PHY 303, I-Semester 2023/24, Tutorial 5 solution

Stage 1 **(Postulates)** Consider an arbitrary time-independent Hamiltonian, with eigenvalue problem

$$\hat{H}|\,\phi_n\,\rangle = E_n|\,\phi_n\,\rangle, \tag{1}$$

where there is no degeneracy (or $E_n \neq E_m$ for $n \neq m$). The system is in the quantum state

$$|\,\Psi\,\rangle = \frac{1}{2}|\,\phi_1\,\rangle + \frac{1}{\sqrt{2}}|\,\phi_2\,\rangle + \frac{1}{2}|\,\phi_3\,\rangle \tag{2}$$

and assume $E_1 = 1$ eV, $E_2 = 2$ eV, $E_3 = 8$ eV.

(a) Check that the state is correctly normalized.
Solution: We have, $|\,\Psi\,\rangle = \frac{1}{2}|\,\phi_1\,\rangle + \frac{1}{\sqrt{2}}|\,\phi_2\,\rangle + \frac{1}{2}|\,\phi_3\,\rangle$*, where* $|\,\phi_n\,\rangle$ *are eigenstates of Hamitonian* $\hat{H}$*. Now to check the normalization of* $|\,\Psi\,\rangle$*, we compute the inner product* $\langle\Psi|\Psi\rangle$*:*

$$\langle\Psi|\Psi\rangle = \left\{\frac{1}{2}\langle\phi_1| + \frac{1}{\sqrt{2}}\langle\phi_2| + \frac{1}{2}\langle\phi_3|\right\}\left\{\frac{1}{2}|\phi_1\rangle + \frac{1}{\sqrt{2}}|\phi_2\rangle + \frac{1}{2}|\phi_3\rangle\right\}, \tag{3}$$

from the orthonormality relation of the eigenstates , $\langle\phi_m|\phi_n\rangle = \delta_{mn}$ *we can simpilify the above as*

$$\langle\Psi|\Psi\rangle = \frac{1}{4} + \frac{1}{2} + \frac{1}{4} = 1.$$

Hence, the state is normalized.

(b) We now repeatedly create the state (2) and then measure the energy of the system. Find the expectation value of this measurement, all possible results of of a single measurement and the most likely result of a measurement. With which probability will a single measurement result be the same as the expectation value?
Solution: The superposition state only contains the eigenstates $|\,\phi_1\,\rangle$*,* $|\,\phi_2\,\rangle$*,* $|\,\phi_3\,\rangle$*, hence the only possible results for the energy measurement are* E_1*,* E_2 *and* E_3*. If we denote by* p_1, p_2*, and* p_3 *the probabilities of measuring energy eigenvalues* E_1, E_2*, and* E_3 *respectively, we can calcluate all possible results of a single measurements with corresponding probabilities using:*

$$p_n = |c_n|^2 = |\langle\phi_n|\Psi\rangle|^2 \tag{4}$$

$$\begin{aligned} p_1 &= \frac{1}{4}, E_1 = 1eV \\ p_2 &= \frac{1}{2}, E_2 = 2eV \\ p_3 &= \frac{1}{4}, E_3 = 8eV. \end{aligned} \tag{5}$$

Now we see that E_2 is the most likely outcome of the measurement with the highest probability.
To find the expectation value of energy, we use

$$\langle \hat{H} \rangle = \langle \Psi | \hat{H} | \Psi \rangle = \left\{ \frac{1}{2}\langle\phi_1| + \frac{1}{\sqrt{2}}\langle\phi_2| + \frac{1}{2}\langle\phi_3| \right\} \hat{H} \left\{ \frac{1}{2}|\phi_1\rangle + \frac{1}{\sqrt{2}}|\phi_2\rangle + \frac{1}{2}|\phi_3\rangle \right\}, \quad (6)$$

$$= \left\{ \frac{1}{2}\langle\phi_1| + \frac{1}{\sqrt{2}}\langle\phi_2| + \frac{1}{2}\langle\phi_3| \right\} \left\{ \frac{1}{2}E_1|\phi_1\rangle + \frac{1}{\sqrt{2}}E_2|\phi_2\rangle + \frac{1}{2}E_3|\phi_3\rangle \right\} \quad (7)$$

which due to orthonormality of the eigenvectors

$$\langle E \rangle = p_1 E_1 + p_2 E_2 + p_3 E_3 = \frac{13}{4} eV. \quad (8)$$

This is of course also the mathematical probability theory result for the expectation value of realisations of a random variable with three outcomes E_k and probabilities p_k.
Note that the expectation value is not one of the possible measurement outcomes, thus the probability that a single measurement result is the same as the expectation value is zero.

(c) Suppose in a first measurement we have found energy E_2. Now we do a second measurement on the same system without re-initialising the quantum state. Answer all the questions in (b) again.
Solution: In a first measurement, if the measurement result is E_2, the state is collapsed to eigenstate $|\phi_2\rangle$ i.e. now $|\Psi\rangle = |\phi_2\rangle$. So, if we perform a second measurement on the same system without re-initialising the state, we get the energy E_2 with the probability 1, and hence, it will be the expectation value (do the same calculation as above) and most likely value of the energy. In this case of course the probability that a single measurement result is the same as the expectation value is one.

(d) Now consider the Hermitian operator

$$\hat{O} = \sum_{n=0}^{\infty} o_n \left(|\phi_{n+1}\rangle\langle\phi_n| + |\phi_n\rangle\langle\phi_{n+1}| \right). \quad (9)$$

with some constants o_n. What is the expectation value of measurements of this operator in the state (2)?
Solution: The operation of $\hat{O}$ on state $|\Psi\rangle$ can be expressed as

$$\hat{O}|\Psi\rangle = \textstyle\sum_{n=0}^{\infty} o_n \left(|\phi_{n+1}\rangle\langle\phi_n| + |\phi_n\rangle\langle\phi_{n+1}| \right) |\Psi\rangle \quad (10)$$

Using orthonormality of the states $\langle\phi_m|\phi_n\rangle = \delta_{mn}$, we can simplify the outcome as

$$\hat{O}|\Psi\rangle = \tfrac{1}{\sqrt{2}} o_1 |\phi_1\rangle + \left(\tfrac{1}{2} o_1 + \tfrac{1}{2} o_2\right) |\phi_2\rangle + \tfrac{1}{\sqrt{2}} o_2 |\phi_3\rangle + \tfrac{1}{2} o_3 |\phi_4\rangle \quad (11)$$

Hence, we can write the expectation value of operator $\hat{O}|\,\Psi\,\rangle$ as

$$
\begin{aligned}
\langle\,\Psi\,|\hat{O}|\,\Psi\,\rangle = &\left\{\frac{1}{2}\langle\phi_1| + \frac{1}{\sqrt{2}}\langle\phi_2| + \frac{1}{2}\langle\phi_3|\right\} \\
&\left\{\frac{1}{\sqrt{2}}o_1|\,\phi_1\,\rangle + \left(\frac{1}{2}o_1 + \frac{1}{2}o_2\right)|\,\phi_2\,\rangle + \frac{1}{\sqrt{2}}o_2|\,\phi_3\,\rangle + \frac{1}{2}o_3|\,\phi_4\,\rangle\right\} \\
&= \frac{1}{\sqrt{2}}o_1 + \frac{1}{\sqrt{2}}o_2 = \frac{1}{\sqrt{2}}(o_1 + o_2).
\end{aligned}
$$

Stage 2 (Commutators) Show the relation (3.41): $\big[\hat{A}, \hat{B}\hat{C}\big] = \big[\hat{A}, \hat{B}\big]\hat{C} + \hat{B}\big[\hat{A}, \hat{C}\big]$.
Solution:

$$\big[\hat{A}, \hat{B}\hat{C}\big] = \hat{A}\hat{B}\hat{C} - \hat{B}\hat{C}\hat{A}$$

on adding and subtracting $\hat{B}\hat{A}\hat{C}$,

$$
\begin{aligned}
\big[\hat{A}, \hat{B}\hat{C}\big] &= \hat{A}\hat{B}\hat{C} - \hat{B}\hat{A}\hat{C} + \hat{B}\hat{A}\hat{C} - \hat{B}\hat{C}\hat{A} \\
&= \left[\hat{A}\hat{B} - \hat{B}\hat{A}\right]\hat{C} + \hat{B}\left[\hat{A}\hat{C} - \hat{C}\hat{A}\right] \\
&= \big[\hat{A}, \hat{B}\big]\hat{C} + \hat{B}\big[\hat{A}, \hat{C}\big]. \qquad (12)
\end{aligned}
$$

Then evaluate the following commutators:

(i) $\big[m\omega^2\hat{x}^2 + \hat{p}^2, \hat{x}\big]$
Solution:

$$
\begin{aligned}
\big[m\omega^2\hat{x}^2 + \hat{p}^2, \hat{x}\big] &\overset{\text{Eq. (3.41)}}{=} \big[m\omega^2\hat{x}^2, \hat{x}\big] + \big[\hat{p}^2, \hat{x}\big] \\
&\overset{\text{Eq. 12}}{=} m\omega^2\left\{\big[\hat{x}, \hat{x}\big]\hat{x} + \hat{x}\big[\hat{x}, \hat{x}\big]\hat{x}\right\} + \big[\hat{p}, \hat{x}\big]\hat{p} + \hat{p}\big[\hat{p}, \hat{x}\big]\hat{p} \\
&= \big[\hat{p}, \hat{x}\big]\hat{p} + \hat{p}\big[\hat{p}, \hat{x}\big]\hat{p} \\
&\overset{\text{Eq. (2.46)}}{=} -i\hbar\hat{p}.
\end{aligned}
$$

(ii) Consider operators $\hat{\sigma}_x$, $\hat{\sigma}_y$ and $\hat{\sigma}_z$. Assume a Hilbertspace with only two basis states $|\,1\,\rangle$ and $|\,2\,\rangle$. In this basis, let the matrix representations of those operators be

$$\underline{\underline{\sigma_x}} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \underline{\underline{\sigma_y}} = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \underline{\underline{\sigma_z}} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \qquad (13)$$

Find the matrix representation of all commutators $\big[\hat{\sigma}_k, \hat{\sigma}_n\big]$, and try to find a single neat expression for them.

Solution: First we could show that if $\left[\hat{A},\hat{B}\right]=\hat{C}$*, then the matrix representation of* $\hat{C}$ *fulfills* $\underline{\underline{C}}=\underline{\underline{A}}\,\underline{\underline{B}}-\underline{\underline{B}}\,\underline{\underline{A}}$*. Using that result, we just evaluate matrix products of the matrices in Eq. (13) in the two different orderings and substract.*
The matrix representation of commutators that we find are then

$$\begin{aligned}\left[\hat{\sigma}_x,\hat{\sigma}_y\right] &= 2i\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}=2i\hat{\sigma}_z,\\ \left[\hat{\sigma_y},\hat{\sigma_z}\right] &= \begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}=2i\hat{\sigma_x},\\ \left[\hat{\sigma_z},\hat{\sigma_x}\right] &= \begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}=2i\hat{\sigma_y}\end{aligned}$$

Hence, a single expression can be written as $\left[\hat{\sigma}_k,\hat{\sigma}_n\right]=2i\epsilon_{knm}\hat{\sigma}_m$.

Stage 3 (Uncertainty relations)

(i) Consider the anharmonic oscillator Hamiltonian

$$\hat{H}=\frac{\hat{p}^2}{2m}+\chi\hat{x}^4. \tag{14}$$

Can one simultaneously know the momentum and energy? If not, what is the uncertainty relation between these two observables?
Solution: No. The uncertainty relation between these two observables is defined as $\sigma_{\hat{H}}\sigma_{\hat{p}}=\sqrt{\left(\frac{1}{2i}\langle\left[\hat{H},\hat{p}\right]\rangle\right)^2}$ *, so first we calculate* $\left[\hat{H},\hat{p}\right]$*:*

$$\begin{aligned}\left[\hat{H},\hat{p}\right] &= \left[\frac{\hat{p}^2}{2m}+\chi\hat{x}^4,\hat{p}\right]\\ &= \frac{1}{2m}\left[\hat{p}^2,\hat{p}\right]+\chi\left[\hat{x}^4,\hat{p}\right]\\ &= \chi\left[\hat{x}^4,\hat{p}\right]\\ &= 4i\hbar\chi\hat{x}^3,\end{aligned}$$

where we have used the identity $\left[\hat{A}^n,B\right]=n\hat{A}^{n-1}\left[\hat{A},\hat{B}\right]$*, which follows through repeated application of Eq. 12.*
The uncertainty relation that we seek thus reads

$$\sigma_{\hat{H}}\sigma_{\hat{p}} = \sqrt{\left(\frac{1}{2i}\langle(4i\hbar\chi\hat{x}^3)\rangle\right)^2}=\left|2\hbar\chi\langle\hat{x}^3\rangle\right|. \tag{15}$$

Note, that unlike the basic HUP, the RHS still contains the expectation value $\langle\hat{x}^3\rangle$*. In particular this means that the answer depends on the* <u>*state*</u>*. For example in an eigenstate* $\phi_n(x)$ *of* $\hat{H}$ $\langle\hat{x}^3\rangle$ *will be zero since* $|\phi_n(x)|^2$ *is even (Assignment 3, Q1b) and* x^3 *is odd. This makes sense since* $\sigma_{\hat{H}}=0$ *and* $\sigma_{\hat{p}}>0$ *but finite, so the LHS of Eq. 15 is also zero.*

(ii) For which of the following tasks can you use the energy-time uncertainty relation (and why or why not)? What does it tell you if yes?

(a) A harmonic oscillator is in eigenstate $\phi_5(x)$. We want to know the period of oscillations of the complex phase of the wavefunction.
Solution: We cannot use energy-time HUP, since that discusses the rate of change of observables, which do not change if the system is in a stationary state, like in this case.

(b) A harmonic oscillator is in a superposition of eigenstates $\phi_5(x)$, $\phi_6(x)$ and $\phi_7(x)$. We want to approximate the time-scale of oscillations of the expectation value of momentum $\langle\, \hat{p}\, \rangle$.
Solution: Yes. This has to do with a time-dependent scenario and we ask for the time-scale of change of an observable, so it perfectly matches the scenario for which we derived this HUP. To check you can write the state as $\Psi(x,t) = \sum_{n=5}^{7} c_n \phi_n(x) e^{-iE_n t/\hbar}$ and calculate $\langle \hat{p} \rangle$ using $\langle \Psi|\hat{p}|\psi \rangle \sim \langle \Psi|(\hat{a}^\dagger - \hat{a})|\Psi\rangle$ to get the period of oscillations $T = \frac{2\pi\hbar}{|E_n - E_{n+1}|} = \frac{2\pi\hbar}{\Delta E}$ as characteristic time scale of oscillations of the expectation value of momentum and see how it relates to the one predicted by the HUP.

(c) A quantum superposition state at time $t = 0$

$$|\, \Psi(0)\, \rangle = \sum_n c_n |\, \phi_n\, \rangle \tag{16}$$

contains a superposition of a larger number of basis states as shown in the figure below (left). Because of all the different phase factors $e^{-iE_n t/\hbar}$ in the corresponding time evolving state, the expectation value of some (unspecified) operator $\langle\, \hat{O}\, \rangle$ quickly decays to near zero as also shown in the figure (right). However let this be a case where all the energies E_n are rational multiples of each other, then there is a time t_{rev} called "revival time", where $\langle\, \hat{O}\, \rangle$ returns to its initial value because <u>all</u> $e^{-iE_n t_{\text{rev}}/\hbar} = 1$.
You want to know the timescale of this revival and the timescale it takes for $\langle\, \hat{O}\, \rangle$ to decay to near zero (answer for both of these separately).
Solution: We can use it to find the decay time (in the drawing the time it takes for $\langle\, \hat{O}\, \rangle$ to reach zero or almost zero), since this also is clearly related to the "characteristic time on which the expectation value $\langle\, \hat{O}\, \rangle$ changes, as drawn and discussed near Eq. (3.52). To find it, we would first have to evaluate ΔE for the state Eq. 16, which is straightforward if we know the Hamiltonian and all the c_n. We <u>cannot</u> use the HUP to find the revival time, since that time-scale does not match the definition of the one to which the HUP applies. t_{rev} will be related to the least common multiple of all the E_n, and thus is a subtle function of all the <u>details of the spectrum of the Hamiltonian</u>. This is meant as a

warning that in order to apply the energy-time HUP, one has to pay careful attention to what energies and what times are being considered. Bonus: To see how a revival can come about: if there is a finite number of basis states in a superposition, we can write the time-evolving quantum state as

$$| \Psi(t) \rangle = \sum_{n=0}^{M} c_n e^{-iE_n t/hbar} | \phi_n \rangle, \tag{17}$$

as usual. If now the energies of these states are related by <u>*rational numbers*</u>*, this means we can write all of them as* $E_n = CP_n/Q_n$*, for integers* P_n *and* Q_n*. Then there exists a time* $t = t_{rev}$ *called "revival time", where all the complex exponential functions will reach the value* 1 *simultaneously. Thus the state will be the* <u>*same*</u> *state as at the initial time, and therefore any expectation value must take the same value as at the initial time.*
You can then show that that time is

$$t_{rev} = \frac{2\pi\hbar}{L_{cd}[P]C} L_{cm}[Q], \tag{18}$$

where $L_{cm}[Q]$ *is the lowest common multiple of the* Q_n *and* $L_{cd}[P]$ *the greatest common divisor of the* P_n*. (see also Wikipedia, Quantum revival). Both,* $L_{cm}[Q]$*,* $L_{cd}[P]$ *depend on all sorts of details of the allowed energies, and not only on the energy uncertainty.*