3D-Central Force Problems I

Read: C-TDL, pages 643-660 for next lecture.

**All 2-Body, 3-D problems can be reduced to**

* a 2-D angular part that is exactly and universally soluble
* a 1-D radial part that is system-specific and soluble by 1-D techniques in which you are now expert

**Next 3 lectures:**

- Correspondence Principle
- Commutation Rules

→ all matrix elements

**Roadmap**

1. define radial momentum \( \mathbf{p}_r = r^{-1}(\mathbf{q} \cdot \mathbf{p} - i\hbar) \)

2. define orbital angular momentum \( \mathbf{L} = \mathbf{\bar{q}} \times \mathbf{\bar{p}} \)

   - also \( \mathbf{L} \times \mathbf{L} = i\hbar\mathbf{L} \) and \( [\mathbf{L}_i, \mathbf{L}_j] = i\hbar \sum_k \varepsilon_{ijk} \mathbf{L}_k \)

3. separate \( \mathbf{p}^2 \) into radial and angular terms: \( \mathbf{p}^2 = \mathbf{p}_r^2 + r^{-2}\mathbf{L}^2 \)

4. find Complete Set of Commuting Observables (CSCO) useful for block-diagonalizing \( \mathbf{H} \)

   \[
   [\mathbf{H}, \mathbf{L}^2] = [\mathbf{H}, \mathbf{L}_i] = [\mathbf{L}^2, \mathbf{L}_i] = 0 \quad \mathbf{H}, \mathbf{L}^2, \mathbf{L}_i \quad \text{CSCO}
   \]

   - \( [\mathbf{L}, M_L] \) universal basis set

5. separate radial part of \( \mathbf{H} \):

   \[
   \mathbf{H}_\ell(r) = \frac{\mathbf{p}_r^2}{2\mu} + V(r) + \frac{\hbar^2 \ell(\ell + 1)}{2\mu r^2} \quad \text{effective radial potential}
   \]

6. ALL Matrix Elements of Angular Momentum Components Derived from Commutation Rules.

7. Spherical Tensor Classification of all operators.

8. Wigner-Eckart Theorem → all angular matrix elements of all operators.

I hate differential operators. Replace them using exclusively simple Commutation Rule based Operator Algebra.
Lots of derivations based on classical VECTOR ANALYSIS — much will be set aside as NONLECTURE

Central Force Problems: 2 bodies where interaction force is along the vector \( \vec{r}_{12} \)

\[
\vec{q}_1 = \vec{q}_1 - \vec{q}_{cm}
\]

\[
\vec{q}_2 = \vec{q}_1 + \vec{q}_{12}
\]

\[
\vec{q}_{12} = \vec{q}_2 - \vec{q}_1 = \hat{i}(x_2 - x_1) + \hat{j}(y_2 - y_1) + \hat{k}(z_2 - z_1)
\]

\[
r = |\vec{q}_{12}| = \left[ (x_2 - x_1)^2 + (y_2 - y_1)^2 + (z_2 - z_1)^2 \right]^{1/2}
\]

also C.M. Coordinate system

\[
\vec{r}_1 = \vec{q}_1 - \vec{r}_{cm}
\]

\[
[l/r = m_2/M]
\]

\[
\vec{r}_2 = \vec{q}_2 - \vec{q}_{cm}
\]

\[
[l/r = m_1/M]
\]

\[
\mathbf{H} = \mathbf{H}_{\text{translation}} + \mathbf{H}_{\text{center of mass}}
\]

motion of fictitious

free translation of C of M of system of mass \( \mu = \frac{m_1m_2}{m_1 + m_2} \)

in coordinate system with origin at C of M (CTDL page 713)

LAB

\[
\mathbf{H}_{\text{translation}}^f = \frac{\mathbf{p}_{\text{trans}}^2}{2(m_1 + m_2)} + \mathbf{V}_{\text{constant}}
\]

free translation of system with respect to lab (not interesting)

BODY

\[
\mathbf{H}_{\text{C.M.}}^f = \frac{1}{2\mu} \mathbf{p}_{\text{cm}}^2 + \mathbf{V}(\mathbf{r})
\]

motion of particle of mass \( \mu \) with respect to origin at c. of m.

GOAL IS TO SIMPLIFY \( \mathbf{p}_{\text{cm}}^2 \)

because that is only place where \( \theta, \phi \) degrees of freedom appear.
1. Define Radial Component of $P_{cm}$

Correspondence Principle

* classical mechanics
* Cartesian Coordinates
* symmetrize to avoid failure to satisfy Commutation Rules

** verify that all three derived operators, $p$, $p_r$, and $L$
  * are Hermitian
  * satisfy $[q, p] = i\hbar$

Purpose of this lecture is to walk you through the standard vector analysis and Quantum Mechanics Correspondence Principle procedures

$q = \hat{i}x + \hat{j}y + \hat{k}z$

$p = \hat{i}p_x + \hat{j}p_y + \hat{k}p_z$

$r = \sqrt{x^2 + y^2 + z^2} = \frac{1}{2}[q \cdot q]^{1/2} = |q|$

find radial (i.e. along $q$)-part of $p$

project $\vec{p}$ onto $q$

$q \cdot p = |q||p|\cos \theta$

$\cos(q, p) = \frac{q \cdot p}{|q||p|}$

radial component of $p$ is obtained by projecting $\vec{p}$ onto $\vec{q}$

$p_r = |p|\cos \theta = \frac{|q \cdot p|}{|q||p|} = \frac{q \cdot p}{r}$

so from standard vector analysis we get $p_r = r^{-1}q \cdot \vec{p}$
This is a trial form for \( p_r \), but it is necessary, according to Correspondence Principle, to symmetrize it.

\[
p_r = \frac{1}{4} \left[ r^{-1} (q \cdot p + p \cdot q) + (q \cdot p + p \cdot q) r^{-1} \right]
\]

arrange terms in all possible orders!

**NONLECTURE (except for Eq. (4))**

SIMPLIFY ABOVE Definition to

\[
p_r = r^{-1} (q \cdot p - i\hbar) \quad (r \text{ is not a vector})
\]

\[
[q, p] = [x, p_x] + [y, p_y] + [z, p_z] = 3i\hbar
\]

\[
\therefore p \cdot q = q \cdot p - [q, p]
\]

\[
p_r = \frac{1}{4} \left[ r^{-1} (2q \cdot p - [q, p]) + (2q \cdot p - [q, p]) r^{-1} \right] \tag{1}
\]

\[
= \frac{1}{4} \left[ r^{-1} 4q \cdot p - r^{-1} 2q \cdot p + 2q \cdot pr^{-1} - 6i\hbar r^{-1} \right] \tag{2}
\]

\[
= r^{-1} q \cdot p - \frac{3}{2} i\hbar r^{-1} + \frac{1}{2} [q \cdot p, r^{-1}] \tag{3}
\]

**LEMMA:** need more general Commutation Rule for which \([q \cdot p, r^{-1}]\) is a special case

1st simplify: \([f(r), q \cdot p] = q \cdot [f(r), p] + [f(r), q] \cdot p\)
but, from 1-D, we could have shown

\[ [f(x), p] \phi = f(x) \frac{\hbar}{i} \frac{\partial}{\partial x} \phi - \frac{\hbar}{i} \frac{\partial}{\partial x} (f(x) \phi) \]

\[ = \frac{\hbar}{i} [f(x) \phi' - f' \phi - f \phi'] = i\hbar f'(x) \phi \]

\[ [f(x), p] = i\hbar \frac{\partial f}{\partial x} \] for 1-D

Thus, in 3-D, the chain rule gives

\[ [f(r), \vec{p}] = i\hbar \left[ \frac{\partial f}{\partial r} \frac{\partial r}{\partial x} + \frac{\partial f}{\partial r} \frac{\partial r}{\partial y} + \frac{\partial f}{\partial r} \frac{\partial r}{\partial z} \right] \]

evaluate these first

\[ \frac{\partial r}{\partial x} = \frac{\partial}{\partial x} \left[ x^2 + y^2 + z^2 \right]^{1/2} = x / r \]

\[ \text{etc. for } \frac{\partial r}{\partial y} \text{ & } \frac{\partial r}{\partial z} \]

Thus \[ [f(r), \vec{p}] = i\hbar \frac{\partial f}{\partial r} \left[ \frac{x}{r} + \frac{y}{r} + \frac{z}{r} \right] = i\hbar \frac{\partial f}{\partial r} \frac{\vec{q}}{\vec{r}} \]

\[ [f(r), \vec{q} \cdot \vec{p}] = \vec{q} \cdot [f(r), p] = i\hbar \frac{\partial f}{\partial r} \left( \frac{x^2 + y^2 + z^2}{r} \right) = i\hbar \frac{\partial f}{\partial r} \frac{\vec{r}}{r} \]

\[ [f(r), \vec{q} \cdot \vec{p}] = i\hbar \frac{\partial f}{\partial \vec{r}} \cdot \vec{r} \] this is a scalar, not a vector, equation (4)

But we wanted to evaluate the commutation rule for \( f(r) = r^{-1} \)

\[ \left[ r^{-1}, \vec{q} \cdot \vec{p} \right] = i\hbar \frac{\partial}{\partial r} \left( \frac{1}{r} \right) \vec{r} = -i\hbar r^{-1} \]

plug this result into (3)

\[ p_r = r^{-1} \vec{q} \cdot \vec{p} - \frac{3}{2} i\hbar r^{-1} + \frac{1}{2} (i\hbar r^{-1}) \]

This is the compact but non-symmetric result we got starting with a carefully symmetrized starting point – as required by Correspondence Principle.
This result is identical to result obtained from standard vector analysis IN THE LIMIT OF $h \to 0$.

Still must do 2 things: show $[r, p_r] = i\hbar$
show $p_r$ is Hermitian

$$[r, p_r] = [r, r^{-1}(q \cdot p - i\hbar)] - 0\ 0$$
$$= r^{-1}[r, q \cdot p] - r^{-1}[i\hbar] + [r, r^{-1}](q \cdot p - i\hbar)$$
$$= r^{-1}[r, q \cdot p]$$
Use Eq. (4)

$$[r, q \cdot p] = i\hbar r$$

$$\therefore [r, p_r] = i\hbar$$

* we do not need to confirm that $p_r$ is Hermitian because it was constructed from a symmetrized form which is guaranteed to be Hermitian.

Correspondence Principle!

2. Verify that Classical Definition of Angular Momentum is Appropriate for QM.

$$\vec{L} = \vec{q} \times \vec{p} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix}$$

We will see that this definition of an angular momentum is acceptable as far as the correspondence principle is concerned, but it is not sufficiently general.

NONLECTURE

What about symmetrizing $\vec{L}$?

$$L_x = y p_z - z p_y = p_z y - p_y z$$

PRODUCTS OF NON-CONJUGATE QUANTITIES

$$= -(\vec{p} \times \vec{q})_x$$

$$\therefore p \times q = -L$$
5.73 Lecture #21

\[ q \times p + p \times q = 0 \]  
\[ q \times p - p \times q = 2\vec{L} \]

symmetrization is impossible!

antisymmetrization is unnecessary!

But is \( \vec{L} \) Hermitian as defined?

BE CAREFUL: \( (q \times p)\dagger \neq p\dagger \times q\dagger \)!

\[
\begin{align*}
L_x &= yp_z - zp_y \\
L_x\dagger &= p_z\dagger y - p_y\dagger z = p_z y - p_y z = y p_z - z p_y = L_x
\end{align*}
\]

\( (p,q \text{ are Hermitian}) \)

\[ \therefore \vec{L} \text{ is Hermitian as defined.} \]

RESUME

3A. Separate \( p^2 \) into radial and angular terms.

GOAL:

\[
p^2 = p_r^2 + r^{-2}L^2
\]  
\[ \vec{p} = \vec{p}_\parallel + \vec{p}_\perp \]

\( (\parallel \text{ and } \perp \text{ with respect to } \vec{q}) \)

Classically

\[
\vec{p} = r^{-2} \left[ \vec{q}(\vec{q} \cdot \vec{p}) - \vec{q} \times (\vec{q} \times \vec{p}) \right]
\]

component \parallel \text{ to } \vec{q} \quad \text{ component in } \vec{q} \cdot \vec{p}

plane which is \perp \text{ to } \vec{q} \quad \text{(is the sign correct?)}

\( r^{-2} \) is needed in both terms to remain dimensionally correct.
talk through this vector identity

1st term ($\mathbf{p}_1$): \[ \mathbf{q} \cdot \mathbf{p} = |\mathbf{q}| |\mathbf{p}| \cos \theta \]
\[ \frac{\mathbf{q}}{|\mathbf{q}|} = \text{unit vector along } \mathbf{q} \]

2nd term ($\mathbf{p}_\perp$): \[ \mathbf{q} \times \mathbf{p} \text{ points } \perp \text{ up out of paper} \]

\[ \text{thumb} \quad \text{finger} \quad \text{palm} \]

\[ \text{thumb} \quad \mathbf{q} \times \mathbf{p} \text{ finger} \]
\[ \text{is in plane of paper in opposite direction of } \mathbf{p}_\perp, \]
\[ \text{hence minus sign.} \]

Is it necessary to symmetrize Eq. (9)?

NONLECTURE

Examine Eq. (9) for QM consistency

x component

\[ p_x = r^{-2} \left[ x(xp_x + yp_y + zp_z) - (yL_z - zL_y) \right] \]

but \[ yL_z - zL_y = y(xp_y - yp_x) + z(xp_z - zp_x) \]
\[ p_x = r^{-2} \left[ (x^2 + y^2 + z^2) p_x + (xy - yx)p_y + (xz - zx)p_z \right] = p_x \]

similarly for $p_y, p_z$

Symmetrize? No, because 2 parts of $\vec{p}$

are already shown to be Hermitian.

RESUME
5.73 Lecture #21

3B. Evaluate $\mathbf{p} \cdot \mathbf{p}$

$$
\mathbf{p}^2 = \mathbf{p}\mathbf{r}^{-2}\left[\mathbf{q}(\mathbf{q} \cdot \mathbf{p}) - \mathbf{q} \times (\mathbf{q} \times \mathbf{p})\right]
$$

[goal is $\mathbf{p}^2 = \mathbf{p}_r^2 + r^{-2}\mathbf{L}^2$] (10)

commute $\mathbf{\bar{p}}$ through $r^{-2}$ to be able to take advantage of classical vector triple product

NONLECTURE

$$
\left[\mathbf{\bar{p}}, r^{-2}\right] = -i\hbar\left[\hat{i} \frac{\partial}{\partial x} r^{-2} + \hat{j} \frac{\partial}{\partial y} r^{-2} + \hat{k} \frac{\partial}{\partial z} r^{-2}\right]
$$

$$
= 2i\hbar r^{-4}\hat{q}
$$

Recall $\left[f(x), \mathbf{p}_x\right] = i\hbar \frac{\partial f}{\partial x}$

because $\frac{\partial}{\partial x} r^{-2} = -2r^{-3} \frac{\partial r}{\partial x} = -2r^{-3}\left(\frac{1}{2}\right)\frac{2x}{r} = -2x/r^4$

thus $\mathbf{\bar{p}} r^{-2} = r^{-2}\left(\mathbf{\bar{p}} + 2i\hbar r^{-2}\hat{q}\right)$ (11)

$$
\mathbf{p}^2 = r^{-2}\left(\mathbf{\bar{p}} + 2i\hbar r^{-2}\hat{q}\right)[\mathbf{q}(\mathbf{q} \cdot \mathbf{p}) - \mathbf{q} \times (\mathbf{q} \times \mathbf{p})]
$$

(12)

get 4 terms

$$
\mathbf{p}^2 = r^{-2}(\mathbf{p} \cdot \mathbf{q})(\mathbf{q} \cdot \mathbf{p}) - r^{-2}\mathbf{p} \cdot [\mathbf{q} \times (\mathbf{q} \times \mathbf{p})] + r^{-2}(2i\hbar) r^{-2}(\mathbf{q} \cdot \mathbf{q})(\mathbf{q} \cdot \mathbf{p}) - r^{-2}(2i\hbar) r^{-2}\mathbf{q} \cdot [\mathbf{q} \times (\mathbf{q} \times \mathbf{p})]
$$

I II III IV

$$
\begin{align*}
I &= r^{-2}(\mathbf{q} \cdot \mathbf{p} - 3i\hbar)(\mathbf{q} \cdot \mathbf{p}) \\
III &= r^{-2}(2i\hbar)(\mathbf{q} \cdot \mathbf{p}) \\
II &= -r^{-2}(\mathbf{p} \times \mathbf{q}) \cdot (\mathbf{q} \times \mathbf{p}) = -r^{-2}(\pm \mathbf{L}^2) = r^{-2}\mathbf{L}^2 \\
IV &= -r^4(2i\hbar)(\mathbf{q} \times \mathbf{q})^0(\mathbf{q} \times \mathbf{p}) \\
\end{align*}
$$

$$
\mathbf{p}^2 = r^{-1}\mathbf{p}_r(\mathbf{r}\mathbf{p}_r + i\hbar) + r^{-2}\mathbf{L}^2 = r^{-1}[\mathbf{r}\mathbf{p}_r - i\hbar]\mathbf{p}_r + r^{-1}\mathbf{p}_r i\hbar + r^{-2}\mathbf{L}^2 = \mathbf{p}_r^2 + r^{-2}\mathbf{L}^2
$$

(13)
RESUME

This $p^2 = p_r^2 + r^{-2}L^2$ equation
is a very useful and simple form for $p^2$ – separated into additive radial and angular terms! If $H$ can be separated into additive terms, then the eigenvectors can be factored.

SUMMARY

$p_r = r^{-1}(q \cdot p - ih)$  
radial momentum

$p^2 = p_r^2 + r^{-2}L^2$  
separation of radial and angular terms

$H = \frac{p_r^2}{2\mu} + \left[ \frac{L^2}{2\mu r^2} + V(r) \right]$  

eventually $V_\ell(r) = \frac{\hbar^2 \ell(\ell + 1)}{2\mu r^2} + V(r)$

Next: properties of $L_i, \ L^2 \longrightarrow$ CSCO