8.05 Fall 2024

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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 bases $\{v_1, v_2, \ldots\}$. 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? I 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 eignvalue 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 nontrivial, 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 chose $v = \begin{pmatrix} -a \\ 1/b \end{pmatrix}$.
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 dimentional 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,

$$\langle j|T_1 1\rangle = \lambda_1\langle k|1\rangle = \lambda_1\delta 1j$$

$$\langle 1|T_1 j\rangle = (\langle j|T_1^\dagger 1\rangle)^* = \langle j|\lambda_1^* 1\rangle^* = \lambda_1\delta_{1j}$$

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

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

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

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

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 distinguised? 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 wan 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 Hammiltonians 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 reversability, 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:

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

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 $\langle u|(|v\rangle) = \langle u, v\rangle$. 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

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

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

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 preleminary form of the uncertainty principle.

Now,

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

We can get

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

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

Similarly,

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

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

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

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

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

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

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

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,

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

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

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

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

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

Our result is that

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

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

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

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

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

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

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

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

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

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

$$\langle\lambda|\lambda|\lambda\rangle = \lambda$$

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

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

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

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

Similarly, we can derive that

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

Therefore, $a^\dagger|\lambda\rangle$ 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 $|\lambda_{\min}\rangle$ such that $a|\lambda_{\min}\rangle = 0$.

Since we know that

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

Therefore, the eigenvalues of $|\lambda_{\min}\rangle$ 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 $|0\rangle, |1\rangle, |2\rangle, \ldots$. 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 $a|\lambda\rangle = 0$ has only one unique $|\lambda\rangle$. We get

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

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

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 Hesienberg 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 quanta 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:

$$|\psi(t)\rangle = e^{-i\omega t\left(\hat{N}+\frac{1}{2}\right)}\sum_{n=0}^{\infty}\frac{1}{\sqrt{n!}}\alpha_0^n|n\rangle = e^{-i\omega t/2}\sum_{n=0}^{\infty}\frac{1}{\sqrt{n!}}e^{-i\omega tn}\alpha_0^n|n\rangle = e^{-i\omega t/2}|\alpha = \alpha_0 e^{-i\omega t}\rangle$$

For today, we can ignore this global phase, but in the future, it may become relevant. To summarize:

$$|\alpha_0, t\rangle = |\alpha = \alpha_0 e^{-i\omega t}\rangle e^{-i\omega t/2}$$

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 dissapear 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

$$|\psi(t)\rangle = e^{-i\omega t/2}\int \mathrm{d}^2\alpha\Phi_0(\alpha)|\alpha e^{-i\omega t}\rangle$$

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 nontrivial 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 qunatized, 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 $1.26\,\text{cm}$, 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 inhomogenous 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

$$|\tilde{\psi}(t)\rangle = (U_0(t))^\dagger U(t)|\psi(0)\rangle$$

where $U_0(t) = e^{i\nu t S_z/\hbar}$. Let's try to find an equation of motion for $|\tilde{\psi}(t)\rangle$.

$$\frac{\mathrm{d}}{\mathrm{d}t}|\tilde{\psi}(t)\rangle = \frac{\mathrm{d}}{\mathrm{d}t}(U_0(t))^\dagger|\psi(t)\rangle + U_0^\dagger(t)\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle$$

$$= \left(\frac{\mathrm{d}}{\mathrm{d}t}U_0^\dagger(t)\right)U_0(t)U_0^\dagger(t)|\psi(t)\rangle - iU_0^\dagger(t)\frac{H(t)}{\hbar}|\psi(t)\rangle$$

$$= \frac{i\nu S_z}{\hbar}U_0^\dagger(t)|\psi(t)\rangle - iU_0^\dagger(t)H(t)U_0(t)U_0^\dagger(t)|\psi(t)\rangle$$

$$= \frac{i\nu S_z}{\hbar}|\tilde{\psi}(t)\rangle - iU_0^\dagger(t)H(t)U_0(t)|\tilde{\psi}(t)\rangle$$

So

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

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.