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:

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

    - 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, 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

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

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

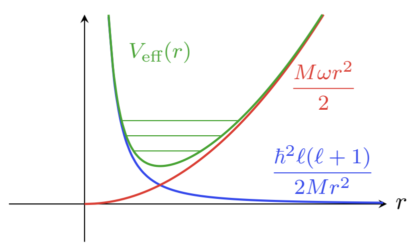

Figure 7.1: Spherically symmetric harmonic oscillator potential.

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

- In this case, the solution is proportional to

$$U_{n\ell} \propto C r^{\ell+1}$$

- This is because

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

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

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

- In this case, the solution is proportional to

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

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

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

– 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

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

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

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

– 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 κ_{II}^{-1} is the idea that if we have a value that's very large (like κ_{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 ϵ 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.
    $$x = x_0 + \epsilon x_1 + \epsilon^2 x_2 + \cdots$$

7.3 Spherically Symmetric Harmonic Oscillator

2/14:

- Review.
  - Recall that the 3D case we're considering corresponds to the Hamiltonian
    $$\hat{H} = -\frac{\hbar^2}{2M}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + \frac{M\omega^2}{2}(x^2 + y^2 + z^2)$$
    - For this Hamiltonian, we are trying to solve the Eigenvalue equation
      $$\hat{H}\psi(x,y,z) = E\psi(x,y,z)$$
    - The solution may be obtained in Cartesian coordinates as a limiting case of the asymmetric harmonic oscillator, i.e., via the separation of variables
      $$\psi(x,y,z) = X(x)Y(y)Z(z)$$

- This results in the solutions

$$\psi(x,y,z)=\prod_{i=1}^{3}H_{n_i}(\xi_i)\mathrm{e}^{-\xi_i^2/2}c_{n_i} \qquad E_{n_1n_2n_3}=\hbar\omega\left(n_1+n_2+n_3+\frac{3}{2}\right)$$

where $\xi_i=x_i\sqrt{m\omega/\hbar}$ and $x_1,x_2,x_3=x,y,z$, respectively.

– Recall also the polar coordinates r,θ,ϕ. The solution may be obtained here as well.
- In polar coordinates, we can see that the potential described above is central.
- Thus, we have that

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

and

$$\hat{L}_zY_{\ell m}(\theta,\phi)=\hbar mY_{\ell m}(\theta,\phi)$$

and

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

where $-\ell\leq m\leq\ell$ and thus there is a $2\ell+1$ degeneracy of $E_{n\ell}$ associated with different m.

➢ Recall that

$$R_{n\ell}(r)=\frac{U_{n\ell}(r)}{r}$$

- Substituting in

$$V(r)=\frac{M\omega^2r^2}{2}$$

we obtain the effective potential described in Figure 7.1.

- Limiting cases then lead us to construct the ansatz

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

- Now propose that

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

- Recall that we may obtain the differential equation

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

- We must set $a_1=0$.
- Moving on, we obtain

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

- We now begin on new content, continuing the same derivation from above.
- We can further simplify the above equation by solving for a_{j+2} in terms of a_j.
  – Begin by bringing all r's into the summations and running all sums from 0 to ∞ with no terms that go to zero so that every term is in r^j.

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

 - Combine the summations.

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

 - Simplify and combine terms.

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

 - Because each term in the above summation is affixed to a different power of r, meaning that no two terms can cancel, not only is the entire sum above equal to zero, but each individual term in it is equal to zero, too.
 - Thus, for all $j\in\mathbb{Z}_{\geq 0}$,

$$\begin{aligned}0&=(j+2)(j+2\ell+3)a_{j+2}+\left(\frac{M\omega}{\hbar}(2j+2\ell+3)-\frac{2ME_{n\ell}}{\hbar^2}\right)a_j\\a_{j+2}&=\frac{\frac{2ME_{n\ell}}{\hbar^2}-\frac{M\omega}{\hbar}(2j+2\ell+3)}{(j+2)(j+2\ell+3)}a_j\end{aligned}$$

- This combined with the fact that $a_1=0$ means that *all odd a_j equal zero.*
 - It follows that $f_{n\ell}$ can be viewed as a function of r^2, not just r, since this fact means that the power series will be of the form

$$f_{n\ell}(r)=a_0+a_2r^2+a_4r^4+a_6r^6+\cdots+a_{2n}r^{2n}+\cdots$$

- Now observe that in the limit of large j (i.e., as $j\to\infty$),

$$a_{j+2}\approx\frac{\frac{M\omega}{\hbar}(2j)}{j^2+2j}$$

and thus[1]

$$f_{n\ell}(r)\approx\mathrm{e}^{M\omega r^2/\hbar}$$

 - This, in turn, would lead to an exponential growth of $U_{n\ell}$ as $r\to\infty$ and hence a non-renormalizable solution.
 - Consequently, there must be some maximum value of j which we will denote by $n:=j_{\max}$.
 - In particular, n will be the value of j such that the numerator of the expression above giving $a_{j+2}(a_j)$ equals zero. This will guarantee that $a_{n+2}=0$ and hence all $a_j=0$ for $j>n$.
 - Solving for this n, we have that

$$\begin{aligned}\frac{2ME_{n\ell}}{\hbar^2}&=\frac{M\omega}{\hbar}(2n+2\ell+3)\\E_{n\ell}&=\hbar\omega\left(n+\ell+\frac{3}{2}\right)\end{aligned}$$

   - Recall that n is even; $n\geq 0$; $\ell\geq 0$; and for each ℓ, we have $2\ell+1$ solutions with $-\ell\leq m\leq\ell$ where $\hbar m$ are the eigenvalues of $\hat{L}_z$.

- Notice the remarkable similarity between the energy equations for the spherically symmetric harmonic oscillator in Cartesian coordinates (left below) and polar coordinates (right below).

$$E_{n_1n_2n_3}=\hbar\omega\left(\bar{n}+\frac{3}{2}\right)\qquad\qquad E_{\bar{n}}=\hbar\omega\left(\bar{n}+\frac{3}{2}\right)$$

[1]How did we get this transformation to exponential growth??

  - On the left above, $\bar{n} = n_1 + n_2 + n_3$. On the right above, $\bar{n} = n + \ell$.

- Now let's investigate some particular solutions in both cases.
- $\bar{n} = 0$.
  - Cartesian: The only possible values are $n_1 = n_2 = n_3 = 0$, corresponding to

$$\mathrm{e}^{-M\omega(x^2+y^2+z^2)/2\hbar}$$

  - Polar: The only possible values are $n = \ell = 0$, corresponding to

$$\mathrm{e}^{-M\omega r^2/2\hbar}$$

  - In both cases, there is only one solution, and the solutions are mathematically equivalent.
- $\bar{n} = 1$.
  - Cartesian: We could have $n_1 = 1$, $n_2 = n_3 = 0$; $n_2 = 1$, $n_1 = n_3 = 0$; or $n_3 = 1$, $n_2 = n_3 = 0$; corresponding to

$$x\mathrm{e}^{-M\omega r^2/2\hbar} \qquad y\mathrm{e}^{-M\omega r^2/2\hbar} \qquad z\mathrm{e}^{-M\omega r^2/2\hbar}$$

  - Polar: We have $n = 0$; $\ell = 1$; and $m = 1$, $m = 0$, or $m = -1$; corresponding to

$$r\mathrm{e}^{-M\omega r^2/2\hbar}\underbrace{\sin\theta\mathrm{e}^{i\phi}}_{(x+iy)/r} \qquad r\mathrm{e}^{-M\omega r^2/2\hbar}\cos\theta \qquad r\mathrm{e}^{-M\omega r^2/2\hbar}\underbrace{\sin\theta\mathrm{e}^{-i\phi}}_{(x-iy)/r}$$

  - In both cases, there are three solutions, and the solutions are mathematically equivalent (up to linear combinations).
- A pattern is emerging: Naturally, it makes sense that the coordinate system chosen should not affect the solutions.
- $\bar{n} = 2$.

n_1	n_2	n_3
0	0	2
0	2	0
2	0	0
0	1	1
1	0	1
1	1	0

(a) Cartesian coordinates.

n	ℓ	m
0	2	2
0	2	1
0	2	0
0	2	-1
0	2	-2
2	0	0

(b) Spherical coordinates.

Table 7.1: Spherically symmetric harmonic oscillator solutions ($\bar{n} = 2$).

  - In both cases, there are six solutions.
  - Note that we do not consider the case where $n = \ell = 1$ in Table 7.1b because this would mean that $j_{\max} = n = 1$ is an odd number, which is not allowed.