U\rho(0)U^\dagger H \end{aligned}$$

Therefore,

$$i\hbar\frac{\mathrm{d}\rho}{\mathrm{d}t} = [H,\rho]$$

Let's also think about the time evolution of the purity:

$$\xi(t) = \operatorname{Tr}(\rho(t)^2)$$

$$\frac{\mathrm{d}\xi(t)}{\mathrm{d}t} = 2\operatorname{Tr}\left(\rho(t)\frac{\mathrm{d}\rho(t)}{\mathrm{d}t}\right) = 2\operatorname{Tr}(\rho[H,\rho]) = 2\operatorname{Tr}(\rho H\rho - \rho\rho H) = 0$$

because of the cyclic property of the trace. Therefore, the purity is conserved.

51.4 Bipartite Systems

Say we have a Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$. For pure states ψ_{AB} that are entangled, there is no $|\psi_A\rangle$ that describes A. By this, we mean that for operators Q_A, we want to find a ψ_A such that

$$\langle\psi_A| Q_A |\psi_A\rangle = \langle\psi_{AB}| Q_A \otimes I_B |\psi_{AB}\rangle$$

In general, it is not possible to find such a $|\psi_A\rangle$. However, it is possible to find a density matrix that describes the subsystem A.

Let's briefly talk about partial traces: given vector spaces V and W with orthonormal bases $|e_i\rangle$ and $|f_j\rangle$, then for a linear operator $\theta \in \mathcal{L}_{V\otimes W}$,

$$\operatorname{Tr}_W \theta = \sum_j \langle f_j| \theta |f_j\rangle \in \mathcal{L}_V$$

and

$$\operatorname{Tr}_V \theta = \sum_i \langle e_i| \theta |e_i\rangle \in \mathcal{L}_W$$

Furthermore,

$$\operatorname{Tr}(\theta) = \operatorname{Tr}_V \operatorname{Tr}_W \theta = \operatorname{Tr}_W \operatorname{Tr}_V \theta$$

The main result using this is: Let ρ_{AB} be the density matrix for they composite system AB. Now, define $\rho_A = \operatorname{Tr}_B \rho_{AB}$, and $\rho_B = \operatorname{Tr}_A \rho_{AB}$. Then,

$$\rho_A = \sum_j \left\langle e_j^B\right| \rho_{AB} \left|e_j^B\right\rangle \in \mathcal{L}_A$$

$$\rho_B \sum_i \left\langle e_i^A\right| \rho_{AB} \left|e_i^A\right\rangle \in \mathcal{L}_B$$

It turns out that for an operator θ_A in the A system,

$$\operatorname{Tr}(\rho_{AB}(\theta_A \otimes I)) = \operatorname{Tr}_A(\rho_A\theta_A)$$

Therefore, ρ_A is the density matrix that describes the subsystem A.

52 Recitation 26 (2024-12-10)

This recitation, we reviewed the density matrix.

Let's also introduce Schmidt Decomposition. If we have a composite state

$$|\psi_{AB}\rangle = \sum_{i,j} c_{ij} |i_A\rangle |j_B\rangle$$

, we can decompose it into

$$|\psi_{AB}\rangle = \sum_{\mu=1}^{x} \lambda_\mu |\phi_\mu\rangle_A |\psi_\mu\rangle_B$$

where x is known as the Schmidt rank.