The Dirac Notation

Integrals of the type $\int f^* g dq$ or $\int f^* \hat{O} g dq$ appear frequently in quantum mechanics. These are scalar product integrals.

The reason for the name may be understood if we expand the functions in an orthonormal basis $\{u_i\}$:

$$f = \sum_i a_i u_i; \quad g = \sum_i b_i u_i$$

$$\int f^* g dq = \sum_i \sum_j a_i^* b_j \int u_i^* u_j dq = \sum_i \sum_j a_i^* b_j \delta_{ij} = \sum_i a_i^* b_i,$$

which is a generalization of a scalar product of two vectors,

$$\vec{a} \cdot \vec{b} = a_x b_x + a_y b_y + a_z b_z.$$

Dirac proposed a notation where a function f is denoted by $|f\rangle$.

$$f \rightarrow |f\rangle; \quad \int f^* g dq \rightarrow \langle f|g\rangle.$$

$\langle f|g\rangle$ is, in general, a complex number. $\langle f|$ is called a bra, and $|g\rangle$ is a ket.

What is $|g\rangle\langle f|$? It is an operator, because operating on a ket $|k\rangle$ it gives a ket:

$$(|g\rangle\langle f|)\,|k\rangle = |g\rangle\langle f|k\rangle.$$

Projection operator: $(|f\rangle\langle f|)|\psi\rangle = |f\rangle\langle f|\psi\rangle$. This is the projection of $|\psi\rangle$ on $|f\rangle$.

If $|f\rangle$ is normalized, then
$(|f\rangle\langle f|)(|f\rangle\langle f|) = |f\rangle\langle f|f\rangle\langle f| = |f\rangle\langle f|$.
This property (idempotency) is a characteristic feature of projection operators, because a second projection with the same operator does nothing.

Basis set $\{|u_i\rangle\}$. Orthogonality: $\langle u_i|u_j\rangle = \delta_{ij}$.

Expansion of an arbitrary function: $|\psi\rangle = \sum_i |u_i\rangle c_i$.

Finding expansion coefficients: $\langle u_j|\psi\rangle = \sum_i \langle u_j|u_i\rangle c_i = c_j$

$$|\psi\rangle = \sum_i |u_i\rangle\langle u_i|\psi\rangle.$$

$\sum_i |u_i\rangle\langle u_i|$ is therefore a unit operator.

Given the basis $\{|u_i\rangle\}$, $|\psi\rangle$ may be represented by the expansion coefficients c_i:

$$\begin{pmatrix} \langle u_1|\psi\rangle \\ \langle u_2|\psi\rangle \\ . \\ . \end{pmatrix} \text{ or } \begin{pmatrix} c_1 \\ c_2 \\ . \\ . \end{pmatrix}$$

A ket is thus represented by a column vector, a bra by a row vector $(c_1^* \, c_2^* \, \cdots)$, and an operator $\hat{A}$ by a matrix with elements $\langle u_i|\hat{A}|u_j\rangle$. The results obtained in this representation must be the same as in the usual function space: if $\psi' = \hat{A}\psi$, then

$$\begin{pmatrix} c_1' \\ c_2' \\ \cdot \\ \cdot \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} & \cdots \\ a_{21} & a_{22} & \cdots \\ \cdot & \cdot & \cdots \\ \cdot & \cdot & \cdots \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \cdot \\ \cdot \end{pmatrix}.$$

Proof:

$$|\psi'\rangle = A|\psi\rangle = \sum_j A|u_j\rangle\langle u_j|\psi\rangle,$$

where the unit operator was inserted. Multiplying by $\langle u_i|$,

$$\langle u_i|\psi'\rangle = \sum_j \langle u_i|A|u_j\rangle\langle u_j|\psi\rangle, \text{or } c_i' = \sum_j a_{ij}c_j,$$

showing that the vector corresponding to ψ' is obtained by multiplying the matrix of $\hat{A}$ by the vector of ψ.

Similarly, the operator $\widehat{AB}$ is represented by the product of the matrices of $\hat{A}$ and $\hat{B}$:

$$(\widehat{AB})_{ij} = \langle u_i|\widehat{AB}|u_j\rangle = \sum_k \langle u_i|\hat{A}|u_k\rangle\langle u_k|\hat{B}|u_j\rangle = \sum_k a_{ik}b_{kj}.$$

Basis set transformation

Going from the old basis $\{|u_i\rangle\}$ to a new basis $\{|t_k\rangle\}$. Both are orthonormal. The motivation will become clear later.

The transformation is $|t_k\rangle = \sum_i |u_i\rangle S_{ik}$, where S is the transformation matrix.

Using the unit operator, we can write $|t_k\rangle = \sum_i |u_i\rangle\langle u_i|t_k\rangle$. Comparing with the previous eq'n, we get $S_{ik} = \langle u_i|t_k\rangle$.

If the two bases are orthonormal, S must be a unitary matrix, meaning $S^\dagger S = SS^\dagger = I$ (the Hermitian conjugate $S^\dagger$ is the transpose of the complex conjugate, $S^\dagger = \tilde{S}^*$):

$$(S^\dagger S)_{kl} = \sum_i S^\dagger_{ki} S_{il} = \sum_i S^*_{ik} S_{il} = \sum_i \langle t_k|u_i\rangle\langle u_i|t_l\rangle = \langle t_k|t_l\rangle = \delta_{kl}.$$

Representation of the ket $|\psi\rangle$:

$$\langle t_k|\psi\rangle = \sum_i \langle t_k|u_i\rangle\langle u_i|\psi\rangle = \sum_i S^\dagger_{ki}\langle u_i|\psi\rangle$$

$$\langle u_i|\psi\rangle = \sum_k \langle u_i|t_k\rangle\langle t_k|\psi\rangle = \sum_k S_{ik}\langle t_k|\psi\rangle.$$

Operator:

$$A_{kl} = \langle t_k|A|t_l\rangle = \sum_{ij} \langle t_k|u_i\rangle\langle u_i|A|u_j\rangle\langle u_j|t_l\rangle = \sum_{ij} S^\dagger_{ki} A_{ij} S_{jl}.$$

The representation of the operator is $S^\dagger A S$, where A is the matrix in the old basis and S the basis transformation matrix.

If A is Hermitian, there is a unitary matrix S for which $D \equiv S^\dagger A S$ is diagonal. This process of diagonalizing Hermitian matrices is very important in physics, and highly efficient computational algorithms have been devised, which can handle very large matrices.

The eigenvalues and eigenfunction of $\hat{A}$:
$\hat{A}|\psi\rangle = \lambda|\psi\rangle$. Using the basis $\{|u_i\rangle\}$, $\langle u_i|\hat{A}|\psi\rangle = \lambda\langle u_i|\psi\rangle$, leading to
$\sum_j \langle u_i|\hat{A}|u_j\rangle\langle u_j|\psi\rangle = \lambda\langle u_i|\psi\rangle$. or $\sum_j A_{ij}c_j = \lambda c_i, \quad \Rightarrow$
$\sum_j \left(A_{ij} - \lambda\delta_{ij}\right) c_j = 0$.
Taking a finite, N-dimensional space, we get N linear equations (the secular equations) in N unknowns. The trivial solution (all $c_i = 0$) is not acceptable physically, and an additional, nontrivial solution exists only of the equations are linearly dependent, which occurs if the determinant of the coefficients (secular determinant) vanishes,

$$\det|A - \lambda I| = 0.$$

This gives an equation of order N for λ, which yields in general N eigenvalues. Substituting these eigenvalues in the secular equations gives the corresponding eigenvectors.

Note: if the basis is composed of the eigenfunctions of $\hat{A}$, $\langle t_k|A|t_l\rangle = a_l\delta_{kl}$. The matrix of $\hat{A}$ is diagonal, with the eigenvalues appearing in the diagonal. Therefore, diagonalizing the matrix of an operator in a given basis gives its eigenvalues and eigenvectors. (Example in class.)

Uncertainty principle – a generalization.

Definition of uncertainty: an observable A is measured in many equivalent systems. The average is $\langle A\rangle$, the deviation from average is $A - \langle A\rangle$. The uncertainty is defined as the root-mean-square of the deviation,

$$\Delta A \equiv \sqrt{\langle (A - \langle A\rangle)^2\rangle}.$$

$$(\Delta A)^2 = \langle A^2 - 2A\langle A\rangle + \langle A\rangle^2\rangle = \langle A^2\rangle - 2\langle A\rangle^2 + \langle A\rangle^2 = \langle A^2\rangle - \langle A\rangle^2.$$

Let us take two Hermitian operators P, Q, which satisfy
$[Q, P] = i\hbar$ (an example is given by x and $-i\hbar\partial/\partial x$).

Define $|\varphi\rangle = (Q + i\lambda P)|\psi\rangle$,
where $|\psi\rangle$ is the normalized wavefunction and λ an arbitrary real number.
$\langle\varphi| = |\varphi\rangle^\dagger = \langle\psi|(Q - i\lambda P)$

$$\begin{aligned} 0 \le \langle\varphi|\varphi\rangle &= \langle\psi|(Q - i\lambda P)(Q + i\lambda P)|\psi\rangle = \\ &= \langle\psi|Q^2|\psi\rangle + \langle\psi|i\lambda QP - i\lambda PQ|\psi\rangle + \langle\psi|\lambda^2 P^2|\psi\rangle = \\ &= \langle Q^2\rangle + i\lambda\langle[Q, P]\rangle + \lambda^2\langle P^2\rangle = \langle Q^2\rangle - \lambda\hbar + \lambda^2\langle P^2\rangle. \end{aligned}$$

This quadratic expression in λ is ≥ 0 for all λ, and its discriminant must therefore be ≤ 0.

$$\hbar^2 - 4\langle P^2\rangle\langle Q^2\rangle \le 0 \quad \Rightarrow \quad \langle P^2\rangle\langle Q^2\rangle \ge \frac{\hbar^2}{4}.$$

Let us define $P' \equiv P - \langle P\rangle$ and $Q' \equiv Q - \langle Q\rangle$.
$[Q', P'] = [Q, P] = i\hbar$, therefore $\langle P'^2\rangle\langle Q'^2\rangle \ge \hbar^2/4$.
Since $\Delta P = \sqrt{\langle P'^2\rangle}$ and $\Delta Q = \sqrt{\langle Q'^2\rangle}$, we get $\Delta P\Delta Q \ge \frac{1}{2}\hbar$.