# 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 $\psi, E$.
  - There are three compatible operators:

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

    - 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 $(r,\theta,\phi)$.

• 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*

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

  - 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

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

    we may write

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

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

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

    - 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

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

    - 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

$$E = E_{n_1n_2n_3} = \hbar\omega_1\left(n_1 + \frac{1}{2}\right) + \hbar\omega_2\left(n_2 + \frac{1}{2}\right) + \hbar\omega_3\left(n_3 + \frac{1}{2}\right)$$

  - 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 $n_1 \to n_2$, $x \to y$, and $\omega_1 \to \omega_2$?
  - 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
$$\hat{\vec{L}}^2 Y_{\ell m}(\theta,\phi) = \hbar^2\ell(\ell+1)Y_{\ell m}(\theta,\phi)$$
and
$$\hat{L}_z Y_{\ell m}(\theta,\phi) = \hbar m Y_{\ell m}(\theta,\phi)$$
and
$$-\frac{\hbar^2}{2M}\frac{\mathrm{d}^2}{\mathrm{d}r^2}[U_{n\ell}(r)] + \underbrace{\left[V(r) + \frac{\hbar^2\ell(\ell+1)}{2Mr^2}\right]}_{V_{\text{eff}}(r)} U_{n\ell}(r) = E_{n\ell}U_{n\ell}(r)$$
- 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*
$$V_{\text{eff}}(r) = \frac{M\omega^2 r^2}{2} + \frac{\hbar^2\ell(\ell+1)}{2Mr^2}$$

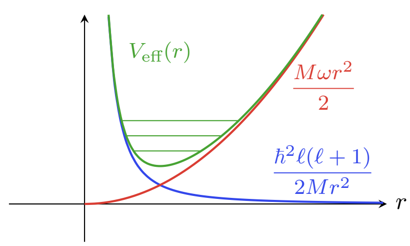


Figure 7.1: Spherically symmetric harmonic oscillator potential.

  - The problem we have to solve here is
$$-\frac{\hbar^2}{2M}\frac{\mathrm{d}^2}{\mathrm{d}r^2}[U_{n\ell}(r)] + \left[\frac{M\omega r^2}{2} + \frac{\hbar^2\ell(\ell+1)}{2Mr^2}\right] U_{n\ell}(r) = E_{n\ell}U(r)$$
  - Recall that
$$\psi(r,\theta,\phi) = R_{n\ell}(r)Y_{\ell m}(\theta,\phi) \qquad\qquad R_{n\ell}(r)r = U_{n\ell}(r)$$
  - 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 ($r\to 0$), we can approximate the potential as giving us
$$-\frac{\hbar^2}{2M}\frac{\mathrm{d}^2U_{n\ell}}{\mathrm{d}r^2} + \frac{\hbar^2\ell(\ell+1)}{2Mr^2}U_{n\ell} + \cdots = 0$$

  - In this case, the solution is proportional to

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

  - This is because

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

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

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

  - In this case, the solution is proportional to

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

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

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

- 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

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

  - 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

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

- Make a change of variables $j \to j+2$ 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.

## 7.2 Office Hours (Yunjia)

2/13: - PSet 2, Q2c.
  - If we can get up to Equation 12 in the answer key, that's full credit.
  - The thing with $\kappa_{II}^{-1}$ is the idea that if we have a value that's very large (like $\kappa_{II}$ will be as $V_0 \to \infty$ since $\kappa_{II} \propto V_0^{1/2}$), then we can Taylor expand in its reciprocal.
    - We cannot Taylor expand in the large values; we can only Taylor expand in small values.
    - This technique is called **perturbation theory** and will be a major topic of QMechII; Yunjia's use of it here was admittedly a bit extra.
- A brief introduction to perturbation theory.
  - Suppose we seek to solve an equation
    $$f(x,\epsilon) = 0$$
    where $\epsilon$ is small.
  - We can approximate the solution in the form
    $$f^{(0)}(x) + f^{(1)}(x)\epsilon + f^{(2)}(x)\epsilon^2 = 0$$
    where the digit superscripts in parentheses just denote different functions, not derivatives or anything like that. For example, we could equally well have used the notation $f,g,h$; it's just that this is less general.
  - To solve the original equation, we first solve
    $$f^{(0)}(x_0) = 0$$
    for $x_0$.
  - Then we solve
    $$f^{(0)}(x_0 + \epsilon x_1) + \epsilon f^{(1)}(x_0) = 0$$
    for $x_1$.
  - Continuing in this fashion, our solution takes on the following form and is progressively refined as more terms are calculated.
    $$x = x_0 + \epsilon x_1 + \epsilon^2 x_2 + \cdots$$