

## 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:  $\left[ \begin{array}{l} \text{Correspondence Principle} \\ \text{Commutation Rules} \end{array} \right] \longrightarrow$  all matrix elements

Roadmap

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

2. define orbital angular momentum  $\vec{\mathbf{L}} = \vec{\mathbf{q}} \times \vec{\mathbf{p}}$

general definition of angular momentum and of "vector operators"

$$\left( \text{also } \mathbf{L} \times \mathbf{L} = i\hbar\mathbf{L} \text{ and } [\mathbf{L}_i, \mathbf{L}_j] = i\hbar \sum_k \epsilon_{ijk} \mathbf{L}_k \right)$$

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

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

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

$|\mathbf{L}, M_L\rangle$  universal basis set

5. separate radial part of  $\mathbf{H}$ :  $\mathbf{H}_\ell(\mathbf{r}) = \frac{\mathbf{p}_r^2}{2\mu} + V(\mathbf{r}) + \underbrace{\frac{\hbar^2 \ell(\ell+1)}{2\mu r^2}}_{V_\ell(\mathbf{r})}$  effective radial potential

1-D Schröd Eq.

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

7. Spherical Tensor Classification of **all** operators.

↓

8. Wigner-Eckart Theorem  $\rightarrow$  all angular matrix elements of all operators.

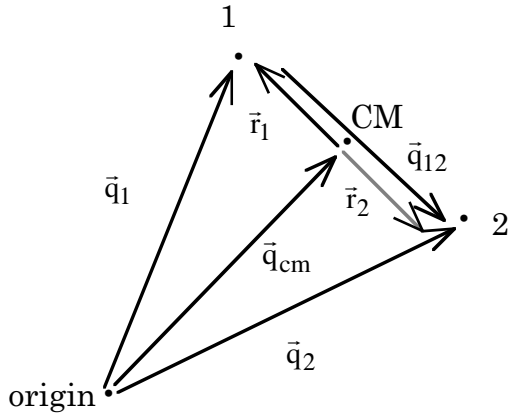
I hate differential operators. Replace them using exclusively simple Commutation Rule based Operator Algebra.

# 5.73 Lecture #21

# 21 - 2

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  $\vec{q}_1 - \vec{q}_2$



$$\vec{q}_2 = \vec{q}_1 + \vec{q}_{12}$$

$$\vec{q}_{12} = \vec{q}_2 - \vec{q}_1$$

$$= \hat{i}(x_2 - x_1) + \hat{j}(y_2 - y_1) + \hat{k}(z_2 - z_1)$$

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

also C.M. Coordinate system

$$\vec{r}_1 = \vec{q}_1 - \vec{q}_{cm} \quad [ |r_1|/r = m_2/M ]$$

$$\vec{r}_2 = \vec{q}_2 - \vec{q}_{cm} \quad [ |r_2|/r = m_1/M ]$$

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

motion of fictitious

free translation of C of M of system of mass  $M = m_1 + m_2$  particle of mass  $\mu = \frac{m_1 m_2}{m_1 + m_2}$

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

LAB  $\mathbf{H}_{\text{translation}} = \frac{\mathbf{P}_{\text{trans}}^2}{2(m_1 + m_2)} + \mathbf{V}_{\text{constant}}$  free translation of system with respect to lab (not interesting)

BODY  $\mathbf{H}_{\text{C.M.}} = \frac{1}{2\mu} \mathbf{P}_{\text{cm}}^2 + \underbrace{\mathbf{V}(\mathbf{r})}_{\text{free rotation (no } \theta, \phi \text{ dependence)}}$  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.

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### 1. Define Radial Component of $\vec{P}_{cm}$

Correspondence Principle

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

- \*\* verify that all three derived operators,  $\mathbf{p}$ ,  $\mathbf{p}_r$  and  $\mathbf{L}$
- are Hermitian
  - satisfy  $[\mathbf{q}, \mathbf{p}] = i\hbar$

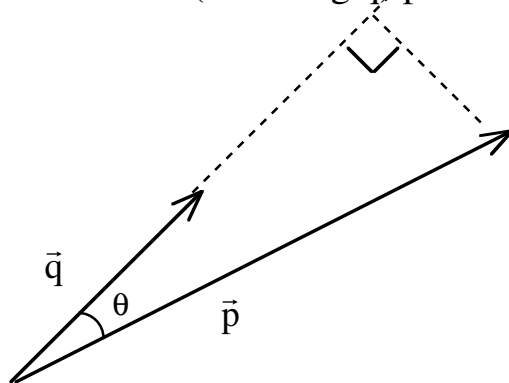
Purpose of this lecture is to walk you through the standard vector analysis and Quantum Mechanics Correspondence Principle procedures

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

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

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

find radial (i.e. along  $\vec{q}$ ) part of  $\vec{p}$



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

$$\mathbf{q} \cdot \mathbf{p} = |\mathbf{q}||\mathbf{p}|\cos\theta$$

$$\cos(\underbrace{\mathbf{q}, \mathbf{p}}_{\theta}) = \frac{\mathbf{q} \cdot \mathbf{p}}{|\mathbf{q}||\mathbf{p}|}$$

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

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

so from standard vector analysis we get  $p_r = r^{-1}\vec{q} \cdot \vec{p}$

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This is a trial form for  $p_r$ , but it is necessary, according to Correspondence Principle, to symmetrize it.

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

arrange terms in all possible orders!

NONLECTURE (except for Eq. (4))

SIMPLIFY ABOVE Definition to  $p_r = r^{-1} (\mathbf{q} \cdot \mathbf{p} - i\hbar)$  ( $\mathbf{r}$  is not a vector)

$[\vec{q}, \vec{p}]$  is a vector commutator — be careful

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

$$\therefore \mathbf{p} \cdot \mathbf{q} = \mathbf{q} \cdot \mathbf{p} - [\vec{q}, \vec{p}]$$

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

$$= \frac{1}{4} \left[ \underbrace{r^{-1} 4\mathbf{q} \cdot \mathbf{p} - r^{-1} 2\mathbf{q} \cdot \mathbf{p}}_{\text{add and subtract } 2r^{-1}\mathbf{q} \cdot \mathbf{p}} + 2\mathbf{q} \cdot \mathbf{p} r^{-1} - 6i\hbar r^{-1} \right] \quad (2)$$

$$= r^{-1} \mathbf{q} \cdot \mathbf{p} - \frac{3}{2} i\hbar r^{-1} + \frac{1}{2} [\mathbf{q} \cdot \mathbf{p}, r^{-1}] \quad (3)$$

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

$$\text{1st simplify: } [f(\mathbf{r}), \mathbf{q} \cdot \mathbf{p}] = \mathbf{q} \cdot [f(\mathbf{r}), \vec{p}] + [f(\mathbf{r}), \vec{q}] \cdot \vec{p}$$

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but, from 1-D, we could have shown

$$\begin{aligned} [f(\mathbf{x}), \mathbf{p}] \phi &= f(\mathbf{x}) \frac{\hbar}{i} \frac{\partial}{\partial \mathbf{x}} \phi - \frac{\hbar}{i} \frac{\partial}{\partial \mathbf{x}} (f(\mathbf{x}) \phi) \\ &= \frac{\hbar}{i} [f(\mathbf{x}) \phi' - f' \phi - f \phi'] = i \hbar f'(\mathbf{x}) \phi \\ [f(\mathbf{x}), \mathbf{p}] &= i \hbar \frac{\partial f}{\partial \mathbf{x}} \quad \text{for 1-D} \end{aligned}$$

Thus, in 3-D, the chain rule gives

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

evaluate these first

$$\begin{aligned} \frac{\partial \mathbf{r}}{\partial \mathbf{x}} &= \frac{\partial}{\partial \mathbf{x}} [x^2 + y^2 + z^2]^{1/2} = x [x^2 + y^2 + z^2]^{-1/2} = \mathbf{x} / r \\ \text{etc. for } \frac{\partial \mathbf{r}}{\partial \mathbf{y}} &\text{ \& } \frac{\partial \mathbf{r}}{\partial \mathbf{z}} \end{aligned}$$

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

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

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

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

$$\left[ r^{-1}, \mathbf{q} \cdot \mathbf{p} \right] = i \hbar \frac{\partial}{\partial \mathbf{r}} \left( \frac{1}{r} \right) \mathbf{r} = -i \hbar \mathbf{r}^{-1} \quad (5)$$

plug this result into (3)

$$\mathbf{p}_r = r^{-1} \mathbf{q} \cdot \mathbf{p} - \frac{3}{2} i \hbar r^{-1} + \frac{1}{2} (i \hbar r^{-1})$$

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RESUME  
HERE  $\mathbf{p}_r = r^{-1} (\mathbf{q} \cdot \mathbf{p} - i \hbar)$  (6)

This is the compact but non-symmetric result we got starting with a carefully symmetrized starting point – as required by Correspondence Principle.

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- \* This result is identical to result obtained from standard vector analysis IN THE LIMIT OF  $\hbar \rightarrow 0$ .

Still must do 2 things: show  $[\mathbf{r}, \mathbf{p}_r] = i\hbar$   
show  $\mathbf{p}_r$  is Hermitian

$$\begin{aligned} [\mathbf{r}, \mathbf{p}_r] &= [\mathbf{r}, \mathbf{r}^{-1}(\mathbf{q} \cdot \mathbf{p} - i\hbar)] \\ &= \mathbf{r}^{-1}[\mathbf{r}, \mathbf{q} \cdot \mathbf{p}] - \mathbf{r}^{-1}[\mathbf{r}, i\hbar] + [\mathbf{r}, \mathbf{r}^{-1}](\mathbf{q} \cdot \mathbf{p} - i\hbar) \\ &= \mathbf{r}^{-1}[\mathbf{r}, \mathbf{q} \cdot \mathbf{p}] \quad \text{Use Eq. (4)} \end{aligned}$$

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

$$\therefore [\mathbf{r}, \mathbf{p}_r] = i\hbar$$

\*

- \* we do not need to confirm that  $\mathbf{p}_r$  is Hermitian because it was constructed from a symmetrized form which is guaranteed to be Hermitian.

Correspondence Principle!

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

$$\vec{L} = \vec{q} \times \vec{p} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix} \quad (7)$$

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.

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NONLECTURE

What about symmetrizing  $\vec{L}$ ?

$$\begin{aligned} L_x &= yp_z - zp_y = p_z y - p_y z \\ &= -(\vec{p} \times \vec{q})_x \end{aligned}$$

$$\therefore \mathbf{p} \times \mathbf{q} = -\mathbf{L}$$

PRODUCTS OF  
NON-CONJUGATE  
QUANTITIES

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$$\begin{aligned} \mathbf{q} \times \mathbf{p} + \mathbf{p} \times \mathbf{q} &= 0 && \text{symmetrization is impossible!} \\ \mathbf{q} \times \mathbf{p} - \mathbf{p} \times \mathbf{q} &= 2\vec{\mathbf{L}} && \text{antisymmetrization is unnecessary!} \end{aligned}$$

But is  $\vec{\mathbf{L}}$  Hermitian as defined?

BE CAREFUL:  $(\mathbf{q} \times \mathbf{p})^\dagger \neq \mathbf{p}^\dagger \times \mathbf{q}^\dagger!$

go back to definition of vector cross product

$$\begin{aligned} L_x &= y p_z - z p_y \\ L_x^\dagger &= p_z^\dagger y^\dagger - p_y^\dagger z^\dagger = p_z y - p_y z = y p_z - z p_y = L_x \\ &(\mathbf{p}, \mathbf{q} \text{ are Hermitian}) \end{aligned}$$

$\therefore \vec{\mathbf{L}}$  is Hermitian as defined.

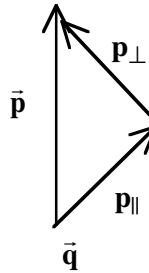
### RESUME

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3A. Separate  $\mathbf{p}^2$  into radial and angular terms.

GOAL:  $\mathbf{p}^2 = \mathbf{p}_r^2 + r^{-2} \mathbf{L}^2$  (8)

vector analysis  $\vec{\mathbf{p}} = \vec{\mathbf{p}}_{\parallel} + \vec{\mathbf{p}}_{\perp}$  (|| and  $\perp$  with respect to  $\vec{\mathbf{q}}$ )



Classically 
$$\vec{\mathbf{p}} = \mathbf{r}^{-2} \left[ \underbrace{\vec{\mathbf{q}}(\mathbf{q} \cdot \mathbf{p})}_{\text{component || to } \vec{\mathbf{q}}} - \underbrace{\vec{\mathbf{q}} \times (\overbrace{\mathbf{q} \times \mathbf{p}}^{\vec{\mathbf{L}}})}_{\text{component in } \vec{\mathbf{q}}, \vec{\mathbf{p}} \text{ plane which is } \perp \text{ to } \vec{\mathbf{q}}} \right]$$
 (9)

(is the sign correct?)

$\mathbf{r}^{-2}$  is needed in both terms to remain dimensionally correct.

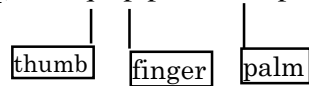
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talk through this vector identity

1st term ( $\mathbf{p}_{\parallel}$ ):  $\mathbf{q} \cdot \mathbf{p} = |\mathbf{q}||\mathbf{p}|\cos\theta$   
 $\vec{q}/|\mathbf{q}| = \text{unit vector along } \vec{q}$

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



$\vec{q} \times \underbrace{\mathbf{q} \times \mathbf{p}}_{\text{finger}}$  is in plane of paper in opposite direction of  $\mathbf{p}_{\perp}$ ,  
 hence minus sign.

Is it necessary to symmetrize Eq. (9)?

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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  $yL_z - zL_y = y(xp_y - yp_x) + z(xp_z - zp_x)$

$$p_x = r^{-2} \left[ (x^2 + y^2 + z^2)p_x + \cancel{(xy - yx)^0}p_y + \cancel{(xz - zx)^0}p_z \right] = p_x$$

similarly for  $p_y, p_z$

Symmetrize? No, because 2 parts of  $\vec{p}$   
 are already shown to be Hermitian.

RESUME

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

$$\mathbf{p}^2 = \bar{\mathbf{p}} \mathbf{r}^{-2} [\mathbf{q}(\mathbf{q} \cdot \mathbf{p}) - \mathbf{q} \times (\mathbf{q} \times \mathbf{p})] \quad (10)$$

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

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

### NONLECTURE

$$\begin{aligned} [\bar{\mathbf{p}}, \mathbf{r}^{-2}] &= -i\hbar \left[ \hat{i} \frac{\partial}{\partial x} \mathbf{r}^{-2} + \hat{j} \frac{\partial}{\partial y} \mathbf{r}^{-2} + \hat{k} \frac{\partial}{\partial z} \mathbf{r}^{-2} \right] \\ &= 2i\hbar \mathbf{r}^{-4} \bar{\mathbf{q}} \end{aligned} \quad \left[ \text{Recall } [f(\mathbf{x}), \mathbf{p}_x] = i\hbar \frac{\partial f}{\partial x} \right]$$

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

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

$$\mathbf{p}^2 = \mathbf{r}^{-2} (\bar{\mathbf{p}} + 2i\hbar \mathbf{r}^{-2} \bar{\mathbf{q}}) [\mathbf{q}(\mathbf{q} \cdot \mathbf{p}) - \mathbf{q} \times (\mathbf{q} \times \mathbf{p})] \quad (12)$$

get 4 terms

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

I
II
III
IV

$$\begin{aligned} \text{I} &= \mathbf{r}^{-2} (\mathbf{q} \cdot \mathbf{p} - 3i\hbar) (\mathbf{q} \cdot \mathbf{p}) \\ \text{III} &= \mathbf{r}^{-2} (2i\hbar) (\mathbf{q} \cdot \mathbf{p}) \end{aligned} \left. \vphantom{\begin{aligned} \text{I} \\ \text{III} \end{aligned}} \right\} \mathbf{r}^{-2} (\mathbf{q} \cdot \mathbf{p} - i\hbar) (\mathbf{q} \cdot \mathbf{p}) = \mathbf{r}^{-1} \mathbf{p}_r (\mathbf{q} \cdot \mathbf{p})$$

$\mathbf{r} \mathbf{p}_r + i\hbar$

$$\begin{aligned} \text{II} &= -\mathbf{r}^{-2} (\mathbf{p} \times \mathbf{q}) \cdot (\mathbf{q} \times \mathbf{p}) = -\mathbf{r}^{-2} (\pm \mathbf{L}^2) = \mathbf{r}^{-2} \mathbf{L}^2 \\ \text{IV} &= -\mathbf{r}^{-4} (2i\hbar) (\mathbf{q} \times \bar{\mathbf{q}}) \cdot (\mathbf{q} \times \mathbf{p}) \\ \mathbf{p}^2 &= \mathbf{r}^{-1} \mathbf{p}_r (\mathbf{r} \mathbf{p}_r + i\hbar) + \mathbf{r}^{-2} \mathbf{L}^2 = \mathbf{r}^{-1} [\mathbf{r} \mathbf{p}_r - i\hbar] \mathbf{p}_r + \mathbf{r}^{-1} \mathbf{p}_r i\hbar + \mathbf{r}^{-2} \mathbf{L}^2 = \mathbf{p}_r^2 + \mathbf{r}^{-2} \mathbf{L}^2 \end{aligned} \quad (13)$$

$\mathbf{r} \mathbf{p}_r \cdot [\mathbf{r}, \mathbf{p}_r]$

RESUME

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This  $\mathbf{p}^2 = \mathbf{p}_r^2 + r^{-2}\mathbf{L}^2$  equation

is a very useful and simple form for  $\mathbf{p}^2$  – separated into additive radial and angular terms! If  $\mathbf{H}$  can be separated into additive terms, then the eigenvectors can be factored.

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## SUMMARY

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

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

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

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

Next: properties of  $\mathbf{L}_i$ ,  $\mathbf{L}^2 \longrightarrow$  CSCO