

Week 7

Spin, Fermions, and Bosons

7.1 Three-Dimensional Harmonic Oscillator

2/12: • Last time.

- We discussed some of the problems we face in 3D.
- The Hamiltonian is now

$$\hat{H} = -\frac{\hbar^2}{2m} \left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right] + V(x, y, z)$$

- Derivatives in three coordinates.
- The potential is time-independent.
- If the potential does not depend on anything more specific (e.g., is not central, for instance), then only \hat{H} is conserved.
- We solve

$$\hat{H}\psi(x, y, z) = E\psi(x, y, z)$$

for ψ, E .

- There are three compatible operators:

$$\hat{H}, \hat{L}^2, \hat{L}_z$$

- The z -angular momentum operator, in particular, has the form

$$\hat{L}_z = -i\hbar \frac{\partial}{\partial \phi}$$

which is analogous to the form $\hat{p}_z = -i\hbar(\partial/\partial z)$.

- The potential is central, i.e.,

$$V(x, y, z) = V(r) = V(\sqrt{x^2 + y^2 + z^2})$$

- If the potential is depends on r , we solve the ODE in polar coordinates (r, θ, ϕ) .
- There are also many cases when we only have

$$V(x, y, z) = V(\sqrt{x^2 + y^2})$$

- In this case, $\hat{H}, \hat{L}_z, \hat{p}_z$ will all be compatible.

- If the potential depends via

$$V(x, y, z) = V(\sqrt{x^2 + y^2}, z)$$

then we will conserve \hat{H}, \hat{L}_z .

- We will play with this in the problem set.

- Today, we begin with the **asymmetric harmonic oscillator**.
- **Asymmetric harmonic oscillator:** A particle subject to the following three-dimensional potential.
Constraint

$$V(x, y, z) = \frac{M\omega_1^2 x^2}{2} + \frac{M\omega_2^2 y^2}{2} + \frac{M\omega_3^2 z^2}{2}$$

- This potential is special in the sense that it allows us to solve by separation of variables.
- In other words, since we can write the ODE in the form

$$\left[-\frac{\hbar^2}{2M} \frac{\partial^2 \psi}{\partial x^2} + \frac{M\omega_1^2 x^2}{2} \psi \right] + \left[-\frac{\hbar^2}{2M} \frac{\partial^2 \psi}{\partial y^2} + \frac{M\omega_2^2 y^2}{2} \psi \right] + \left[-\frac{\hbar^2}{2M} \frac{\partial^2 \psi}{\partial z^2} + \frac{M\omega_3^2 z^2}{2} \psi \right] = E\psi$$

we may write

$$\psi(x, y, z) = X(x)Y(y)Z(z)$$

- This allows us to algebraically manipulate the ODE into the form

$$\frac{1}{X} \left[-\frac{\hbar^2}{2M} \frac{d^2 X}{dx^2} + \frac{M\omega_1^2 x^2}{2} X \right] + \frac{1}{Y} \left[-\frac{\hbar^2}{2M} \frac{d^2 Y}{dy^2} + \frac{M\omega_2^2 y^2}{2} Y \right] + \frac{1}{Z} \left[-\frac{\hbar^2}{2M} \frac{d^2 Z}{dz^2} + \frac{M\omega_3^2 z^2}{2} Z \right] = E$$

- We switch from partial to total derivatives here because now each function is only a function of one variable (e.g., $X(x)$ depends only on x)!
- Since the sum of these three independent terms is equal to a constant, each term must equal a constant!
- Splitting the above equation into three, we obtain

$$\begin{aligned} -\frac{\hbar^2}{2M} \frac{d^2 X}{dx^2} + \frac{M\omega_1^2 x^2}{2} X &= E_{n_1} X \\ -\frac{\hbar^2}{2M} \frac{d^2 Y}{dy^2} + \frac{M\omega_2^2 y^2}{2} Y &= E_{n_2} Y \\ -\frac{\hbar^2}{2M} \frac{d^2 Z}{dz^2} + \frac{M\omega_3^2 z^2}{2} Z &= E_{n_3} Z \end{aligned}$$

- It follows that

$$E = E_{n_1} + E_{n_2} + E_{n_3}$$

- We already know the solution to each of these three ODEs! They are just quantum harmonic oscillators. Thus,

$$E_{n_i} = \hbar\omega_i \left(n_i + \frac{1}{2} \right)$$

and

$$E = E_{n_1 n_2 n_3} = \hbar\omega_1 \left(n_1 + \frac{1}{2} \right) + \hbar\omega_2 \left(n_2 + \frac{1}{2} \right) + \hbar\omega_3 \left(n_3 + \frac{1}{2} \right)$$

- Additionally, it follows that the wave functions of each direction are of the form (for example)

$$X_{n_1}(x) = \left(\frac{M\omega_1}{\hbar\pi} \right)^{1/4} \frac{H_{n_1}(\xi_1)}{\sqrt{2^{n_1} n_1!}} \exp \left[-\frac{\xi_1^2}{2} \right]$$

where $\xi_1 = x\sqrt{M\omega_1/\hbar}$.

- What happens to $X_{n_1}(x), Y_{n_2}(y)$ in the limiting case that $n_1 \rightarrow n_2$, $x \rightarrow y$, and $\omega_1 \rightarrow \omega_2$?
 - We start approaching something interesting.
 - We need to go a bit further, though.

- Now consider the limiting case where

$$\omega_1 = \omega_2 = \omega_3 = \omega$$

- Herein, the Hamiltonian becomes

$$\begin{aligned}\hat{H} &= -\frac{\hbar^2}{2M}\vec{\nabla}^2 + \frac{M\omega^2}{2}(x^2 + y^2 + z^2) \\ &= -\frac{\hbar^2}{2M}\vec{\nabla}^2 + \frac{M\omega^2 r^2}{2}\end{aligned}$$

- In this *central potential*, recall that we have

$$\hat{L}^2 Y_{\ell m}(\theta, \phi) = \hbar^2 \ell(\ell + 1) Y_{\ell m}(\theta, \phi)$$

and

$$\hat{L}_z Y_{\ell m}(\theta, \phi) = \hbar m Y_{\ell m}(\theta, \phi)$$

and

$$-\frac{\hbar^2}{2M} \frac{d^2}{dr^2} [U_{n\ell}(r)] + \underbrace{\left[V(r) + \frac{\hbar^2 \ell(\ell + 1)}{2Mr^2} \right]}_{V_{\text{eff}}(r)} U_{n\ell}(r) = E_{n\ell} U_{n\ell}(r)$$

- This leads directly into our discussion of the **spherically symmetric harmonic oscillator**.
- **Spherically symmetric harmonic oscillator:** A particle subject to the following one-dimensional effective potential. *Constraint*

$$V_{\text{eff}}(r) = \frac{M\omega^2 r^2}{2} + \frac{\hbar^2 \ell(\ell + 1)}{2Mr^2}$$

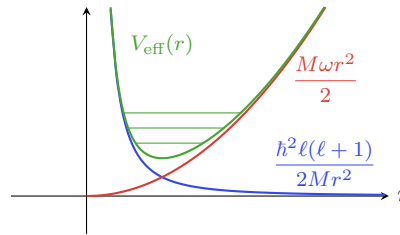


Figure 7.1: Spherically symmetric harmonic oscillator potential.

- The problem we have to solve here is

$$-\frac{\hbar^2}{2M} \frac{d^2}{dr^2} [U_{n\ell}(r)] + \left[\frac{M\omega r^2}{2} + \frac{\hbar^2 \ell(\ell + 1)}{2Mr^2} \right] U_{n\ell}(r) = E_{n\ell} U_{n\ell}(r)$$

- Recall that

$$\psi(r, \theta, \phi) = R_{n\ell}(r) Y_{\ell m}(\theta, \phi) \quad R_{n\ell}(r) r = U_{n\ell}(r)$$

- In the effective potential, we have the interplay of two peaking potentials as in Figure 7.1.

■ The particle will have certain energy states within the well.

- In the limiting case that r is small ($r \rightarrow 0$), we can approximate the potential as giving us

$$-\frac{\hbar^2}{2M} \frac{d^2 U_{n\ell}}{dr^2} + \frac{\hbar^2 \ell(\ell + 1)}{2Mr^2} U_{n\ell} + \dots = 0$$

- In this case, the solution is proportional to

$$U_{n\ell} \propto Cr^{\ell+1}$$

- This is because

$$\begin{aligned}\frac{d}{dr}(Cr^{\ell+1}) &= (\ell+1)Cr^{\ell} \\ \frac{d^2}{dr^2}(Cr^{\ell+1}) &= \ell(\ell+1)C\frac{r^{\ell+1}}{r^2}\end{aligned}$$

- In the limiting case that r is large ($r \rightarrow \infty$), we can approximate the potential as giving us

$$-\frac{\hbar^2}{2M}\frac{d^2U_{n\ell}}{dr^2} + \frac{M\omega^2r^2}{2}U_{n\ell} + \dots = 0$$

- In this case, the solution is proportional to

$$U_{n\ell} = Ce^{-M\omega r^2/\hbar}$$

- Thus, we combine the two partial solutions to propose the overall ansatz

$$U_{n\ell} = f_{n\ell}r^{\ell+1}e^{-M\omega r^2/\hbar}$$

- Substituting back into the original ODE, we obtain the differential equation

$$f_{n\ell}'' + 2\left(\frac{\ell+1}{r} - \frac{M\omega r}{\hbar}\right)f_{n\ell}' + \left[\frac{2ME_{n\ell}}{\hbar^2} - \frac{(2\ell+3)M\omega}{\hbar}\right]f_{n\ell} = 0$$

- As we have previously, propose that

$$f_{n\ell}(r) = \sum_j a_j r^j$$

- But there's a problem: $f_{n\ell}'(r=0) = a_1$, and this would allow the $(\ell+1)/r$ term to diverge and make the differential equation blow up.
- Thus, we choose $a_1 = 0$ and proceed.

- Substituting this power series into the differential equation, we obtain

$$\sum_j j(j-1)a_j r^{j-2} + 2\left(\frac{\ell+1}{r} - \frac{M\omega r}{\hbar}\right)\sum_j ja_j r^{j-1} + \left[\frac{2ME_{n\ell}}{\hbar^2} - \frac{(2\ell+3)M\omega}{\hbar}\right]\sum_j a_j r^j = 0$$

- Make a change of variables $j \rightarrow j+2$ so that we can start the sum from zero.

$$\begin{aligned}\sum_{j=0}^{\infty} (j+2)(j+1)a_{j+2}r^j + 2\left(\frac{\ell+1}{r} - \frac{M\omega r}{\hbar}\right)\sum_{j=0}^{\infty} (j+2)a_{j+2}r^{j+1} \\ + \left[\frac{2ME_{n\ell}}{\hbar^2} - \frac{(2\ell+3)M\omega}{\hbar}\right]\sum_{j=0}^{\infty} a_{j+2}r^{j+2} = 0\end{aligned}$$

- We will finish this derivation on Wednesday.