QM1 Problem Set 3 solutions — Mike Saelim

If you find any errors with these solutions, please email me at mjs496@cornell.edu.

1 **(a)** We're given a Hamiltonian here, so we should try to figure out how best to use it. H has the nice property that, whenever it sits next to $|\phi\rangle$, it pulls out the energy of the state and becomes a nice commuting c-number. So, let's try to relate x and p using a commutator:

$$[x, H] = [x, \frac{p^2}{2m}] = i\hbar \frac{p}{m}$$
$$p = \frac{m}{i\hbar}[x, H].$$

Note that this is very nice for us! The H's will invariably end up next to bras and kets, leaving us with only x inside the product. Trying to do this with $[p, H]$ is not so nice for us, because you end up getting derivatives of $V(x)$. Continuing,

$$\langle \phi_n | p | \phi_{n'} \rangle = \frac{m}{i\hbar} \langle \phi_n | xH - Hx | \phi_{n'} \rangle = \frac{im}{\hbar}(E_n - E_{n'}) \langle \phi_n | x | \phi_{n'} \rangle.$$

(b) We can use the result of part (a) here, starting with the right-hand side.

$$\begin{aligned}
\langle \phi_n | p^2 | \phi_n \rangle &= \sum_{n'} \langle \phi_n | p | \phi_{n'} \rangle \langle \phi_{n'} | p | \phi_n \rangle \\
&= \sum_{n'} |\langle \phi_n | p | \phi_{n'} \rangle|^2 \\
&= \sum_{n'} \frac{m^2}{\hbar^2} (E_n - E_{n'})^2 |\langle \phi_n | x | \phi_{n'} \rangle|^2
\end{aligned}$$
$$\Longrightarrow \sum_{n'} (E_n - E_{n'})^2 |\langle \phi_n | x | \phi_{n'} \rangle|^2 = \frac{\hbar^2}{m^2} \langle \phi_n | p^2 | \phi_n \rangle$$

2 **Canonical transformation and simple harmonic motion**

(a) We straightforwardly compute the derivatives and solve for q and p:

$$\begin{cases} p = \dfrac{\partial F_1}{\partial q} = m\omega q \cot \bar{q} \\ -\bar{p} = \dfrac{\partial F_1}{\partial \bar{q}} = -\dfrac{m}{2}\omega q^2 \csc^2 \bar{q} \end{cases} \quad \Longrightarrow \quad \begin{cases} q = \sqrt{\dfrac{2\bar{p}}{m\omega}} \sin \bar{q} \\ p = \sqrt{2\bar{p} m\omega} \cos \bar{q} \end{cases}$$

Since F_1 has no t-dependence,

$$K(\bar{q}, \bar{p}) = H(q, p) = \omega \bar{p} \cos^2 \bar{q} + \omega \bar{p} \sin^2 \bar{q} = \omega \bar{p}.$$

(b) The equations of motion are

$$\dot{\bar{q}} = \frac{\partial K}{\partial \bar{p}} = \omega \qquad \dot{\bar{p}} = -\frac{\partial K}{\partial \bar{q}} = 0.$$

(c) $\bar{q}(t) = \omega t + \bar{q}_0$ is like a phase that increases linearly with time, and $\bar{p}(t) = \bar{p}_0$ is some conserved quantity of the system.

(d) Using the results of part (a),

$$q(t) = \sqrt{\frac{2\bar{p}_0}{m\omega}} \sin(\omega t + \bar{q}_0) \qquad\qquad p(t) = \sqrt{2\bar{p}_0 m\omega} \cos(\omega t + \bar{q}_0).$$

This confirms our thinking from part (c).

3 Expectation value

(a) We can solve this problem with a neat property of Fourier transforms. Let's first expand the position-space wavefunction in the momentum basis, for a state vector $|\xi\rangle$:

$$\psi(x') = \langle x'|\xi\rangle = \int_{-\infty}^{\infty} dp' \langle x'|p'\rangle\langle p'|\xi\rangle = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dp'\, e^{ip'x'/\hbar}\phi(p').$$

The momentum-space wavefunction is simply the coefficients of the Fourier expansion of the position-space wavefunction. But, since $\psi(x')$ is restricted to real values, the values of the coefficients $\phi(p')$ are also restricted!

How? Let's expand the other way, with the momentum-space wavefunction in the position basis:

$$\phi(p') = \langle p'|\xi\rangle = \int_{-\infty}^{\infty} dx' \langle p'|x'\rangle\langle x'|\xi\rangle = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dx'\, e^{-ip'x'/\hbar}\psi(x').$$

Now let's take the complex conjugate of this:

$$\begin{aligned} \phi^*(p') &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dx'\, e^{ip'x'/\hbar}\psi^*(x') \\ &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dx'\, e^{ip'x'/\hbar}\psi(x') \\ &= \phi(-p'). \end{aligned}$$

This restriction turns the Fourier expansion of $\psi(x')$ into

$$\psi(x') = \frac{1}{\sqrt{2\pi\hbar}} \int_{0}^{\infty} dp'\, [e^{ip'x'/\hbar}\phi(p') + \text{complex conjugate}],$$

which is an integral of strictly real integrands.

We can also use this restriction to solve our problem. As the prompt suggests, consider the probability density for the momentum to be observed at some particular value. We get

$$|\phi(-p')|^2 = \phi^*(-p')\phi(-p') = \phi(p')\phi^*(p') = |\phi(p')|^2,$$

so it's equally likely to observe momentum p' as it is to observe $-p'$, loosely speaking. Formally,

$$\langle p\rangle = \int_{-\infty}^{\infty} dp' \langle\xi|p|p'\rangle\langle p'|\xi\rangle = \int_{-\infty}^{\infty} dp'\, p'\, |\phi(p')|^2 = \int_{0}^{\infty} dp'\, p'(|\phi(p')|^2 - |\phi(-p')|^2) = 0.$$

We can generalize to the case where $\psi(x') = c\psi_r(x') \Longrightarrow |\xi\rangle = c|\xi_r\rangle$:

$$\langle p\rangle = \langle\xi|p|\xi\rangle = |c|^2\langle\xi_r|p|\xi_r\rangle = 0.$$

So, introducing a phase to the wavefunction won't change anything.

(b) Let $\psi(x') = \langle x'|\xi\rangle$ have expectation value $\langle p\rangle = \langle\xi|p|\xi\rangle$. Also, note that $e^{ip_0x'/\hbar}\psi(x') = \langle x'|e^{ip_0x/\hbar}|\xi\rangle$ and we have the commutator

$$[p, e^{ip_0x/\hbar}] = -i\hbar\frac{\partial}{\partial x}e^{ip_0x/\hbar} = p_0e^{ip_0x/\hbar}.$$

So,

$$\langle\xi|e^{-ip_0x/\hbar}\, p\, e^{ip_0x/\hbar}|\xi\rangle = \langle\xi|p|\xi\rangle + \langle\xi|e^{-ip_0x/\hbar}\,[p, e^{ip_0x/\hbar}]|\xi\rangle = \langle p\rangle + p_0.$$

4 Harmonic oscillator

We'll tackle this problem by solving the equation that defines the time evolution of these operators in the Heisenberg picture: $i\hbar\frac{dX}{dt} = [X, H]$.

$$\begin{aligned}\frac{d}{dt}a &= \frac{-i}{\hbar}[a, H] = \frac{-i}{\hbar}[a, \hbar\omega(a^\dagger a + 1/2)] = -i\omega a \\ \implies a(t) &= a(0)e^{-i\omega t} \\ \implies \langle a(t)\rangle &= \langle a(0)\rangle e^{-i\omega t}.\end{aligned}$$

The derivation of the other equation is analogous.

5 Sakurai p.64, #1.18

(a) This inequality obviously holds, since $|\alpha\rangle + \lambda|\beta\rangle$ itself is a ket, and the quantity on the left-hand side is the inner product of that ket with itself. Expanding,

$$\langle\alpha|\alpha\rangle + |\lambda|^2\langle\beta|\beta\rangle + \lambda\langle\alpha|\beta\rangle + \lambda^*\langle\beta|\alpha\rangle \geq 0.$$

From here, you can go about this two ways. If you simply just choose $\lambda = -\frac{\langle\beta|\alpha\rangle}{\langle\beta|\beta\rangle}$, you easily recover the Schwarz inequality. And that's completely fine. But some of you might feel unsatisfied with that.

To derive the inequality naturally, one strategy is to complete the square in λ. Since that square will be positive and we have the freedom to choose any λ we want, we can choose a λ that makes the square go away, leaving us with a stricter inequality.

$$\begin{aligned}\langle\beta|\beta\rangle\left(|\lambda|^2 + \lambda\frac{\langle\alpha|\beta\rangle}{\langle\beta|\beta\rangle} + \lambda^*\frac{\langle\beta|\alpha\rangle}{\langle\beta|\beta\rangle} + \frac{|\langle\alpha|\beta\rangle|^2}{\langle\beta|\beta\rangle^2} - \frac{|\langle\alpha|\beta\rangle|^2}{\langle\beta|\beta\rangle^2} + \frac{\langle\alpha|\alpha\rangle}{\langle\beta|\beta\rangle}\right) &\geq 0 \\ \langle\beta|\beta\rangle\left|\lambda + \frac{\langle\beta|\alpha\rangle}{\langle\beta|\beta\rangle}\right|^2 + \left(\langle\alpha|\alpha\rangle - \frac{|\langle\alpha|\beta\rangle|^2}{\langle\beta|\beta\rangle}\right) &\geq 0\end{aligned}$$

The first term here must strictly be greater than or equal to zero, so we choose whatever λ makes it zero, which puts the strictest bounds on the second term. The second term then becomes

$$\begin{aligned}\langle\alpha|\alpha\rangle - \frac{|\langle\alpha|\beta\rangle|^2}{\langle\beta|\beta\rangle} &\geq 0 \\ \langle\alpha|\alpha\rangle\langle\beta|\beta\rangle &\geq |\langle\alpha|\beta\rangle|^2.\end{aligned}$$

Note that the choice of λ that sets the squared term to zero is naturally the same as the ad hoc choice we made above.

(b) The generalized uncertainty relation is

$$\langle(\Delta A)^2\rangle\langle(\Delta B)^2\rangle \geq \frac{1}{4}|\langle[A, B]\rangle|^2.$$

If $\Delta A|\alpha\rangle = \lambda\,\Delta B|\alpha\rangle$, the left-hand side becomes

$$\langle(\Delta A)^2\rangle\langle(\Delta B)^2\rangle = |\lambda|^2\langle(\Delta B)^2\rangle^2.$$

while the right-hand side becomes

$$\begin{aligned}
\frac{1}{4}|\langle[A,B]\rangle|^2 &= \frac{1}{4}|\langle[A,B]\rangle - [\langle A\rangle, B] - [A, \langle B\rangle] + [\langle A\rangle, \langle B\rangle]|^2 \\
&= \frac{1}{4}|\langle[\Delta A, \Delta B]\rangle|^2 \\
&= \frac{1}{4}|\lambda^*\langle(\Delta B)^2\rangle - \lambda\langle(\Delta B)^2\rangle|^2 \\
&= \frac{1}{4}|2\lambda\langle(\Delta B)^2\rangle|^2 \\
&= |\lambda|^2\langle(\Delta B)^2\rangle^2.
\end{aligned}$$

(c) All we need to do is insert a complete set of position eigenstates into $\langle x'|\Delta p|\alpha\rangle$ so that we can use the position wavefunction for our Gaussian wavepacket.

$$\begin{aligned}
\langle x'|\Delta p|\alpha\rangle &= \int dx''\, \langle x'|p - \langle p\rangle|\alpha\rangle \\
&= \left(-i\hbar\frac{\partial}{\partial x'} - \langle p\rangle\right)\langle x'|\alpha\rangle \\
&= \left[-i\hbar\left(\frac{i\langle p\rangle}{\hbar} - \frac{x' - \langle x\rangle}{2d^2}\right) - \langle p\rangle\right]\langle x'|\alpha\rangle \\
&= \frac{i\hbar}{2d^2}(x' - \langle x\rangle)\langle x'|\alpha\rangle \\
&= \frac{i\hbar}{2d^2}\langle x'|\Delta x|\alpha\rangle.
\end{aligned}$$

Thus, $\langle x'|\Delta x|\alpha\rangle = -i\frac{2d^2}{\hbar}\langle x'|\Delta p|\alpha\rangle$.

6 Sakurai p.142, #2.1

We plug and chug with the Heisenberg equation of motion, which tells us how Heisenberg operators evolve with time:

$$\begin{aligned}
\frac{dS_x}{dt} &= \frac{1}{i\hbar}[S_x, H] = -\omega S_y \\
\frac{dS_y}{dt} &= \frac{1}{i\hbar}[S_y, H] = \omega S_x \\
\frac{dS_z}{dt} &= \frac{1}{i\hbar}[S_z, H] = 0
\end{aligned}$$

Obviously, $S_z(t) = S_{z0} = \frac{\hbar}{2}\sigma_3$ is a constant. The other two observables give us two coupled first-order differential equations... which is most easily resolved (in my opinion) by figuring out what the second derivatives are:

$$\begin{aligned}
\frac{d^2S_x}{dt^2} &= \frac{1}{i\hbar}\left[\frac{dS_x}{dt}, H\right] = -\omega^2 S_x \\
\frac{d^2S_y}{dt^2} &= \frac{1}{i\hbar}\left[\frac{dS_y}{dt}, H\right] = -\omega^2 S_y.
\end{aligned}$$

Now we have two decoupled second-order differential equations, subject to the conditions

$$\begin{aligned}
\frac{dS_x}{dt} &= -\omega S_y & \qquad S_x(0) &= S_{x0} = \frac{\hbar}{2}\sigma_1 \\
\frac{dS_y}{dt} &= \omega S_x & \qquad S_y(0) &= S_{y0} = \frac{\hbar}{2}\sigma_2.
\end{aligned}$$

We can easily solve this to get

$$S_x(t) = S_{x0}\cos(\omega t) - S_{y0}\sin(\omega t)$$
$$S_y(t) = S_{x0}\sin(\omega t) + S_{y0}\cos(\omega t)$$
$$S_z(t) = S_{z0}.$$

7 Hamilton-Jacobi equation

(a) We plug the ansatz $S(q,\alpha,t) = W(q,\alpha) - \alpha t$ into the Hamilton-Jacobi equation,

$$\frac{1}{2m}\left(\frac{\partial W}{\partial q}\right)^2 + \frac{1}{2}m\omega^2 q^2 - \alpha = 0,$$

which we can rearrange to get

$$\frac{\partial W}{\partial q} = \pm\sqrt{2m\alpha - m^2\omega^2 q^2} = \pm\sqrt{2m\alpha}\sqrt{1 - \frac{m\omega^2}{2\alpha}q^2}.$$

This result is prone to integration via trig substitution, which gives us

$$W(q,\alpha) = \pm\left\{\frac{\alpha}{\omega}\sin^{-1}\left(\sqrt{\frac{m\omega^2}{2\alpha}}q\right) + \frac{q}{2}\sqrt{2m\alpha - m^2\omega^2 q^2} + C(\alpha)\right\}$$
$$S(q,\alpha,t) = \pm\left\{\frac{\alpha}{\omega}\sin^{-1}\left(\sqrt{\frac{m\omega^2}{2\alpha}}q\right) + \frac{q}{2}\sqrt{2m\alpha - m^2\omega^2 q^2} + C(\alpha)\right\} - \alpha t$$

Note that the integration constant C can still be α-dependent!

(b) We get a nice cancellation once we take the derivative:

$$\bar{q} = \frac{\partial S}{\partial \alpha} = \pm\left\{\frac{1}{\omega}\sin^{-1}\left(\sqrt{\frac{m\omega^2}{2\alpha}}q\right) + \frac{\alpha}{\omega}\frac{1}{\sqrt{1 - \frac{m\omega^2}{2\alpha}q^2}} \cdot -\frac{1}{2}q\sqrt{\frac{m\omega^2}{2}}\alpha^{-3/2} + \frac{q}{2}\frac{2m}{2\sqrt{2m\alpha - m^2\omega^2 q^2}} + \frac{\partial C}{\partial \alpha}\right\} - t$$
$$= \pm\left[\frac{1}{\omega}\sin^{-1}\left(\sqrt{\frac{m\omega^2}{2\alpha}}q\right) + \frac{\partial C}{\partial \alpha}\right] - t$$

(c) We invert the equation from part (b) to get

$$q(t) = \pm\frac{1}{\omega}\sqrt{\frac{2\alpha}{m}}\sin\left[\omega\left(t + \bar{q} \mp \frac{\partial C}{\partial \alpha}\right)\right].$$

We see now that $\bar{q} \mp \frac{\partial C}{\partial \alpha}$ seems to play the role of a time offset, which is a constant of the motion. If you let $t = 0$, you can easily see that this expression sets the initial phase of the harmonic oscillator: whether it starts all the way to one side, in the middle, or wherever. The $\pm$ ambiguity can be fixed with a sufficient choice of initial conditions. The term $\frac{\partial C}{\partial \alpha}$ reflects the ambiguity in how we match up $\bar{q}$ with the initial phase of the harmonic oscillator: I can just as easily say that $\bar{q} = 0$ corresponds to starting the oscillator in the middle as I can say that $\bar{q} = 0$ corresponds to halfway between the middle and the end of the swing, with sufficient choice of $\frac{\partial C}{\partial \alpha}$. Of course, this choice is reflected in our canonical transformation generator $S(q,\alpha,t)$.

(d) With these initial conditions, we can now write the Hamilton-Jacobi equation at $t = 0$,

$$0 + \frac{1}{2}m\omega^2[q(0)]^2 - \alpha = 0,$$

so that $\bar{p} = \alpha = \frac{1}{2}m\omega^2[q(0)]^2$. This is simply the energy of the system, which is a constant of the motion. Plugging this into our equation for $\bar{q}$,

$$\begin{aligned}
\bar{q} &= \pm\left[\frac{1}{\omega}\sin^{-1}\left(\frac{q(0)}{q(0)}\right) + \frac{\partial C}{\partial \alpha}\right] - 0 \\
&= \pm\left[\frac{(4n+1)\pi}{2\omega} + \frac{\partial C}{\partial \alpha}\right] \quad ; \quad n \in Z
\end{aligned}$$

which is indeed the offset, in time, of the sine function at $t = 0$ for the given initial conditions. Note that, in addition to the ambiguity you get from $\frac{\partial C}{\partial \alpha}$ allowing you to define $\bar{q}$ however you want by changing your canonical transformation, you also get an ambiguity from the periodicity of the system. You can choose both $\frac{\partial C}{\partial \alpha}$ and n to be 0 in order to get the vanilla $\bar{q} = \frac{\pi}{2\omega}$, which would be your first guess for the time offset that allows the position of the oscillator to go as $q \sim \cos(\omega t)$.

The canonical transformation you witnessed here is an example of transforming from our usual variables (p, the momentum, and q, the position) to action-angle variables ($\bar{p}$, the total energy, and $\bar{q}$, the initial time offset). These action-angle variables are constants of the motion, and still completely define our harmonic oscillator just as well as the time-dependent position and momentum.

If you want to try to visualize these action-angle variables, envision the phase space plane for this harmonic oscillator: the position q lies on the x-axis, say, and the momentum p lies on the y-axis. At any point in time, this system is at some point in the phase space (q, p). But our Hamiltonian restricts the system to certain orbits around the phase space, which take the form of concentric ellipses that have their major and minor axes flush with the x- and y-axes. So we can fully describe our system by saying which ellipse we're on (which corresponds to the total energy in the system, $\bar{p}$, our action variable) and where we started at $t = 0$ (which corresponds to the time offset $\bar{q}$, our angle variable). The Hamiltonian tells us how the system time evolves, so we don't need to say anything further. That's your action-angle variables for you.