Lesson 14: Vector spaces, operators and matrices

Quantum Mechanics for Electronical And Electronics Engineerings

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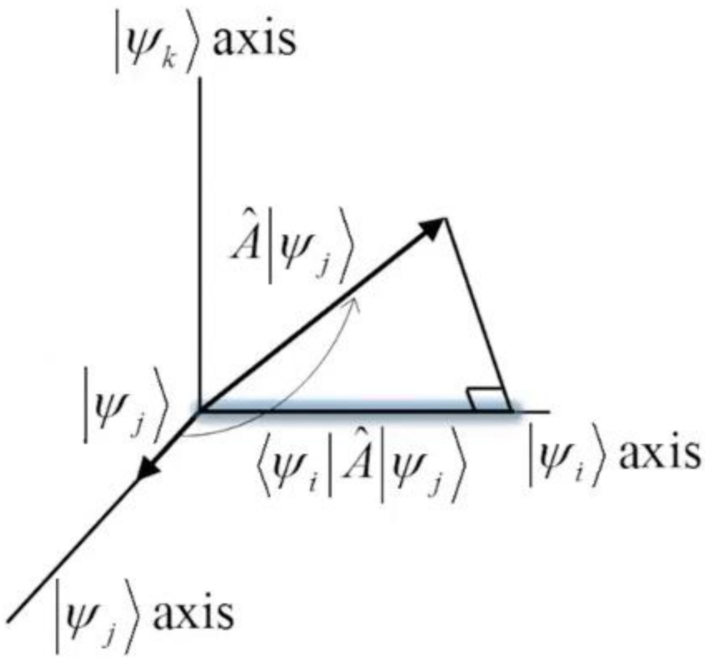

$$\hat{A} \equiv \begin{bmatrix} \langle\psi_1|\hat{A}|\psi_1\rangle & \langle\psi_1|\hat{A}|\psi_2\rangle & \langle\psi_1|\hat{A}|\psi_3\rangle & \cdots \\ \langle\psi_2|\hat{A}|\psi_1\rangle & \langle\psi_2|\hat{A}|\psi_2\rangle & \langle\psi_2|\hat{A}|\psi_3\rangle & \cdots \\ \langle\psi_3|\hat{A}|\psi_1\rangle & \langle\psi_3|\hat{A}|\psi_2\rangle & \langle\psi_3|\hat{A}|\psi_3\rangle & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

Vector Spaces

- We need a “space” in which our vectors exist for a vector with three components.

$$\begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix}$$

- The vector can be visualized as a line starting from the origin with projected lengths a_1, a_2, and a_3 along the x, y, and z axes respectively.

- For a function express as its value at a set of points, instead of 3 axes labeled x, y, and z

- We may have an infinite number of **orthogonal axes** labeled with their associated basis function e.g., ψ_n

- Just as we label axes in conventional space with unit vectors, one notation is x, y, and z for the unit vectors

- So also here we label the axes with the kets $|\psi_n>$

Mathematical properties – existence of inner product

- Geometrical space has a vector dot product that defines both the **orthogonality** of the axes.

$$\hat{\mathbf{x}} \cdot \hat{\mathbf{y}} = 0$$

- And the components of a vector along those axes

$$f = f_x \hat{\mathbf{x}} + f_y \hat{\mathbf{y}} + f_z \hat{\mathbf{z}} \quad \text{with} \quad f_x = f \cdot \hat{\mathbf{x}}$$

- And similarly for the other components.

- Our vector space has an inner product that defines both the **orthogonality of the basis functions**

$$\boxed{\langle \psi_m | \psi_n \rangle = \delta_{nm}}$$

- As well as the components $c_m = \langle \psi_m | f \rangle$

Mathematical properties – addition of vectors, linearity

- With respect to addition of vectors, both geometrical space and our vector space are **commutative**.

$$\mathbf{a}+\mathbf{b}=\mathbf{b}+\mathbf{a} \qquad |f\rangle+|g\rangle=|g\rangle+|f\rangle$$

  and **associate**

$$\mathbf{a}+(\mathbf{b}+\mathbf{c})=(\mathbf{a}+\mathbf{b})+\mathbf{c} \qquad |f\rangle+\left(|g\rangle+|h\rangle\right)=\left(|f\rangle+|g\rangle\right)+|h\rangle$$

- Both the geometrical space and our vector space are linear in **multiplying by constants**.

$$c(\mathbf{a}+\mathbf{b})=c\mathbf{a}+c\mathbf{b} \qquad c\left(|f\rangle+|g\rangle\right)=c|f\rangle+c|g\rangle$$

- Our constants may be **complex**

- And the inner product is linear both in multiplying by constants.

$$\mathbf{a}\cdot(c\mathbf{b})=c(\mathbf{a}\cdot\mathbf{b}) \qquad \langle f|cg\rangle=c\langle f|g\rangle$$

- And in **superposition of vectors**

$$\langle f|\left(|g\rangle+|h\rangle\right)=\langle f|g\rangle+\langle f|h\rangle$$

Mathematical properties – norm of a vector, completeness

- There is a well-define “length” to a vector formally a “norm”

$$\|\mathbf{a}\| = \sqrt{(\mathbf{a} \cdot \mathbf{a})}$$

$$\| f \| = \sqrt{\langle f \mid f \rangle}$$

- In both cases, any vector in the space can be represented to an arbitrary degree of accuracy.

- As a linear combination of the basis vectors, this is the completeness requirement on the basis set

- In vector spaces this property of the vector space itself is sometimes described as “**completeness**.”

Mathematical properties – commutation and inner product

- In geometrical space, the length a_x, a_y, and a_z of the vector's components are real, so the inner product (vector dot product) is **commutative**

$$\mathbf{a} \cdot \mathbf{b} = \mathbf{b} \cdot \mathbf{a}$$

- But with complex coefficients rather than real lengths, we choose a non-commutative inner product of the form

$$\langle f | g \rangle = \langle g | f \rangle^*$$

- This ensures that $\langle f | f \rangle$ is real even if we word with complex numbers as required for it to form a useful norm.

Operators

- A **function** turns one number, the argument into another the result.

- An **operator** turns one function into another in the vector space representation of a function.

- An **operator** turns one vector into another.

- Suppose that we are constructing the new function *g*(*y*) from the function *f*(*x*) by acting an *f*(*x*) with the operator $\hat{A}$

- The variable *x* and *y* might be the same kind of variable as in the case where the operator corresponds to differentiation of the function

$$g(x) = \frac{d}{dx} f(x)$$

Operators

- The variable *x* and *y* might be quite different as in the case of a **Fourier transform operation** where *x* might represent time and *y* might represent frequency.

- A standart notation for writing any such operation on a function is

$$g(y)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(x)\exp(-iyx)dx$$

- This should be read as $\hat{A}$ operating on *f*(*x*)

$$g(y)=\hat{A}f(x)$$

- For A to be the most general operation possible, it should be possible for the value of g(y)

Linear operators

- We are interested here solely in **linear operators**

- They are the only ones we will use in quantum mechanics, because of the fundamental linearity of quantum mechanics

- A linear operator has the following characteristics

$$\hat{A}\left[f(x)+h(x)\right]=\hat{A}f(x)+\hat{A}h(x)$$

$$\hat{A}\left[cf(x)\right]=c\hat{A}f(x)$$

for any complex number *c*

- Let us consider the most general way we could have the function $g(y)$ at some specific value y_1 of its argument.

- That is, $g(y_1)$ be related to the values of $f(x)$ for possibly all values of x and still retain the linearity properties for this relation.

Consequences of linearity for operators

- Think of the function $f(x)$
- As being represented by a list of values $f(x_1)$, $f(x_2)$, $f(x_3)$,… just as we did when considering $f(x)$ as a vector
- We can take the values of x to be as closely spaced as a we want.
- We believe that this representation can give us as accurate a representation of $f(x)$ for any calculation we need to perform.
- Then we propose that for a linear operation the value of $g(y_1)$ might be related to the values of $f(x)$ by a relation of the form

$$g(y_1) = a_{11} f(x_1) + a_{12} f(x_2) + a_{13} f(x_3) + \dots$$

where the a_{ij} are complex constants

Consequences of linearity for operators

- This form shows the linearity behavior we want

$$g(y_1) = a_{11} f(x_1) + a_{12} f(x_2) + a_{13} f(x_3) + \dots$$

- If we replaced *f*(*x*) by *f*(*x*)+*h*(*x*) ,then we would have

$$\begin{aligned} g(y_1) &= a_{11}\left[f(x_1) + h(x_1)\right] + a_{12}\left[f(x_2) + h(x_2)\right] + a_{13}\left[f(x_3) + h(x_3)\right] + \dots \\ &= a_{11} f(x_1) + a_{12} f(x_2) + a_{13} f(x_3) + \dots \\ &\quad + a_{11} h(x_1) + a_{12} h(x_2) + a_{13} h(x_3) + \dots \end{aligned}$$

- As required for a linear operator relation from

$$\hat{A}\left[f(x) + h(x)\right] = \hat{A} f(x) + \hat{A} h(x)$$

Consequences of linearity for operators

- And, in this form $g(y_1) = a_{11} f(x_1) + a_{12} f(x_2) + a_{13} f(x_3) + \ldots$

- If we replaced *f*(*x*) by *cf*(*x*), then we would have

$$g(y_1) = a_{11} c f(x_1) + a_{12} c f(x_2) + a_{13} c f(x_3) + \ldots$$

$$= c\left[a_{11} f(x_1) + a_{12} f(x_2) + a_{13} f(x_3) + \ldots\right]$$

- As required for a linear operator relation from

$$\hat{A}\left[c f(x)\right] = c \hat{A} f(x)$$

Consequences of linearity for operators

- Now consider whether this form

$$g(y_1) = a_{11} f(x_1) + a_{12} f(x_2) + a_{13} f(x_3) + \ldots$$

is as general as it could be and still be a linear relation.

- We can see this by trying to add other powers and “cross terms” of $f(x)$

- Any more complicated relation of $g(y_1)$ to f(x) could presumably be written as a power series in $f(x)$ possibly involving $f(x)$ for different values of x that is, “cross terms”

- If we were to add higher powers of $f(x)$ such as $[f(x)]^2$, or cross terms such as $f(x_1)f(x_2)$ in the series, it would no longer have the required linear behavior of

$$\hat{A}[f(x) + h(x)] = \hat{A}f(x) + \hat{A}h(x)$$

- We also cannot add a constant term to this series, that would violate the second linearity condition

$$\hat{A}[cf(x)] = c\hat{A}f(x)$$

Generality of the proposed linear operation

- Hence we conclude

$$g(y_1) = a_{11} f(x_1) + a_{12} f(x_2) + a_{13} f(x_3) + \ldots$$

is the most general form possible for the relation between $g(y_1)$ and $f(x)$, if this relation is to correspond to a linear operator.

- To construct the entire function $g(y)$, we should construct series like for each value of y

- If we write $f(x)$ and $g(y)$ as vectors then we can write all these series at once

$$\begin{bmatrix} g(y_1) \\ g(y_2) \\ g(y_3) \\ \vdots \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots \\ a_{21} & a_{22} & a_{23} & \cdots \\ a_{31} & a_{32} & a_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} f(x_1) \\ f(x_2) \\ f(x_3) \\ \vdots \end{bmatrix}$$

Construction of the entire operator

- We see that

$$\begin{bmatrix} g(y_1) \\ g(y_2) \\ g(y_3) \\ \vdots \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots \\ a_{21} & a_{22} & a_{23} & \cdots \\ a_{31} & a_{32} & a_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} f(x_1) \\ f(x_2) \\ f(x_3) \\ \vdots \end{bmatrix}$$

- Can be written as $g(y) = \hat{A} f(x)$

- Where the operator $\hat{A}$ can be written as a matrix

$$\hat{A} = \begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots \\ a_{21} & a_{22} & a_{23} & \cdots \\ a_{31} & a_{32} & a_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

Bra-ket notation and operators

- Presuming functions can be represented as vectors, then linear operators can be represented by matrices.

- In Bra-ket notation, we can write $g(y) = \hat{A}f(x)$ as

$$|g\rangle = \hat{A}|f\rangle$$

if we regard the ket as a vector

- We now regard the (linear) operator A as a matrix

Consequences of linear operator algebra

- Because of the mathematical equivalence of matrices and linear operators, the algebra for such operators is identical to that of matrices

- In particular operators do not in general commute

  $\hat{A}\hat{B}|f\rangle$ is not in general equal to $\hat{B}\hat{A}|f\rangle$ for any arbitrary $|f\rangle$

- Whether or not operators commute is very important in quantum mechanics

- We discussed operators for the case of functions of position (e.g., *x*)

- But we can also use expansion coefficients on the basis sets

Generalization to expansion coefficients

- We expanded $f(x) = \sum_n c_n \psi_n(x)$ and $g(x) = \sum_n d_n \psi_n(x)$

- We could have followed a similar argument requiring each expansion coefficient d_i depends linearly on all the expansion coefficients c_n

- By similar arguments, we would deduce the most general linear relation between the vectors of expansion coefficients could be represented as a matrix.

$$\begin{bmatrix} d_1 \\ d_2 \\ d_3 \\ \vdots \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} & A_{13} & \cdots \\ A_{21} & A_{22} & A_{23} & \cdots \\ A_{31} & A_{32} & A_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{bmatrix}$$

- The bra-ket statement of the relation between *f*, *g*, and $\hat{A}$ remains unchanged as

$$|g\rangle = \hat{A}|f\rangle$$

Evaluating the matrix elements of an operator

- Quite generally when writing an operator $\hat{A}$ as a matrix when using a basis set $|\psi_j\rangle$

- The matrix elements of that operator are $A_{ij} = \langle \psi_i | A | \psi_j \rangle$

- We can now turn any linear operator into a matrix or example, for a simple one-dimensional spatial case

$$A_{ij} = \int \psi_i^*(x) \hat{A} \psi_j(x) dx$$

- Operator $\hat{A}$ acting on the unit vector $|\psi_j\rangle$ generates the vector $\hat{A}|\psi_j\rangle$ with generally a new length and direction.

- The matrix element $\langle \psi_i | \hat{A} | \psi_j \rangle$ is the projection of $\hat{A}|\psi_j\rangle$ onto the $|\psi_j\rangle$ axis