Problem One

If $\hat{Q}$ is an observable that does not depend explicitly on time, show that the expectation value of $\hat{Q}$ in an eigenstate $|u_n\rangle$ of the Hamiltonian $\hat{H}$ of the system is time-independent.

Solution:
Since the observable $\hat{Q}$ does not depend explicitly on time, the equation-of-motion of its expectation value is given by

$$\begin{aligned}\frac{d}{dt}\left\langle \hat{Q}\right\rangle &= \frac{i}{\hbar}\left\langle [\hat{H},\hat{Q}]\right\rangle = \frac{i}{\hbar}\langle u_n|\left(\hat{H}\hat{Q}-\hat{Q}\hat{H}\right)|u_n\rangle \\ &= \frac{i}{\hbar}\left(E_n\langle u_n|\hat{Q}|u_n\rangle - E_n\langle u_n|\hat{Q}|u_n\rangle\right) = 0,\end{aligned}$$

where E_n is the energy eigenvalue corresponding to the eigenstate $|u_n\rangle$.

Problem Two

Show that the density operator $\hat{\rho(t)} \equiv |\psi(t)\rangle\langle\psi(t)|$ satisfies the equation-of-motion

$$i\hbar\frac{d}{dt}\hat{\rho(t)} = [\hat{H},\hat{\rho(t)}].$$

Solution:

$$i\hbar\frac{d}{dt}\left(|\psi(t)\rangle\langle\psi(t)|\right) = \left(i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle\right)\langle\psi(t)| + |\psi(t)\rangle\left(i\hbar\frac{\partial}{\partial t}\langle\psi(t)|\right).$$

Recalling that from the Schrödinger equation, we have the relations

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle \qquad \text{and} \qquad -i\hbar\frac{\partial}{\partial t}\langle\psi(t)| = \langle\psi(t)|\hat{H},$$

the expression can be simplified to yield

$$i\hbar\frac{d}{dt}\hat{\rho(t)} = \hat{H}|\psi(t)\rangle\langle\psi(t)| - |\psi(t)\rangle\langle\psi(t)|\hat{H} = \hat{H}\hat{\rho(t)} - \hat{\rho(t)}\hat{H} = [\hat{H},\hat{\rho(t)}].$$

Problem Three

(a) Calculate the commutator $[\hat{x}, \hat{T}_a]$, where $\hat{T}_a \equiv e^{-ia\hat{p}/\hbar}$.

Solution:
All functions F that can be expressed as a power series in its argument satisfy the generalised commutation relation

$$[\hat{x}, F(\hat{p})] = i\hbar \frac{\partial F}{\partial \hat{p}}.$$

Hence,

$$[\hat{x}, \hat{T}_a] = i\hbar \frac{\partial \hat{T}_a}{\partial \hat{p}} = i\hbar \frac{\partial}{\partial \hat{p}}(e^{-ia\hat{p}/\hbar}) = a e^{-ia\hat{p}/\hbar} = a\hat{T}_a.$$

(b) Show that

$$\hat{T}_a \, \hat{x} \, \hat{T}_a^\dagger = \hat{x} - a\hat{I}.$$

Solution:

$$\hat{T}_a \, \hat{x} \, \hat{T}_a^\dagger = \left(\hat{x}\hat{T}_a - [\hat{x}, \hat{T}_a]\right) \hat{T}_a^\dagger = \hat{x}\hat{T}_a\hat{T}_a^\dagger - a\hat{T}_a\hat{T}_a^\dagger = \hat{x} - a\hat{I},$$

where $\hat{T}_a\hat{T}_a^\dagger = \hat{\mathcal{I}}$ since $\hat{T}_a$ is unitary.

Alternatively, we can also use the Baker–Campbell–Hausdorff lemma

$$e^{\hat{Y}} \, \hat{X} \, e^{-\hat{Y}} = \hat{X} + [\hat{Y}, \hat{X}] + \frac{1}{2!}[\hat{Y}, [\hat{Y}, \hat{X}]] + \frac{1}{3!}[\hat{Y}, [\hat{Y}, [\hat{Y}, \hat{X}]]] + \cdots ,$$

which yields

$$\begin{aligned} \hat{T}_a \, \hat{x} \, \hat{T}_a^\dagger &= \hat{x} + [-ia\hat{p}/\hbar, \hat{x}] + \frac{1}{2!}[-ia\hat{p}/\hbar, [-ia\hat{p}/\hbar, \hat{x}]] + \cdots \\ &= \hat{x} - a\hat{I}, \end{aligned}$$

recognising that the order two and higher commutators all vanish.

Problem Four

A particle is described by the (position-space) wavefunction

$$\psi(x) = \frac{1}{(x - ic)(x + ic)} e^{isx}.$$

Calculate the expectation values of its position and momentum, and show that the uncertainty in the momentum cannot be zero.

Solution:
The probability density is given by

$$|\psi(x)|^2 = \frac{1}{(x^2 + c^2)^2},$$

which is evidently symmetric about $x = 0$, and hence it follows that the expectation value $\langle \hat{x} \rangle$ is zero. For the momentum, we invoke Ehrenfest's theorem,

$$\langle \hat{p} \rangle = m \frac{d}{dt} \langle \hat{x} \rangle ,$$

and find that (unsurprisingly), $\langle \hat{p} \rangle = 0$ as well.

Let us consider the standard deviation of the position of the particle, $\sigma_x \equiv \sqrt{\langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2}$. If σ_x is finite-valued, then by Heisenberg's uncertainty principle, σ_p cannot be zero. Since $\langle \hat{x} \rangle = 0$, it suffices to examine the value of $\langle \hat{x}^2 \rangle$. We have

$$\langle \hat{x}^2 \rangle = \int_{-\infty}^{\infty} \frac{x^2}{(x^2 + c^2)^2} \mathrm{d}x < \int_{-\infty}^{\infty} \frac{x^2 + c^2}{(x^2 + c^2)^2} \mathrm{d}x = \int_{-\infty}^{\infty} \frac{1}{(x^2 + c^2)} \mathrm{d}x = \frac{\pi}{|c|}.$$

Hence, σ_x is finite and we are done.

Problem Five

Evaluate the expression $\langle x;-|\exp\left[i\frac{\pi}{2\hbar}\hat{S}_y\right]$ and express the result in terms of the z-eigenbasis $\langle z;+|$ and $\langle z;-|$.

Solution:

$$\exp\left[i\frac{\pi}{2\hbar}\hat{S}_y\right]=\exp\left[i\frac{\pi}{4}\hat{\sigma}_y\right]=\hat{\mathcal{I}}\cos\left(\frac{\pi}{4}\right)+i\hat{\sigma}_y\sin\left(\frac{\pi}{4}\right)=\frac{1}{\sqrt{2}}\left(\hat{\mathcal{I}}+i\hat{\sigma}_y\right)$$

Casting the desired expression in explicit matrix form, with $\{\langle z;+|,\langle z;-|\}$ as the basis, we obtain

$$\langle x;-|\exp\left[i\frac{\pi}{2\hbar}\hat{S}_y\right]\widehat{=}\frac{1}{\sqrt{2}}\begin{pmatrix}1 & -1\end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ -1 & 1\end{pmatrix}=\begin{pmatrix}1 & 0\end{pmatrix}\equiv\langle z;+|$$

This result could have been anticipated by considering the conjugate expression

$$\left(\langle x;-|\exp\left[i\frac{\pi}{2\hbar}\hat{S}_y\right]\right)^\dagger=\exp\left[-i\frac{\pi}{2\hbar}\hat{S}_y\right]|x;-\rangle=\exp\left[-i\frac{\pi/2}{2}\hat{\sigma}_y\right]|x;-\rangle=\hat{R}_y\left(\pi/2\right)|x;-\rangle,$$

which corresponds to rotating the vector $|x;-\rangle$ clockwise by an angle of $\pi/2$ about the y-axis, and (obviously) results in $|z;+\rangle$.

Problem Six

For the quantum harmonic oscillator, show that the relation $\hat{a}|n\rangle=\gamma|n-1\rangle$ with $\gamma>0$ must imply that $\gamma=\sqrt{n}$.

Solution:
We consider the norm of both sides of the relation to obtain

$$\langle n-1|\gamma^*\gamma|n-1\rangle=|\gamma|^2 \qquad\text{and}\qquad \langle n|\hat{a}^\dagger\hat{a}|n\rangle=\langle n|\hat{n}|n\rangle=n,$$

where $\hat{n}\equiv\hat{a}^\dagger\hat{a}$ is the number operator.

Without any loss of generality, we assume that γ is real and positive, and hence arrive at $\gamma=\sqrt{n}$.

Problem Seven

For a simplified model of a triatomic molecule, the Hamiltonian and position operators have the matrix representations (in the $\{|x_1\rangle, |x_2\rangle, |x_3\rangle\}$ basis)

$$\hat{H} \,\widehat{=}\, \hbar\beta \begin{bmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{bmatrix} \qquad \text{and} \qquad \hat{X} \,\widehat{=}\, a \begin{bmatrix} -1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

The system was prepared in the initial state $|\psi(t=0)\rangle = |x_1\rangle$.

(a) Find the possible energy values and corresponding probabilities at $t = 0$.

Solution:
The eigenvalues and eigenstates of the Hamiltonian are

$$E_1 = -\hbar\beta, |E_1\rangle \,\widehat{=}\, \frac{1}{\sqrt{6}} \begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix}; E_2 = \hbar\beta, |E_2\rangle \,\widehat{=}\, \frac{1}{\sqrt{2}} \begin{bmatrix} -1 \\ 0 \\ 1 \end{bmatrix}; E_3 = 2\hbar\beta, |E_3\rangle \,\widehat{=}\, \frac{1}{\sqrt{3}} \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

Hence the possible measurement outcomes and corresponding probabilities are

$$\begin{aligned} P(E = -\hbar\beta) &= |\langle E_1|\psi(0)\rangle|^2 = 1/6 \\ P(E = \hbar\beta) &= |\langle E_2|\psi(0)\rangle|^2 = 1/2 \\ P(E = 2\hbar\beta) &= |\langle E_3|\psi(0)\rangle|^2 = 1/3 \end{aligned}$$

(b) Find the expectation value and uncertainty of the energy at $t = 0$

Solution:

$$\begin{aligned} \langle \hat{H} \rangle &= (1/6)(-\hbar\beta) + (1/2)(\hbar\beta) + (1/3)(2\hbar\beta) = \hbar\beta \\ \langle \hat{H}^2 \rangle &= (1/6)(-\hbar\beta)^2 + (1/2)(\hbar\beta)^2 + (1/3)(2\hbar\beta)^2 = 2(\hbar\beta)^2 \\ \delta H &\equiv \sqrt{\langle \hat{H}^2 \rangle - \langle \hat{H} \rangle^2} = \hbar\beta \end{aligned}$$

(c) Compute the probability of finding the electron at atom 2 at a later time t.

Solution:

$$|\psi(t)\rangle = \exp\left[-i\hat{H}t/\hbar\right] |\psi(0)\rangle = \sum_i \exp\left[-iE_i t/\hbar\right] |E_i\rangle \langle E_i|\psi(0)\rangle$$

$$\Rightarrow |\langle x_2|\psi(t)\rangle|^2 = \left| \sum_i \exp\left[-iE_i t/\hbar\right] \langle x_2|E_i\rangle \langle E_i|x_1\rangle \right|^2 = \left| -\frac{1}{3}\exp[i\beta t] + \frac{1}{3}\exp[-2i\beta t] \right|^2$$

$$= \frac{2}{9} - \frac{2}{9}\cos(3\beta t) = \frac{4}{9}\sin^2\left(\frac{3}{2}\beta t\right)$$

(d) Find the expectation value and uncertainty of the energy at time t.

Solution:
By conservation of energy, it is quite evident that the expectation value and uncertainty in the energy are independent of time and hence the answer is the same as in part (i).

(e) Are there other times $t > 0$ at which a position measurement will yield $x = -1$ (atom 1) with absolute certainty?

Solution:

$$P(x=-1) = |\langle x_1|\psi(t)\rangle|^2 = \left|\sum_i \exp\left[-iE_i t/\hbar\right] \langle x_1|E_i\rangle \langle E_i|x_1\rangle\right|^2$$

In order for the expression to be unity, we require that all the components share the same phase, that is

$$\exp\left[i\beta t\right] = \exp\left[-i\beta t\right] = \exp\left[-2i\beta t\right]$$

This clearly occurs when $t = 2n\pi/\beta$, $n \in \mathbb{Z}$.

(f) If the system is projected into the most likely energy state at $t = 0$, what is the expectation value of the position?

Solution:
After the measurement, the electron is in the state $|E_2\rangle = \left(-|x_1\rangle + |x_3\rangle\right)/\sqrt{2}$. Since there is equal probability of finding the electron at $x = -1$ (atom 1) and $x = 1$ (atom 3), the expectation value of the position is obviously 0.

Problem Eight

(a) Consider a particle in the ground state in an infinite square square well potential in the region $0 < x < a$. Write down the corresponding normalized wavefunction and energy.

Solution:

$$\psi_1(x) = \begin{cases} \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right) & 0 < x < a \\ 0 & \text{otherwise} \end{cases} \qquad \text{and} \qquad E_1 = \frac{\pi^2 \hbar^2}{2ma^2}$$

(b) The left wall is diabatically moved to the position $x = -a$ so that the well becomes twice as wide.

(i) Write down the eigenfunctions and energies of the particle in the new potential.

Solution:

$$\phi_n(x) = \begin{cases} \sqrt{\frac{1}{a}} \sin\left(\frac{n\pi x}{2a} + \frac{n\pi}{2}\right) & -a < x < a \\ 0 & \text{otherwise} \end{cases} \qquad \text{and} \qquad \mathcal{E}_n = \frac{n^2 \pi^2 \hbar^2}{8ma^2}$$

(ii) Find the probability of finding the particle in the ground state of the new potential

Solution:

$$\begin{aligned} \int_{-a}^{a} \phi_1^*(x)\psi_1(x)\,\mathrm{d}x &= \frac{\sqrt{2}}{a} \int_0^a \cos\left(\frac{\pi x}{2a}\right) \sin\left(\frac{\pi x}{a}\right) \mathrm{d}x = \frac{1}{a\sqrt{2}} \int_0^a \sin\left(\frac{\pi x}{2a}\right) + \sin\left(\frac{3\pi x}{2a}\right) \mathrm{d}x \\ &= \frac{1}{a\sqrt{2}} \left(\frac{2a}{\pi} + \frac{2a}{3\pi}\right) = \frac{4\sqrt{2}}{3\pi} \end{aligned}$$

Hence the probability is given by

$$\text{Prob} = \frac{32}{9\pi^2} \approx 0.360$$

(iii) Find the probability of finding the particle with an energy that is not higher than the original energy it had before the wall was moved.

Solution:
Only the states $\phi_1(x)$ and $\phi_2^{(}x)$ correspond to energies lower than or equal to the original energy. Hence,

$$\text{Prob} = \left| \int_{-a}^{a} \phi_1^*(x)\psi_1(x)\,\mathrm{d}x \right|^2 + \left| \int_{-a}^{a} \phi_2^*(x)\psi_1(x)\,\mathrm{d}x \right|^2 .$$

The first term had already been evaluated in Part (ii). Evaluating the second term explicitly yields

$$\begin{aligned} \int_{-a}^{a} \phi_2^*(x)\psi_1(x)\,\mathrm{d}x &= \frac{\sqrt{2}}{a} \int_0^a -\sin\left(\frac{\pi x}{a}\right) \sin\left(\frac{\pi x}{a}\right) \mathrm{d}x = -\frac{\sqrt{2}}{a} \int_0^a \sin^2\left(\frac{\pi x}{a}\right) \mathrm{d}x \\ &= \frac{\sqrt{2}}{a}\left(\frac{a}{2}\right) = \frac{1}{\sqrt{2}} \end{aligned}$$

Therefore,

$$\text{Prob} = \frac{32}{9\pi^2} + \frac{1}{2} \approx 0.860.$$

Problem Nine

(a) Spin-1/2 particles initially prepared in the state $|y,-\rangle$ are passed through a sequence of Stern-Gerlach selectors picking out the $|x,+\rangle$, $|n,+\rangle$ and $|z,+\rangle$ states respectively, where the second selector is oriented along the direction $\mathbf{n} = \sin\theta\,\mathbf{u}_x + \cos\theta\,\mathbf{u}_y$. What is the fraction of particles leaving the last selector for (i) $\theta = 0$, (ii) $\theta = \pi$ and (iii) $\theta = \pi/2$?

Solution:
The fraction of particles leaving the last selector is given by

$$|\langle y,-|x,+\rangle\,\langle x,+|n,+\rangle\,\langle n,+|z,+\rangle|^2 = \frac{1}{4}\,|\langle x,+|n,+\rangle|^2\,,$$

since $|\langle y,-|x,+\rangle|^2 = |\langle n,+|z,+\rangle|^2 = 1/2$, as $\mathbf{n}$ is orthogonal to the z-axis.

(i) $\theta = 0:\ |\langle x,+|n,+\rangle|^2 = |\langle x,+|y,+\rangle|^2 = 1/2 \Rightarrow \text{Fraction} = 1/8$

(ii) $\theta = \pi:\ |\langle x,+|n,+\rangle|^2 = |\langle x,+|y,-\rangle|^2 = 1/2 \Rightarrow \text{Fraction} = 1/8$

(iii) $\theta = \pi/2:\ |\langle x,+|n,+\rangle|^2 = |\langle x,+|x,+\rangle|^2 = 1 \Rightarrow \text{Fraction} = 1/4$

(b) The atoms leaving the last Stern-Gerlach selector travel at a constant velocity v_0 and enter a box of length L where they are subjected to a magnetic field described by the Hamiltonian $\hat{H} = (\hbar\omega_0/2)\,\hat{\sigma}_y$. What length L is required for all atoms leaving the box to be in the state $|x,+\rangle$?

Solution:

$$\begin{aligned}|\psi(t)\rangle &= \exp\left[i(\omega_0/2)t\right]|y,-\rangle\,\langle y,-|z,+\rangle + \exp\left[-i(\omega_0/2)t\right]|y,+\rangle\,\langle y,+|z,+\rangle \\ &= \frac{1}{\sqrt{2}}\,|y,+\rangle + \left(\exp\left[i\omega_0 t\right]|y,-\rangle\right)\exp\left[-i(\omega_0/2)t\right]\end{aligned}$$

Expressing $|x,+\rangle$ in terms of $|y,\pm\rangle$, we have

$$|x,+\rangle = \frac{1-i}{2}\,|y,+\rangle + \frac{1+i}{2}\,|y,-\rangle = \frac{1}{\sqrt{2}}\left(|y,+\rangle + i\,|y,-\rangle\right)\exp[-i\pi/4]$$

Evidently, we require that $\exp\left[i\omega_0 t\right] = i \ \Rightarrow\ \omega_0 t = (2n+1/2)\pi$ and the required length is

$$L = v_0 t = (2n+1/2)\pi\frac{v_0}{\omega_0}$$

(c) Inside the box, are any of the spin projections a constant of the motion?

Solution:
The spin projection along the y-axis is clearly a constant of the motion since $[\hat{H},\hat{S}_y] = 0$, while the other two are not as $[\hat{H},\hat{S}_x] \neq 0$ and $[\hat{H},\hat{S}_z] \neq 0$. Physically, the Hamiltonian causes the spin to precess about the y-axis.

