PH 500 Problem Set #3

We've established the language of states, operators, and probabilities that describes a quantum system. In this and the next problem set, we put the system in motion. Again, the things I want you to do are in **bold**.

I said that when we take a quantum state |ψ⟩ and measure the physical quantity corresponding to the operator Ô, the result will always be an eigenvalue λ_i of Ô, and the probability of a given λ_i is |⟨λ_i|ψ⟩|² where |λ_i⟩ is the corresponding eigenstate. There's one more twist to the story: after the measurement, the system will no longer be in the state |ψ⟩. Instead it will be in the state |λ_i⟩! (Rigorously speaking, |ψ⟩ gets projected onto the subspace spanned by all eigenstates with eigenvalue λ_i.) In particular, if we measure Ô again right away, we will always get the same result as we got the first time. In quantum mechanics, the act of measurement changes the system.

Start with our favorite state

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

In an earlier problem set, you calculated the probabilities of each possible result of measuring $\hat{\sigma}_z$. Now imagine that you first measure $\hat{\sigma}_x$ and *then* measure $\hat{\sigma}_z$. Find the probability of each possible result of the $\hat{\sigma}_z$ measurement. Note that you have to sum over both possible results you could have gotten for $\hat{\sigma}_x$.

2. Even if we don't make a measurement, the system doesn't stand still. So next we turn to *time dependence*.

Time dependence is governed by the Schrödinger equation:

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \hat{\mathcal{H}} |\psi(t)\rangle$$
 (2)

Let's understand this equation one piece at a time:

- \mathcal{H} is a Hermitian operator, called the *Hamiltonian*. It is the operator corresponding to the *energy* of the system. In classical mechanics, if I tell you the energy function for a particle as a function of where it is on a hill, and I tell you where it is and how fast it's going at t = 0, you can determine its motion as it rolls down the hill. Similarly, by specifying the energy *operator* in quantum mechanics, we determine the evolution of the quantum state given the initial quantum state.
- The *i* indicates that the equation is inherently complex. That's why we have considered complex vector spaces from the start you can't get dynamics with real states alone.

- \hbar is a new fundamental constant, with units energy time. (As an aside, note that these are the same units as angular momentum. That's actually the underlying reason why the Bohr model for hydrogen in which angular momentum is quantized in integer units worked even though Bohr didn't know anything about the Schrödinger equation.)
- Besides these two constants, the left-hand side is the *change* in the state $|\psi(t)\rangle$ per unit time, which is another state in the same vectorspace. To start with, I would like to assume that the operator $\hat{\mathcal{H}}$ does not depend on time *explicitly*. For example, we could be talking about the energy of a particle in an electromagnetic field. Just as in classical mechanics, the state of the particle can (and will) change as the field acts on it. But we will not change the background electromagnetic field itself. So the operator $\hat{\mathcal{H}}$ corresponding to the energy will not change, but the *state* of a particular particle will change, according to the Schrödinger equation. Later, we will loosen this restriction and see the additional effect of letting $\hat{\mathcal{H}}$ depend on time explicitly as well.
- The Schrödinger equation is *linear*, so that if we have two solutions $|\psi_1(t)\rangle$ and $|\psi_2(t)\rangle$, any linear combination $c_1|\psi_1(t)\rangle + c_2|\psi_2(t)\rangle$ of these solutions is also a solution (where the coefficients c_1 and c_2 are time-independent).
- Unless |ψ⟩ happens to be an eigenstate of Ĥ, Ĥ|ψ⟩ will point in a different direction than |ψ⟩. So over time, one state can evolve into a completely different state. Eigenvectors of Ĥ are special because they do not evolve into different states.

Suppose that at t = 0, the system is in the state $|E\rangle$, which is an eigenstate of $\hat{\mathcal{H}}$ with eigenvalue E, and suppose we let the system evolve without disturbing it. Show that the state of the system at time t is $|\psi(t)\rangle = e^{-iEt/\hbar}|E\rangle$. Show that for any operator $\hat{\mathcal{O}}$ (including $\hat{\mathcal{H}}$ itself!), the expectation value of $\hat{\mathcal{O}}$ for a system initially in the state $|E\rangle$ is time independent.

3. Starting again with our favorite state

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

at t = 0, take the Hamiltonian to be $\hat{\mathcal{H}} = \gamma B \frac{\hbar}{2} \hat{\sigma}_z$ where γ and B are constants (the reason for including all these arbitrary constants will be explained later). Find the expectation values of $\hat{\sigma}_x$, $\hat{\sigma}_y$ and $\hat{\sigma}_z$ as functions of time. Hint: write $|\psi\rangle$ as a linear combination of the eigenvectors of $\hat{\mathcal{H}}$. Then each eigenvector has a simple time dependence. Do the same for $\hat{\mathcal{H}} = \gamma B \frac{\hbar}{2} \hat{\sigma}_x$.

4. Suppose I have a system with Hamiltonian $\hat{\mathcal{H}}$, start in a state $|\psi\rangle$, and compute the expectation value of some other Hermitian operator $\hat{\mathcal{O}}$ as a function of time.

Show that adding a *constant* to the energy — which means adding an operator proportional to the identity to $\hat{\mathcal{H}}$ — does not affect the expectation value of $\hat{\mathcal{O}}$.

- Suppose that some Hermitian operator Ô commutes with Ĥ, that is,
 [Ĥ, Ô] = ĤÔ ÔĤ = 0. Show that the expectation value of Ô is time independent. In this case, we say that Ô is conserved.
- 6. The Schrödinger equation looks a little bit like the ordinary differential equation

$$i\hbar \frac{d}{dt}f(t) = Ef(t) \tag{4}$$

for which the solution is $f(t) = e^{-\frac{iEt}{\hbar}} f(t=0)$. Of course, it isn't so simple, since it's a vector equation involving matrices, but we can nonetheless define similar concepts.

We define the exponential of an operator as follows:

$$e^{\hat{A}} = \sum_{n=0}^{\infty} \frac{\hat{A}^n}{n!} = 1 + \hat{A} + \frac{\hat{A}^2}{2} + \frac{\hat{A}^3}{6} + \dots$$
(5)

All we have done is to plug the operator \hat{A} into the Taylor series for e^x . Technically, we should worry about whether the infinite series converges, but we will always assume it does (this is generally correct, and certainly rigorous for finite-dimensional matrices, but we won't bother to prove it).

Show the following properties of the exponential:

- (a) If $|\lambda_i\rangle$ is an eigenstate of \hat{A} with eigenvalue λ_i , then it is also an eigenstate of $e^{\hat{A}}$, with eigenvalue e^{λ_i} .
- (b) If $[\hat{A}, \hat{B}] = 0$, $e^{\hat{A}+\hat{B}} = e^{\hat{A}}e^{\hat{B}}$. Hint: You may assume that since \hat{A} and \hat{B} commute, you can work in a basis consisting of vectors that are eigenstates of both operators.
- (c) If $\hat{\mathcal{O}}$ is Hermitian, then $e^{i\hat{\mathcal{O}}}$ is unitary. (This is analogous to the statement that the exponential of *i* times a real number is a complex number of magnitude 1.)
- (d) Given the initial state $|\psi(t=0)\rangle$, the solution to the Schrödinger equation is given by

$$|\psi(t)\rangle = e^{-\frac{i\mathcal{H}t}{\hbar}}|\psi(t=0)\rangle \tag{6}$$

7. Prove that the normalization of the state is preserved under time evolution.

- 8. Another prescription for defining functions like the exponential on matrices is as follows:
 - Change to a basis of eigenvectors so that the matrix is diagonal.
 - Act with the function on each eigenvalue.
 - Go back to the original basis.

(This procedure is only strictly valid for *diagonalizable* matrices, but we have seen that all Hermitian matrices are diagonalizable, and all unitary matrices are diagonalizable as well. In fact any matrix can be expressed as the limit of a sequence of diagonalizable matrices, which allows us to extend this procedure to all matrices. But for the purposes of this problem just assume we are always working with diagonalizable matrices.)

- (a) Show that our earlier definition of the exponential is equivalent to this definition.
- (b) Show that $\operatorname{Tr} \log \hat{A} = \log \det \hat{A}$.

Hint: Remember that $\operatorname{Tr} \hat{A}\hat{B}\hat{C} = \operatorname{Tr} \hat{C}\hat{A}\hat{B}$ and $\det \hat{A}\hat{B} = \det \hat{A} \det \hat{B}$.