Exam 1

1. (5+5+5=15 pts) Let’s say A is the value of various dollar bills. Actual allowed “eigenvalues” are $a_0 = 1$, $a_1 = 5$, $a_2 = 10$, $a_3 = 20$, etc. You have a single $1 bill, two $5 bills, four $20 bills.

a. What are the probabilities $P(a_0 = 1)$, $P(a_1 = 5)$, $P(a_2 = 10)$, and $P(a_3 = 20)$ of pulling a bill from your collection randomly out of your wallet?

b. What is the formula for the average value of a dollar bill $<A>$ in terms of the allowed “eigenvalues” and the probability for each eigenvalue?

c. What is the average $<A>$?

Solution:

a. We have 7 total bills, and so the probability of pulling each bill randomly from your wallet is

$$P(a_0 = 1) = 1/7 = 0.143 \text{ (single$1 bill)}$$
$$P(a_1 = 5) = 2/7 = 0.286 \text{ (two$5 bills)}$$
$$P(a_2 = 10) = 0/7 = 0 \text{ (no$10 bill)}$$
$$P(a_3 = 20) = 4/7 = 0.571 \text{ (four$20 bills)}$$

b. $\langle A \rangle = \sum_n a_n P(A = a_n)$

c. $\langle A \rangle = 1 \left(\frac{1}{7}\right) + 5 \left(\frac{2}{7}\right) + 10 \left(\frac{0}{7}\right) + 20 \left(\frac{4}{7}\right) = 13$

2. (10 pts) Consider a particle in a 3-D cubic box, at an energy level given by

$$E = \frac{26 \hbar^2}{8mL^2},$$

where $L$ is the length of each side. What is the degeneracy of this state, that is, how many different combinations of the $n_x$, $n_y$, $n_z$ quantum numbers can you have, that all lie at this exact energy?

Solution: The energy for a cubic box is given by

$$E = E_x + E_y + E_z = \frac{(n_x^2 + n_y^2 + n_z^2)\hbar^2}{8mL^2}$$

(1)

So we need to find out how many different combinations of $n_x$, $n_y$, $n_z$ satisfy

$$n_x^2 + n_y^2 + n_z^2 = 26$$

(2)

The most expedient way to do this is by simple logic and guess/check. We see that the n’s need to take values 1, 3 and 4, resulting in

$$1^2 + 3^2 + 4^2 = 26$$

(3)
There are 3! = 6 different combinations of $n_x, n_y, n_z$ that satisfy eq. (5). They are listed below:

\begin{align*}
&n_x = 1, n_y = 3, n_z = 4 \\
&n_x = 1, n_y = 4, n_z = 3 \\
&n_x = 3, n_y = 1, n_z = 4 \\
&n_x = 3, n_y = 4, n_z = 1 \\
&n_x = 4, n_y = 1, n_z = 3 \\
&n_x = 4, n_y = 3, n_z = 1
\end{align*}

Thus the degeneracy is 6.

3. (5+5+5=15 pts) Use postulate (4) of quantum mechanics to prove that the energy of a quantum particle with stationary state wavefunction $\psi(x, t) = \Psi_n(x)e^{-\frac{iE_nt}{\hbar}}$ is simply $E_n$ with 100% probability.

Postulate (4): If an observable $A$ is measured, its value MUST BE one of the solutions of the equation $\hat{A}\varphi_n(x) = a_n\varphi_n(x)$. In this equation, $a_n$ is called an “eigenvalue” of the operator $\hat{A}$ for the observable $A$, and $\varphi_n(x)$ is called an “eigenfunction.” The probability of measuring that “nth” eigenvalue as the actual value of $A$ is $P(A = a_n) = \int dx \varphi_n^*(x)\psi(x, t)$. 

a. Insert the stationary state into the time-dependent Schrödinger equation $\hat{H}\psi(x, t) = i\hbar\frac{\partial\psi(x, t)}{\partial t}$ and take the time derivative to write down the eigenvalue equation for the specific case where $A$ is the energy. Call the eigenvalues $E_n$ and the eigenfunctions $\Psi_n(x)$.

b. For the SPECIFIC case where $A$ is the energy, write down the formula for the probability $P(E = E_n)$.

c. Now assume that the wavefunction $\psi(x, t)$ in your probability formula is not just any function, but the stationary state $\psi(x, t) = \Psi_n(x)e^{-\frac{iE_nt}{\hbar}}$. Simplify the probability formula from (b) to prove that for stationary state $\Psi_n(x)e^{-\frac{iE_nt}{\hbar}}$, $P(E = E_n) = 1$.

Solution:

a. 

$$\hat{H}\Psi_n(x)e^{-\frac{iE_nt}{\hbar}} = i\hbar\frac{\partial}{\partial t}\Psi_n(x)e^{-\frac{iE_nt}{\hbar}}$$

Therefore

$$\hat{H}\Psi_n(x) = E_n\Psi_n(x)$$

b. Now, the particle has the wavefunction $\psi(x, t) = \Psi_n(x)e^{-\frac{iE_nt}{\hbar}}$.

Therefore $P(E = E_n) = |\int dx \psi_n^*(x)\psi(x, t)|^2$ according to postulate (4).
c. We can simplify this special case by realizing that $e^{-\frac{iE_nt}{\hbar}}$ is independent of $x$, so we can pull it out of the integral. Also $|a|^2$ is just $a^*$, so $|e^{-\frac{iE_n t}{\hbar}}|^2$ is just $e^{-\frac{iE_n t}{\hbar}} e^{\frac{iE_n t}{\hbar}}$.

Therefore $P(E = E_n) = | \int dx \Psi_n^*(x)\Psi_n(x)e^{-\frac{iE_n t}{\hbar}} |^2$

$$= e^{-\frac{iE_n t}{\hbar}} e^{\frac{iE_n t}{\hbar}} | \int dx \Psi_n^*(x)\Psi_n(x) |^2$$

$$= 1$$

The third line is obtained because $e^{a}e^{a^*}=1$ for any number, and because $\Psi_n^*(x)$ is normalized. Thus, the stationary state is guaranteed (100% probable) to have energy $E_n$.

4. (5+5+5=15 pts) On the homework, you expressed the Hamiltonian of the Harmonic Oscillator in terms of the raising operator $\hat{a}^+ = (\frac{m\omega}{2\hbar})^{\frac{1}{2}} (x - \frac{i\hat{p}}{m\omega})$ and lowering operator $\hat{a} = (\frac{m\omega}{2\hbar})^{\frac{1}{2}} (x + \frac{i\hat{p}}{m\omega})$ proving that $\hat{H} = \hbar\omega \left( \hat{a} \hat{a}^+ - \frac{1}{2} \right)$

a. **Multiply out** $\hat{a}^+ \hat{a} = ?$ to write down the explicit formula in terms of $x$ and $\hat{p}$.

b. Use $x\hat{p} - \hat{p}x = i\hbar$ to **simplify the formula** in (a) so only $x^2$ and $p^2$ and constants show up on the right hand side.

c. Remembering that $\omega^2 = k/m$, **show that**

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{k}{2} x^2 = \hbar\omega \left( \hat{a} \hat{a}^+ + \frac{1}{2} \right).$$

**Solution:**

a. Multiplying together,

$$\hat{a}^+ \hat{a} = (\frac{m\omega}{2\hbar})^{\frac{1}{2}} (x - \frac{i\hat{p}}{m\omega}) (\frac{m\omega}{2\hbar})^{\frac{1}{2}} (x + \frac{i\hat{p}}{m\omega})$$

$$\hat{a}^+ \hat{a} = (\frac{m\omega}{2\hbar}) \left\{ x^2 + \frac{i}{m\omega} (x\hat{p} - \hat{p}x) + \frac{\hat{p}^2}{m^2\omega^2} \right\} \quad (1)$$

b. We use $(x\hat{p} - \hat{p}x) = i\hbar$ and substitute into eq. (2)

$$\hat{a}^+ \hat{a} = (\frac{m\omega}{2\hbar}) \left\{ x^2 - \frac{\hbar}{m\omega} + \frac{\hat{p}^2}{m^2\omega^2} \right\}$$

$$\hat{a}^+ \hat{a} = (\frac{m\omega}{2\hbar}) \left\{ x^2 - \frac{\hbar}{m\omega} + \frac{\hat{p}^2}{m^2\omega^2} \right\} \quad (3)$$
c. Now, distribute \( \left( \frac{m\omega^2}{2} \right) \) through the brackets in (3) to obtain

\[
\hat{a}^{\dagger} \hat{a} = \left( \frac{1}{\hbar \omega} \right) \left\{ \left( \frac{m\omega^2}{2} \right) x^2 - \frac{\hbar \omega}{2} + \frac{\hat{p}^2}{2m} \right\}.
\] (4)

Multiply both sides by \( \hbar \omega \), move the constant to the left side, and recall that \( k = m\omega^2 \) to write

\[
\hbar \omega \hat{a}^{\dagger} \hat{a} - \frac{\hbar \omega}{2} \left\{ \frac{\hat{p}^2}{2m} + \frac{k}{2} x^2 \right\} = \hat{H}
\] (5)

This proves the desired result,

\[
\hat{H} = \hbar \omega \left( \hat{a}^{\dagger} \hat{a} + \frac{1}{2} \right)
\]

5. \( 5+5+5=15 \) pts) According to postulate (5), the wavefunction satisfies the two equations

\[
+ \frac{\partial \Psi^{(r)}}{\partial t} = \frac{\hat{H}}{\hbar} \Psi^{(i)}
\]

\[- \frac{\partial \Psi^{(i)}}{\partial t} = \frac{\hat{H}}{\hbar} \Psi^{(r)},
\]

from which we derived the time-dependent Schrödinger equation in class.

a. Replace the time derivative in both equations by a finite difference involving \( \Psi^{(r \ or \ i)}(t+\Delta t) \), \( \Psi^{(r \ or \ i)}(t) \) and \( \Delta t \), and write down the resulting two finite-difference equations.

b. Solve the two equations for \( \Psi^{(r \ or \ i)}(t+\Delta t) \) to obtain

\[
\Psi^{(r)}(t+\Delta t) = (1)
\]

\[
\Psi^{(i)}(t+\Delta t) = (2)
\]

with explicit equations in place of (1) and (2).

c. Now assume we get even lazier than baby calculus and on the computer, after we calculate \( \Psi^{(r)}(t+\Delta t) \) from \( \Psi^{(r)}(t) \) in the first line (1), we store the new value \( \Psi^{(r)}(t+\Delta t) \) ON TOP OF the old value \( \Psi^{(r)}(t) \), erasing it. How does that modify (2)?

Congrats, you have derived the SUR algorithm for moving the wavefunction forward in time on a computer.

**Solution:**

\[
+ \frac{\partial \Psi^{(r)}}{\partial t} = \frac{\hat{H}}{\hbar} \Psi^{(i)} \rightarrow \frac{\Psi^{(r)}(t+\Delta t) - \Psi^{(r)}(t)}{\Delta t} = \frac{\hat{H}}{\hbar} \Psi^{(i)}(t)
\] (1)
\[ -\frac{\partial \psi^{(i)}}{\partial t} = \frac{\hat{H}}{\hbar} \psi^{(r)} \rightarrow -\frac{\psi^{(i)}(t + \Delta t) - \psi^{(i)}(t)}{\Delta t} = \frac{\hat{H}}{\hbar} \psi^{(r)}(t) \]  

(2)

b)

\[ \psi^{(r)}(t + \Delta t) = \psi^{(r)}(t) + \frac{1}{\hbar} \hat{H} \psi^{(i)}(t) \Delta t \]  

(3)

\[ \psi^{(i)}(t + \Delta t) = \psi^{(i)}(t) - \frac{1}{\hbar} \hat{H} \psi^{(r)}(t) \Delta t \]  

(4)

c)

Now, we store the new value of \( \psi^{(r)}(t + \Delta t) \) on top of the old value \( \psi^{(r)}(t) \) and place this into equation (4) yielding

\[ \psi^{(i)}(t + \Delta t) = \psi^{(i)}(t) - \frac{1}{\hbar} \hat{H} \psi^{(r)}(t + \Delta t) \Delta t \]  

(5)

This the SUR algorithm takes the wavefunction from time \( t \) to time \( t + \Delta t \) in two steps of code,

\[ \psi^{(r)}(t + \Delta t) = \psi^{(r)}(t) + \frac{1}{\hbar} \hat{H} \psi^{(i)}(t) \Delta t \]

\[ \psi^{(i)}(t + \Delta t) = \psi^{(i)}(t) - \frac{1}{\hbar} \hat{H} \psi^{(r)}(t + \Delta t) \Delta t \]