Quantum Physics II (8.05) Fall 2004
Assignment 3

Massachusetts Institute of Technology
Physics Department
September 23, 2004

Due September 30, 2004
7:00pm

This week we continue to study the basic principles of quantum mechanics, particularly hermitian operators and compatible and incompatible observables. We will then discuss the operator treatment of the harmonic oscillator and perhaps start time evolution.

Reading Assignment for week three

- (continued from last week) Basic foundations of quantum mechanics: **Griffiths Ch.3**. For further reading see **Ohanian Ch.4**, **Shankar Ch.4**, and **Cohen-Tannoudji Ch.II & III**.
- **Griffiths §2.3.1** on the algebraic treatment of the harmonic oscillator. Griffiths' treatment is quite brief, but every modern quantum mechanics textbook treats this subject, so you can choose your favorite.

Problem Set 3

1. **Trace and determinant of an operator** [10 points]

   Consider a Hilbert space spanned by an orthonormal basis $\{|n\rangle\}$, and assume that we have a second complete orthonormal basis with kets $\{|n'\rangle\}$. Recall that there is a unitary operator $\hat{U}$ such that $\hat{U}|n\rangle = |n'\rangle$.

   A linear operator $\hat{A}$ can be represented by a matrix with elements $A_{mn} = \langle m|\hat{A}|n\rangle$. In the primed basis $A'_{mn} = \langle m'|\hat{A}|n'\rangle$. The trace and determinant of an operator are defined as the trace and determinant of the matrix that represents the operator. The object of this problem is to show that the trace and determinant of $\hat{A}$ are *independent of the choice of basis used for the matrix representation.*

   (a) Prove that the trace is independent of the choice of basis, i.e. that

   $$\sum_n \langle n|\hat{A}|n\rangle = \sum_{n'} \langle n'|\hat{A}|n'\rangle$$

   [The trace is the sum of the diagonal elements, $\text{Tr}\hat{A} = \sum_n A_{nn}$.] Hint: Insert the identity operator.

   (b) Show that as a matrix equation $A' = U^\dagger A U$.

(c) It is a well known property of the determinant of finite matrices that $\det AB = \det A \det B$. This result can be extended to infinite dimensional matrices as well. Use this fact to show that $\det A' = \det A$. [Hint: First show that $|\det U| = 1$.]

(d) Let $\hat{A}$ be hermitian and prove that its trace and determinant are the sum and product of its eigenvalues respectively, $\mathrm{Tr}\,\hat{A} = \sum_a \lambda_a$, $\det \hat{A} = \prod_a \lambda_a$.

2. **Position and momentum operators** [10 points]

(a) Calculate the action of the operators $\hat{x}$, $\hat{p}^2$, $\hat{x}\hat{p}$, $\hat{p}\hat{x}$ and $\hat{p}\hat{x}^2$ on the state ket $|\psi\rangle$ in the x-representation. That is, calculate $\langle x|\hat{A}|\psi\rangle$ for $\hat{A}$ given by each of the operators listed.

(b) Show that the position operator $\hat{x}$ can be represented as $i\hbar d/dp$ in the momentum representation. That is, show that

$$\langle p|\hat{x}|\psi\rangle = i\hbar \frac{d}{dp}\langle p|\psi\rangle \ .$$

[Hint: Remember how we showed $\langle x|\hat{p}|\psi\rangle = -i\hbar \frac{d}{dx}\langle x|\psi\rangle$.]

(c) Calculate the action of the operator $[\hat{x}, \hat{p}]$ on the state ket $|\psi\rangle$ in the *momentum* representation.

3. **The parity operator** [10 points]

Define the parity operator $\hat{\Pi}$ by

$$\hat{\Pi}|x\rangle = |-x\rangle \ .$$

(a) Using an appropriate identity operator write $\hat{\Pi}|\psi\rangle$ in the $\{|x\rangle\}$ basis, and then compute $\langle x|\hat{\Pi}|\psi\rangle$.

(b) Prove that $\hat{\Pi}$ is hermitian. Is $\hat{\Pi}$ unitary?

(c) When $\hat{\Pi}$ acts on $|p\rangle$ what ket does it give?

(d) Consider an infinite square well, with the potential

$$V(x) = \begin{cases} \infty & x \leq -L/2 \text{ or } x \geq L/2 \\ 0 & -L/2 < x < L/2 \end{cases} \ .$$

Denote the energy eigenstates by $\{|n\rangle\}$ and write down the wavefunctions $\langle x|n\rangle$. Are the kets $|n\rangle$ eigenstates of $\hat{\Pi}$? If so, what are their eigenvalues?

4. **Hermitian operators?** [10 points]

   Consider the *space of complex valued functions*, $\{f(r)\}$, defined on the interval $0 \le r < \infty$.

   (a) Suppose we demand that the functions are all square integrable,

   $$\int_0^\infty dr |f(r)|^2 < \infty. \tag{1}$$

   and that $f(0)$ exists. Define the *inner product* on this space by

   $$(f_1, f_2) \equiv \int_0^\infty dr f_1^*(r) f_2(r) \tag{2}$$

   i. Show that the operator $-i\frac{d}{dr}$ *is not* hermitian on this space.
   ii. Show that the same operator will be hermitian if we add the requirement $f(0) = 0$ to the definition of the space of functions.

   Comment: This tells us that if we try to do quantum mechanics on a space with a boundary, we have to specify how the wavefunction behaves at the boundary.

   (b) Suppose, instead, that we add a factor of r^2 to the integration measure. This is what would occur if r is actually the radial coordinate and $f(r)$ is the radial wavefunction in three dimensions, because $\mathrm{d}^3x = r^2 \mathrm{d}r\, \mathrm{d}\cos\theta\, \mathrm{d}\phi$.

   Define an *inner product* on this space,

   $$(f_1, f_2) \equiv \int_0^\infty dr\, r^2 f_1^*(r) f_2(r). \tag{3}$$

   and assume $f(0)$ exists.

   i. Show that the operator $-i\frac{d}{dr}$ *is not* hermitian with respect to this inner product on this function space.
   ii. Now show that the operator $-i\frac{d}{dr} - i/r$ is hermitian on this space.

   Comment: The coordinate space representation of operators cannot always be naively taken from one context to another. In this case the "radial component of momentum", p_r, is not just $-i\hbar d/dr$ as you might have expected.

5. **The Levi-Civita Symbol** [5 points]

   You are familiar with the Kronecker delta, δ_{ij}. The Levi-Civita symbol, ε_{ijk}, is a similar object that plays an important role in several places in quantum mechanics (as well as in tensor analysis and group theory). We will encounter ε_{ijk} in studying two state systems and a little bit later when we do three dimensional rotations. The object of this problem is to familiarize you with ε and work out some standard properties.

Note: In this problem, i, j, k, *etc.* take on the values 1,2 or 3. Also a summation convention is understood: any *repeated* index, i, j, k, *etc.* is understood to be summed over the values 1, 2 and 3. For example, $\epsilon_{ijk}\, a_i = \sum_{i=1}^{3} \epsilon_{ijk}\, a_i$.

ε_{ijk} is defined as follows:

- $\varepsilon_{123} = 1$
- ε_{ijk} changes sign whenever any two indices are interchanged.

(a) Write down all non-zero values of ε_{ijk}.

(b) If $\vec{a}$ and $\vec{b}$ are vectors in 3-space, and if $\vec{c} = \vec{a} \times \vec{b}$ is their vector cross product, prove

$$c_i = \varepsilon_{ijk} a_j b_k \tag{4}$$

(c) A useful identity is

$$\varepsilon_{ijk}\varepsilon_{\ell mn} = \begin{vmatrix} \delta_{i\ell} & \delta_{im} & \delta_{in} \\ \delta_{j\ell} & \delta_{jm} & \delta_{jn} \\ \delta_{k\ell} & \delta_{km} & \delta_{kn} \end{vmatrix} \tag{5}$$

Use it to derive expressions for the following sums of products of ε symbols *in terms of Kronecker δ_{ij}'s and their products.* [The first one is given to show you what I mean (with unknown coefficients A and B for you to determine).]

$$\begin{aligned} \varepsilon_{ijk}\varepsilon_{imn} &= A\delta_{jm}\delta_{kn} + B\delta_{jn}\delta_{km} \\ \varepsilon_{ijk}\varepsilon_{ijn} &= \ldots \\ \varepsilon_{ijk}\varepsilon_{ijk} &= \ldots \end{aligned} \tag{6}$$

[Note the use of the summation convention.]

6. **Operators in a two-dimensional Hilbert space** (15 points)

Consider a two-dimensional Hilbert space spanned by the orthonormal basis $\{|+\rangle, |-\rangle\}$. In this basis, the matrix representation of the operators $\hat{S}_x$, $\hat{S}_y$, and $\hat{S}_z$ are given in terms of the Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \; ; \; \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \; ; \; \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

by

$$\hat{S}_i = \frac{\hbar}{2}\sigma_i \; .$$

(Throughout this problem, the indices i, j, k run over x, y, z.)

(a) Write the operators $\hat{S}_x$, $\hat{S}_y$, and $\hat{S}_z$ in Dirac notation using $|+\rangle$, $|-\rangle$, $\langle+|$, and $\langle-|$. Are these operators Hermitian?

(b) Consider the state

$$|\psi\rangle = \frac{1}{\sqrt{3}}|+\rangle + \frac{\sqrt{2}}{\sqrt{3}}|-\rangle \ .$$

Find $\langle\psi|\hat{S}_z|\psi\rangle$, the expectation value for the measurement of the z-component of the spin on an ensemble of atoms each in the state $|\psi\rangle$. Is the expectation value given by one of the eigenvalues of $\hat{S}_z$? [Note: When it is understood what state is being discussed, one often writes $\langle\psi|\hat{S}_z|\psi\rangle$ as just $\langle\hat{S}_z\rangle$.]

(c) Since the state $|\psi\rangle$ is not an eigenstate of $\hat{S}_z$, we cannot predict the result of a measurement of the z-component of the spin with certainty. Having calculated the mean value of the probability distribution for this measurement, let us now calculate the uncertainty. Define

$$\Delta A \equiv \sqrt{\left\langle \left(\hat{A} - \langle\hat{A}\rangle\right)^2 \right\rangle} = \sqrt{\langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2} \ . \tag{7}$$

Demonstrate the second equality in (7). Show that if $|\psi\rangle$ were an eigenstate of $\hat{A}$, then ΔA would be zero. Now take the state given in part (b) and find ΔS_z.

(d) Prove that

$$\left[\hat{S}_i, \hat{S}_j\right] = i\hbar\varepsilon_{ijk}\hat{S}_k \ . \tag{8}$$

Here ε_{ijk} is the same as the Levi-Civita symbol from problem 5, except with 1,2,3 replaced by x,y,z. [Note the use of the summation convention.]

(e) Prove that an arbitrary hermitian operator (in the two-dimensional Hilbert space considered in this problem) can be expressed as a linear combination of the identity operator and the three operators represented by the Pauli matrices σ_i, with real coefficients.

(f) Find a unitary matrix U such that $U^\dagger\sigma_y U = \sigma_z$. Find a different unitary matrix such that $U^\dagger\sigma_z U = \sigma_x$.

Comment: The two unitary matrices you have constructed are examples of "rotation matrices".