Quantum Mechanics II, Coursework 1

Jiaru (Eric) Li (CID: 02216531)

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Question 1

(a) We are given that $\phi(x) = Axe^{-x^2/a^2}$, which must satisfy the normalisation condition

$$\int_{-\infty}^{\infty} |\phi(x)|^2 \mathrm{d}x = 1.$$

We have $|\phi(x)|^2 = A^2x^2e^{-2x^2/a^2}$, and by setting $\alpha = 2/a^2$, we get

$$\begin{aligned}\int_{-\infty}^{\infty} A^2x^2e^{-2x^2/a^2}\mathrm{d}x &= A^2\int_{-\infty}^{\infty} x^2e^{-\alpha x^2}\mathrm{d}x \\ &= -A^2\int_{-\infty}^{\infty} \frac{\mathrm{d}}{\mathrm{d}\alpha}\left(e^{-\alpha x^2}\right)\mathrm{d}x \\ &= -A^2\frac{\mathrm{d}}{\mathrm{d}\alpha}\int_{-\infty}^{\infty} e^{-\alpha x^2}\mathrm{d}x,\end{aligned}$$

where we recall the Gaussian integral

$$\int_{-\infty}^{\infty} e^{-\alpha x^2}\mathrm{d}x = \sqrt{\frac{\pi}{\alpha}}.$$

This gives

$$\frac{\mathrm{d}}{\mathrm{d}\alpha}\int_{-\infty}^{\infty} e^{-\alpha x^2}\mathrm{d}x = -\frac{\sqrt{\pi}}{2}\alpha^{-3/2} = -\frac{a^3\sqrt{\pi}}{2^{5/2}}.$$

Substituting into the normalisation condition gives

$$\begin{aligned}\left(-A^2\right)\left(-\frac{a^3\sqrt{\pi}}{2^{5/2}}\right) &= 1 \\ A^2 &= \frac{2^{5/2}}{a^3\sqrt{\pi}},\end{aligned}$$

so we take A to be

$$\boxed{A = \frac{2^{5/4}}{a^{3/2}\pi^{1/4}}}.$$

(b) To compute $\tilde{\phi}(p)$ in the momentum basis, we use the Fourier transform relation, namely

$$\tilde{\phi}(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} \phi(x)e^{-\mathrm{i}xp/\hbar}\mathrm{d}x.$$

Recall the standard definition of Fourier transform in the form of

$$\mathcal{F}\{f(x)\}(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(x)e^{-\mathrm{i}kx}\mathrm{d}x.$$

Therefore, by setting $k = p/\hbar$, we get

$$\tilde{\phi}(p) = \frac{1}{\sqrt{\hbar}} \mathcal{F}\{\phi(x)\}(k).$$

To compute the Fourier transform of $\phi(x) = Ax\mathrm{e}^{-x^2/a^2}$, we recall a property of Fourier transform

$$\mathcal{F}\{xf(x)\}(k) = \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}k} \left(\mathcal{F}\{f(x)\}(k)\right),$$

and we already know the Fourier transform of a Gaussian function $f(x) = \mathrm{e}^{-\alpha x^2}$ as

$$\mathcal{F}\{f(x)\}(k) = \sqrt{\frac{1}{2\alpha}} \mathrm{e}^{-k^2/4\alpha}.$$

We then have

$$\begin{aligned}
\mathcal{F}\{\phi(x)\}(k) &= \mathrm{i}A\frac{\mathrm{d}}{\mathrm{d}k} \left(\mathcal{F}\left\{\mathrm{e}^{-x^2/a^2}\right\}(k)\right) \\
&= \mathrm{i}A\frac{\mathrm{d}}{\mathrm{d}k} \left(\frac{a}{\sqrt{2}}\mathrm{e}^{-a^2k^2/4}\right) \\
&= \mathrm{i}A\frac{a}{\sqrt{2}}\mathrm{e}^{-a^2k^2/4}\left(-\frac{a^2k}{2}\right),
\end{aligned}$$

so by plugging A from part (a) in, we get

$$\begin{aligned}
\mathcal{F}\{\phi(x)\}(k) &= -\mathrm{i}\frac{2^{5/4}}{a^{3/2}\pi^{1/4}} \frac{a}{\sqrt{2}} \frac{a^2}{2} \cdot k\mathrm{e}^{-a^2k^2/4} \\
&= -\mathrm{i}\frac{a^{3/2}}{(2\pi)^{1/4}} k\mathrm{e}^{-a^2k^2/4} \\
&= -\mathrm{i}\frac{a^{3/2}}{\hbar\,(2\pi)^{1/4}} p\mathrm{e}^{-a^2p^2/4\hbar^2},
\end{aligned}$$

which gives the final answer

$$\boxed{\tilde{\phi}(p) = -\mathrm{i}\frac{(a/\hbar)^{3/2}}{(2\pi)^{1/4}} p\mathrm{e}^{-a^2p^2/4\hbar^2}}.$$

(c) Again recall the Fourier transform relation between $\phi(x)$ and $\tilde{\phi}(p)$ given as

$$\tilde{\phi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \phi(x)\mathrm{e}^{-\mathrm{i}xp/\hbar}\mathrm{d}x.$$

Therefore, we have

$$\tilde{\phi}(-p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \phi(x)\mathrm{e}^{\mathrm{i}xp/\hbar}\mathrm{d}x,$$

so if we substitute $x = -u$ into the integral and use the identity $\phi(x) = \phi(-x)$ given, we get

$$\begin{aligned}
\tilde{\phi}(-p) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{\infty}^{-\infty} \phi(-u)\mathrm{e}^{-\mathrm{i}up/\hbar}(-\mathrm{d}u) \\
&= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \phi(u)\mathrm{e}^{-\mathrm{i}up/\hbar}\mathrm{d}u \\
&= \tilde{\phi}(p),
\end{aligned}$$

which implies that $\boxed{\tilde{\phi}(p) \text{ is also even}}$.

(d) We are now given the condition $\phi(x) = [\phi(-x)]^*$ where a^* denotes the complex conjugate of a. Recall again that

$$\tilde{\phi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \phi(x) \mathrm{e}^{-\mathrm{i}xp/\hbar} \mathrm{d}x.$$

The complex conjugate of $\tilde{\phi}(p)$ is given by

$$\begin{aligned}
\left[\tilde{\phi}(p)\right]^* &= \left[\frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \phi(x) \mathrm{e}^{-\mathrm{i}xp/\hbar} \mathrm{d}x\right]^* \\
&= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \left[\phi(x) \mathrm{e}^{-\mathrm{i}xp/\hbar}\right]^* \mathrm{d}x \\
&= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} [\phi(x)]^* \, \mathrm{e}^{\mathrm{i}xp/\hbar} \mathrm{d}x,
\end{aligned}$$

where we have used the identity $(e^z)^* = e^{z^*}$.

We can then substitute $x = -u$ into the integral, giving

$$\begin{aligned}
\left[\tilde{\phi}(p)\right]^* &= \frac{1}{\sqrt{2\pi\hbar}} \int_{\infty}^{-\infty} [\phi(-u)]^* \, \mathrm{e}^{-\mathrm{i}up/\hbar} (-\mathrm{d}u) \\
&= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \phi(u) \mathrm{e}^{-\mathrm{i}up/\hbar} \mathrm{d}u,
\end{aligned}$$

which is precisely the definition of $\tilde{\phi}(p)$.

This implies that the complex conjugate of $\tilde{\phi}(p)$ equals to itself, i.e., $\boxed{\tilde{\phi}(p) \text{ is real}}$.

Question 2

(a) The rotation operator $\hat{R}$ is given by $\hat{R} = |3\rangle\langle 1| + |1\rangle\langle 2| + |2\rangle\langle 3|$, so its Hermitian conjugate $\hat{R}^\dagger$ is $\hat{R}^\dagger = |1\rangle\langle 3| + |2\rangle\langle 1| + |3\rangle\langle 2|$.

By using the basic fact that $\langle a|b\rangle = 1$ when $a = b$ and 0 otherwise, we can then verify that

$$\begin{aligned}
\hat{R}^\dagger \hat{R} &= (|3\rangle\langle 1| + |1\rangle\langle 2| + |2\rangle\langle 3|) \cdot (|1\rangle\langle 3| + |2\rangle\langle 1| + |3\rangle\langle 2|) \\
&= |3\rangle\langle 1|1\rangle\langle 3| + |3\rangle\langle 1|2\rangle\langle 1| + |3\rangle\langle 1|3\rangle\langle 2| + \\
&\quad |1\rangle\langle 2|1\rangle\langle 3| + |1\rangle\langle 2|2\rangle\langle 1| + |1\rangle\langle 2|3\rangle\langle 2| + \\
&\quad |2\rangle\langle 3|1\rangle\langle 3| + |2\rangle\langle 3|2\rangle\langle 1| + |2\rangle\langle 3|3\rangle\langle 2| \\
&= |3\rangle\langle 3| + |1\rangle\langle 1| + |2\rangle\langle 2| = I.
\end{aligned}$$

Similarly, the reflection operator $\hat{\sigma} = |1\rangle\langle 2| + |2\rangle\langle 1| + |3\rangle\langle 3|$ has Hermitian conjugate $\hat{\sigma}^\dagger = |2\rangle\langle 1| + |1\rangle\langle 2| + |3\rangle\langle 3|$ and satisfies

$$\begin{aligned}
\hat{\sigma}^\dagger \hat{\sigma} &= (|1\rangle\langle 2| + |2\rangle\langle 1| + |3\rangle\langle 3|)(|2\rangle\langle 1| + |1\rangle\langle 2| + |3\rangle\langle 3|) \\
&= |1\rangle\langle 2|2\rangle\langle 1| + |1\rangle\langle 2|1\rangle\langle 2| + |1\rangle\langle 2|3\rangle\langle 3| + \\
&\quad |2\rangle\langle 1|2\rangle\langle 1| + |2\rangle\langle 1|1\rangle\langle 2| + |2\rangle\langle 1|3\rangle\langle 3| + \\
&\quad |3\rangle\langle 3|2\rangle\langle 1| + |3\rangle\langle 3|1\rangle\langle 2| + |3\rangle\langle 3|3\rangle\langle 3| \\
&= |1\rangle\langle 1| + |2\rangle\langle 2| + |3\rangle\langle 3| = I.
\end{aligned}$$

We have therefore shown that $\boxed{\hat{R}, \hat{\sigma} \text{ are unitary}}$.

To prove commutativity with the Hamiltonian $\hat{\mathcal{H}}$ given, recall that

$$\hat{\mathcal{H}} = -w[|1\rangle\langle 2| + |2\rangle\langle 3| + |3\rangle\langle 1| + \text{h.c.}].$$

Note that we have

$$\hat{R}\,|1\rangle = (|3\rangle\langle 1| + |1\rangle\langle 2| + |2\rangle\langle 3|)\,|1\rangle = |3\rangle\,,$$
$$\hat{R}\,|2\rangle = (|3\rangle\langle 1| + |1\rangle\langle 2| + |2\rangle\langle 3|)\,|2\rangle = |1\rangle\,,$$
$$\hat{R}\,|3\rangle = (|3\rangle\langle 1| + |1\rangle\langle 2| + |2\rangle\langle 3|)\,|3\rangle = |2\rangle\,,$$

so $\hat{R}$ is essentially a cyclic permutation that maps $\{1,2,3\}$ to $\{3,1,2\}$, leaving $\hat{\mathcal{H}}$ unchanged.
Intuitively, if we think of $\hat{\mathcal{H}}$ as describing a particle that can jump between vertices of an equilateral triangle, as given in the problem, then $\hat{R}$ is a 120° rotation.
Similarly, we can also write

$$\hat{\sigma}\,|1\rangle = (|1\rangle\langle 2| + |2\rangle\langle 1| + |3\rangle\langle 3|)\,|1\rangle = |2\rangle\,,$$
$$\hat{\sigma}\,|2\rangle = (|1\rangle\langle 2| + |2\rangle\langle 1| + |3\rangle\langle 3|)\,|2\rangle = |1\rangle\,,$$
$$\hat{\sigma}\,|3\rangle = (|1\rangle\langle 2| + |2\rangle\langle 1| + |3\rangle\langle 3|)\,|3\rangle = |3\rangle\,,$$

so $\hat{\sigma}$ only swaps 1 and 2, which again preserves the symmetry of $\hat{\mathcal{H}}$.
Intuitively, $\hat{\sigma}$ is a reflection with the axis being the median from the vertex with label 3.

We have now proven that $\boxed{\hat{R}, \hat{\sigma} \text{ commutes with } \hat{\mathcal{H}}}$.

From the geometric picture given, and by looking at the structure of the Hamiltonian, we could find another two distinct unitary symmetry operators, which are basically the other two reflections,

$$\hat{\sigma}_1 = |2\rangle\langle 3| + |3\rangle\langle 2| + |1\rangle\langle 1|\,,$$
$$\hat{\sigma}_2 = |1\rangle\langle 3| + |3\rangle\langle 1| + |2\rangle\langle 2|\,,$$

in addition to the (trivial) identity operator.

(In fact, in the language of group theory, these symmetries form a dihedral group of order 6*,* D_6*. This group has* 6 *elements: one identity; two* 120° *rotations, clockwise and anticlockwise (corresponding to* $\hat{R}$ *and* $\hat{R}^\dagger$*); and three reflections. The fact that* D_6 *is isomorphic to the symmetric group of order 3,* S_3*, tells us about the symmetry of the Hamiltonian in an elegant way.)*

(b) From part (a), we can write $\hat{R}$ and $\hat{\sigma}$ in matrix form with respect to the given basis $\{|1\rangle, |2\rangle, |3\rangle\}$ as permutation matrices,

$$\hat{R} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \quad \hat{\sigma} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

To find the eigenvalues of $\hat{R}$, we compute

$$\begin{aligned} \det\left(\hat{R} - \lambda I\right) &= \begin{vmatrix} -\lambda & 1 & 0 \\ 0 & -\lambda & 1 \\ 1 & 0 & -\lambda \end{vmatrix} \\ &= -\lambda \begin{vmatrix} -\lambda & 1 \\ 0 & -\lambda \end{vmatrix} - \begin{vmatrix} 0 & 1 \\ 1 & -\lambda \end{vmatrix} \\ &= -\lambda^3 + 1, \end{aligned}$$

whose roots are the third roots of unity $\boxed{1, \omega, \omega^2}$ where $\omega = \mathrm{e}^{2\pi \mathrm{i}/3}$. These are the eigenvalues required.

The corresponding eigenvectors v_i for $i = 1,2,3$ must satisfy $\hat{R}v_i = \lambda v_i$, and so by letting $v_i = \begin{pmatrix} a \\ b \\ c \end{pmatrix}$, we get $\hat{R}v_i = \begin{pmatrix} c \\ a \\ b \end{pmatrix}$ and $\lambda v_i = \begin{pmatrix} \lambda a \\ \lambda b \\ \lambda c \end{pmatrix}$, and we have

$$\begin{cases} c = \lambda a, \\ a = \lambda b, \\ b = \lambda c. \end{cases}$$

For $\lambda = 1$, one possible solution is $(a, b, c) = (1, 1, 1)$. For $\lambda = \omega$, one possible solution is $(a, b, c) = \left(1, \omega, \omega^2\right)$. For $\lambda = \omega^2$, one possible solution is $(a, b, c) = \left(1, \omega^2, \omega\right)$.

The eigenstates of $\hat{R}$ can therefore be expressed as

$$\begin{aligned}
|\phi_1\rangle &= |1\rangle + |2\rangle + |3\rangle\,, \\
|\phi_2\rangle &= |1\rangle + \omega\,|2\rangle + \omega^2\,|3\rangle\,, \\
|\phi_3\rangle &= |1\rangle + \omega^2\,|2\rangle + \omega\,|3\rangle\,,
\end{aligned}$$

so an eigenbasis is given by $\boxed{\{|\phi_1\rangle\,, |\phi_2\rangle\,, |\phi_3\rangle\}}$.

Now we return to the Hamiltonian given,

$$\hat{\mathcal{H}} = -w[|1\rangle\langle 2| + |2\rangle\langle 3| + |3\rangle\langle 1| + \text{h.c.}].$$

We observe that this can alternatively be written as $\hat{\mathcal{H}} = -w\left(\hat{R} + \hat{R}^\dagger\right) = -w\left(\hat{R} + \hat{R}^2\right)$.

Therefore, we have

$$\begin{aligned}
\hat{\mathcal{H}}\,|\phi_i\rangle &= -w\left(\hat{R} + \hat{R}^2\right)|\phi_i\rangle \\
&= -w\left(\lambda + \lambda^2\right)|\phi_i\rangle\,.
\end{aligned}$$

Since $\lambda + \lambda^2$ can take values of $1 + 1^2 = 2, \omega + \omega^2 = -1$ and $\omega^2 + \left(\omega^2\right)^2 = -1$, the three eigenvalues of $\hat{\mathcal{H}}$ are given by $\boxed{-2w, w, w}$ under the same eigenbasis.

We then return our attention to $\hat{\sigma} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$. This matrix has eigenvalues μ such that

$$\begin{aligned}
\det\left(\hat{\sigma} - \mu I\right) &= \begin{vmatrix} -\mu & 1 & 0 \\ 1 & -\mu & 0 \\ 0 & 0 & 1-\mu \end{vmatrix} \\
&= -\mu\begin{vmatrix} -\mu & 0 \\ 0 & 1-\mu \end{vmatrix} - \begin{vmatrix} 1 & 0 \\ 0 & 1-\mu \end{vmatrix} \\
&= \mu^2(1-\mu) - (1-\mu) \\
&= -(1-\mu)^2(1+\mu),
\end{aligned}$$

which has roots $\mu = 1, 1, -1$. These correspond to eigenvectors $u_i = \begin{pmatrix} a \\ b \\ c \end{pmatrix}$, so $\hat{\sigma} u_i = \begin{pmatrix} b \\ a \\ c \end{pmatrix}$ and $\mu u_i = \begin{pmatrix} \mu a \\ \mu b \\ \mu c \end{pmatrix}$, and we have

$$\begin{cases} b = \mu a, \\ a = \mu b, \\ c = \mu c. \end{cases}$$

For $\mu = 1$, we have $a = b$ and c is arbitrary. For $\mu = -1$, we need $a = -b$ and $c = 0$. Therefore, the eigenstates of $\hat{\sigma}$ takes the form of $|\psi_1\rangle = |1\rangle - |2\rangle$ and $|\psi_{2,3}\rangle = a(|1\rangle + |2\rangle) + b\,|3\rangle$, where a and b are constants.

We now compute

$$\begin{aligned}
\hat{\mathcal{H}}\,|\psi_{2,3}\rangle &= -w[|1\rangle\langle 2| + |2\rangle\langle 3| + |3\rangle\langle 1| + \text{h.c.}][a(|1\rangle + |2\rangle) + b\,|3\rangle] \\
&= -w(a\,|1\rangle\langle 2|1\rangle + a\,|1\rangle\langle 2|2\rangle + b\,|1\rangle\langle 2|3\rangle + a\,|2\rangle\langle 3|1\rangle + a\,|2\rangle\langle 3|2\rangle + b\,|2\rangle\langle 3|3\rangle + \\
&\qquad a\,|3\rangle\langle 1|1\rangle + a\,|3\rangle\langle 1|2\rangle + b\,|3\rangle\langle 1|3\rangle + a\,|2\rangle\langle 1|1\rangle + a\,|2\rangle\langle 1|2\rangle + b\,|2\rangle\langle 1|3\rangle + \\
&\qquad a\,|3\rangle\langle 2|1\rangle + a\,|3\rangle\langle 2|2\rangle + b\,|3\rangle\langle 2|3\rangle + a\,|1\rangle\langle 3|1\rangle + a\,|1\rangle\langle 3|2\rangle + b\,|1\rangle\langle 3|3\rangle \\
&= -w((a+b)\,|1\rangle + (a+b)\,|2\rangle + 2a\,|3\rangle).
\end{aligned}$$

Within the same eigenbasis, we have $\hat{\mathcal{H}}\,|\psi_{2,3}\rangle = \lambda\,|\psi_{2,3}\rangle$. By comparison, we get $\lambda a = -w(a+b)$ and $\lambda b = -2aw$. Recall that the three eigenvalues of $\hat{\mathcal{H}}$ are given by $-2w, w, w$. For $\lambda = -2w$, the solutions are $b = a$; for $\lambda = w$, the solutions are $b = -2a$.

The eigenstates of $\hat{\sigma}$ can therefore be expressed as

$$\begin{aligned} |\psi_1\rangle &= |1\rangle - |2\rangle\,, \\ |\psi_2\rangle &= |1\rangle + |2\rangle + |3\rangle\,, \\ |\psi_2\rangle &= |1\rangle + |2\rangle - 2\,|3\rangle\,, \end{aligned}$$

so an eigenbasis is given by $\boxed{\{|\psi_1\rangle\,, |\psi_2\rangle\,, |\psi_3\rangle\}}$.

(c) We have already calculated that

$$\hat{R} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \quad \hat{\sigma} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

so we could compute

$$\hat{R}\hat{\sigma} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \hat{\sigma}\hat{R} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix},$$

and therefore

$$\left[\hat{R}, \hat{\sigma}\right] = \hat{R}\hat{\sigma} - \hat{\sigma}\hat{R} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} = \boxed{\begin{pmatrix} 1 & 0 & -1 \\ 0 & -1 & 1 \\ -1 & 1 & 0 \end{pmatrix}}.$$

Note that $|\phi\rangle = |1\rangle + |2\rangle + |3\rangle$ is a common eigenstate for both $\hat{R}$,$\hat{\mathcal{H}}$ and $\hat{\sigma}$,$\hat{\mathcal{H}}$. We have

$$\begin{pmatrix} 1 & 0 & -1 \\ 0 & -1 & 1 \\ -1 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix},$$

So we have $\boxed{\left[\hat{R}, \hat{\sigma}\right] |\phi\rangle = 0}$. This is consistent with Section 3.2 of the notes: while $\left[\hat{R}, \hat{\sigma}\right] \neq 0$, we do have $\left[\hat{R}, \hat{\sigma}\right] |\phi\rangle = 0$ for the non-degenerate eigenstate $|\phi\rangle$, verifying the relation between symmetry and degeneracy.

Question 3

(a) We start with the 1d harmonic oscillator Hamiltonian

$$\hat{\mathcal{H}} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right),$$

where the ladder operators $\hat{a}^\dagger$ and $\hat{a}$ satisfy $\left[\hat{a}, \hat{a}^\dagger\right] = 1$.

Therefore, we have

$$\left[\hat{a}, \hat{\mathcal{H}}\right] = \hbar\omega\left[\hat{a}, \hat{a}^\dagger\hat{a}\right] = \hbar\omega\left(\left[\hat{a}, \hat{a}^\dagger\right]\hat{a} + \hat{a}^\dagger\left[\hat{a}, \hat{a}\right]\right) = \hbar\omega\hat{a}.$$

In the Heisenberg picture, the equation of motion for the ladder operator $\hat{a}_{\mathrm{H}}$ is given by

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\hat{a}_{\mathrm{H}}(t) = \hat{\mathcal{U}}^\dagger\left[\hat{a}, \hat{\mathcal{H}}\right]\hat{\mathcal{U}} = \hbar\omega\hat{\mathcal{U}}^\dagger\hat{a}\hat{\mathcal{U}} = \hbar\omega\hat{a}_{\mathrm{H}}(t), \quad \hat{a}_{\mathrm{H}}(0) = \hat{a},$$

which can be solved to give $\hat{a}_{\mathrm{H}}(t) = \mathrm{e}^{-\mathrm{i}\omega t}\hat{a}$. Thus, we also have $\hat{a}_{\mathrm{H}}^{\dagger}(t) = \mathrm{e}^{\mathrm{i}\omega t}\hat{a}^{\dagger}$.

Recall that we have

$$\hat{a}\left|\phi_0\right\rangle = 0, \quad \hat{a}\left|\phi_1\right\rangle = \left|\phi_0\right\rangle, \quad \hat{a}^{\dagger}\left|\phi_0\right\rangle = \left|\phi_1\right\rangle, \quad \hat{a}^{\dagger}\left|\phi_1\right\rangle = \sqrt{2}\left|\phi_2\right\rangle,$$

where $\left|\phi_0\right\rangle$ and $\left|\phi_1\right\rangle$ are the ground and first excited states of the Hamiltonian.

Therefore, we have

$$\left\langle\phi_0\right|\hat{a}\left|\phi_0\right\rangle = \left\langle\phi_1\right|\hat{a}\left|\phi_1\right\rangle = \left\langle\phi_1\right|\hat{a}\left|\phi_0\right\rangle = 0, \quad \left\langle\phi_0\right|\hat{a}\left|\phi_1\right\rangle = \left\langle\phi_0|\phi_0\right\rangle = 1,$$
$$\left\langle\phi_0\right|\hat{a}^{\dagger}\left|\phi_0\right\rangle = \left\langle\phi_1\right|\hat{a}^{\dagger}\left|\phi_1\right\rangle = \left\langle\phi_0\right|\hat{a}^{\dagger}\left|\phi_1\right\rangle = 0, \quad \left\langle\phi_1\right|\hat{a}^{\dagger}\left|\phi_0\right\rangle = \left\langle\phi_1|\phi_1\right\rangle = 1.$$

Since the initial state is given as $\left|\psi(0)\right\rangle = \left(\left|\phi_0\right\rangle + \left|\phi_1\right\rangle\right)/\sqrt{2}$, the expectation value of $\hat{a}$ and $\hat{a}^{\dagger}$ at time t can be found as

$$\begin{aligned}
\left\langle\hat{a}\right\rangle(t) &= \left\langle\psi(0)\right|\hat{a}_{\mathrm{H}}(t)\left|\psi(0)\right\rangle = \mathrm{e}^{-\mathrm{i}\omega t}\left\langle\psi(0)\right|\hat{a}\left|\psi(0)\right\rangle = \frac{\mathrm{e}^{-\mathrm{i}\omega t}}{2}\left\langle\left(\left|\phi_0\right\rangle + \left|\phi_1\right\rangle\right)\right|\hat{a}\left|\left(\left|\phi_0\right\rangle + \left|\phi_1\right\rangle\right)\right\rangle \\
&= \frac{\mathrm{e}^{-\mathrm{i}\omega t}}{2}\left(\left\langle\phi_0\right|\hat{a}\left|\phi_0\right\rangle + \left\langle\phi_1\right|\hat{a}\left|\phi_1\right\rangle + \left\langle\phi_0\right|\hat{a}\left|\phi_1\right\rangle + \left\langle\phi_1\right|\hat{a}\left|\phi_0\right\rangle\right) \\
&= \frac{\mathrm{e}^{-\mathrm{i}\omega t}}{2}(0+0+1+0) = \frac{\mathrm{e}^{-\mathrm{i}\omega t}}{2}, \\
\left\langle\hat{a}^{\dagger}\right\rangle(t) &= \left\langle\psi(0)\right|\hat{a}_{\mathrm{H}}^{\dagger}(t)\left|\psi(0)\right\rangle = \mathrm{e}^{\mathrm{i}\omega t}\left\langle\psi(0)\right|\hat{a}^{\dagger}\left|\psi(0)\right\rangle = \frac{\mathrm{e}^{\mathrm{i}\omega t}}{2}\left\langle\left(\left|\phi_0\right\rangle + \left|\phi_1\right\rangle\right)\right|\hat{a}^{\dagger}\left|\left(\left|\phi_0\right\rangle + \left|\phi_1\right\rangle\right)\right\rangle \\
&= \frac{\mathrm{e}^{\mathrm{i}\omega t}}{2}\left(\left\langle\phi_0\right|\hat{a}^{\dagger}\left|\phi_0\right\rangle + \left\langle\phi_1\right|\hat{a}^{\dagger}\left|\phi_1\right\rangle + \left\langle\phi_0\right|\hat{a}^{\dagger}\left|\phi_1\right\rangle + \left\langle\phi_1\right|\hat{a}^{\dagger}\left|\phi_0\right\rangle\right) \\
&= \frac{\mathrm{e}^{\mathrm{i}\omega t}}{2}(0+0+0+1) = \frac{\mathrm{e}^{\mathrm{i}\omega t}}{2}.
\end{aligned}$$

Recall that the position operator $\hat{x}$ and the momentum operator $\hat{p}$ can be represented as

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^{\dagger}), \quad \hat{p} = -\mathrm{i}\sqrt{\frac{m\hbar\omega}{2}}(\hat{a} - \hat{a}^{\dagger}).$$

By linearity of expectation, we could therefore determine the expectation of $\hat{x}$ as

$$\left\langle\hat{x}\right\rangle(t) = \sqrt{\frac{\hbar}{2m\omega}}\left(\left\langle\hat{a}\right\rangle(t) + \left\langle\hat{a}^{\dagger}\right\rangle(t)\right) = \sqrt{\frac{\hbar}{2m\omega}}\left(\frac{\mathrm{e}^{-\mathrm{i}\omega t}}{2} + \frac{\mathrm{e}^{\mathrm{i}\omega t}}{2}\right) = \boxed{\sqrt{\frac{\hbar}{2m\omega}}\cos\omega t},$$

where we have used the identities $\mathrm{e}^{\mathrm{i}\omega t} = \cos\omega t + \mathrm{i}\sin\omega t$ and $\mathrm{e}^{-\mathrm{i}\omega t} = \cos\omega t - \mathrm{i}\sin\omega t$.

(b) Similarly, we have

$$\left\langle\hat{p}\right\rangle(t) = -\mathrm{i}\sqrt{\frac{m\hbar\omega}{2}}\left(\left\langle\hat{a}\right\rangle(t) - \left\langle\hat{a}^{\dagger}\right\rangle(t)\right) = -\mathrm{i}\sqrt{\frac{m\hbar\omega}{2}}\left(\frac{\mathrm{e}^{-\mathrm{i}\omega t}}{2} - \frac{\mathrm{e}^{\mathrm{i}\omega t}}{2}\right) = -\sqrt{\frac{m\hbar\omega}{2}}\sin\omega t.$$

To determine the variance, we also need to calculate the expectation of $\hat{x}^2$ and $\hat{p}^2$.

We have

$$\begin{aligned}
\hat{x}^2 &= \frac{\hbar}{2m\omega}\left(\hat{a} + \hat{a}^{\dagger}\right)^2 = \frac{\hbar}{2m\omega}\left(\hat{a}^2 + \hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a} + \hat{a}^{\dagger 2}\right), \\
\hat{p}^2 &= -\frac{m\hbar\omega}{2}\left(\hat{a} - \hat{a}^{\dagger}\right)^2 = -\frac{m\hbar\omega}{2}\left(\hat{a}^2 - \hat{a}\hat{a}^{\dagger} - \hat{a}^{\dagger}\hat{a} + \hat{a}^{\dagger 2}\right).
\end{aligned}$$

Note that, by definition, we have

$$\hat{a}^2\left|\phi_0\right\rangle = 0, \quad \hat{a}^2\left|\phi_1\right\rangle = \hat{a}\left|\phi_0\right\rangle = 0, \quad \hat{a}^{\dagger 2}\left|\phi_0\right\rangle = \hat{a}^{\dagger}\left|\phi_1\right\rangle = \left|\phi_2\right\rangle, \quad \hat{a}^{\dagger 2}\left|\phi_1\right\rangle = \sqrt{2}\hat{a}^{\dagger}\left|\phi_2\right\rangle = \sqrt{6}\left|\phi_3\right\rangle,$$

so we must have $\left\langle\hat{a}^2\right\rangle(t) = 0$ since both states result in 0 and $\left\langle\hat{a}^{\dagger 2}\right\rangle(t) = 0$ for any time t since both states are outside of (orthogonal to) the original states.

For the number operator $\hat{a}^\dagger \hat{a}$, we have

$$\hat{a}^\dagger \hat{a} \left|\phi_0\right\rangle = 0, \quad \hat{a}^\dagger \hat{a} \left|\phi_1\right\rangle = \left|\phi_1\right\rangle, \quad \left(\hat{a}^\dagger \hat{a}\right)_{\mathrm{H}} = \hat{a}^\dagger_{\mathrm{H}} \hat{a}_{\mathrm{H}}(t) = \mathrm{e}^{\mathrm{i}\omega t} \hat{a}^\dagger \mathrm{e}^{-\mathrm{i}\omega t} \hat{a} = \hat{a}^\dagger \hat{a},$$

so its expectation is

$$\begin{aligned}
\left\langle \hat{a}^\dagger \hat{a} \right\rangle (t) &= \left\langle \psi(0) \right| \left(\hat{a}^\dagger \hat{a}\right)_{\mathrm{H}} \left|\psi(0)\right\rangle = \left\langle \psi(0) \right| \hat{a}^\dagger \hat{a} \left|\psi(0)\right\rangle = \frac{1}{2} \left\langle (\left|\phi_0\right\rangle + \left|\phi_1\right\rangle) \right| \hat{a}^\dagger \hat{a} \left| (\left|\phi_0\right\rangle + \left|\phi_1\right\rangle) \right\rangle \\
&= \frac{1}{2} \left(\left\langle \phi_0 \right| \hat{a}^\dagger \hat{a} \left|\phi_0\right\rangle + \left\langle \phi_1 \right| \hat{a}^\dagger \hat{a} \left|\phi_1\right\rangle + \left\langle \phi_0 \right| \hat{a}^\dagger \hat{a} \left|\phi_1\right\rangle + \left\langle \phi_1 \right| \hat{a}^\dagger \hat{a} \left|\phi_0\right\rangle \right) \\
&= \frac{1}{2} (0 + 1 + 0 + 0) = \frac{1}{2}.
\end{aligned}$$

By the identity $\left[\hat{a}, \hat{a}^\dagger\right] = \hat{a}\hat{a}^\dagger - \hat{a}^\dagger \hat{a} = 1$, we have

$$\left\langle \hat{a}\hat{a}^\dagger \right\rangle (t) = 1 + \left\langle \hat{a}^\dagger \hat{a} \right\rangle (t) = 1 + \frac{1}{2} = \frac{3}{2}.$$

Finally, we are able to compute

$$\begin{aligned}
\left\langle \hat{x}^2 \right\rangle (t) &= \frac{\hbar}{2m\omega} \left(\left\langle \hat{a}^2 \right\rangle (t) + \left\langle \hat{a}\hat{a}^\dagger \right\rangle (t) + \left\langle \hat{a}^\dagger \hat{a} \right\rangle (t) + \left\langle \hat{a}^{\dagger 2} \right\rangle (t) \right) = \frac{\hbar}{2m\omega} \left(0 + \frac{3}{2} + \frac{1}{2} + 0 \right) = \frac{\hbar}{m\omega}, \\
\left\langle \hat{p}^2 \right\rangle (t) &= -\frac{m\hbar\omega}{2} \left(\left\langle \hat{a}^2 \right\rangle (t) - \left\langle \hat{a}\hat{a}^\dagger \right\rangle (t) - \left\langle \hat{a}^\dagger \hat{a} \right\rangle (t) + \left\langle \hat{a}^{\dagger 2} \right\rangle (t) \right) = -\frac{m\hbar\omega}{2} \left(0 - \frac{3}{2} - \frac{1}{2} + 0 \right) = m\hbar\omega.
\end{aligned}$$

The variance the position and momentum at time t are, respectively,

$$\begin{aligned}
\sigma_x^2(t) &= \left\langle \hat{x}^2 \right\rangle (t) - \left(\left\langle \hat{x} \right\rangle (t) \right)^2 = \frac{\hbar}{m\omega} - \left(\sqrt{\frac{\hbar}{2m\omega}} \cos \omega t \right)^2 = \boxed{\frac{\hbar}{m\omega} \left(1 - \frac{1}{2} \cos^2 \omega t \right)}, \\
\sigma_p^2(t) &= \left\langle \hat{p}^2 \right\rangle (t) - \left(\left\langle \hat{p} \right\rangle (t) \right)^2 = m\hbar\omega - \left(-\sqrt{\frac{m\hbar\omega}{2}} \sin \omega t \right)^2 = \boxed{m\hbar\omega \left(1 - \frac{1}{2} \sin^2 \omega t \right)}.
\end{aligned}$$

The product between these variances is

$$\begin{aligned}
\sigma_x^2(t)\sigma_p^2(t) &= \frac{\hbar}{m\omega} \left(1 - \frac{1}{2} \cos^2 \omega t \right) \cdot m\hbar\omega \left(1 - \frac{1}{2} \sin^2 \omega t \right) \\
&= \frac{\hbar^2}{4} \left(2 - \cos^2 \omega t \right) \left(2 - \sin^2 \omega t \right),
\end{aligned}$$

and because $\cos^2 \omega t, \sin^2 \omega t \le 1$ for $t \in \mathbb{R}$, we have

$$\sigma_x^2(t)\sigma_p^2(t) \ge \frac{\hbar^2}{4} (2 - 1)(2 - 1) = \frac{\hbar^2}{4},$$

which is indeed $\boxed{\text{consistent with the Heisenberg uncertainty principle}}$.

In fact, for this case, we can calculate the lower bound of the variance product $\sigma_x^2(t)\sigma_p^2(t)$ by using $\cos^2 x + \sin^2 x = 1$ where $x = \omega t$, so that

$$\begin{aligned}
\left(2 - \cos^2 x\right)\left(2 - \sin^2 x\right) &= (2 - \cos^2 x)(1 + \cos^2 x) \\
&= 2 + \cos^2 x - \cos^4 x = \frac{9}{4} - \left(\cos^2 x - \frac{1}{2} \right)^2,
\end{aligned}$$

which is minimised when $\cos^2 x = 0$ or $\cos^2 x = 1$ since $0 \le \cos^2 x \le 1$, with minimum $9/4 - 1/4 = 2$. This corresponds to the cases where $x = k\pi$ or $x = k\pi + \pi/2$ where $k \in \mathbb{Z}$, i.e.,

$$t = \frac{k\pi}{\omega} \quad \text{or} \quad \frac{k\pi + \pi/2}{\omega}.$$

At these times, the variance product is minimised at $\boxed{\left(\sigma_x^2(t)\sigma_p^2(t)\right)_{\min} = \hbar^2/2}$.