1. Find allowed energies of the *half* harmonic oscillator

$$V(x) = \begin{cases} \frac{1}{2}m\omega^2 x^2, & x > 0, \\ \infty, & x < 0. \end{cases}$$

2. A charged particle (mass m, charge q) is moving in a simple harmonic potential (frequency $\omega/2\pi$). In addition, an external electric field $\mathcal{E}_0$ is also present. Write down the hamiltonian of this particle. Find the energy eigenvalues, eigenfunctions. Find the average position of the particle, when it is in one of the stationary states.

3. Assume that the atoms in a CO molecule are held together by a spring. The spacing between the lines of the spectrum of CO molecule is $2170\,\mathrm{cm}^{-1}$. Estimate the spring constant.

4. If the hermite polynomials $H_n(x)$ are defined using the generating function $G(x,s) = \exp\left(-s^2 + 2xs\right)$, that is

$$\exp\left(-s^2 + 2xs\right) = \sum_n \frac{H_n(x)}{n!} s^n,$$

   (a) Show that the Hermite polynomials obey the differential equation

$$H_n''(x) - 2xH_n'(x) + 2nH_n(x) = 0$$

   and the recurrence relation

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x).$$

   (b) Derive Rodrigues' formula

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}.$$

5. Let ϕ_n be the nth stationary state of a particle in harmonic oscillator potential. Given that the lowering operator is

$$\hat{a} = \frac{1}{\sqrt{2\hbar m\omega}} \left(m\omega\hat{X} + i\hat{P}\right).$$

   and $\xi = \sqrt{m\omega/\hbar}x$,

   (a) show that

$$\hat{a} = \frac{1}{\sqrt{2}} \left(\xi + \frac{d}{d\xi}\right).$$

   (b) Show that

$$\hat{a}\phi_n(\xi) = \sqrt{n}\phi_{n-1}(\xi)$$

6. Let $B = \{\phi_n \,|\, n = 0, 1, \ldots\}$ be the set of energy eigenfunctions of the harmonic oscillator. Find the matrix elements of $\hat{X}$ and $\hat{P}$ wrt to basis B

7. Suppose that a harmonic oscillator is in its n^{th} stationary state.

(a) Compute uncertainties σ_x and σ_P in position and momentum. [Hint: To calculate expectation values, first write $\hat{X}$ and $\hat{P}$ in terms of the lowering operator $\hat{a}$ and its adjoint.]

(b) Show that the average kinetic energy is equal to the average potential energy (Virial Theorem).

8. A particle of mass m in the harmonic oscillator potential, starts out at $t = 0$, in the state

$$\Psi(x, 0) = A\,(1 - 2\xi)^2\, e^{-\xi^2}$$

where A is a constant and $\xi = \sqrt{m\omega/\hbar}x$.

(a) What is the average value of energy?

(b) After time T, the wave function is

$$\Psi(x, T) = B\,(1 + 2\xi)^2\, e^{-\xi^2}$$

for some constant B. What is the smallest value of T?

9. Let ϕ_n be eigenstates of the harmonic oscillator. For a given complex number μ, let

$$\chi_\mu = e^{-\frac{|\mu|}{2}} \sum_{n=0}^{\infty} \frac{\mu^n}{\sqrt{n!}} \phi_n.$$

Such states are called *coherent* states.

(a) Show that

$$\hat{a}\chi_\mu = \mu\chi_\mu$$

that is χ_μ is an eigenstate of $\hat{a}$.

(b) If the state of the oscillator is χ_μ, then show that $\sigma_x\sigma_p = \hbar/2$.

(c) The state of the oscillator $\Psi(t = 0) = \chi_\mu$, then show that

$$\Psi(t) = \chi_{\mu'}$$

where $\mu' = e^{-i\omega t}\mu$. That means, if the state of the system, at an instant is a coherent state, then it is a coherent state at all times.

(d) Optional: If you choose the hilbert space to be $L_2(R)$, then show that $|\Psi(x, t)|^2$ is a gaussian wave packet and the wave packet performs a harmonic oscillations without changing the shape.

Solutions:

1. Since $V(x) = \infty$ for $x \leq 0$, $\psi(x) = 0$ for $x \leq 0$. The Schrodinger time-independent equation is then

$$\begin{aligned} -\frac{\hbar^2}{2m}\psi'' + \frac{1}{2}m\omega^2 x^2\psi &= E\psi \qquad x \geq 0 \\ \psi(0) &= 0 \end{aligned}$$

and ψ must be square integrable. This problem is same as usual harmonic oscillator except that we must choose only those eigenfunction which satisfy the bc of the half harmonic oscillator, that is $\psi(0) = 0$. If $\phi_n(x) = H_n(\xi)\exp(-\xi^2/2)$, then we know that ϕ_n satisfies the above de and bc if n is odd. Thus, the energy eigenvalues of the half harmonic oscillator are

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \qquad n = 1, 3, 5, \ldots$$

2. The potential energy can be written as

$$
\begin{aligned}
V(x) &= \frac{1}{2}m\omega^2 x^2 - q\mathcal{E}_0 x \\
&= \frac{1}{2}m\omega^2\left(x - \frac{q\mathcal{E}_0}{m\omega^2}\right)^2 - \frac{q^2\mathcal{E}_0^2}{m\omega^2}
\end{aligned}
$$

Let $x_0 = q\mathcal{E}_0/m\omega^2$ and $H_0 = -q^2\mathcal{E}_0^2/m\omega^2$. Let $x - x_0 = z$ and $H_1 = H - H_0$. Then the hamiltonian

$$H_1 = \frac{P^2}{2m} + \frac{1}{2}m\omega^2 z^2.$$

The eigenvalues of H_1 are $E_n = \left(n + \frac{1}{2}\right)\hbar\omega$, then the eigenvalues of H are $E_n + H_0$. Note H_0 is just a number.

3. Then $\hbar\omega = 2170\,\mathrm{cm}^{-1} = 2170 \times 1.24 \times 10^{-4}\,\mathrm{eV}$. Calculate force constant $K = m\omega^2$.

4. See Arfken.

5. Prove this by using the recurrence relations given in problem 4.

6. Note

$$
\begin{aligned}
\hat{X} &= \sqrt{\frac{\hbar}{2m\omega}}\left(a + a^\dagger\right) \\
\hat{P} &= \tfrac{1}{i}\sqrt{\frac{m\omega\hbar}{2}}\left(a - a^\dagger\right)
\end{aligned}
$$

The matrix elements are

$$
\begin{aligned}
\hat{X}_{mn} &= \left\langle \phi_m, \hat{X}\phi_n \right\rangle \\
&= \sqrt{\frac{\hbar}{2m\omega}}\left\langle \phi_m, \left(a + a^\dagger\right)\phi_n \right\rangle \\
&= \sqrt{\frac{\hbar}{2m\omega}}\left\langle \phi_m, \left(\sqrt{n}\phi_{n-1} + \sqrt{n+1}\phi_{n+1}\right)\right\rangle \\
&= = \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n}\delta_{m,n-1} + \sqrt{n+1}\delta_{m,n+1}\right)
\end{aligned}
$$

Simillarly

$$
\begin{aligned}
\hat{P}_{m,n} &= \left\langle \phi_m, \hat{P}\phi_n \right\rangle \\
&= \sqrt{\frac{m\omega\hbar}{2}}(-i)\left(\sqrt{n}\delta_{m,n-1} - \sqrt{n+1}\delta_{m,n+1}\right)
\end{aligned}
$$

7. Note

$$
\begin{aligned}
\hat{X} &= \sqrt{\frac{\hbar}{2m\omega}}\left(a + a^\dagger\right) \\
\hat{P} &= \tfrac{1}{i}\sqrt{\frac{m\omega\hbar}{2}}\left(a - a^\dagger\right).
\end{aligned}
$$

Then

$$\left\langle \hat{X} \right\rangle = \hat{X}_{n,n} = 0$$

and

$$\left\langle \hat{P} \right\rangle = \hat{P}_{n,n} = 0.$$

Now

$$\begin{aligned}
\left\langle \hat{X}^2 \right\rangle &= \frac{\hbar}{2m\omega} \left\langle \phi_n, \left(a + a^\dagger\right) \left(a + a^\dagger\right) \phi_n \right\rangle \\
&= \frac{\hbar}{2m\omega} \left\langle \phi_n, \left(a^2 + a^{\dagger 2} + aa^\dagger + a^\dagger a\right) \phi_n \right\rangle \\
&= \frac{\hbar}{2m\omega} \left(0 + 0 + (n+1) + n\right) = \frac{\hbar}{2m\omega}(2n+1).
\end{aligned}$$

Simillarly

$$\left\langle \hat{P}^2 \right\rangle = \frac{\hbar m\omega}{2}(2n+1)$$

(a) Thus,

$$\sigma_X \sigma_P = \left(n + \frac{1}{2}\right)\hbar$$

(b) Note:

$$\langle K \rangle = \frac{1}{2m} \left\langle \hat{P}^2 \right\rangle = \frac{\hbar\omega}{2}(n + \frac{1}{2})$$

and

$$\langle V \rangle = \frac{1}{2} m\omega^2 \left\langle \hat{X}^2 \right\rangle = \frac{\hbar\omega}{2}(n + \frac{1}{2})$$

8. Now,

$$\psi(x, 0) = \frac{1}{5}\left(3\phi_0 - 2\sqrt{2}\phi_1 + 2\sqrt{2}\phi_2\right)$$

where ϕ_n is the nth eigenfunction of energy operator.

(a) The average energy

$$\begin{aligned}
\langle E \rangle &= \frac{1}{25}\left(9E_0 + 8E_1 + 8E_2\right) \\
&= \left(\frac{1}{2} + \frac{24}{25}\right)\hbar\omega.
\end{aligned}$$

(b) After time T

$$\begin{aligned}
\psi(x, T) &= B\left(1 + 2\xi^2\right)e^{-\xi^2} \\
\frac{1}{5}\left(3\phi_0 e^{-i\omega T/2} - 2\sqrt{2}\phi_1 e^{-i\omega 3T/2} + 2\sqrt{2}\phi_2 e^{-i\omega 5T/2}\right) &= \frac{1}{5}\left(3\phi_0 + 2\sqrt{2}\phi_1 + 2\sqrt{2}\phi_2\right)
\end{aligned}$$

Must find T such that $e^{-i\omega T/2} = e^{-i5\omega T/2} = 1$ and $e^{-i3\omega T/2} = -1$. when, $\omega T = \pi$,

$$\begin{aligned}
\exp\left(-i\omega T/2\right) &= -i \\
\exp\left(-i3\omega T/2\right) &= i \\
\exp\left(-i\omega T/2\right) &= -i
\end{aligned}$$

This will do.

9. Given:

$$\chi_\mu = e^{-\frac{|\mu|^2}{2}} \sum_{n=0}^{\infty} \frac{\mu^n}{\sqrt{n!}}\phi_n$$

(a) Now

$$\begin{aligned}
\hat{a}\chi_\mu &= e^{-\frac{|\mu|^2}{2}} \sum_{n=0}^{\infty} \frac{\mu^n}{\sqrt{n!}} \hat{a}\phi_n \\
&= e^{-\frac{|\mu|^2}{2}} \sum_{n=1}^{\infty} \frac{\mu^n}{\sqrt{n!}} n\phi_{n-1} \\
&= \mu e^{-\frac{|\mu|^2}{2}} \sum_{n=1}^{\infty} \frac{\mu^{n-1}}{\sqrt{(n-1)!}} \phi_{n-1} \\
&= \mu\chi_\mu
\end{aligned}$$

Interestingly, χ_μ is not an eigenstate of $\hat{a}^\dagger$.

(b) First note:

$$\begin{aligned}
\langle \chi_\mu, \chi_\mu \rangle &= e^{-|\mu|^2} \sum_{n=0}^{\infty} \frac{(\bar{\mu})^n}{\sqrt{n!}} \frac{\mu^m}{\sqrt{m!}} \langle \phi_n, \phi_m \rangle \\
&= e^{-|\mu|^2} \sum_{n=0}^{\infty} \frac{(\bar{\mu})^n}{\sqrt{n!}} \frac{\mu^m}{\sqrt{m!}} \delta_{m,n} \\
&= e^{-|\mu|^2} \sum_{n=0}^{\infty} \frac{|\mu|^{2n}}{n!} = 1
\end{aligned}$$

Then,

$$\begin{aligned}
\langle \chi_\mu, \hat{a}\chi_\mu \rangle &= \mu \\
\left\langle \chi_\mu, \hat{a}^\dagger \chi_\mu \right\rangle &= \langle \hat{a}\chi_\mu, \chi_\mu \rangle = \bar{\mu}.
\end{aligned}$$

Now, $\hat{X} = \sqrt{\frac{\hbar}{2m\omega}} \left(\hat{a} + \hat{a}^\dagger\right)$,

$$\begin{aligned}
\left\langle \chi_\mu, \hat{X}\chi_\mu \right\rangle &= \sqrt{\frac{\hbar}{2m\omega}} \left\langle \chi_\mu, \left(\hat{a} + \hat{a}^\dagger\right) \chi_\mu \right\rangle \\
&= \sqrt{\frac{\hbar}{2m\omega}} \left(\mu + \bar{\mu}\right) = \sqrt{\frac{2\hbar}{m\omega}} \left(\mathrm{Re}\mu\right)
\end{aligned}$$

And, $\hat{X}^2 = \frac{\hbar}{2m\omega} \left(\hat{a} + \hat{a}^\dagger\right)^2 = \frac{\hbar}{2m\omega} \left(\hat{a}^2 + \left(\hat{a}^\dagger\right)^2 + 2\hat{a}^\dagger\hat{a} + 1\right)$, so

$$\begin{aligned}
\left\langle \hat{X}^2 \right\rangle &= \frac{\hbar}{2m\omega} \left(\mu^2 + \bar{\mu}^2 + 2|\mu|^2 + 1\right) \\
&= \frac{\hbar}{2m\omega} \left((2\mathrm{Re}\mu)^2 + 1\right)
\end{aligned}$$

Finally,

$$\begin{aligned}
\sigma_x^2 &= \frac{\hbar}{2m\omega} \left((2\mathrm{Re}\mu)^2 + 1\right) - \frac{2\hbar}{m\omega} \left(\mathrm{Re}\mu\right)^2 \\
&= \frac{\hbar}{2m\omega}
\end{aligned}$$

Now, simillary, $\sigma_p^2 = \frac{\hbar^2}{2} \left(\frac{m\omega}{\hbar}\right)$ and

$$\sigma_x \sigma_p = \frac{\hbar}{2}.$$

Here the product of uncertainties is as minimum as it can get!

(c) If $\Psi(0) = \chi_\mu$, then

$$\begin{aligned}
\Psi(t) &= e^{-\frac{|\mu|^2}{2}} \sum_{n=0}^{\infty} \frac{\mu^n}{\sqrt{n!}} e^{-i\omega(n+\frac{1}{2})t} \phi_n \\
&= e^{-i\omega t/2} e^{-\frac{|\mu|^2}{2}} \sum_{n=0}^{\infty} \frac{\left(\mu e^{-i\omega t}\right)^n}{\sqrt{n!}} \phi_n \\
&= e^{-i\omega t/2} \chi_{\mu'}
\end{aligned}$$

where $\mu' = \mu e^{-i\omega t}$.

(d) Now if we write $\chi_\mu(x)$ in space represenetation, we need to substitute

$$\begin{aligned}
\phi_n(x) &= \left(\frac{\alpha}{\sqrt{\pi}}\right)^{1/2} \frac{1}{\sqrt{2^n n!}} e^{-\xi^2/2} H_n(\xi) \\
&= = \left(\frac{\alpha}{\sqrt{\pi}}\right)^{1/2} \frac{(-1)^n}{\sqrt{2^n n!}} e^{\xi^2/2} \frac{d^n}{dx^n} e^{-\xi^2}
\end{aligned}$$

using Rodrigue's formular for Hermite polynomials.

$$\begin{aligned}
\Psi(x,t) &= \left(\frac{\alpha}{\sqrt{\pi}}\right)^{1/2} e^{-i\omega t/2} e^{-\frac{|\mu|^2}{2}} e^{\xi^2/2} \sum_{n=0}^{\infty} \frac{(-1)^n}{\sqrt{2^n n!}} \frac{\left(\mu e^{-i\omega t}\right)^n}{\sqrt{n!}} \frac{d^n}{dx^n} e^{-\xi^2} \\
&= \left(\frac{\alpha}{\sqrt{\pi}}\right)^{1/2} e^{-i\omega t/2} e^{-\frac{|\mu|^2-\xi^2}{2}} e^{-(\xi-\eta)^2}
\end{aligned}$$

Use Taylor expansion for the last step and $\eta = |\mu| \exp(-i(\omega t - x))/\sqrt{2}$. Now

$$\begin{aligned}
|\Psi(x,t)|^2 &= \frac{\alpha}{\sqrt{\pi}} e^{-|\mu|^2+\xi^2} e^{-(\xi-\eta)^2} e^{-(\xi-\bar{\eta})^2} \\
&= \frac{\alpha}{\sqrt{\pi}} e^{-\left(\xi-\sqrt{2}|\mu|\cos(\omega t - \mathrm{Arg}\mu)\right)^2}
\end{aligned}$$

This is a gaussian wave packet performing simple harmonic motion with frequency ω and amplitude $A = \sqrt{2\hbar/m\omega}|\mu|$. Now show that the average energy of this state is

$$E_\Psi - \frac{1}{2}\hbar\omega = \frac{1}{2} m\omega^2 A^2.$$