Physics 741 – Graduate Quantum Mechanics 1

Homework Set O

Due Wednesday, October 15

1. **[10] Two particles interacting via a spherically symmetric relative potential have Hamiltonian**

$$H = \frac{\mathbf{P}_1^2}{2m_1} + \frac{\mathbf{P}_2^2}{2m_2} + V\left(\left|\mathbf{Q}_1 - \mathbf{Q}_2\right|\right)$$

Define new operators

$$\mathbf{P} \equiv \mathbf{P}_1 + \mathbf{P}_2 \qquad \mathbf{Q} \equiv \left(m_1\mathbf{Q}_1 + m_2\mathbf{Q}_2\right)/\left(m_1 + m_2\right)$$
$$\mathbf{p} \equiv \left(m_2\mathbf{P}_1 - m_1\mathbf{P}_2\right)/\left(m_1 + m_2\right) \qquad \mathbf{q} \equiv \mathbf{Q}_1 - \mathbf{Q}_2$$

(a) [4] Find the commutation relations for these operators with each other, *i.e.*, find

$$\left[Q_i, P_j\right], \quad \left[Q_i, p_j\right], \quad \left[q_i, P_j\right], \quad \text{and} \quad \left[q_i, p_j\right]$$

This is pretty straightforward, we simply write down each of the commutators and work them out:

$$\left[Q_i, P_j\right] = \frac{\left[m_1Q_{1i} + m_2Q_{2i}, P_{1j} + P_{2j}\right]}{m_1 + m_2} = \frac{m_1\left[Q_{1i}, P_{1j}\right] + m_2\left[Q_{2i}, P_{2j}\right]}{m_1 + m_2} = \frac{m_1 + m_2}{m_1 + m_2} i\hbar\delta_{ij} = i\hbar\delta_{ij}$$

$$\left[q_i, p_j\right] = \frac{\left[Q_{1i} - Q_{2i}, m_2P_{1j} - m_1P_{2j}\right]}{m_1 + m_2} = \frac{m_2\left[Q_{1i}, P_{1j}\right] + m_2\left[Q_{2i}, P_{2j}\right]}{m_1 + m_2} = \frac{m_2 + m_1}{m_1 + m_2} i\hbar\delta_{ij} = i\hbar\delta_{ij}$$

$$\left[q_i, P_j\right] = \left[Q_{1i} - Q_{2i}, P_{1j} + P_{2j}\right] = \left[Q_{1i}, P_{1i}\right] - \left[Q_{1i}, P_{2j}\right] = i\hbar\delta_{ij} - i\hbar\delta_{ij} = 0$$

$$\left[Q_i, p_j\right] = \frac{\left[m_1Q_{1i} + m_2Q_{2i}, m_2P_{1j} - m_1P_{2j}\right]}{\left(m_1 + m_2\right)^2} = \frac{m_1m_2\left(\left[Q_{1i}, P_{1i}\right] - \left[Q_{1i}, P_{2j}\right]\right)}{\left(m_1 + m_2\right)^2} = 0$$

(b) [6] Write the Hamiltonian in terms of these new operators, and in terms of the constants

$$M = m_1 + m_2 \quad \text{and} \quad \mu = \frac{m_1m_2}{m_1 + m_2}$$

The potential term is trivial. For the kinetic term, we first note that

$$\left(m_1 + m_2\right)\mathbf{p} + m_1\mathbf{P} = m_2\mathbf{P}_1 - m_1\mathbf{P}_2 + m_1\mathbf{P}_1 + m_1\mathbf{P}_2 = \left(m_1 + m_2\right)\mathbf{P}_1 \quad \Rightarrow \quad \mathbf{P}_1 = \frac{m_1}{M}\mathbf{P} + \mathbf{p}$$

$$m_2\mathbf{P} - \left(m_1 + m_2\right)\mathbf{p} = m_2\mathbf{P}_1 + m_2\mathbf{P}_2 - m_2\mathbf{P}_1 + m_1\mathbf{P}_2 = \left(m_1 + m_2\right)\mathbf{P}_2 \quad \Rightarrow \quad \mathbf{P}_2 = \frac{m_2}{M}\mathbf{P} - \mathbf{p}$$

We now substitute these in for each of the kinetic terms.

$$H = \frac{1}{2m_1}\left(\frac{m_1}{M}\mathbf{P}+\mathbf{p}\right)^2 + \frac{1}{2m_2}\left(\frac{m_2}{M}\mathbf{P}-\mathbf{p}\right)^2 + V\left(|\mathbf{q}|\right)$$
$$= \frac{m_1}{2M^2}\mathbf{P}^2 + \frac{1}{M}\mathbf{P}\cdot\mathbf{p} + \frac{1}{2m_1}\mathbf{p}^2 + \frac{m_2}{2M^2}\mathbf{P}^2 - \frac{1}{M}\mathbf{P}\cdot\mathbf{p} + \frac{1}{2m_2}\mathbf{p}^2 + V\left(|\mathbf{q}|\right)$$
$$= \frac{m_1+m_2}{2M^2}\mathbf{P}^2 + \frac{1}{2}\left(\frac{1}{m_1}+\frac{1}{m_2}\right)\mathbf{p}^2 + V\left(|\mathbf{q}|\right) = \frac{\mathbf{P}^2}{2M} + \frac{\mathbf{p}^2}{2\mu} + V\left(|\mathbf{q}|\right)$$

where in the last step we defined $\mu^{-1} = m_1^{-1} + m_2^{-1}$, which is equivalent to the given definition.

2. **[15] It is often important to find expectations values of operators like Q_i, which when acting on a wave function ψ yields one of the quantities $\{x, y, z\}$.**
   (a) **[3] Write each of the quantities $\{x, y, z\}$ in spherical coordinates, and then show how each of them can be written as *r* times some linear combination of spherical harmonics. I recommend against trying to "derive" them, just try looking for expressions similar to what you want.**

<u>Warning</u>: Several of the spherical harmonics were incorrectly given in the notes, which could be problematic. For this reason, your answers will probably differ from mine.

These are given in many sources in spherical coordinates, where we have

$$x = r\sin\theta\cos\phi, \quad y = r\sin\theta\sin\phi, \quad z = r\cos\theta$$

Now, glancing at the spherical harmonics, we see that reasonable functions to try would be the Y_1^m's for which we have

$$rY_1^0\left(\theta,\phi\right) = r\tfrac{1}{2}\sqrt{\tfrac{3}{\pi}}\cos\theta = \tfrac{1}{2}\sqrt{\tfrac{3}{\pi}}z$$
$$rY_1^{\pm1}\left(\theta,\phi\right) = \mp r\tfrac{1}{2}\sqrt{\tfrac{3}{2\pi}}\sin\theta e^{\pm i\phi} = \mp r\tfrac{1}{2}\sqrt{\tfrac{3}{2\pi}}\sin\theta\left(\cos\phi \pm i\sin\phi\right) = \tfrac{1}{2}\sqrt{\tfrac{3}{2\pi}}\left(\mp x - iy\right)$$

It is pretty easy to see how to write *z* in terms of Y_1^0. For the other two, we note

$$rY_1^1\left(\theta,\phi\right) + rY_1^{-1}\left(\theta,\phi\right) = \tfrac{1}{2}\sqrt{\tfrac{3}{2\pi}}\left(-x-iy+x-iy\right) = -i\sqrt{\tfrac{3}{2\pi}}y$$
$$rY_1^{-1}\left(\theta,\phi\right) - rY_1^1\left(\theta,\phi\right) = \tfrac{1}{2}\sqrt{\tfrac{3}{2\pi}}\left(x-iy+x+iy\right) = \sqrt{\tfrac{3}{2\pi}}x$$

So in summary, we have

$$x = \sqrt{\tfrac{2\pi}{3}}r\left[Y_1^{-1}\left(\theta,\phi\right) - Y_1^1\left(\theta,\phi\right)\right]$$
$$y = \sqrt{\tfrac{2\pi}{3}}ir\left[Y_1^1\left(\theta,\phi\right) + Y_1^{-1}\left(\theta,\phi\right)\right]$$
$$z = 2\sqrt{\tfrac{\pi}{3}}rY_1^0\left(\theta,\phi\right)$$

(b) [12] Show that the six quantities $\{x^2, y^2, z^2, xy, xz, yz\}$ can similarly be written as r^2 times various combinations of spherical harmonics.

Inspired by our previous successes, this time we try using the Y_2^m's times r^2. Writing them out, we have

$$r^2 Y_2^0(\theta,\phi) = r^2 \tfrac{1}{4}\sqrt{\tfrac{5}{\pi}}\left(3\cos^2\theta - 1\right) = \tfrac{1}{4}\sqrt{\tfrac{5}{\pi}}\left(3z^2 - r^2\right) = \tfrac{1}{4}\sqrt{\tfrac{5}{\pi}}\left(2z^2 - x^2 - y^2\right)$$
$$r^2 Y_2^{\pm1}(\theta,\phi) = \mp r^2 \tfrac{1}{2}\sqrt{\tfrac{15}{2\pi}}\sin\theta\cos\theta e^{\pm i\phi} = \mp\tfrac{1}{2}\sqrt{\tfrac{15}{2\pi}} zr\sin\theta\left(\cos\phi \pm i\sin\phi\right) = \tfrac{1}{2}\sqrt{\tfrac{15}{2\pi}} z\left(\mp x - iy\right)$$
$$r^2 Y_2^{\pm2}(\theta,\phi) = r^2 \tfrac{1}{4}\sqrt{\tfrac{15}{2\pi}}\sin^2\theta e^{\pm 2i\phi} = \tfrac{1}{4}\sqrt{\tfrac{15}{2\pi}}\left[r\sin\theta\left(\cos\phi \pm i\sin\phi\right)\right]^2 = \tfrac{1}{4}\sqrt{\tfrac{15}{2\pi}}\left(x \pm iy\right)^2$$

The cross terms aren't too hard to work out, for example

$$r^2\left[Y_2^1(\theta,\phi) + Y_2^{-1}(\theta,\phi)\right] = \tfrac{1}{2}\sqrt{\tfrac{15}{2\pi}} z\left(-x - iy + x - iy\right) = -i\sqrt{\tfrac{15}{2\pi}} yz$$
$$r^2\left[Y_2^{-1}(\theta,\phi) - Y_2^1(\theta,\phi)\right] = \tfrac{1}{2}\sqrt{\tfrac{15}{2\pi}} z\left(x + iy + x - iy\right) = \sqrt{\tfrac{15}{2\pi}} xz$$
$$r^2\left[Y_2^2(\theta,\phi) - Y_2^{-2}(\theta,\phi)\right] = \tfrac{1}{4}\sqrt{\tfrac{15}{2\pi}}\left[\left(x + iy\right)^2 - \left(x - iy\right)^2\right] = i\sqrt{\tfrac{15}{2\pi}} xy$$

From these we see that

$$xy = i\sqrt{\tfrac{2\pi}{15}} r^2\left[Y_2^{-2}(\theta,\phi) - Y_2^2(\theta,\phi)\right]$$
$$xz = \sqrt{\tfrac{2\pi}{15}} r^2\left[Y_2^{-1}(\theta,\phi) - Y_2^1(\theta,\phi)\right]$$
$$yz = i\sqrt{\tfrac{2\pi}{15}} r^2\left[Y_2^1(\theta,\phi) + Y_2^{-1}(\theta,\phi)\right]$$

The problem is the other ones. We notice quickly that we can write

$$2z^2 - x^2 - y^2 = 4\sqrt{\tfrac{\pi}{5}} r^2 Y_2^0(\theta,\phi)$$
$$x^2 - y^2 = 2\sqrt{\tfrac{2\pi}{15}} r^2\left[Y_2^2(\theta,\phi) + Y_2^{-2}(\theta,\phi)\right]$$

Unfortunately, we can find none of the desired quantities using only these. Hunting around through the other choices, we see that

$$r^2 = x^2 + y^2 + z^2 = 2\sqrt{\pi} r^2 Y_0^0(\theta,\phi)$$

At this point it doesn't take a genius to see that we can get any combination we want by taking combinations of these three expressions. We have

$$\begin{aligned} x^2 &= \tfrac{1}{3}\left(x^2 + y^2 + z^2\right) - \tfrac{1}{6}\left(2z^2 - x^2 - y^2\right) + \tfrac{1}{2}\left(x^2 - y^2\right) \\ &= \tfrac{2}{3}\sqrt{\pi} r^2 Y_0^0(\theta,\phi) - \tfrac{2}{3}\sqrt{\tfrac{\pi}{5}} r^2 Y_2^0(\theta,\phi) + \sqrt{\tfrac{2\pi}{15}} r^2\left[Y_2^2(\theta,\phi) + Y_2^{-2}(\theta,\phi)\right], \\ y^2 &= \tfrac{1}{3}\left(x^2 + y^2 + z^2\right) - \tfrac{1}{6}\left(2z^2 - x^2 - y^2\right) - \tfrac{1}{2}\left(x^2 - y^2\right) \\ &= \tfrac{2}{3}\sqrt{\pi} r^2 Y_0^0(\theta,\phi) - \tfrac{2}{3}\sqrt{\tfrac{\pi}{5}} r^2 Y_2^0(\theta,\phi) - \sqrt{\tfrac{2\pi}{15}} r^2\left[Y_2^2(\theta,\phi) + Y_2^{-2}(\theta,\phi)\right], \end{aligned}$$

$$z^2 = \tfrac{1}{3}\left(x^2 + y^2 + z^2\right) + \tfrac{1}{3}\left(2z^2 - x^2 - y^2\right) = \tfrac{2}{3}\sqrt{\pi}r^2 Y_0^0\left(\theta,\phi\right) + \tfrac{4}{3}\sqrt{\tfrac{\pi}{5}}r^2 Y_2^0\left(\theta,\phi\right)$$