3 The Harmonic Oscillator

1/26: **1.** Harmonic oscillator in Earth's gravity.

In class, we solved the Harmonic Oscillator Problem, which has the potential

$$V(x) = \frac{m\omega^2 x^2}{2} \tag{3.1}$$

with $\omega = \sqrt{k/m}$ being the classical frequency. Now assume that x is a vertical direction and that we place the harmonic oscillator close to the Earth's surface. Now, if x grows upwards, the potential will be

$$V(x) = \frac{m\omega^2 x^2}{2} + mgx + C \tag{3.2}$$

with $g = 9.8\,\mathrm{m/s^2}$ and C an arbitrary (and irrelevant) constant.

a) First, think about the classical problem. The equilibrium point is no longer at $x = 0$, but a displaced point where the tension and gravity forces are equilibrated. Find that point and rewrite the potential in terms of a new variable representing departures from the equilibrium point. What would be the motion of a classical particle under the potential given in Eq. 3.2?

Answer. The equilibrium point x_{eq} will correspond to a minimum of V. Thus, we may solve

$$V'(x_{\text{eq}}) = 0$$

for x_{eq}. Doing this, we obtain

$$\begin{aligned}
0 &= \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{m\omega^2 x^2}{2} + mgx + C\right)\bigg|_{x_{\text{eq}}} \\
&= m\omega^2 x_{\text{eq}} + mg \\
&\boxed{x_{\text{eq}} = -\frac{g}{\omega^2}}
\end{aligned}$$

Let

$$u := x - x_{\text{eq}}$$

Then $x = u + x_{\text{eq}}$, so

$$\begin{aligned}
V(u) &= \frac{m\omega^2 (u + x_{\text{eq}})^2}{2} + mg(u + x_{\text{eq}}) + C \\
&= \frac{m\omega^2 u^2}{2} + m\omega^2 x_{\text{eq}} u + mgu + \frac{m\omega^2 x_{\text{eq}}^2}{2} + mgx_{\text{eq}} + C \\
V(u) &= \frac{m\omega^2 u^2}{2} + m\omega^2\left(-\frac{g}{\omega^2}\right)u + mgu + C \\
&\boxed{V(u) = \frac{m\omega^2 u^2}{2} + C}
\end{aligned}$$

Note that we combine all constants from the second to the third line above, which we may do because only relative — not absolute — values of the potential matter.

This result reveals that the motion of a classical particle under the potential given in Eq. 3.2 is $\boxed{\text{simple harmonic motion about } x_{\text{eq}}.}$ □

b) Now think about the quantum problem. Without gravity, the energy eigenvalues are given by $E_n^{\text{HO}} = \hbar\omega(n+1/2)$ and the corresponding wave functions ψ_n^{HO} can be written in terms of odd and even Hermite polynomials and a Gaussian function of x. (Here, HO means "harmonic oscillator.") Using these results, derive the new energy eigenvalues E_n and eigenfunctions ψ_n in the presence of gravity, Eq. 3.2. *Hint*: Can you make a similar redefinition of the coordinates as you did in the classical case?

Answer. To derive E_n, ψ_n, we must solve the following ODE.

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi_n(x) + \left[\frac{m\omega^2x^2}{2} + mgx + C\right]\psi_n(x) = E_n\psi_n(x)$$

Define u as in part (a). Fold C into the energy to get rid of it, and substitute $\psi_n(u)$ and $x = u + x_{\text{eq}}$ into the above equation.

$$\begin{aligned}
-\frac{\hbar^2}{2m}\frac{\mathrm{d}}{\mathrm{d}x}\left[\frac{\mathrm{d}}{\mathrm{d}x}\psi_n(u)\right] + \frac{m\omega^2u^2}{2}\psi_n(u) &= E_n\psi_n(u) \\
-\frac{\hbar^2}{2m}\frac{\mathrm{d}}{\mathrm{d}x}\left[\frac{\mathrm{d}}{\mathrm{d}u}\psi_n(u)\cdot\underbrace{\frac{\mathrm{d}u}{\mathrm{d}x}}_{1}\right] + \frac{m\omega^2u^2}{2}\psi_n(u) &= E_n\psi_n(u) \\
-\frac{\hbar^2}{2m}\frac{\mathrm{d}}{\mathrm{d}u}\left[\frac{\mathrm{d}}{\mathrm{d}u}\psi_n(u)\right]\cdot\underbrace{\frac{\mathrm{d}u}{\mathrm{d}x}}_{1} + \frac{m\omega^2u^2}{2}\psi_n(u) &= E_n\psi_n(u) \\
-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}u^2}\psi_n(u) + \frac{m\omega^2u^2}{2}\psi_n(u) &= E_n\psi_n(u)
\end{aligned}$$

We worked out the solutions to this equation already in class. They are

$$\psi_n(u) = \psi_n^{\text{HO}}(u) \qquad\qquad E_n - C = E_n^{\text{HO}}$$

It follows by returning the substitution that

$$\boxed{\psi_n(x) = \psi_n^{\text{HO}}(x - x_{\text{eq}})} \qquad\qquad \boxed{E_n = E_n^{\text{HO}} + C}$$

□

c) What would be the mean value of x and p in this system (for a given energy eigenstate, not a generic state)? What would be the mean value of x^2 and p^2 in the ground state of the system? *Hint*: Use properties of the wave functions under displacements from the equilibrium point, and write $x = x_{\text{eq}} + (x - x_{\text{eq}})$, where x_{eq} is the equilibrium point.

Answer. Piggybacking off of the results from class, we will have

$$\boxed{\langle\psi_n|\hat{x}|\psi_n\rangle = x_{\text{eq}}} \qquad\qquad \boxed{\langle\psi_n|\hat{p}|\psi_n\rangle = 0}$$

In the ground state of the system, we have (taking the hint) that

$$\begin{aligned}
\langle\psi_0|\hat{x}^2|\psi_0\rangle &= \int \psi_0^*(x)x^2\psi_0(x)\,\mathrm{d}x \\
&= \int [\psi_0^{\text{HO}}]^*(u)(x_{\text{eq}} + u)^2\psi_0^{\text{HO}}(u)\,\mathrm{d}u \\
&= x_{\text{eq}}^2\int [\psi_0^{\text{HO}}]^*(u)\psi_0^{\text{HO}}(u)\,\mathrm{d}u + 2x_{\text{eq}}\int [\psi_0^{\text{HO}}]^*(u)u\psi_0^{\text{HO}}(u)\,\mathrm{d}u \\
&\quad + \int [\psi_0^{\text{HO}}]^*(u)u^2\psi_0^{\text{HO}}(u)\,\mathrm{d}u
\end{aligned}$$

The leftmost integral above evaluates to 1. The middle integral above evaluates to zero because its integrand is an odd function (the product of an odd and even function). The right integral expands to

$$\int_{-\infty}^{\infty} u^2 \left(\frac{m\omega}{\hbar\pi}\right)^{1/2} \mathrm{e}^{-m\omega u^2/\hbar}\,\mathrm{d}u = \frac{\hbar}{2m\omega}$$

upon plugging in the harmonic oscillator's ground state wave function, and may be evaluated using computational software. Thus, altogether,

$$\boxed{\langle\psi_0|\hat{x}^2|\psi_0\rangle = x_{\text{eq}}^2 + \frac{\hbar}{2m\omega}}$$

Similar explicit computations for the mean value of p^2 yield

$$\boxed{\langle\psi_0|\hat{p}^2|\psi_0\rangle = \frac{\hbar m\omega}{2}}$$

□

d) Think about the uncertainty principle. What is the value of $\sigma_x\sigma_p$ in the ground state of this system? Does it differ from the value we obtained in the absence of gravity?

Answer. We have that

$$\sigma_x^2 = \langle\psi_0|\hat{x}^2|\psi_0\rangle - (\langle\psi_0|\hat{x}|\psi_0\rangle)^2 = x_{\text{eq}}^2 + \frac{\hbar}{2m\omega} - x_{\text{eq}}^2 = \frac{\hbar}{2m\omega}$$

and

$$\sigma_p^2 = \langle\psi_0|\hat{p}^2|\psi_0\rangle - (\langle\psi_0|\hat{p}|\psi_0\rangle)^2 = \frac{\hbar m\omega}{2}$$

Therefore, the value of $\sigma_x\sigma_p$ in the ground state of this system is

$$\begin{aligned}\sigma_x^2 \cdot \sigma_p^2 &= \frac{\hbar}{2m\omega} \cdot \frac{\hbar m\omega}{2} \\ &= \frac{\hbar^2}{4} \\ \boxed{\sigma_x\sigma_p = \frac{\hbar}{2}}\end{aligned}$$

This $\boxed{\text{does not differ}}$ from the value we obtained in the absence of gravity in class on 1/22. □

2. Bouncing harmonic oscillator.

Assume now that we add an infinite potential floor just at the equilibrium point, so that the particle can no longer go below it. Under this modification, the new potential is

$$V(x) = \begin{cases} \frac{m\omega^2x^2}{2} + mgx + C & x > x_{\text{eq}} \\ \infty & x \leq x_{\text{eq}} \end{cases} \tag{3.3}$$

where x_{eq} is the equilibrium point. Classically, every time the particle hits the floor, it will bounce back with the same modulus of the momentum, but in the upwards direction.

a) What is the mathematical description of $x(t)$ of the classical motion? *Hint*: Think about the oscillator without a floor and the symmetry regarding displacements in the positive and negative directions from the equilibrium point.

Answer. The motion will be identical for $x \geq x_{\text{eq}}$, but instead of continuing past x_{eq}, the particle will elastically reflect back. Mathematically, if motion in Q1a was described by

$$x(t) = A\sin(\omega t) + B\cos(\omega t) + x_{\text{eq}}$$

then motion now is described by

$$\boxed{x(t) = |A\sin(\omega t) + B\cos(\omega t)| + x_{\text{eq}}}$$

$\square$

b) Now go back to the quantum mechanical problem. Similarly to the infinite square well that we solved last week, what should happen to the wave functions at $x = x_{\text{eq}}$ and why?

Answer. At and below $x = x_{\text{eq}}$, the potential goes to infinity, so just like in the infinite square well, the particle no longer has a probability of existing there so the wave function $\boxed{\text{must go to zero.}}$ $\square$

c) Now look at the Schrödinger equation for positive values of the displacement with respect to the equilibrium point. Does it change from the one we had without the floor? Find the energy eigenvalues and the corresponding functions ψ_n to this problem. *Hint*: Observe that the boundary condition at $x = x_{\text{eq}}$ eliminates some solutions.

Answer. The Schrödinger equation for positive values of the displacement with respect to the equilibrium point $\boxed{\text{does not}}$ change from the one we had without the floor because the potential in that region has not changed.

Since the Schrödinger equation does not change, we can solve it as in Q1b. However, taking the hint, only the odd solutions will be allowed by the boundary condition. Additionally, allowable space has halved from $(-\infty, \infty)$ to $[x_{\text{eq}}, \infty)$, so we must renormalize the odd eigenstates. Fortunately, this is fairly straightforward since $|\psi_n|^2$ is even, so

$$\begin{aligned}
1 &= \int_{x_{\text{eq}}}^{\infty} |\psi_n(x - x_{\text{eq}})|^2 \,\mathrm{d}x \\
&= \frac{1}{2}\int_{-\infty}^{\infty} |\psi_n(x - x_{\text{eq}})|^2 \,\mathrm{d}x \\
&= \frac{1}{2}\int_{-\infty}^{\infty} |A\psi_n^{\text{HO}}(x - x_{\text{eq}})|^2 \,\mathrm{d}x \\
2 &= A^2 \\
A &= \sqrt{2}
\end{aligned}$$

Thus, the energy eigenvalues and corresponding functions are

$$\boxed{\psi_n(x) = \sqrt{2}\psi_n^{\text{HO}}(x - x_{\text{eq}}) \qquad E_n = E_n^{\text{HO}} + C \qquad n = 1, 3, 5, \ldots}$$

$\square$

d) What is the minimal energy solution once we add the floor to the system? Is it the same as the system without the floor? What is the corresponding eigenfunction of this solution?

Answer. The minimal energy is now that which corresponds to the new smallest eigenstate, i.e.,

$$\boxed{E_1 = \frac{3\hbar\omega}{2} + C}$$

This is $\boxed{\text{not}}$ the same as the system without the floor, which had minimal energy $\hbar\omega/2 + C$. The corresponding eigenfunction is $\boxed{\psi_1(x).}$ $\square$

e) Find σ_x and σ_p for the minimum energy solution. Is $\sigma_x\sigma_p$ the same as in the system without the wall?

Answer. Per part (d), the minimum energy solution is the wave function

$$\begin{aligned}
\psi_1(x) &= \sqrt{2}\psi_1^{\text{HO}}(x - x_{\text{eq}}) \\
&= \sqrt{2}\left(\frac{m\omega}{\hbar\pi}\right)^{1/4}\frac{H_1(\xi)}{\sqrt{2^1 1!}}\mathrm{e}^{-\xi^2/2} \\
&= \left(\frac{m\omega}{\hbar\pi}\right)^{1/4}\left[(-1)^1\mathrm{e}^{\xi^2}\cdot\frac{\mathrm{d}}{\mathrm{d}\xi}\left(\mathrm{e}^{-\xi^2}\right)\right]\mathrm{e}^{-\xi^2/2} \\
&= \left(\frac{m\omega}{\hbar\pi}\right)^{1/4}\left[-\mathrm{e}^{\xi^2}\cdot -2\xi\mathrm{e}^{-\xi^2}\right]\mathrm{e}^{-\xi^2/2} \\
&= 2\left(\frac{m\omega}{\hbar\pi}\right)^{1/4}\xi\mathrm{e}^{-\xi^2/2} \\
&= 2\left(\frac{m\omega}{\hbar\pi}\right)^{1/4}u\left(\frac{m\omega}{\hbar}\right)^{1/2}\mathrm{e}^{-m\omega u^2/2\hbar} \\
&= \frac{2}{\pi^{1/4}}\left(\frac{m\omega}{\hbar}\right)^{3/4}(x - x_{\text{eq}})\mathrm{e}^{-m\omega(x - x_{\text{eq}})^2/2\hbar}
\end{aligned}$$

From here, we can use computational software to learn that

$$\begin{aligned}
\langle\psi_1|\hat{x}|\psi_1\rangle &= \int_{x_{\text{eq}}}^{\infty} x\psi_1^2(x)\,\mathrm{d}x = \int_0^{\infty}(u + x_{\text{eq}})\psi_1^2(u + x_{\text{eq}})\,\mathrm{d}u = 2\sqrt{\frac{\hbar}{m\omega\pi}} + x_{\text{eq}} \\
\langle\psi_1|\hat{x}^2|\psi_1\rangle &= x_{\text{eq}}^2 + \frac{3\hbar}{2m\omega} + 4x_{\text{eq}}\sqrt{\frac{\hbar}{m\omega\pi}} \\
\langle\psi_1|\hat{p}|\psi_1\rangle &= 0 \\
\langle\psi_1|\hat{p}^2|\psi_1\rangle &= \frac{3\hbar m\omega}{2}
\end{aligned}$$

Thus,

$$\sigma_x^2 = \left(x_{\text{eq}}^2 + \frac{3\hbar}{2m\omega} + 4x_{\text{eq}}\sqrt{\frac{\hbar}{m\omega\pi}}\right) - \left(2\sqrt{\frac{\hbar}{m\omega\pi}} + x_{\text{eq}}\right)^2 = \frac{3\hbar}{2m\omega} - \frac{4\hbar}{m\omega\pi}$$

and

$$\sigma_p^2 = \frac{3\hbar m\omega}{2}$$

so

$$\sigma_x\sigma_p = \sqrt{\left(\frac{3\hbar}{2m\omega} - \frac{4\hbar}{m\omega\pi}\right)\left(\frac{3\hbar m\omega}{2}\right)} = \hbar\sqrt{\frac{9}{4} - \frac{6}{\pi}} \approx 0.58\hbar$$

Since $0.58\hbar \neq \hbar/2$ (the answer to Q1d), $\boxed{\text{no,}}$ $\sigma_x\sigma_p$ is not the same as in the system without the wall. □

3. For the harmonic oscillator, consider the ladder operators $a_\pm = (\mp ip + m\omega x)/\sqrt{2\hbar m\omega}$. Recall that $[a_-, a_+] = 1$, the Hamiltonian may be written as $\hat{H} = \hbar\omega(a_+a_- + 1/2)$, and the eigenfunctions describing the eigenstates of energy $E_n = \hbar\omega(n + 1/2)$ are related by $a_+\psi_n = \sqrt{n+1}\psi_{n+1}$ and $a_-\psi_n = \sqrt{n}\psi_{n-1}$.

a) Compute the mean value of x and p in the energy eigenstates described by ψ_n.

Answer. We have that

$$\langle \psi_n | \hat{\vec{x}} | \psi_n \rangle = \sqrt{\frac{\hbar}{2m\omega}} \left[\langle \psi_n | a_+ | \psi_n \rangle + \langle \psi_n | a_- | \psi_n \rangle \right]$$

$$= \sqrt{\frac{\hbar}{2m\omega}} \left[\sqrt{n+1} \underbrace{\langle \psi_n | \psi_{n+1} \rangle}_{0} + \sqrt{n} \underbrace{\langle \psi_n | \psi_{n-1} \rangle}_{0} \right]$$

$$\boxed{\langle \psi_n | \hat{\vec{x}} | \psi_n \rangle = 0}$$

and

$$\langle \psi_n | \hat{\vec{p}} | \psi_n \rangle = i\sqrt{\frac{\hbar m\omega}{2}} \left[\langle \psi_n | a_+ | \psi_n \rangle - \langle \psi_n | a_- | \psi_n \rangle \right]$$

$$= i\sqrt{\frac{\hbar m\omega}{2}} \left[\sqrt{n+1} \underbrace{\langle \psi_n | \psi_{n+1} \rangle}_{0} - \sqrt{n} \underbrace{\langle \psi_n | \psi_{n-1} \rangle}_{0} \right]$$

$$\boxed{\langle \psi_n | \hat{\vec{p}} | \psi_n \rangle = 0}$$

□

b) Compute the mean value of x^2 and p^2 in these states.

Answer. As derived in class,[1] we have that

$$\left\langle \psi_n \middle| \frac{k\hat{x}^2}{2} \middle| \psi_n \right\rangle = \frac{E_n}{2} \qquad \left\langle \psi_n \middle| \frac{\hat{p}^2}{2m} \middle| \psi_n \right\rangle = \frac{E_n}{2}$$

Therefore,

$$\langle \psi_n | \hat{x}^2 | \psi_n \rangle = \frac{2}{k} \cdot \frac{E_n}{2} \qquad \langle \psi_n | \hat{p}^2 | \psi_n \rangle = 2m \cdot \frac{E_n}{2}$$

$$\boxed{\langle \psi_n | \hat{x}^2 | \psi_n \rangle = \frac{\hbar\omega}{k} \left(n + \frac{1}{2} \right)} \qquad \boxed{\langle \psi_n | \hat{p}^2 | \psi_n \rangle = \hbar\omega m \left(n + \frac{1}{2} \right)}$$

□

c) What would the uncertainty principle tell me about $\sigma_x \sigma_p$?

Answer. Since[2]

$$\sigma_x^2 = \langle \psi_n | \hat{\vec{x}}^2 | \psi_n \rangle - (\langle \psi_n | \hat{\vec{x}} | \psi_n \rangle)^2 \qquad \sigma_p^2 = \langle \psi_n | \hat{\vec{p}}^2 | \psi_n \rangle - (\langle \psi_n | \hat{\vec{p}} | \psi_n \rangle)^2$$

we have that

$$\sigma_x^2 \cdot \sigma_p^2 = \hbar^2 \left(n + \frac{1}{2} \right)^2$$

$$\boxed{\sigma_x \sigma_p = \frac{\hbar}{2}(2n+1)}$$

□

d) Verify that the uncertainty principle is fulfilled for the energy eigenstates.

[1] For future reference, they would have liked me to show this derivation and I did lose points for just stating this result.

[2] There is an entirely different derivation of these facts in the solutions key; one that works directly from the formal commutator definition of the uncertainty principle. Pretty cool!

Answer. Per part (c), we have that

$$\sigma_x\sigma_p = \frac{\hbar}{2}(2n+1) \geq \frac{\hbar}{2}$$

for all $n \geq 0$, as desired. ☐

e) Write a formal expression for the mean value of the position and the momentum for the general solution $\psi(x,t)$. Work it out as much as you can, using the orthonormality of the wave functions ψ_n.

Hint: For instance, the mean value of the operators x^q and p^q can be obtained by computing

$$\langle x^q \rangle = \left(\frac{\hbar}{2m\omega}\right)^{q/2} \int \psi(x)^*(a_+ + a_-)^q \psi(x)\,\mathrm{d}x \tag{3.4}$$

and

$$\langle p^q \rangle = i^q \left(\frac{\hbar}{2m\omega}\right)^{q/2} \int \psi(x)^*(a_+ - a_-)^q \psi(x)\,\mathrm{d}x \tag{3.5}$$

Observe that due to orthonormality of the real functions ψ_n and the fact that $a_\pm$ are ladder operators, the only nonvanishing contributions are

$$\begin{aligned}
\int \psi_m(x) a_+^q \psi_n(x)\,\mathrm{d}x & \qquad \text{Non-vanishing for } m = n+q \\
\int \psi_m(x) a_-^q \psi_n(x)\,\mathrm{d}x & \qquad \text{Non-vanishing for } m = n-q \\
\int \psi_m(x) a_-^q a_+^r \psi_n(x)\,\mathrm{d}x & \qquad \text{Non-vanishing for } m = n+r-q \\
\int \psi_m(x) a_+^q a_-^r \psi_n(x)\,\mathrm{d}x & \qquad \text{Non-vanishing for } m = n-r+q
\end{aligned} \tag{3.6}$$

Two useful cases, as follows from the above, are $\langle \psi_n | a_+ a_- | \psi_n \rangle = n$ and $\langle \psi_n | a_- a_+ | \psi_n \rangle = n+1$.

Answer. See Lecture 4.2. ☐