PHYSICS 204A: MATH METHODS

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Lecture 1.

Wednesday, September 25, 2019

Reading assignment: read Ch. 2 and 3 of the course text (Arfken/Weber). This is basic linear algebra and vector analysis.

The purpose of this course is to learn formal aspects of quantum mechanics. We'll focus on doing analysis in Hilbert space. It's a remarkable fact about the natural world that most of our physical world is well-approximated by linear systems.

In the simplest form, we may think of vectors as arrays of numbers,

$$(v_1, v_2, \ldots). \tag{1.1}$$

But we can also think of some real function $f(x) : \mathbb{R} \to \mathbb{R}$ as a collection of numbers too, just by taking its values at arbitrarily close points.

Definition 1.2. A *linear vector space* over a field F, denoted $L(F)$, is a set $\{|v\rangle\}$ with an addition operation $+$ such that

- for $|v\rangle, |u\rangle \in L, |u\rangle + |v\rangle = |w\rangle \in L$ (closure)
- for $c \in F$, $c|v\rangle \in L$ (scalar multiplication).

These axioms directly imply that any linear combination of vectors in L is also in the vector space:

$$c_v|v\rangle + c_u|u\rangle \in L. \tag{1.3}$$

This leads us naturally to the notion of *linear (in)dependence*. Suppose we take some vectors $|v_k\rangle \in L$ and make a linear combo,

$$\sum_k c_k|v_k\rangle. \tag{1.4}$$

Definition 1.5. A set of vectors $\{|v_k\rangle\}$ is *linearly dependent* if there exists some $\{c_k\}$ not all zero such that

$$\sum_k c_k|v_k\rangle = |0\rangle, \tag{1.6}$$

and such that $|0\rangle \notin \{|v_k\rangle\}$.

We need this last condition because otherwise we could simply take the coefficient of the $|0\rangle$ vector to be 1 and then arrive at a trivial solution.

Definition 1.7. If a set of vectors is not linearly dependent, it is *linearly independent*.

The next question we might ask is as follows: what is the size of the biggest set of linearly independent vectors we can construct for a given vector space?

Definition 1.8. The maximum number of linearly independent vectors associated to a given vector space is called the *dimension*.

Example 1.9. We may consider an infinitely differentiable (C^∞) function. It has a Taylor expansion

$$f(x) = \sum \frac{f^{(n)}(0}{n!} x^n, \tag{1.10}$$

which we may think of as an expansion in the basis $(1, x, x^2, \ldots)$.

So this is a vector space with countably infinite dimension. But we can have uncountably infinite-dimensional spaces too, e.g. the space of Fourier-transformable functions in a basis $e^{ikx}, k \in \mathbb{R}$. These factors are not just linearly independent; introducing an appropriate inner product, they are orthogonal.

It follows that for a vector space L_D of dimension D, any set with more than D vectors must be linearly dependent, i.e. $\exists \bar{c}_v, \bar{c}_k$ not all zero such that

$$\bar{c}_v |v\rangle + \sum_k \bar{c}_k |v_k\rangle = 0. \tag{1.11}$$

Moreover $\bar{c}_v \neq 0$ or else the original set $|v_k\rangle$ would be linearly dependent. Hence we can divide through, define $\hat{c}_k = \bar{c}_k / \bar{c}_v$, and write

$$|v\rangle = \sum_k \hat{c}_k |v_k\rangle. \tag{1.12}$$

That is, we have *decomposed* a general vector $|v\rangle$ in terms of its components $\hat{c}_k$ with respect to a basis $|v_k\rangle$.

We might now be interested in adding more structure to our vector space. Consider L_D with $|v\rangle, |u\rangle$.

Definition 1.13. We define an *inner product* by

$$\langle v|u\rangle : (|v\rangle, |u\rangle) \to F \tag{1.14}$$

as a map from the input vectors to the field over which the vector space is defined, with the following properties:

- $\langle u|(\lambda|v_1\rangle + \mu|v_2\rangle) = \lambda\langle u|v_1\rangle + \mu\langle u|v_2\rangle$ (linearity)
- $\langle v|u\rangle = \langle u|v\rangle^*$
- $\langle v|v\rangle \geq 0$, with equality only for the zero vector (positive semi-definite).

If we choose a basis $\{|v_k\rangle\}$, then if our vectors $|u\rangle, |v\rangle$ have some expansion in this basis then by linearity that

$$\langle u|v\rangle = \sum_k \hat{c}_k^v \langle u|v_k\rangle, \tag{1.15}$$

and we can expand each of these inner products as

$$\langle u|v_k\rangle = (\langle v_k|u\rangle)^* = \sum_n c_n^{u*} \langle v_n|v_k\rangle. \tag{1.16}$$

It follows that we can write a general inner product as

$$\langle u|v\rangle = \sum_{n,k} = c_k^v c_n^{u*} \langle v_n|v_k\rangle. \tag{1.17}$$

Moreover if we could choose a nice basis which had a special property of *orthogonality* or better yet *orthonormality*, we could reduce this to a single sum

$$\langle u|v\rangle = \sum_k c_k^v c_k^* \tag{1.18}$$

in terms of the components alone.

Lecture 2.

Monday, September 30, 2019

Last time, we wrote a general form for the dot (inner) product,

$$\langle u|v\rangle = \sum_{n,m} c_n^{*u} c_m^v \langle \phi_n|\phi_m\rangle, \tag{2.1}$$

where the $|\phi\rangle$s are basis vectors and u, v have expansions

$$|u\rangle = \sum_n c_n^u |\phi_n\rangle. \tag{2.2}$$

This is some quadratic form (it depends only quadratically on the components). And indeed it would be very nice if we could define $\langle \phi_N|\phi_m\rangle = \delta_{nm}$, so that our double-sum collapses to a single sum.

Orthonormality Let us suppose we start with a basis $\{|\phi_n\rangle\}$ for a vector space L_D. We shall show that we can construct a new basis $\{|\chi_n\rangle\}^D$ such that $\langle \chi_m|\chi_n\rangle = \delta_{mn}$ has the desired property.

WLOG let us number the basis vectors $|\phi_1\rangle, |\phi_2\rangle, \ldots$ and consider some inner products. The inner product

$$\langle \phi_1|\phi_1\rangle = N_1 \tag{2.3}$$

is some value N_1. If $N_1 = 1$ then we are done; otherwise, define

$$|\chi_1\rangle \equiv \frac{1}{\sqrt{N_1}}|\phi_1\rangle \tag{2.4}$$

so that

$$\langle \chi_1|\chi_1\rangle = \frac{\langle \phi_1|\phi_1\rangle}{N_1} = 1. \tag{2.5}$$

Hence $|\chi_1\rangle$ is a unit vector.

Consider the next vector $|\phi_2\rangle$. If

$$\langle \chi_1|\phi_2\rangle = 0, \tag{2.6}$$

then we can normalize and get

$$|\chi_2\rangle = \frac{|\phi_2\rangle}{\sqrt{N_2}}, \tag{2.7}$$

where $N_2 = \langle \phi_2|\phi_2\rangle$. Otherwise, we first subtract off the projection of the first normalized vector,

$$|\hat{\chi}_2\rangle = |\phi_2\rangle - \langle \chi_1|\phi_2\rangle|\chi_1\rangle, \tag{2.8}$$

so that

$$\langle \chi_1|\hat{\chi}_2\rangle = \langle \chi_1|\phi_2\rangle - \langle \chi_1|\phi_2\rangle \underbrace{\langle \chi_1|\chi_1\rangle}_{=1} = 0. \tag{2.9}$$

Hence by our definition, $|\chi_1\rangle$ and $|\hat{\chi}_2\rangle$ are orthogonal and we can just normalize. Defining

$$\hat{N}_2 = \langle \hat{\chi}_2|\hat{\chi}_2\rangle, \tag{2.10}$$

we have

$$|\chi_2\rangle = \frac{|\hat{\chi}_2\rangle}{\sqrt{\hat{N}_2}}, \tag{2.11}$$

which is a unit vector and normal to $|\chi_1\rangle$.

We continue by induction, subtracting off projections and normalizing. This is the *Gram-Schmidt procedure*.[1] Notice also that because $\langle \phi_n|\phi_m\rangle = \langle \phi_m|\phi_n\rangle^*$, we can consider values of m, n to be entries in a Hermitian matrix. Recalling that $\langle u|u\rangle \geq 0$, the norm is perfectly well-defined and indeed we can see that orthonormalization is equivalent to diagonalizing a Hermitian matrix.

[1] Note that the procedure is a little more subtle in the infinite-dimensional case.

More inner products On a function space, we can define an inner product

$$\langle f|g\rangle = \int_{-\infty}^{\infty} dx\, f^*(x)g(x). \tag{2.12}$$

These inner products come with strings attached; our functions usually have to satisfy some integrability properties in order for the inner products to be well-defined. Often the functions we're interested in come from differential equations. Most of the ones we encounter in physics are second-order so these functions ought to be twice-differentiable.[2] And we should also require that our functions are square-integrable so that the integral is well-defined.

We can then define

$$\begin{aligned}\langle u|u\rangle &= \sum_{n,m} c_n^* c_m \langle\phi_n|\phi_m\rangle \\ &= \sum_n |c_n|^2. \end{aligned} \tag{2.13}$$

And this is none other than the generalization of Pythagoras's theorem.

Schwarz inequality From the axioms, we can prove the following inequality.

$$|\langle f|g\rangle|^2 \le \langle f|f\rangle\langle g|g\rangle. \tag{2.14}$$

We may define the linear combination

$$|f-\lambda g\rangle \tag{2.15}$$

and consider its norm (squared)

$$\langle f-\lambda g|f-\lambda g\rangle = \langle f|f\rangle - \lambda^*\langle g|f\rangle - \lambda\langle f|g\rangle + \lambda\lambda^*\langle g|g\rangle. \tag{2.16}$$

This is obviously non-negative, given the axioms. We can extremize this by taking derivatives with respect to λ, λ^* (which we may treat as linearly independent, since they are complex) and find that

$$\lambda^* = \frac{\langle g|f\rangle}{\langle g|g\rangle}, \quad \lambda = \frac{\langle f|g\rangle}{\langle g|g\rangle}. \tag{2.17}$$

A bit of manipulation yields the Schwarz inequality.

Let us also note that we can in general translate between the ket notation and vector notation. For a ket vector $|u\rangle$ we can associate the bra (row) vector $\langle u| = (c_1^*, c_2^* \ldots, c_D^*)$. Then the vector inner product is the same as old-fashioned row-column multiplication.

Bessel inequality Suppose we rewrite the vector $|u\rangle$ in a weird way, as

$$|u\rangle = \sum_n{}' c_n^u|\phi_n\rangle + |\Delta u\rangle, \tag{2.18}$$

where we take some terms and separate them out (so the sum $\sum'$ omits some indices). We know that

$$|\Delta u\rangle = u - \sum_n{}' c_n^8|\phi_n\rangle \neq 0, \tag{2.19}$$

so that

$$0 < \langle\Delta u|\Delta u\rangle \tag{2.20}$$
$$= \langle u - \sum{}' c_n^u\phi_n|u - \sum{}' c_n^u\phi_n\rangle \tag{2.21}$$
$$= \langle u|u\rangle - \sum{}'|c_n^u|^2. \tag{2.22}$$

Check the cross-terms with the definition of u to get this final term. Rearranging, we get the Bessel inequality, which says that

$$\langle u|u\rangle > \sum{}'|c_n^u|^2, \tag{2.23}$$

i.e. the norm of a vector is greater than the partial sums of the squares of the components.

[2] This is a little too strong, actually. They can have finitely many discontinuities and this is still okay.

Linear operators We are primarily interested in linear operators, i.e. linear maps from the vector space to itself obeying

$$A(\lambda|\phi\rangle + \mu|\chi\rangle) = \lambda A|\phi\rangle + \mu A|\chi\rangle. \tag{2.24}$$

We can define two operators to be equal if they have the same action on all vectors, i.e.

$$A|\phi\rangle = B|\phi\rangle \tag{2.25}$$

for all $\phi \in L$.

In particular there's a nice way that we can rewrite the identity operator, as

$$\mathbb{I} = \sum_n |\phi_n\rangle\langle\phi_n|. \tag{2.26}$$

Let's prove this: by definition, $\mathbb{I}|u\rangle = |u\rangle$. On the other side, we see that

$$\sum_n |\phi_n\rangle\langle u| =\rangle \sum_n c_n^u|\phi_n\rangle \equiv |u\rangle. \tag{2.27}$$

Provided that $\{|\phi_n\rangle\}$ is a complete basis, this operator is indeed the identity.

The delta function The Dirac delta function is defined in such a way that

$$\int_a^b f(t)\delta(x-t)dt = f(x), \tag{2.28}$$

provided that x is in the interval (a,b). We could think of this as an inner product, however. We have a function and its shadow on the delta function picks out a value. The delta function isn't properly square-integrable, but we may consider it as having a good inner product with functions in our function space (as the limit of some sequence of square-integrable functions, if you like).

Now we'll do something strange. Let us express the delta function in a function basis,

$$\delta(x-t) = \sum_n c_n(t)\phi_n(x). \tag{2.29}$$

The t dependence must be in the coefficients since the functions themselves are just given. How do we find the coefficients? Just take the integral

$$\int dx\, \phi_m^*(x)\delta(x-t) = \int dx\, \sum_n c_n(t)\phi_n(x)\phi_n^*. \tag{2.30}$$

This is super easy to evaluate. On the RHS we have a Kronecker delta δ_{nm} by the orthonormality of the basis, and on the left side we have the evaluation of the basis vector ϕ_m^* at t, i.e.

$$c_m(t) = \phi_m^*(t). \tag{2.31}$$

Hence

$$\delta(x-t) = \sum_n \phi_n^*(t)\phi_n(x). \tag{2.32}$$

We can se that this had to be the case by substituting our expression for the delta function into an integral:

$$f(x) = \int dt\, \delta(x-t)f(t) = \sum_n \phi_n(x)\int dt\, \phi_n^*(t)f(t) \tag{2.33}$$

$$= \sum \langle\phi_n|f\rangle\phi_n(x), \tag{2.34}$$

which is none other than the components of f in the basis ϕ_n.

To make our discussion more concrete, let us consider analytic functions which have Taylor expansion

$$f(x) = \sum \frac{f^{(n)}(0)}{n!}x^n, \tag{2.35}$$

defined over the interval $[-1,1]$. Hence $\{1, x, x^2, x^3, \ldots\}$ form a complete basis set for arbitrarily differentiable functions. They are certainly not orthogonal in general, e.g. $\int_{-1}^1 dx\, 1\cdot x^2 \neq 0$. But we can make them orthonormal with Gram-Schmidt.

Under this inner product, we have

$$\int_{-1}^1 dx\, 1\cdot 1 = 2, \tag{2.36}$$

so our first normalized vector is $1/\sqrt{2}$. We can check x:

$$\int_{-1}^{1} dx\, x \cdot x = 2/3, \tag{2.37}$$

so the next normalized vector is $\sqrt{3/2}x$. Continuing this way, we see that x^2 and x are already orthogonal but

$$\int_{-1}^{1} dx\, \frac{1}{\sqrt{2}} x^2 = \frac{2}{3\sqrt{2}}, \tag{2.38}$$

so our first unit vector is not orthogonal to x^2. We can instead define

$$\hat{x}^2 = x^2 - \sqrt{\frac{2}{3}}. \tag{2.39}$$

which is now orthogonal to the first unit vector $1/\sqrt{2}$ and to the second unit vector $\sqrt{3/2}x$. We can normalize $\hat{x}^2$ and determine the third unit vector in this set, which is $\frac{3x^2}{2} - 1$ (we think).

Let us remark that the most general operators that can be diagonalized are *normal* operators, i.e. those satisfying

$$[A, A^\dagger] = 0. \tag{2.40}$$

Clearly, one set of operators that are not normal are the raising and lowering operators, whose commutator is $[a, a^\dagger] = 1$.

Lecture 3.

Wednesday, October 2, 2019

Today we'll continue discussing operators. We've discussed the identity operator,

$$\mathbb{I} = \sum |\phi_i\rangle\langle\phi_i|, \tag{3.1}$$

which maps any vector into itself. More generally, we can define an operator as follows:

Definition 3.2. An *operator* is a map $A : |\psi\rangle \to |\bar{\psi}\rangle$ where $|\psi\rangle, |\bar{\psi}\rangle \in L_D$ are in the same vector space L_D.[3] A *linear operator* is an operator obeying the linearity property

$$A(\mu|\psi\rangle + \nu|\chi\rangle) = \mu A|\psi\rangle + \nu A|\chi\rangle. \tag{3.3}$$

If we have a set of linear operators, we may define an addition operation on operators as

$$(A + B)|\psi\rangle = A|\psi\rangle + B|\psi\rangle \tag{3.4}$$

and scalar multiplication as

$$(kA)|\psi\rangle = k(A|\psi\rangle). \tag{3.5}$$

Hence we can take linear combinations of linear operators as

$$kA + lB, \tag{3.6}$$

and under this definition we see that linear operators form a vector space.

But there's another way to combine operators, namely by *composition*. That is, given operators A and B we can define a new operator AB defined by the composition

$$AB|\psi\rangle = A(B|\psi\rangle). \tag{3.7}$$

Composition must satisfy certain properties with respect to the other operations we've defined, namely distributivity with respect to addition:

$$A(B + C) = AB + AC. \tag{3.8}$$

Let us note that the product of operators (composition) is generally not commutative,

$$AB \neq BA \tag{3.9}$$

in general. We know this from matrix multiplication.

[3] The math-inclined among us may talk about the space of inner automorphisms on the vector space.

Alternately, we could define a composition rule using a commutator (bracket),

$$[A, B] = AB - BA. \tag{3.10}$$

It's not to hard to check that this rule also satisfies distributivity over addition. If we wished, we could also prove (by crunching through the commutators) the Jacobi identity,

$$[[A, B], C] + [[B, C], A] + [[C, A], B] = 0. \tag{3.11}$$

This is related to the Bianchi identity in differential geometry.

Under our standard composition rule, we can define *inverses*. That is, if an operator A acts as

$$|\psi'\rangle = A|\psi\rangle, \tag{3.12}$$

then the inverse A^{-1} (if it exists) is the operator such that

$$A^{-1}|\psi'\rangle = |0\rangle. \tag{3.13}$$

That is, $A^{-1}A|\psi\rangle = |\psi\rangle$.

As we know, not every operator is invertible. Consider the operator which just sends some vector to zero (i.e. it has a null eigenvector). If

$$A|\psi\rangle = 0 \tag{3.14}$$

then the inverse is not well-defined: $A^{-1}|0\rangle =?$.

Definition 3.15. The adjoint $A^\dagger$ of an operator A is defined by

$$\langle\chi|A^\dagger|\psi\rangle = \langle\psi|A|\chi\rangle^*. \tag{3.16}$$

Definition 3.17. If an operator is self-adjoint, $H^\dagger = H$, then we call it Hermitian.

Notice that

$$\langle\psi|H|\psi\rangle = \langle\psi|H^\dagger|\psi\rangle = \langle\psi|H|\psi\rangle^* \tag{3.18}$$

by the definition of the adjoint and hermiticity. Therefore the diagonal matrix elements of H are *real numbers*, i.e. their eigenvalues are real.

We could have also taken an operator which was *anti-Hermitian*, $H^\dagger = -H$, which implies that the diagonal elements are instead purely imaginary by the same argument.

Definition 3.19. A *unitary* operator is an operator obeying the property

$$U^{-1} = U^\dagger. \tag{3.20}$$

It's clear that we can restrict to the real case, in which case Hermitian matrices become symmetric matrices and anti-Hermitian matrices become antisymmetric (sometimes called skew-symmetric). Our unitary matrices reduce to orthogonal matrices.

Example 3.21. Consider the Hilbert space of smooth square-integrable functions over the real line, $f \in L$. Our inner product is the integral

$$\int dx\, f^*(x)g(x). \tag{3.22}$$

Define the operator $D = -\frac{d}{dx}$. What is the adjoint $D^\dagger$? We have

$$\int f^*(-\frac{d}{dx})g = f^*g|_a^b + \int (\frac{d}{dx}f^*)g. \tag{3.23}$$

The boundary term vanishes based on the boundary conditions, i.e. given that f, g vanish at infinity. Taking the complex conjugate to get the adjoint, what is left is

$$\left[\int (\frac{d}{dx}f^*)g\right]^* = -\int g^* Df. \tag{3.24}$$

So D is not Hermitian but iD is (it adds a minus sign to fix the sign in the integration by parts).

Note also that when the integration region is finite, the boundary conditions become nontrivial. However, if f and g vanish at the boundary (e.g. $[-1, 1]$) then we restore hermiticity.

Recall we said that we could assign matrix elements to an operator with respect to some set of vectors,

$$\langle\chi|A|\psi\rangle. \tag{3.25}$$

In fact, it's a Sisyphean task to do this for all sets of vectors, but fortunately (thanks to linearity) it suffices to compute the matrix elements in some (complete) basis. With a basis $|\psi_i\rangle$ we can define

$$\langle\psi_n|A|\psi_k\rangle = A_{nk}. \tag{3.26}$$

For recall that the identity can be written as $\mathbb{I} = \sum_k |\psi_k\rangle\langle\psi_k|$, and suppose $|\psi\rangle$ has some decomposition in the basis

$$|\psi\rangle = \sum_k \langle\psi_k|\psi\rangle|\psi_k\rangle \tag{3.27}$$

Then

$$\begin{aligned} A|\psi\rangle &= \mathbb{I}\mathbb{A}\mathbb{I}|\psi\rangle \\ &= \sum_{k,n} |\psi_k\rangle\langle\psi_k|A|\psi_n\rangle\langle\psi_n|\psi\rangle. \end{aligned}$$

Thus we can recognize the components of $|\psi\rangle$ in our basis, which are given by $\langle\psi_n|\psi\rangle = C_n$. Hence

$$\begin{aligned} A\left(\sum_k \langle\psi_k|\psi\rangle|\psi_k\rangle\right) &= \sum_k |\psi_k\rangle\left(\sum_n \langle\psi_k|A|\psi_n\rangle\langle\psi_n|\psi\rangle\right) \\ &= \sum_k |\psi_k\rangle\left(\sum_n A_{kn}C_n\right) \\ &= \sum |\psi_k\rangle C_k^{\bar{\psi}} \end{aligned}$$

in terms of the components of some new vector $|\bar{\psi}\rangle$. That is, if we know the matrix elements of A in some basis and we know the components of the vector in that basis, we can uniquely determine the components of its image under A in the same basis.

In the end, this is just abstract matrix multiplication. That is,

$$C_n^{\bar{\psi}} = \sum_k A_{nk}C_k^{\psi}. \tag{3.28}$$

We can also write the operator A in terms of its matrix elements:

$$\begin{aligned} A &= \mathbb{I}A\mathbb{I} \\ &= \sum_{n,k} |\psi_k\rangle\langle\psi_k|A|\psi_n\rangle\langle\psi_n| \\ &= \sum_{n,k} A_{kn}|\psi_k\rangle\langle\psi_n|. \end{aligned}$$

This also tells us immediately that the matrix elements of the identity in any orthonormal basis are as we could have guessed– $\mathbb{I}_{nk} = \delta_{nk}$, the Kronecker delta.

It also follows that the matrix elements of the adjoint of an operator obey

$$(A^\dagger)_{nk} = A_{kn}^*. \tag{3.29}$$

This gives us another statement of hermiticity– equivalently, a hermitian operator is one whose matrix elements obey

$$A_{kn}^* = A_{nk}. \tag{3.30}$$

And thus

$$A^\dagger = \sum_{k,n} A_{nk}^*|\psi_k\rangle\langle\psi_n|. \tag{3.31}$$

Let's check that for hermitian operators, the expectation value is non-negative,

$$\langle\psi|A|\psi\rangle \geq 0. \tag{3.32}$$

Writing A in terms of its matrix elements, we have

$$\begin{aligned}\langle\psi|A|\psi\rangle &= \sum_{n,k}\langle\psi|\psi_k\rangle A_{kn}\langle\psi_n|\psi\rangle \\ &= C_k^{*\psi} A_{kn} C_n^{\psi}.\end{aligned}$$

Suppose we have two orthonormal bases for the same space, $\{|\psi_k\rangle\}, \{|\psi'_k\rangle\}$. It follows that the new basis has some decomposition in the old basis. That is, the set $\{|\psi_k\rangle, |\psi'_1\rangle\}$ is linearly dependent and so

$$|\psi'_n\rangle = \sum c_k^{n\prime}|\psi_k\rangle, \tag{3.33}$$

in terms of some coefficients $c_k^{n\prime}$. It's also true that we can go back,

$$|\psi_n\rangle = \sum c_k^{n}|\psi'_k\rangle. \tag{3.34}$$

Certainly we can write this decomposition as the action of an operator U:

$$U|\psi_n\rangle = \sum c_k^{n\prime}|\psi_k\rangle, \tag{3.35}$$

and moreover U must be invertible.

Lecture 4.

Monday, October 7, 2019

When we choose coordinates, the name of the game is to exploit the *symmetries* of the problem. That is, to find coordinates which respect the dynamical symmetries of the Hamiltonian. If we choose our coordinates well enough, the equations of motion become trivial to solve.

Suppose we have two bases $\{|\psi_i\rangle\}, \{|\psi'_i\rangle\}$. Then we can certainly write

$$U|\psi_i\rangle = |\psi'_i\rangle = \sum_j C_{ij}^{\psi'}|\psi_j\rangle \tag{4.1}$$

or equivalently

$$\bar{U}|\psi'_j\rangle = |\psi_j\rangle = \sum_i C_{jk}^{\psi}|\psi'_i\rangle. \tag{4.2}$$

That is, we can express an element of one basis in another basis. It is evident that the inverse exists, since it doesn't matter what we call the first and the second basis. So take the first equation and act on it with U^{-1}. Then

$$|\psi_i\rangle = U^{-1}U|\psi_i\rangle = U^{-1}|\psi'_i\rangle = \sum_j C_{ij}^{\psi'} U^{-1}|\psi_j\rangle. \tag{4.3}$$

What are the matrix elements $\langle\psi_k|U|\psi_i\rangle = \langle\psi_k|\psi'_i\rangle$?

$$\langle\psi_k|\psi'_i\rangle = \sum_j C_{ij}^{\psi'}\langle\psi_k|\psi'_j\rangle, \tag{4.4}$$

or equivalently

$$|\psi'_i\rangle = \sum_j |\psi_j\rangle\langle\psi_j|\psi'_i\rangle. \tag{4.5}$$

Similarly

$$|\psi_j\rangle = \sum_i |\psi'_i\rangle\langle\psi'_i|\psi_j\rangle. \tag{4.6}$$

Notice also that these coefficients are therefore clearly related by

$$\langle\psi'_i|\psi_j\rangle = \langle\psi_j|\psi'_i\rangle^*. \tag{4.7}$$

• Consider now the inner product

$$\begin{aligned}\delta_{kj} &= \langle\psi_k|\psi_j\rangle \\ &= \sum_{i,l}\langle\psi'_l|\psi_k\rangle^* \underbrace{\langle\psi'_l|\psi'_i\rangle}_{\delta_{li}}\langle\psi'_i|\psi_j\rangle \\ &= \sum_i \langle\psi'_i|\psi_k\rangle^*\langle\psi'_i|\psi_j\rangle \\ &= \sum_i \langle\psi_k|\psi'_i\rangle\langle\psi'_i|\psi_j\rangle.\end{aligned}$$

Define

$$U_{ij} = \langle\psi'_i|\psi_j\rangle. \tag{4.8}$$

And similarly

$$\bar{U}_{ki} = \langle\psi_k|\psi'_i\rangle = U^*_{ik}. \tag{4.9}$$

Hence

$$\delta_{kj} = \sum_i U'_{ki}U_{ij}, \tag{4.10}$$

so since $(U^{-1})_{kj} = U^*_{jk}$, we see that transformations between two orthonormal bases are unitary, i.e. they satisfy

$$UU^\dagger = \mathbb{I}. \tag{4.11}$$

We could have seen this in a basis-free way by requiring that inner products do not depend on the choice of basis. Hence

$$\langle\chi'|\psi'\rangle = \langle\chi|U^\dagger U|\psi\rangle = \langle\chi|\psi\rangle = \langle\chi|\mathbb{I}|\psi\rangle, \tag{4.12}$$

and hence it must be that $U^\dagger U = \mathbb{I}$ since they agree on *any* vectors $|\chi\rangle, |\psi\rangle$.

We've concluded that changes of basis can be written as unitary transformations and moreover that inner products must be invariant under such transformations. What about operators? Consider

$$A = \sum_{i,j} a_{ij}|\psi_i\rangle\langle\psi_j|. \tag{4.13}$$

Suppose we have a new vector $|\phi\rangle$ given by

$$|\phi\rangle = \sum_i |\psi_i\rangle\langle\psi_i|\phi\rangle, \tag{4.14}$$

and we act on it with a unitary U to get some new $|\phi'\rangle$. Hence

$$U|\phi\rangle = \sum_i U|\psi_i\rangle\langle\psi_i|\phi\rangle. \tag{4.15}$$

Let U take us between bases, such that $|\psi'_i\rangle = U|\psi_i\rangle$ or equivalently

$$U^\dagger|\psi'_i\rangle = |\psi_i\rangle. \tag{4.16}$$

The easy way to see what happens to operators is to recognize that

$$U|\phi'\rangle = UA|\phi\rangle = UAU^\dagger(U|\phi\rangle), \tag{4.17}$$

so that

$$A' = UAU^\dagger \tag{4.18}$$

is the corresponding operator to A in the new basis. Looking at the spectral decomposition,

$$\begin{aligned}A' = UAU^\dagger &= \sum U|\psi_i\rangle A_{ij}\langle\psi_j|U^\dagger & (4.19)\\ &= \sum |\psi'_i\rangle A_{ij}\langle\psi'_j|, & (4.20)\end{aligned}$$

so the matrix elements are left unchanged in the new basis. In fact, it must have been so, since

$$\langle\psi_i|A|\psi_j\rangle = \left(\langle\psi_i|U^\dagger\right)\left(UAU^\dagger\right)\left(U|\psi_j\rangle\right). \tag{4.21}$$

Let us now make a connection to quantum mechanics. If the Hamiltonian is time-independenct, recall that we can write the solution of

$$i\partial_t|\psi\rangle = H|\psi\rangle \tag{4.22}$$

as

$$|\psi(t)\rangle = e^{-itH}|\psi(0)\rangle. \tag{4.23}$$

That is, we may think of time evolution as a complex rotation of the initial condition.[4]

Consider now a set of vectors which are not orthonormal but are linearly independent, $\{|\chi_i\rangle\}$. By Gram-Schmidt we can therefore define $\{|\psi_\mu\rangle\}$ as the result of acting on $|\psi_i\rangle$ with an operator T such that

$$|\psi_\mu\rangle = \sum_{i=1}^{\mu} T_{\mu i}|\chi_i\rangle. \tag{4.24}$$

In particular we may take $T_{\mu i}$ to be upper-triangular because we limit the sum to run only up to μ.

Now observe that

$$\begin{aligned}
\delta_{\nu\mu} &= \langle\psi_\nu|\psi_\mu\rangle \\
&= \sum_{ij} T^*_{\nu j} T_{\mu i}\langle\chi_j|\chi_i\rangle \\
&= \sum_{ij} T^*_{\nu j}\langle\chi_j|\chi_i\rangle T_{\mu i} \\
&= (T^\dagger S T)_{\nu\mu}.
\end{aligned}$$

These final inner products are in general not 1; they are like a metric, in that they relate the original basis vectors. We see that

$$\mathbb{I} = T^\dagger S T. \tag{4.25}$$

But notice that T is invertible, and therefore so is $T^\dagger$. We find that

$$(T^\dagger)^{-1}T^{-1} = S, \tag{4.26}$$

so the matrix S relating the original vectors can be written in terms of the matrix T which performs the orthonormalization process. In general, this allows us to perform a *similarity transforamation* so that we can write some operator $A' = TAT^{-1}$ and

$$A = (T^\dagger)^{-1}\bar{A}T^{-1}, \tag{4.27}$$

which says that an operator may be written as the product of an upper triangular matrix, a diagonal matrix, and a lower triangular matrix. This is a special case of the Jordan decomposition of an operator.

Notice also that unitaries leave the trace and the determinant unchanged:

$$\mathrm{Tr}(UAU^\dagger) = \mathrm{Tr}(AU^\dagger U) = \mathrm{Tr}(A), \tag{4.28}$$

and determinants are unchanged since

$$UU^\dagger = \mathbb{I} \implies 1 = \det\mathbb{I} = \det U \det U^\dagger = (\det U)(\det U)^*, \tag{4.29}$$

so the determinant of U is a phase $e^{i\delta}$ and

$$\det(UAU^\dagger) = \det(A)\det(U^\dagger U) = \det A. \tag{4.30}$$

This helps our intuition that unitary matrices are really complex generalizations of rotations (orthogonal matrices).

It will often be our interest in quantum mechanics of solving the eigenvector and eigenvalue problem, i.e.

$$A|\phi\rangle = \lambda|\phi\rangle. \tag{4.31}$$

Thanks to the fundamental theorem of algebra, we are guaranteed at least one eigenvalue, some λ satisfying the characteristic equation.

[4] There is a book describing the structure of path integrals in quantum mechanics, by Feynman and Hibbs, related to the exponentiation formula for the Hamiltonian. There is also a text by Messiah which contains lots of good quantum mechanics.