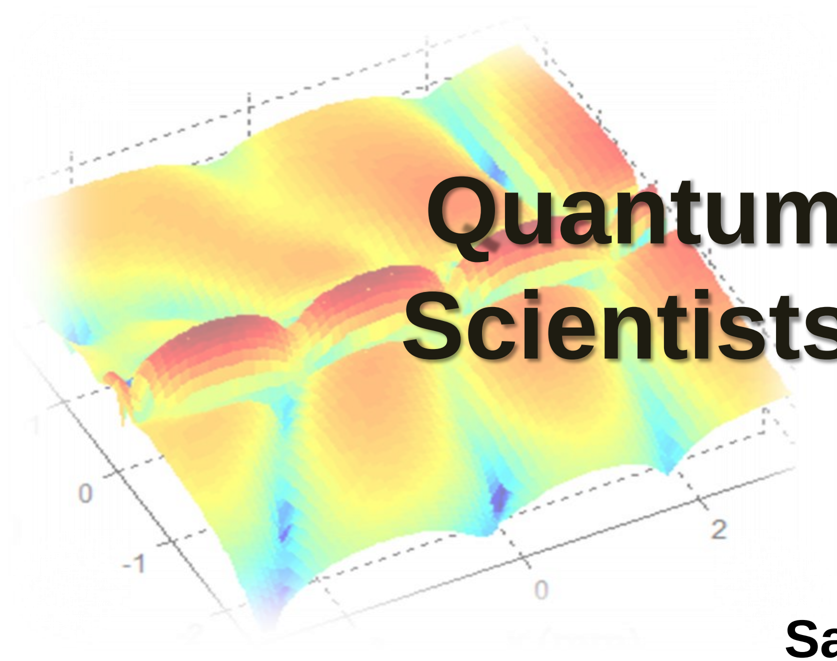

Quantum Mechanics for Scientists and Engineers

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Nov. 14th, 2016

Outline

Quantum Mechanics for Scientists and Engineers

- **Bilinear expansion of linear operators**
- **The identity operator**
- **Inverse and Unitary operators**

Bilinear expansion of linear operators

❖ **Expand functions in a basis set**

$$f(x) = \sum_n c_n \psi_n(x) \quad or \quad |f(x)\rangle = \sum_n c_n |\psi_n(x)\rangle$$

- **By acting with a specific operator** $\hat{A}$

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

- **Expand *g* and *f* on the basis set** ψ_i

$$|g\rangle = \sum_i d_i |\psi_i\rangle \qquad |f\rangle = \sum_j c_j |\psi_j\rangle$$

- **From our matrix representation of** $|g\rangle = \hat{A}|f\rangle$

$d_i = \sum_j A_{ij} c_j$ **we know that** $c_j = \langle \psi_j | f \rangle$ **So,** $d_i = \sum_j A_{ij} \langle \psi_j | f \rangle$

Bilinear expansion of linear operators

❖ **Expand functions in a basis set**

- **Substituting** $d_i = \sum_j A_{ij} \langle \psi_j | f \rangle$ **back into** $|g\rangle = \sum_i d_i |\psi_i\rangle$

$$|g\rangle = \sum_{i,j} A_{ij} \langle \psi_j | f \rangle |\psi_i\rangle$$

- **Remember that** $c_j = \langle \psi_j | f \rangle$ **is simply a number**

- **So, switched multiplicative order**

$$|g\rangle = \sum_{i,j} A_{ij} |\psi_i\rangle \langle \psi_j | f \rangle = \left[\sum_{i,j} A_{ij} |\psi_i\rangle \langle \psi_j | \right] | f \rangle$$

$$\hat{A} \equiv \sum_{i,j} A_{ij} |\psi_i\rangle \langle \psi_j |$$

Bilinear expansion of linear operators

❖ **Expand functions in a basis set**

- **This form** $\hat{A} \equiv \sum_{i,j} A_{ij} |\psi_i\rangle\langle\psi_j|$

  is referred to as a "bilinear expansion" of the operator $\hat{A}$ **on the basis** $|\psi_i\rangle$ **and is analogous to the linear expansion of a vector on a basis**

- **Though the Dirac notation is more general** $g(x) = \int \hat{A} f(x_1) dx_1$

$$\hat{A} \equiv \sum_{i,j} A_{ij} \psi_i(x) \psi_j^*(x_1)$$

Outer product

❖ **Bilinear expansion form**

- **An expression of the form** $\hat{A} \equiv \sum_{i,j} A_{ij} |\psi_i\rangle\langle\psi_j|$

Contains an outer product of two vectors

- **An inner product expression of the form** $\langle g | f \rangle$

➡ **Complex number**

- **An outer product expression of the form** $|g\rangle\langle f|$

➡ **Matrix**

Outer product

$$|g\rangle\langle f| = \begin{bmatrix} d_1 \\ d_2 \\ d_3 \\ \vdots \end{bmatrix} \begin{bmatrix} c_1^* & c_2^* & c_3^* & \cdots \end{bmatrix} = \begin{bmatrix} d_1c_1^* & d_1c_2^* & d_1c_3^* & \cdots \\ d_2c_1^* & d_2c_2^* & d_2c_3^* & \cdots \\ d_3c_1^* & d_3c_2^* & d_3c_3^* & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

- **The specific summation** $\hat{A} \equiv \sum_{i,j} A_{ij} |\psi_i\rangle\langle\psi_j|$

  is actually, then, a sum of matrices

- **In the matrix** $|\psi_i\rangle\langle\psi_j|$

  the element in the *i*th row and the *j*th column is 1, another's are 0

The identity operator

❖ The identity operator $\hat{I}$

- In matrix form, the identity operator is

$$\hat{I} = \begin{bmatrix} 1 & 0 & 0 & \cdots \\ 0 & 1 & 0 & \cdots \\ 0 & 0 & 1 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

- In bra-ket form

The identity operator can be written

$$\hat{I} = \sum_i |\psi_i\rangle\langle\psi_i|$$

where the $|\psi_i\rangle$

form a complete basis for the space

The identity operator

❖ **Proof**

- **For an arbitrary function** $|f\rangle = \sum_i c_i |\psi_i\rangle$ **, we know** $c_m = \langle \psi_m | f \rangle$

  So $|f\rangle = \sum_i \langle \psi_i | f \rangle |\psi_i\rangle$

- **And, the multiplication** $|f\rangle$ **each side of** $\hat{I} = \sum_i |\psi_i\rangle\langle\psi_i|$

$$\hat{I}|f\rangle = \sum_i |\psi_i\rangle\langle\psi_i|f\rangle = \sum_i \langle\psi_i|f\rangle|\psi_i\rangle$$

- **By using,** $|f\rangle = \sum_i \langle\psi_i|f\rangle|\psi_i\rangle$**. So,** $\hat{I}|f\rangle = |f\rangle$

The identity operator

❖ **The statement** $\hat{I} = \sum_i |\psi_i\rangle\langle\psi_i|$

$$|\psi_1\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{bmatrix}$$

So that

$$|\psi_1\rangle\langle\psi_1| = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & \cdots \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & \cdots \\ 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

- **Similarly, we can obtain**

$$\hat{I} = \sum_i |\psi_i\rangle\langle\psi_i| = \begin{bmatrix} 1 & 0 & 0 & \cdots \\ 0 & 1 & 0 & \cdots \\ 0 & 0 & 1 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

Proof that the trace is independent of the basis

- **Consider the sum,** S
  - **of the diagonal elements of an operator** $\hat{A}$
    on some complete orthonormal basis $|\psi_i\rangle$

$$S = \sum_i \langle \psi_i | \hat{A} | \psi_i \rangle$$

  - **And, suppose some other complete orthonormal basis** $|\phi_i\rangle$

$$\hat{I} = \sum_m |\phi_m\rangle\langle\phi_m|$$

  - **In** $S = \sum_i \langle \psi_i | \hat{A} | \psi_i \rangle$ **, we can insert an identity operator just before** $\hat{A}$

$$\hat{I}\hat{A} = \hat{A}$$

$$S = \sum_i \langle \psi_i | \hat{I}\hat{A} | \psi_i \rangle = \sum_i \langle \psi_i | \left(\sum_m |\phi_m\rangle\langle\phi_m| \right) \hat{A} | \psi_i \rangle$$

Proof that the trace is independent of the basis

❖ **Rearranging** $S = \sum_i \langle \psi_i | \hat{I}\hat{A} | \psi_i \rangle = \sum_i \langle \psi_i | \left(\sum_m | \phi_m \rangle \langle \phi_m | \right) \hat{A} | \psi_i \rangle$

reordering the sums $$S = \sum_m \sum_i \langle \psi_i | \phi_m \rangle \langle \phi_m | \hat{A} | \psi_i \rangle$$

moving the number $\langle \psi_i | \phi_m \rangle$ $$= \sum_m \sum_i \langle \phi_m | \hat{A} | \psi_i \rangle \langle \psi_i | \phi_m \rangle$$

moving a sum and associating $$= \sum_m \langle \phi_m | \hat{A} \left(\sum_i | \psi_i \rangle \langle \psi_i | \right) | \phi_m \rangle$$

recognizing $\hat{I} = \sum_i | \psi_i \rangle \langle \psi_i |$ $$= \sum_m \langle \phi_m | \hat{A}\hat{I} | \phi_m \rangle$$

Proof that the trace is independent of the basis

- **So, with now** $S = \sum_i \langle \psi_i | \hat{A} | \psi_i \rangle = \sum_m \langle \phi_m | \hat{A}\hat{I} | \phi_m \rangle$
  - **Using the** $\hat{A}\hat{I} = \hat{A}$

$$S = \sum_i \langle \psi_i | \hat{A} | \psi_i \rangle = \sum_m \langle \phi_m | \hat{A} | \phi_m \rangle$$

  - **Hence the trace of an operator the sum of the diagonal elements is independent of the basis used to represent the operator**

Inverse and projection operator

❖ Inverse operator

- **For an operator $\hat{A}$ operating on an arbitrary function $|f\rangle$**

  The inverse operator $\hat{A}^{-1}$

- **Using the inverse operator** $|f\rangle = \hat{A}^{-1}\hat{A}|f\rangle$

$$\hat{A}^{-1}\hat{A} = \hat{I}$$

❖ Projection operator

- **For example,** $\hat{P} = |f\rangle\langle f|$ **In general has no inverse**

  because it projects all input vectors onto only one axis in the space

  the one corresponding to the specific vector $|f\rangle$

Unitary operator

❖ **Unitary operator** $\hat{U}$

- **One for which** $\hat{U}^{-1} = \hat{U}^{\dagger}$

  That is, its inverse is its Hermitian adjoint

- **The Hermitian adjoint is formed by reflecting on a -45 degree line and taking the complex conjugate**

$$\begin{bmatrix} u_{11} & u_{12} & u_{13} & \cdots \\ u_{21} & u_{22} & u_{23} & \cdots \\ u_{31} & u_{32} & u_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}^{\dagger} = \begin{bmatrix} u_{11}^{*} & u_{21}^{*} & u_{31}^{*} & \cdots \\ u_{12}^{*} & u_{22}^{*} & u_{32}^{*} & \cdots \\ u_{13}^{*} & u_{23}^{*} & u_{33}^{*} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

Unitary operator

- **Conservation of length for unitary operators**
  - **For two matrices $\hat{A}$ and $\hat{B}$** $\left(\hat{A}\hat{B}\right)^\dagger = \hat{B}^\dagger \hat{A}^\dagger$
  - **That is, the Hermitian adjoint of the product is the "flipped round" product of the Hermitian adjoints**
- **Consider the unitary operator $\hat{U}$ and vectors $|f_{old}\rangle$ $|g_{old}\rangle$**
  - **Using the operator** $|f_{new}\rangle = \hat{U}|f_{old}\rangle$ $|g_{new}\rangle = \hat{U}|g_{old}\rangle$
  - **Then,** $\langle g_{new}| = \langle g_{old}|\hat{U}^\dagger$ **So,**

$$\langle g_{new}|f_{new}\rangle = \langle g_{old}|\hat{U}^\dagger\hat{U}|f_{old}\rangle = \langle g_{old}|\hat{U}^{-1}\hat{U}|f_{old}\rangle = \langle g_{old}|\hat{I}|f_{old}\rangle$$
$$= \langle g_{old}|f_{old}\rangle$$

  - **The unitary operation does not change the inner product**
  - **The length of a vector is not changed by a unitary operator**

Thank You for Your Attention,

Do You Have Any Questions?