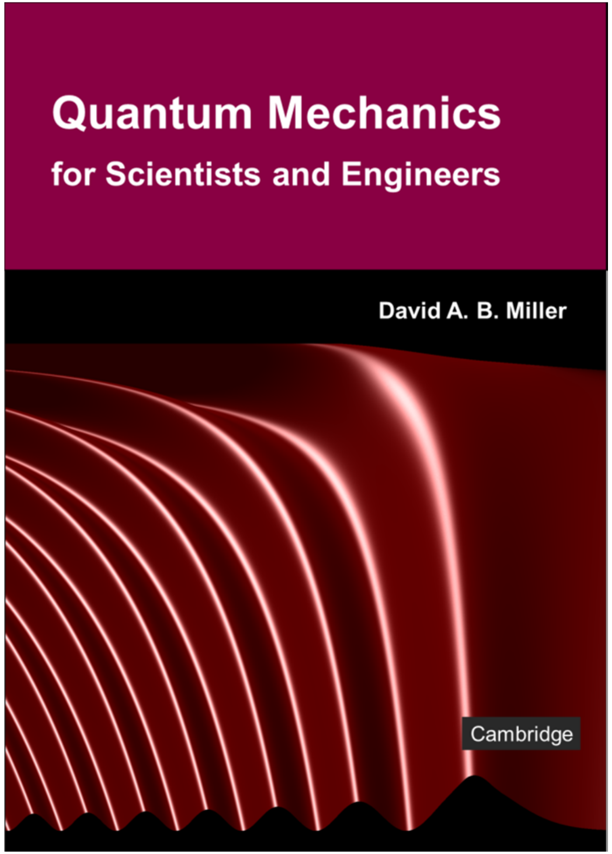
5.3 Vector spaces, operators and matrices

Slides: Video 5.3.1 Vector space

Text reference: Quantum Mechanics for Scientists and Engineers

Section 4.2



Vector spaces, operators and matrices

Vector space

Quantum mechanics for scientists and engineers

David Miller

Vector space

We need a “space” in which our vectors exist

- For a vector with three components $\begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix}$
  - we imagine a three dimensional Cartesian space

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
    - with each of these axes being at right angles

Vector space

For a function expressed 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 $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, and $\hat{\mathbf{z}}$ for the unit vectors

so also here we label the axes with the kets $|\psi_n\rangle$

Either notation is acceptable

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

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

and similarly for the other components

Our vector space has an inner product that defines both

the orthogonality of the basis functions

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

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

Mathematical properties – addition of vectors

With respect to addition of vectors

both geometrical space and our vector space are

commutative

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

$$|f\rangle+|g\rangle=|g\rangle+|f\rangle$$

and associative

$$\mathbf{a}+(\mathbf{b}+\mathbf{c})=(\mathbf{a}+\mathbf{b})+\mathbf{c}$$

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

Mathematical properties - linearity

Both the geometrical space and our vector space are

linear in multiplying by constants

$$c(\mathbf{a}+\mathbf{b}) = c\mathbf{a}+c\mathbf{b}$$

our constants may be complex

$$c(|f\rangle + |g\rangle) = c|f\rangle + c|g\rangle$$

And the inner product is linear

both in multiplying by constants

$$\mathbf{a}\cdot(c\mathbf{b}) = c(\mathbf{a}\cdot\mathbf{b})$$

$$\langle f|cg\rangle = c\langle f|g\rangle$$

and in superposition of vectors

$$\mathbf{a}\cdot(\mathbf{b}+\mathbf{c}) = \mathbf{a}\cdot\mathbf{b}+\mathbf{a}\cdot\mathbf{c}$$

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

Mathematical properties – norm of a vector

There is a well-defined "length" to a vector

formally a "norm"

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

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

Mathematical properties – completeness

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 “compactness”

Mathematical properties – commutation and inner product

In geometrical space, the lengths a_x, a_y, and a_z of a 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

$$\langle f | g \rangle = \left(\langle g | f \rangle \right)^*$$

This ensures that $\langle f | f \rangle$ is real

even if we work with complex numbers

as required for it to form a useful norm