Physics 113 Spring 2010

Quantum Theory Seminar #3

Readings:

Zettili - Chapter(s) - 3 (pages 165-183)
Boccio - Chapter(s) - 5 (pages 26-35), 6(pages 1-30)

Topics:

Maximum Entropy
Formulation of Quantum Mechanics(The Beginnings)

Presentations(15 minutes max):

Maximum Entropy _Dougal_____
Kangaroos and Monkeys
(Chapter 5 - pages 26-35)

Postulates; Density Operators _James______
(Chapter 6 - pages 1-10)

States and Probabilities _Ben________
Transformations of States and Observables
(Chapter 6 - pages 10-16,17-22)

Schrodinger Picture, Heisenberg and
Interaction Pictures _Elizabeth__
(Chapter 6 - pages 16-17,22-30)

Zettili problems:

1. Z3-14(Ed) Time Evolution of Expectation Values
2. Z3-16(Max) Measuring Energy and Other Stuff
3. Z3-17(Sandy) Measuring Energies Ket-Bra Method
4. Z3-17(James) Density Operator Method
4. Z3-18(EVERYONE) Measuring Two Observables
5. Z3-19(Rachael) Measuring Two More Observables
7. Z3-21(Jen) More Measurements
8. Z3-23(Daphne) Energies and Time Evolution

Boccio Problems:

1. Can It Be Written?(Rachael) - Show that a density matrix $\hat{\rho}$ represents a state vector (i.e., it can be written as $|\psi\rangle\langle\psi|$ for some vector $|\psi\rangle$) if, and only if,

$$\hat{\rho}^2 = \hat{\rho}$$

2. Pure and Nonpure States(Ed) - Consider an observable σ that can only take on two values +1 or -1. The eigenvectors of the corresponding operator are denoted by $|+\rangle$ and $|-\rangle$. Now consider the following states.

(a) The one-parameter family of pure states that are represented by the vectors

$$|\theta\rangle = \frac{1}{\sqrt{2}}|+\rangle + \frac{e^{i\theta}}{\sqrt{2}}|-\rangle$$

for arbitrary θ.

(b) the nonpure state

$$\rho = \frac{1}{2}|+\rangle\langle+| + \frac{1}{2}|-\rangle\langle-|$$

Show that $\langle\sigma\rangle = 0$ for all of these states. What, if any, are the physical differences between these various states, and how could they be measured?

3. Probabilities(EVERYONE) - Suppose the operator

$$M = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$

represents an observable. Calculate the probability $\text{Prob}(M = 0 \mid \rho)$ for the following state operators:

$$(a)\ \rho = \begin{bmatrix} \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{4} & 0 \\ 0 & 0 & \frac{1}{4} \end{bmatrix},\ (b)\ \rho = \begin{bmatrix} \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{bmatrix},\ (c)\ \rho = \begin{bmatrix} \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} \end{bmatrix}$$

4. Acceptable Density Operators(Sarah) - Which of the following are acceptable as state operators? Find state vectors for any of them that represent pure states.

$$\rho_1 = \begin{bmatrix} \frac{1}{4} & \frac{3}{4} \\ \frac{3}{4} & \frac{3}{4} \end{bmatrix} \quad , \quad \rho_2 = \begin{bmatrix} \frac{9}{25} & \frac{12}{25} \\ \frac{12}{25} & \frac{16}{25} \end{bmatrix} \quad , \quad \rho_3 = \begin{bmatrix} \frac{1}{2} & 0 & \frac{1}{4} \\ 0 & \frac{1}{2} & 0 \\ \frac{1}{4} & 0 & 0 \end{bmatrix} \quad , \quad \rho_4 = \begin{bmatrix} \frac{1}{2} & 0 & \frac{1}{4} \\ 0 & \frac{1}{4} & 0 \\ \frac{1}{4} & 0 & \frac{1}{4} \end{bmatrix}$$

$$\rho_5 = \frac{1}{3}|u\rangle\langle u| + \frac{2}{3}|v\rangle\langle v| + \frac{\sqrt{2}}{3}|u\rangle\langle v| + \frac{\sqrt{2}}{3}|v\rangle\langle u| \quad , \quad \langle u|u\rangle = \langle v|v\rangle = 1 \text{ and } \langle u|v\rangle = 0$$

5. Is it a Density Matrix?(Sandy) - Let $\hat{\rho}_1$ and $\hat{\rho}_2$ be a pair of density matrices. Show that

$$\hat{\rho} = r\hat{\rho}_1 + (1-r)\hat{\rho}_2$$

is a density matrix for all real numbers r such that $0 \le r \le 1$.

6. Unitary Operators(Jen) - An important class of operators are unitary, defined as those that preserve inner products, i.e., if $|\tilde{\psi}\rangle = \hat{U}|\psi\rangle$ and $|\tilde{\phi}\rangle = \hat{U}|\phi\rangle$, then $\langle\tilde{\phi}|\tilde{\psi}\rangle = \langle\phi|\psi\rangle$ and $\langle\tilde{\psi}|\tilde{\phi}\rangle = \langle\psi|\phi\rangle$.

(a) Show that unitary operators satisfy $\hat{U}\hat{U}^+ = \hat{U}^+\hat{U} = \hat{I}$, i.e., the adjoint is the inverse.

(b) Consider $\hat{U} = e^{i\hat{A}}$, where $\hat{A}$ is a Hermitian operator. Show that $\hat{U}^+ = e^{-i\hat{A}}$ and thus show that $\hat{U}$ is unitary.

(c) Let $\hat{U}(t) = e^{-i\hat{H}t/\hbar}$ where t is time and $\hat{H}$ is the Hamiltonian. Let $|\psi(0)\rangle$ be the state at t = 0. Show that $|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle = e^{-i\hat{H}t/\hbar}|\psi(0)\rangle$ is a solution to the Time-Dependent Schrodinger equation, i.e., the state evolves according to a unitary map. Explain why this is required by the conservation of probability in non-relativistic quantum mechanics.

(d) Let $\{|u_n\rangle\}$ be a complete set of energy eigenfunctions, $\hat{H}|u_n\rangle = E_n|u_n\rangle$. Show that $\hat{U}(t) = \sum_n e^{-iE_nt/\hbar}|u_n\rangle\langle u_n|$. Using this result, show that $|\psi(t)\rangle = \sum_n c_n e^{-iE_nt/\hbar}|u_n\rangle$. What is c_n?

7. More Density Matrices(EVERYONE) - Suppose we have a system with total angular momentum 1. Pick a basis corresponding to the three eigenvectors of the z-component of the angular momentum, J_z, with eigenvalues +1, 0 , _1, respectively. We are given an ensemble described by the density matrix

$$\rho = \frac{1}{4}\begin{pmatrix} 2 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}$$

(a) Is ρ a permissible density matrix? Give your reasoning. For the remainder of this problem, assume that it is permissible. Does it describe a pure or mixed state? Give your reasoning.

(b) Given the ensemble described by ρ, what is the average value of J_z?

(c) What is the spread (standard deviation) in the measured values of J_z?

8. Berger's Burgers (Review of MaxEnt Method)(Dougal) - A fast food restaurant offers three meals: burger, chicken, and fish. The price, Calorie count, and probability of each meal being delivered cold are listed below:

Item	Entree	Cost	Calories	Prob(hot)	Prob(cold)
Meal 1	burger	\$1.00	1000	0.5	0.5
Meal 2	chicken	\$2.00	600	0.8	0.2
Meal 3	fish	\$3.00	400	0.9	0.1

We want to identify the state of the system, i.e., the values of

Prob(Burger) = P(B)
Prob(Chicken) = P(C)
Prob(Fish) = P(F)

Even though the problem has now been set up, we do not know which state the actual state of the system. To express what we do know despite this ignorance, or uncertainty, we assume that each of the possible states A_i has some probability of occupancy $P(A_i)$, where i is an index running over the possible states. As stated above, for the restaurant model, we have three such possibilities, which we have labeled P(B), P(C), and P(F).

A probability distribution $P(A_i)$ has the property that each of the probabilities is in the range $0 \le P(A_i) \le 1$ and since the events are mutually exclusive and exhaustive, the sum of all the probabilities is given by

$$1 = \sum_i P(A_i)$$

Since probabilities are used to cope with our lack of knowledge and since one person may have more knowledge than another, it follows that two observers may, because of their different knowledge, use different probability distributions. In this sense probability, and all quantities that are based on probabilities are **subjective.**

Our uncertainty is expressed quantitatively by the information which we do not have about the state occupied. This information is

$$S = \sum_i P(A_i) \log_2 \left(\frac{1}{P(A_i)} \right)$$

Information if measured in bits because we are using logarithms to base 2.

In physical systems, this uncertainty is known as the **entropy.** Note that the entropy, because it is expressed in terms of probabilities, depends on the observer.

The principle of maximum entropy (MaxEnt) is used to discover the probability distribution which leads to the largest value of the entropy (a maximum), thereby assuring that no information is inadvertently assumed.

If one of the probabilities is equal to 1, the all the other probabilities are equal to 0, and the entropy is equal to 0.

It is a property of the above entropy formula that it has its maximum when all the probabilities are equal (for a finite number of states), which the state of **maximum ignorance.**

If we have no additional information about the system, then such a result seems reasonable. However, if we have additional information, then we should be able to find a probability distribution which is better in the sense that it has less uncertainty.

In this problem we will impose only one constraint. The particular constraint is the known average price for a meal at Berger's Burgers, namely $1.75. This constraint is an example of an expected value.

(a) Express the constraint in terms of the unknown probabilities and the prices for the three types of meals.
(b) Using this constraint and the total probability equal to 1 rule find possible ranges for the three probabilities in the form

$$a \le P(B) \le b$$
$$c \le P(C) \le d$$
$$e \le P(F) \le f$$

(c) Using this constraint, the total probability equal to 1 rule, the entropy formula and the MaxEnt rule, find the value of P(B), P(C) and P(F) which maximize S.
(d) For this state determine the expected value of Calories and the expected number of meals served cold.

In finding the state which maximizes the entropy, we found the probability distribution that is consistent with the constraints and has the largest uncertainty. Thus, we have not inadvertently introduced any biases into the probability estimation.

9. Extended Menu at Berger's Burgers(Dougal) - Suppose now that Berger's extends its menu to include a Tofu option as shown in the table below:

Entree	Cost	Calories	Prob(hot)	Prob(cold)
Burger	$1.00	1000	0.5	0.5
Chicken	$2.00	600	0.8	0.2
Fish	$3.00	400	0.9	0.1
Tofu	$8.00	200	0.6	0.4

Suppose you are now told that the average meal price is $2.50.

Use the method of Lagrange multipliers to determine the state of the system (i.e., P(B), P(C), P(F), and P(T)).

You will need to solve some equations numerically.