

# We will start quantum chemistry today.

policy

- 1 we do not aim at being comprehensive
- 2 we will learn minimum topics to ...

perform astronomical observations

- |                        |  |
|------------------------|--|
| 1 statistic degeneracy | necessary to calculate $N_J$           |
| 2 selection rule       | which transition to look               |
| 3 notation             | J, K, Ka, Kc, m; understand literature |
| 4 nuclear spin         | what is ortho and para?                |

principle

reasons of many things :  
if we think in that way, it matches reality.  
or even have power of prediction.

# 1 statistic degeneracy

$$g_J = 2J + 1$$

$$\frac{N_J}{g_J} = N_0 \exp\left(-\frac{E_J}{kT}\right)$$

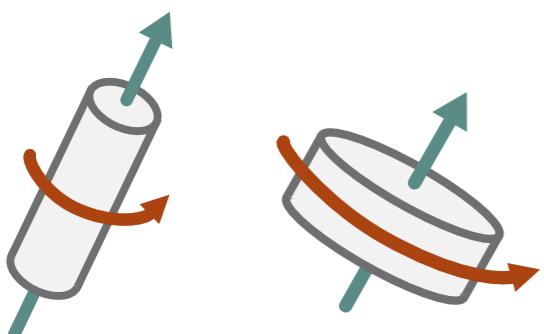
- notation ③
- quantum numbers  
 $J, K, K_a, K_c$

$\phi_r$  wave function

angular momentum  
geometrical view

● spherical harmonics

molecular rotation



prolate

oblate

- 1 statistic degeneracy
- 2 selection rule
- 3 notation
- 4 nuclear spin

# 1 statistic degeneracy

$$g_J = 2J + 1$$

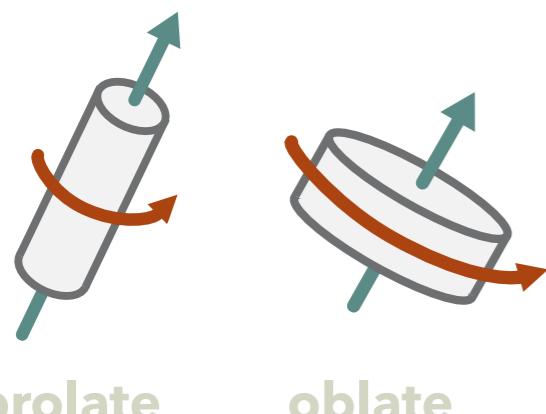
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# 1 statistic degeneracy

- 1 statistic degeneracy
- 2 selection rule
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# 2 selection rule

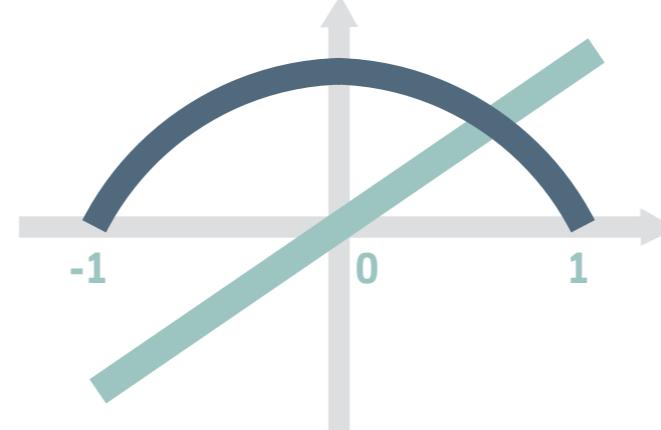
$$\Delta J = 0, \pm 1, 0 \leftrightarrow 0$$

vanishing integral  
 $\langle \phi_i | \mu_e | \phi_f \rangle = 0$

dipole moment

- spherical harmonics
- rotation symmetry group

spherical harmonics



symmetry of wave function

Born-Oppenheimer  
approximation

spherical harmonics

- projection operator
- nuclear spin degeneracy

# 1 statistic degeneracy

$$g_J = 2J + 1$$

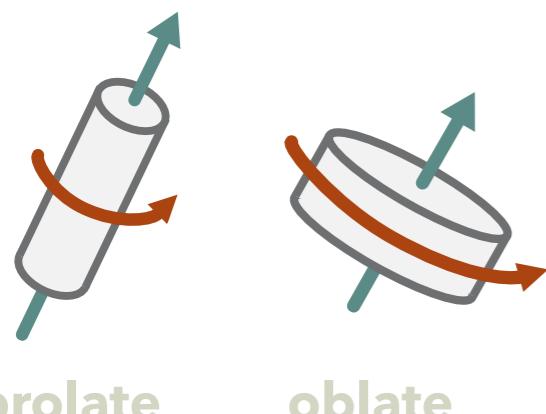
$$\frac{N_J}{g_J} = N_0 \exp\left(-\frac{E_J}{kT}\right)$$

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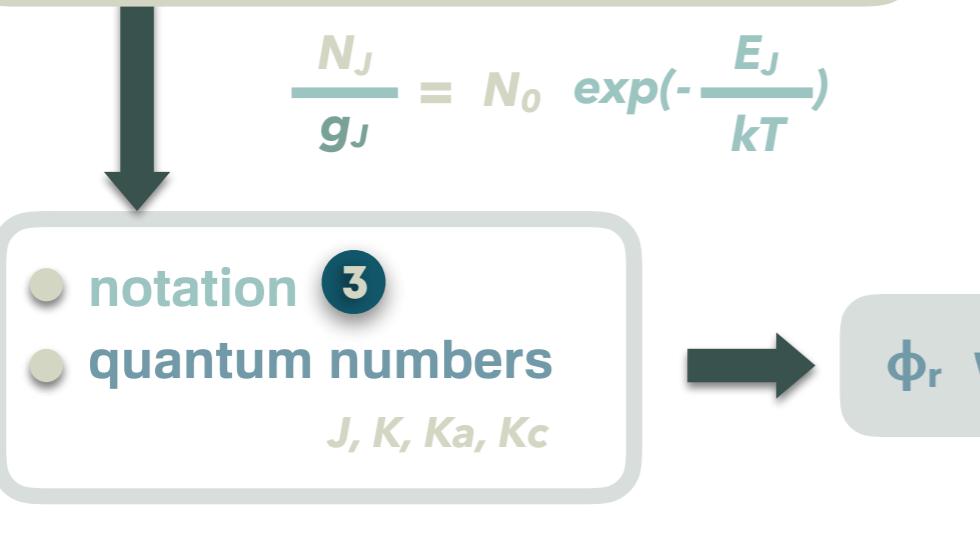
angular momentum  
geometrical view

molecular rotation



prolate

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- 1 statistic degeneracy
- 2 selection rule
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# 2 selection rule

$$\Delta J = 0, \pm 1, 0 \leftrightarrow 0$$

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● spherical harmonics



symmetry of wave function

Born-Oppenheimer  
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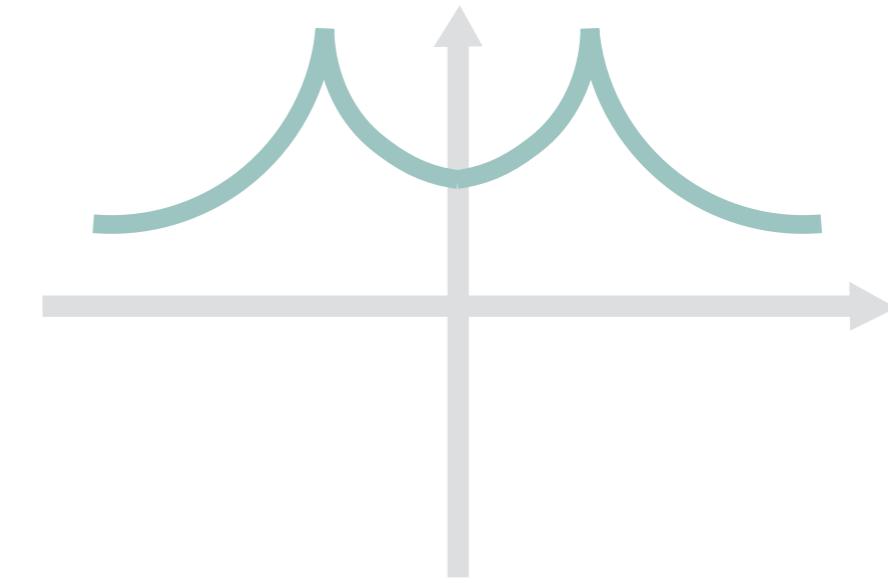
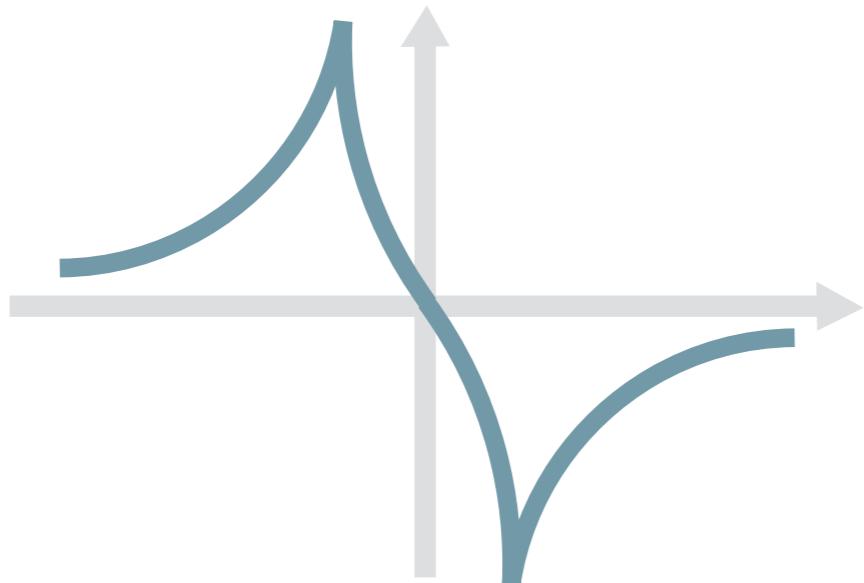
● spherical harmonics

- projection operator
- nuclear spin degeneracy

# Wave function

what do you think is a wavefunction?

- 1 solution of Schrödinger equation
- 2 squared, probability distribution of electron
- 3  $\langle J, K, m | O | J', k', m' \rangle$  bra.
- 4 something related to covalent bond



can we explain what is rotational wavefunction?

# Road to spherical harmonics

- 1 Hamiltonian in central field

$$H = -\frac{\hbar^2}{2\mu} \nabla^2 - \frac{Ze^2}{r}$$

- 2 separate r and  $\theta, \phi$

$$\nabla^2 = \frac{1}{r} \frac{\partial^2}{\partial r^2} r + \frac{1}{r^2} \Lambda^2$$

- 3 Laplacian in polar coordinate

$$\Lambda^2 = \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta}$$

- 
- 4 Legendre differential equation is part of Laplacian

- 5 Rodrigues formula is solution Leibniz rule

- 6 full Laplacian is associated Legendre differential equation

- 7 Derivative of Rodrigues formula is solution

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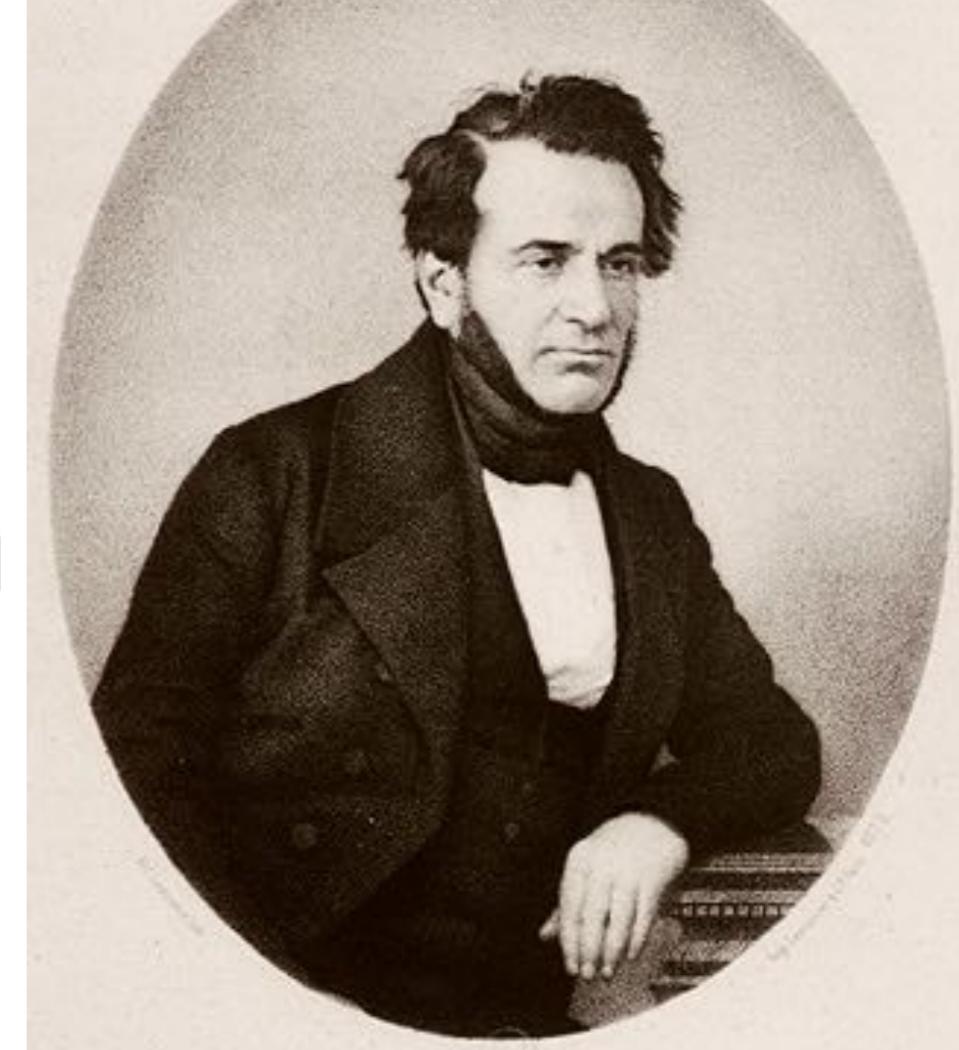
→ spherical harmonics



Pierre-Simon Laplace  
1749-1827



Adrien-Marie Legendre  
1752-1833



Olinde Rodrigues  
1795-1851



Sir William Rowan  
Hamilton  
1805-1865



Gottfried Wilhelm Leibniz  
1646-1715 born in Leipzig

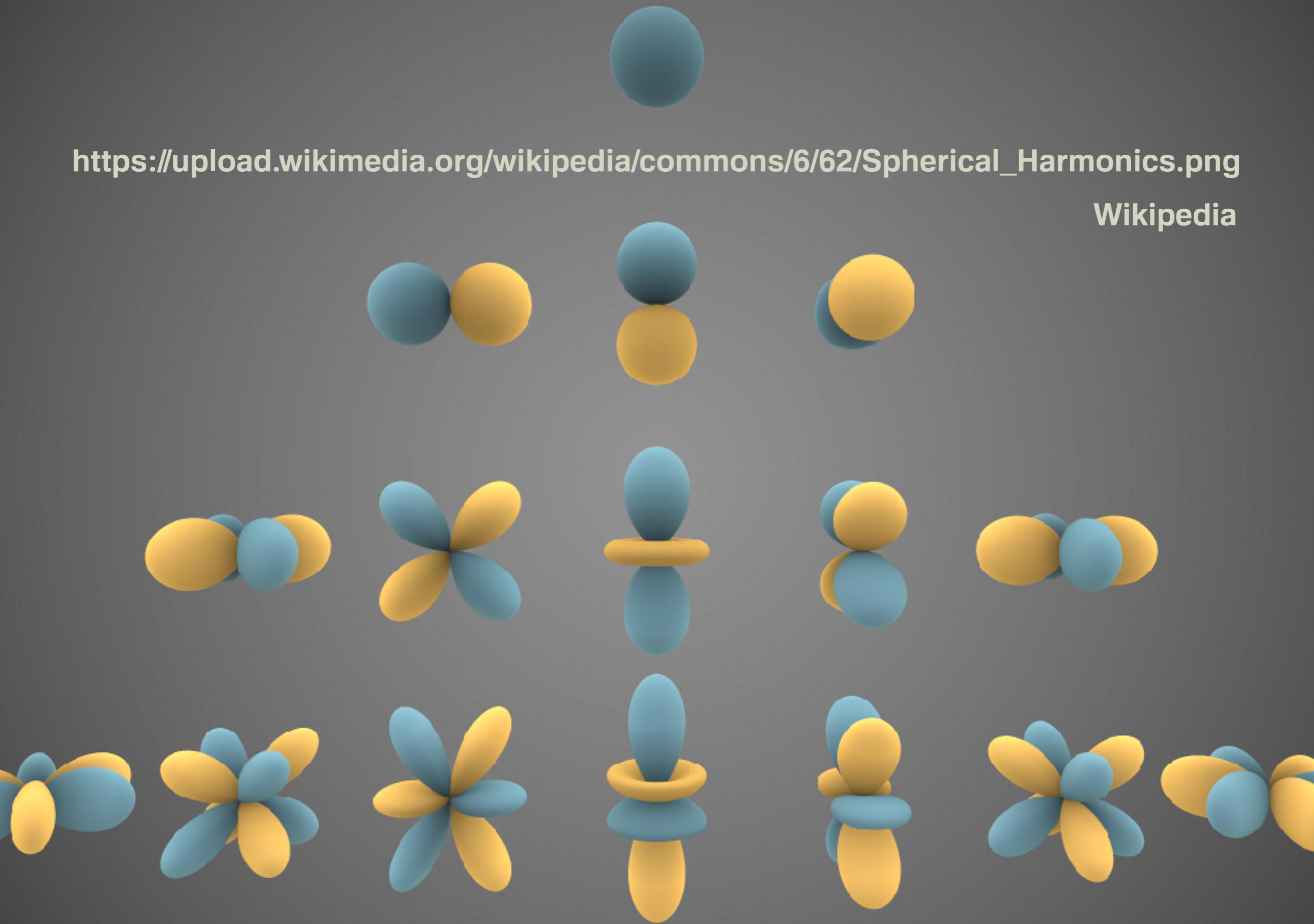
sparing one day  
of your life  
for spherical harmonics  
is not too bad

# Benefits of taking time for spherical harmonics

- 1 it is a wave function**
- 2 angular momentum**  $J, K, K_a, K_c$
- 3 rotational energy**  $E = B\hbar J(J+1)$
- 4 selection rule**  $\Delta J = 0, \pm 1, 0 \leftrightarrow 0$
- 5 parity, symmetry**  $(-1)^J$
- 6 vanishing integral**

[https://upload.wikimedia.org/wikipedia/commons/6/62/Spherical\\_Harmonics.png](https://upload.wikimedia.org/wikipedia/commons/6/62/Spherical_Harmonics.png)

Wikipedia



# Hamiltonian in central field

$$H\Psi = E\Psi$$

$$p = \frac{\hbar}{i} \frac{\partial}{\partial x}$$

$$H = \frac{p^2}{2m} + V(x)$$

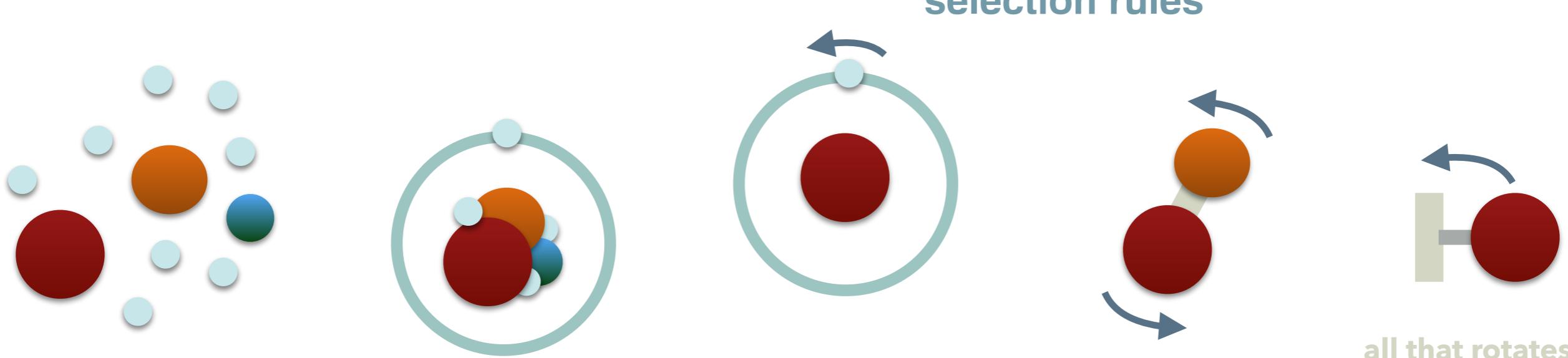
$$= \sum_i^n \frac{p_i^2}{2m_i} + \sum_{i < j}^n \frac{Z_i Z_j e^2}{r_{ij}}$$

kinetic potential

$$H\Psi = E\Psi$$

$$x\Psi = x\Psi$$

$$\mathbf{L}^2\Psi = l(l+1)\Psi$$



$$p_x = \frac{\hbar}{i} \frac{\partial}{\partial x}$$

$$H = \frac{p^2}{2m} + V(x)$$

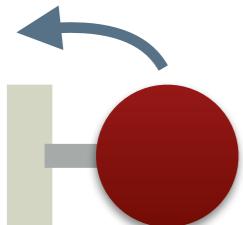
$$p^2 = -\hbar^2 \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right)$$

$$= \sum_i^n \frac{p_i^2}{2m_i} + \sum_{i < j}^n \frac{Z_i Z_j e^2}{r_{ij}}$$

**kinetic**      **potential**

$$H = -\frac{\hbar^2}{2\mu} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) - \frac{Ze^2}{r}$$

$$= -\frac{\hbar^2}{2\mu} \nabla^2 - \frac{Ze^2}{r}$$



**all that rotates**

**Laplacian**

$$\nabla^2 = \frac{1}{r} \frac{\partial^2}{\partial r^2} r + \frac{1}{r^2} \Lambda^2$$

$$\Lambda^2 = \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta}$$

**Legendrian**

$$H\Psi = E\Psi$$

**if**  $\Psi(r, \theta, \phi) = R(r)Y(\theta, \phi)$

$$HRY = -\frac{\hbar^2}{2\mu} \nabla^2 (RY) - \frac{Ze^2}{r} RY$$

$$= -\frac{\hbar^2}{2\mu} \left( \frac{1}{r} \frac{\partial^2}{\partial r^2} r + \frac{1}{r^2} \Lambda^2 \right) RY - \frac{Ze^2}{r} RY$$

$$= -\frac{\hbar^2}{2\mu} \left( Y \frac{1}{r} \frac{\partial^2}{\partial r^2} rR + R \frac{1}{r^2} \Lambda^2 Y \right) - \frac{Ze^2}{r} RY$$


---

**if**  $\Lambda^2 Y = c_1 Y$  **equation involves Y only**

$$Y \frac{1}{r} \frac{\partial^2}{\partial r^2} rR + \frac{R}{r^2} c_1 Y - V(r)RY = -\frac{2\mu}{\hbar^2} ERY$$

$$\frac{1}{r} \frac{\partial^2}{\partial r^2} rR + \frac{R}{r^2} c_1 - V(r)R = -\frac{2\mu}{\hbar^2} ER$$

**equation involves R only**

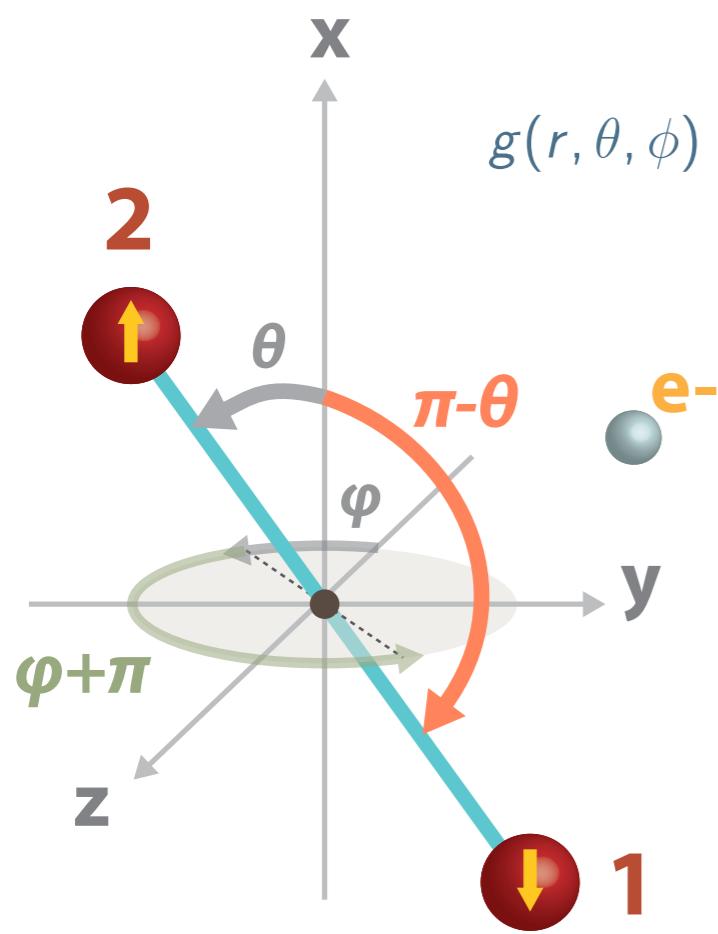
# We left **2** issues behind

①  $\nabla^2 = \frac{1}{r} \frac{\partial^2}{\partial r^2} r + \frac{1}{r^2} \Lambda^2$  Laplacian

$$\Lambda^2 = \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta}$$
 Legendrian

.....

②  $\Lambda^2 Y = c_1 Y$  spherical harmonics



$$x = r \sin \theta \cos \phi$$

$$y = r \sin \theta \sin \phi$$

$$z = r \cos \theta$$

$$g(r, \theta, \phi) = g(r(x, y, z), \theta(x, y, z), \phi(x, y, z)) = f(x, y, z)$$

$$\frac{\partial g}{\partial r} = \frac{\partial f}{\partial x} \frac{\partial x}{\partial r} + \frac{\partial f}{\partial y} \frac{\partial y}{\partial r} + \frac{\partial f}{\partial z} \frac{\partial z}{\partial r}$$

$$g_r = f_x \frac{\partial x}{\partial r} + f_y \frac{\partial y}{\partial r} + f_z \frac{\partial z}{\partial r}$$

our mission here is

to write

$$f_{xx} + f_{yy} + f_{zz}$$

$$\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

in  $g_{rr}$

$$\nabla^2 = \frac{1}{r} \frac{\partial^2}{\partial r^2} r + \frac{1}{r^2} \Lambda^2$$

$$\Lambda^2 = \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta}$$

$g_{\phi\phi}$

$g_\theta$

$$\frac{\partial x}{\partial \phi} = -r \sin \theta \sin \phi$$

$$\frac{\partial y}{\partial \phi} = r \sin \theta \cos \phi$$

$$\frac{\partial z}{\partial \phi} = 0$$

$$\frac{\partial x}{\partial \theta} = r \cos \theta \cos \phi$$

$$\frac{\partial y}{\partial \theta} = r \cos \theta \sin \phi$$

$$\frac{\partial z}{\partial \theta} = -r \sin \theta$$

$$\frac{\partial x}{\partial r} = \sin \theta \cos \phi$$

$$\frac{\partial y}{\partial r} = \sin \theta \sin \phi$$

$$\frac{\partial z}{\partial r} = \cos \theta$$

**without knowing why, let us try**

$$g_r = f_x \frac{\partial x}{\partial r} + f_y \frac{\partial y}{\partial r} + f_z \frac{\partial z}{\partial r}$$

$$g_r = f_x \sin \theta \cos \phi + f_y \sin \theta \sin \phi + f_z \cos \theta$$

1

$$\frac{g_\theta}{r} = f_x \cos \theta \cos \phi + f_y \cos \theta \sin \phi - f_z \sin \theta$$

2

$$\frac{g_\phi}{r \sin \theta} = -f_x \sin \phi + f_y \cos \phi$$

3

1 • sinθ + 2 • cosθ

$$g_r \sin \theta + \frac{g_\theta}{r} \cos \theta$$

$$f_x \sin^2 \theta \cos \phi + f_y \sin^2 \theta \sin \phi + f_x \cos^2 \theta \cos \phi + f_y \cos^2 \theta \sin \phi$$

$$= f_x \cos \phi + f_y \sin \phi$$

$$\frac{\partial x}{\partial \phi} = -r \sin \theta \sin \phi$$

$$\frac{\partial y}{\partial \phi} = r \sin \theta \cos \phi$$

$$\frac{\partial z}{\partial \phi} = 0$$

$$\frac{\partial x}{\partial \theta} = r \cos \theta \cos \phi$$

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$$\frac{\partial y}{\partial r} = \sin \theta \sin \phi$$

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**without knowing why, let us try**

$$g_r = f_x \frac{\partial x}{\partial r} + f_y \frac{\partial y}{\partial r} + f_z \frac{\partial z}{\partial r}$$

$$g_r = f_x \sin \theta \cos \phi + f_y \sin \theta \sin \phi + f_z \cos \theta$$

1

$$\frac{g_\theta}{r} = f_x \cos \theta \cos \phi + f_y \cos \theta \sin \phi - f_z \sin \theta$$

2

$$\frac{g_\phi}{r \sin \theta} = -f_x \sin \phi + f_y \cos \phi$$

3

1 • cosθ - 2 • sinθ

$$g_r \cos \theta - \frac{g_\theta}{r} \sin \theta$$

$$f_x \sin \theta \cos \theta \cos \phi + f_y \sin \theta \cos \theta \sin \phi - f_x \sin \theta \cos \theta \cos \phi - f_y \sin \theta \cos \theta \sin \phi + f_z$$

$$= f_z$$

$$\frac{\partial x}{\partial \phi} = -r \sin \theta \sin \phi$$

$$\frac{\partial y}{\partial \phi} = r \sin \theta \cos \phi$$

$$\frac{\partial z}{\partial \phi} = 0$$

$$\frac{\partial x}{\partial \theta} = r \cos \theta \cos \phi$$

$$\frac{\partial y}{\partial \theta} = r \cos \theta \sin \phi$$

$$\frac{\partial z}{\partial \theta} = -r \sin \theta$$

$$\frac{\partial x}{\partial r} = \sin \theta \cos \phi$$

$$\frac{\partial y}{\partial r} = \sin \theta \sin \phi$$

$$\frac{\partial z}{\partial r} = \cos \theta$$

$$f_z = g_r \cos \theta - \frac{g_\theta}{r} \sin \theta$$

**6**

$$f_x \cos \phi + f_y \sin \phi = g_r \sin \theta + \frac{g_\theta}{r} \cos \theta$$

**4**

$$-f_x \sin \phi + f_y \cos \phi = \frac{g_\phi}{r \sin \theta}$$

**5**

• cosθ

-

• sinθ

• sinθ

+

• cosθ

$$f_x = g_r \sin \theta \cos \phi + \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta}$$

**4**

$$f_y = g_r \sin \theta \sin \phi + \frac{g_\theta}{r} \cos \theta \sin \phi + \frac{g_\phi \cos \phi}{r \sin \theta}$$

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4

$$f_y = g_r \sin \theta \sin \phi + \frac{g_\theta}{r} \cos \theta \sin \phi + \frac{g_\phi \cos \phi}{r \sin \theta}$$

5

$$f_z = g_r \cos \theta - \frac{g_\theta}{r} \sin \theta$$

6

$$f_{xx} = (f_x)_x$$

$$g(r, \theta, \phi) = g(r(x, y, z), \theta(x, y, z), \phi(x, y, z)) = f(x, y, z)$$

$$h(r, \theta, \phi) = h(r(x, y, z), \theta(x, y, z), \phi(x, y, z)) = f_x(x, y, z)$$

$$f_x = g_r \sin \theta \cos \phi + \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta}$$

$$(f_x)_x = h_r \sin \theta \cos \phi + \frac{h_\theta}{r} \cos \theta \cos \phi - \frac{h_\phi \sin \phi}{r \sin \theta}$$

$$f_x = g_r \sin \theta \cos \phi + \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta}$$

**4**

$$f_y = g_r \sin \theta \sin \phi + \frac{g_\theta}{r} \cos \theta \sin \phi + \frac{g_\phi \cos \phi}{r \sin \theta}$$

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$$(f_x)_x = h_r \sin \theta \cos \phi + \frac{h_\theta}{r} \cos \theta \cos \phi - \frac{h_\phi \sin \phi}{r \sin \theta}$$

$$(f_y)_y = \left( g_r \sin \theta \sin \phi + \frac{g_\theta}{r} \cos \theta \sin \phi + \frac{g_\phi \cos \phi}{r \sin \theta} \right)_r \sin \theta \sin \phi$$

$$(f_z)_z = \left( g_r \cos \theta - \frac{g_\theta \sin \theta}{r} \right)_r \cos \theta$$

$$+ \left( g_r \sin \theta \sin \phi + \frac{g_\theta}{r} \cos \theta \sin \phi + \frac{g_\phi \cos \phi}{r \sin \theta} \right)_\theta \frac{\cos \theta \sin \phi}{r}$$

$$- \left( g_r \cos \theta - \frac{g_\theta \sin \theta}{r} \right)_\theta \frac{\sin \theta}{r}$$

$$+ \left( g_r \sin \theta \sin \phi + \frac{g_\theta}{r} \cos \theta \sin \phi + \frac{g_\phi \cos \phi}{r \sin \theta} \right)_\phi \frac{\cos \phi}{r \sin \theta}$$

$$(f_x)_x = \left( g_r \sin \theta \cos \phi + \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta} \right)_r \sin \theta \cos \phi$$

$$+ \left( g_r \sin \theta \cos \phi + \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta} \right)_\theta \frac{\cos \theta \cos \phi}{r}$$

$$- \left( g_r \sin \theta \cos \phi + \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta} \right)_\phi \frac{\sin \phi}{r \sin \theta}$$

$$f_x = g_r \sin \theta \cos \phi + \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta}$$

**4**

$$f_y = g_r \sin \theta \sin \phi + \frac{g_\theta}{r} \cos \theta \sin \phi + \frac{g_\phi \cos \phi}{r \sin \theta}$$

**5**

$$f_z = g_r \cos \theta - \frac{g_\theta}{r} \sin \theta$$

**6**

$$f_{xx} = (f_x)_x$$

$$g(r, \theta, \phi) = g(r(x, y, z), \theta(x, y, z), \phi(x, y, z)) = f(x, y, z)$$

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$$(f_x)_x = \left( g_r \sin \theta \cos \phi + \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta} \right)_r \sin \theta \cos \phi$$

$$+ \left( g_r \sin \theta \cos \phi + \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta} \right)_\theta \frac{\cos \theta \cos \phi}{r}$$

$$- \left( g_r \sin \theta \cos \phi + \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta} \right)_\phi \frac{\sin \phi}{r \sin \theta}$$

$$(f_x)_x = \left( g_r \sin \theta \cos \phi + \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta} \right)_r \sin \theta \cos \phi$$

$$+ \left( g_r \sin \theta \cos \phi + \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta} \right)_\theta \frac{\cos \theta \cos \phi}{r}$$

$$- \left( g_r \sin \theta \cos \phi + \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta} \right)_\phi \frac{\sin \phi}{r \sin \theta}$$

$$f_x = g_r \sin \theta \cos \phi + \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta}$$

4

$$f_y = g_r \sin \theta \sin \phi + \frac{g_\theta}{r} \cos \theta \sin \phi + \frac{g_\phi \cos \phi}{r \sin \theta}$$

5

$$f_z = g_r \cos \theta - \frac{g_\theta}{r} \sin \theta$$

6

$$(f_y)_y = \left( g_r \sin \theta \sin \phi + \frac{g_\theta}{r} \cos \theta \sin \phi + \frac{g_\phi \cos \phi}{r \sin \theta} \right)_r \sin \theta \sin \phi$$

$$+ \left( g_r \sin \theta \sin \phi + \frac{g_\theta}{r} \cos \theta \sin \phi + \frac{g_\phi \cos \phi}{r \sin \theta} \right)_\theta \frac{\cos \theta \sin \phi}{r}$$

$$+ \left( g_r \sin \theta \sin \phi + \frac{g_\theta}{r} \cos \theta \sin \phi + \frac{g_\phi \cos \phi}{r \sin \theta} \right)_\phi \frac{\cos \phi}{r \sin \theta}$$

$$(f_z)_z = \left( g_r \cos \theta - \frac{g_\theta \sin \theta}{r} \right)_r \cos \theta$$

$$- \left( g_r \cos \theta - \frac{g_\theta \sin \theta}{r} \right)_\theta \frac{\sin \theta}{r}$$

$$(f_x)_x = \left( g_r \sin \theta \cos \phi + \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta} \right)_r \sin \theta \cos \phi$$

$$+ \left( g_r \sin \theta \cos \phi + \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta} \right)_\theta \frac{\cos \theta \cos \phi}{r}$$

$$- \left( g_r \sin \theta \cos \phi + \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta} \right)_\phi \frac{\sin \phi}{r \sin \theta}$$

$$(f_y)_y = \left( g_r \sin \theta \sin \phi + \frac{g_\theta}{r} \cos \theta \sin \phi + \frac{g_\phi \cos \phi}{r \sin \theta} \right)_r \sin \theta \sin \phi$$

$$+ \left( g_r \sin \theta \sin \phi + \frac{g_\theta}{r} \cos \theta \sin \phi + \frac{g_\phi \cos \phi}{r \sin \theta} \right)_\theta \frac{\cos \theta \sin \phi}{r}$$

$$+ \left( g_r \sin \theta \sin \phi + \frac{g_\theta}{r} \cos \theta \sin \phi + \frac{g_\phi \cos \phi}{r \sin \theta} \right)_\phi \frac{\cos \phi}{r \sin \theta}$$

$$(f_z)_z = \left( g_r \cos \theta - \frac{g_\theta \sin \theta}{r} \right)_r \cos \theta$$

$$- \left( g_r \cos \theta - \frac{g_\theta \sin \theta}{r} \right)_\theta \frac{\sin \theta}{r}$$

$$f_x = g_r \sin \theta \cos \phi + \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta}$$

4

$$f_y = g_r \sin \theta \sin \phi + \frac{g_\theta}{r} \cos \theta \sin \phi + \frac{g_\phi \cos \phi}{r \sin \theta}$$

5

$$f_z = g_r \cos \theta - \frac{g_\theta}{r} \sin \theta$$

6

$$(f_x)_x = \left( g_r \sin \theta \cos \phi + \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta} \right)_r \sin \theta \cos \phi$$

$$+ \left( g_r \sin \theta \cos \phi + \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta} \right)_\theta \frac{\cos \theta \cos \phi}{r}$$

$$- \left( g_r \sin \theta \cos \phi + \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta} \right)_\phi \frac{\sin \phi}{r \sin \theta}$$

$$(f_y)_y = \left( g_r \sin \theta \sin \phi + \frac{g_\theta}{r} \cos \theta \sin \phi + \frac{g_\phi \cos \phi}{r \sin \theta} \right)_r \sin \theta \sin \phi$$

$$+ \left( g_r \sin \theta \sin \phi + \frac{g_\theta}{r} \cos \theta \sin \phi + \frac{g_\phi \cos \phi}{r \sin \theta} \right)_\theta \frac{\cos \theta \sin \phi}{r}$$

$$+ \left( g_r \sin \theta \sin \phi + \frac{g_\theta}{r} \cos \theta \sin \phi + \frac{g_\phi \cos \phi}{r \sin \theta} \right)_\phi \frac{\cos \phi}{r \sin \theta}$$

$$(f_z)_z = \left( g_r \cos \theta - \frac{g_\theta \sin \theta}{r} \right)_r \cos \theta$$

$$- \left( g_r \cos \theta - \frac{g_\theta \sin \theta}{r} \right)_\theta \frac{\sin \theta}{r}$$

$$f_x = g_r \sin \theta \cos \phi + \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta}$$

$$f_y = g_r \sin \theta \sin \phi + \frac{g_\theta}{r} \cos \theta \sin \phi + \frac{g_\phi \cos \phi}{r \sin \theta}$$

$$f_z = g_r \cos \theta - \frac{g_\theta}{r} \sin \theta$$

4

5

6

our mission here is  
to find  $f_{xx} + f_{yy} + f_{zz}$

how many terms?

$$g_{rr} \quad g_{r\theta} = g_{\theta r} \quad g_r$$

$$g_{\theta\theta} \quad g_{r\phi} = g_{\phi r} \quad g_\theta$$

$$g_{\phi\phi} \quad g_{\theta\phi} = g_{\phi\theta} \quad g_\phi$$

**3 + 3 + 3 = 9 terms**

$$(f_x)_x = \left( g_r \sin \theta \cos \phi + \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta} \right)_r \sin \theta \cos \phi$$

$$+ \left( g_r \sin \theta \cos \phi + \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta} \right)_\theta \frac{\cos \theta \cos \phi}{r}$$

$$- \left( g_r \sin \theta \cos \phi + \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta} \right)_\phi \frac{\sin \phi}{r \sin \theta}$$

$$(f_y)_y = \left( g_r \sin \theta \sin \phi + \frac{g_\theta}{r} \cos \theta \sin \phi + \frac{g_\phi \cos \phi}{r \sin \theta} \right)_r \sin \theta \sin \phi$$

$$+ \left( g_r \sin \theta \sin \phi + \frac{g_\theta}{r} \cos \theta \sin \phi + \frac{g_\phi \cos \phi}{r \sin \theta} \right)_\theta \frac{\cos \theta \sin \phi}{r}$$

$$+ \left( g_r \sin \theta \sin \phi + \frac{g_\theta}{r} \cos \theta \sin \phi + \frac{g_\phi \cos \phi}{r \sin \theta} \right)_\phi \frac{\cos \phi}{r \sin \theta}$$

$$(f_z)_z = \left( g_r \cos \theta - \frac{g_\theta \sin \theta}{r} \right)_r \cos \theta$$

$$- \left( g_r \cos \theta - \frac{g_\theta \sin \theta}{r} \right)_\theta \frac{\sin \theta}{r}$$

$$g_{rr} [\sin^2 \theta \cos^2 \phi + \sin^2 \theta \sin^2 \phi + \cos^2 \theta] = 1$$

$$g_{\theta\theta} \left[ \frac{\cos^2 \theta \cos^2 \phi}{r^2} + \frac{\cos^2 \theta \sin^2 \phi}{r^2} + \frac{\sin^2 \theta}{r^2} \right] = \frac{1}{r^2}$$

$$g_{\phi\phi} \left[ \frac{\sin^2 \phi}{r^2 \sin^2 \theta} + \frac{\cos^2 \phi}{r^2 \sin^2 \theta} \right] = \frac{1}{r^2 \sin^2 \theta}$$

$$(f_x)_x = \left( g_r \sin \theta \cos \phi + \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta} \right)_r \sin \theta \cos \phi$$

$$+ \left( g_r \sin \theta \cos \phi + \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta} \right)_\theta \frac{\cos \theta \cos \phi}{r}$$

$$- \left( g_r \sin \theta \cos \phi + \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta} \right)_\phi \frac{\sin \phi}{r \sin \theta}$$

$$(f_y)_y = \left( g_r \sin \theta \sin \phi + \frac{g_\theta}{r} \cos \theta \sin \phi + \frac{g_\phi \cos \phi}{r \sin \theta} \right)_r \sin \theta \sin \phi$$

$$+ \left( g_r \sin \theta \sin \phi + \frac{g_\theta}{r} \cos \theta \sin \phi + \frac{g_\phi \cos \phi}{r \sin \theta} \right)_\theta \frac{\cos \theta \sin \phi}{r}$$

$$+ \left( g_r \sin \theta \sin \phi + \frac{g_\theta}{r} \cos \theta \sin \phi + \frac{g_\phi \cos \phi}{r \sin \theta} \right)_\phi \frac{\cos \phi}{r \sin \theta}$$

$$(f_z)_z = \left( g_r \cos \theta - \frac{g_\theta \sin \theta}{r} \right)_r \cos \theta$$

$$- \left( g_r \cos \theta - \frac{g_\theta \sin \theta}{r} \right)_\theta \frac{\sin \theta}{r}$$

$$g_{rr} [\sin^2 \theta \cos^2 \phi + \sin^2 \theta \sin^2 \phi + \cos^2 \theta] = 1$$

$$g_{\theta\theta} \left[ \frac{\cos^2 \theta \cos^2 \phi}{r^2} + \frac{\cos^2 \theta \sin^2 \phi}{r^2} + \frac{\sin^2 \theta}{r^2} \right] = \frac{1}{r^2}$$

$$g_{\phi\phi} \left[ \frac{\sin^2 \phi}{r^2 \sin^2 \theta} + \frac{\cos^2 \phi}{r^2 \sin^2 \theta} \right] = \frac{1}{r^2 \sin^2 \theta}$$

$$(f_x)_x = \left( g_r \sin \theta \cos \phi + \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta} \right)_r \sin \theta \cos \phi$$

$$+ \left( g_r \sin \theta \cos \phi + \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta} \right)_\theta \frac{\cos \theta \cos \phi}{r}$$

$$- \left( g_r \sin \theta \cos \phi + \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta} \right)_\phi \frac{\sin \phi}{r \sin \theta}$$

$$(f_y)_y = \left( g_r \sin \theta \sin \phi + \frac{g_\theta}{r} \cos \theta \sin \phi + \frac{g_\phi \cos \phi}{r \sin \theta} \right)_r \sin \theta \sin \phi$$

$$+ \left( g_r \sin \theta \sin \phi + \frac{g_\theta}{r} \cos \theta \sin \phi + \frac{g_\phi \cos \phi}{r \sin \theta} \right)_\theta \frac{\cos \theta \sin \phi}{r}$$

$$+ \left( g_r \sin \theta \sin \phi + \frac{g_\theta}{r} \cos \theta \sin \phi + \frac{g_\phi \cos \phi}{r \sin \theta} \right)_\phi \frac{\cos \phi}{r \sin \theta}$$

$$(f_z)_z = \left( g_r \cos \theta - \frac{g_\theta \sin \theta}{r} \right)_r \cos \theta$$

$$- \left( g_r \cos \theta - \frac{g_\theta \sin \theta}{r} \right)_\theta \frac{\sin \theta}{r}$$

$$g_{rr} [\sin^2 \theta \cos^2 \phi + \sin^2 \theta \sin^2 \phi + \cos^2 \theta] = 1$$

$$g_{\theta\theta} \left[ \frac{\cos^2 \theta \cos^2 \phi}{r^2} + \frac{\cos^2 \theta \sin^2 \phi}{r^2} + \frac{\sin^2 \theta}{r^2} \right] = \frac{1}{r^2}$$

$$g_{\phi\phi} \left[ \frac{\sin^2 \phi}{r^2 \sin^2 \theta} + \frac{\cos^2 \phi}{r^2 \sin^2 \theta} \right] = \frac{1}{r^2 \sin^2 \theta}$$

$$(f_x)_x = \left( g_r \sin \theta \cos \phi + \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta} \right)_r \sin \theta \cos \phi$$

$$+ \left( g_r \sin \theta \cos \phi + \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta} \right)_\theta \frac{\cos \theta \cos \phi}{r}$$

$$- \left( g_r \sin \theta \cos \phi + \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta} \right)_\phi \frac{\sin \phi}{r \sin \theta}$$

$$(f_y)_y = \left( g_r \sin \theta \sin \phi + \frac{g_\theta}{r} \cos \theta \sin \phi + \frac{g_\phi \cos \phi}{r \sin \theta} \right)_r \sin \theta \sin \phi$$

$$+ \left( g_r \sin \theta \sin \phi + \frac{g_\theta}{r} \cos \theta \sin \phi + \frac{g_\phi \cos \phi}{r \sin \theta} \right)_\theta \frac{\cos \theta \sin \phi}{r}$$

$$+ \left( g_r \sin \theta \sin \phi + \frac{g_\theta}{r} \cos \theta \sin \phi + \frac{g_\phi \cos \phi}{r \sin \theta} \right)_\phi \frac{\cos \phi}{r \sin \theta}$$

$$(f_z)_z = \left( g_r \cos \theta - \frac{g_\theta \sin \theta}{r} \right)_r \cos \theta$$

$$- \left( g_r \cos \theta - \frac{g_\theta \sin \theta}{r} \right)_\theta \frac{\sin \theta}{r}$$

**grθ**

$$\left[ \begin{array}{l} \frac{\sin \theta \cos \theta \cos^2 \phi}{r} + \frac{\sin \theta \cos \theta \cos^2 \phi}{r} \\ + \frac{\sin \theta \cos \theta \sin^2 \phi}{r} + \frac{\sin \theta \cos \theta \sin^2 \phi}{r} \\ - \frac{\sin \theta \cos \theta}{r} - \frac{\sin \theta \cos \theta}{r} \end{array} \right] = 0$$

**gθφ**

$$\left[ \begin{array}{l} - \frac{\cos \theta \sin \phi \cos \phi}{r^2 \sin \theta} - \frac{\cos \theta \sin \phi \cos \phi}{r^2 \sin \theta} \\ + \frac{\cos \theta \sin \phi \cos \phi}{r^2 \sin \theta} + \frac{\cos \theta \sin \phi \cos \phi}{r^2 \sin \theta} \end{array} \right] = 0$$

**grφ**

$$\left[ \begin{array}{l} - \frac{\sin \phi \cos \phi}{r} - \frac{\sin \phi \cos \phi}{r} \\ + \frac{\sin \phi \cos \phi}{r} + \frac{\sin \phi \cos \phi}{r} \end{array} \right] = 0$$

$$(f_x)_x = \left( g_r \sin \theta \cos \phi + \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta} \right)_r \sin \theta \cos \phi$$

$$+ \left( g_r \sin \theta \cos \phi + \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta} \right)_\theta \frac{\cos \theta \cos \phi}{r}$$

$$- \left( g_r \sin \theta \cos \phi + \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta} \right)_\phi \frac{\sin \phi}{r \sin \theta}$$

$$(f_y)_y = \left( g_r \sin \theta \sin \phi + \frac{g_\theta}{r} \cos \theta \sin \phi + \frac{g_\phi \cos \phi}{r \sin \theta} \right)_r \sin \theta \sin \phi$$

$$+ \left( g_r \sin \theta \sin \phi + \frac{g_\theta}{r} \cos \theta \sin \phi + \frac{g_\phi \cos \phi}{r \sin \theta} \right)_\theta \frac{\cos \theta \sin \phi}{r}$$

$$+ \left( g_r \sin \theta \sin \phi + \frac{g_\theta}{r} \cos \theta \sin \phi + \frac{g_\phi \cos \phi}{r \sin \theta} \right)_\phi \frac{\cos \phi}{r \sin \theta}$$

$$(f_z)_z = \left( g_r \cos \theta - \frac{g_\theta \sin \theta}{r} \right)_r \cos \theta$$

$$- \left( g_r \cos \theta - \frac{g_\theta \sin \theta}{r} \right)_\theta \frac{\sin \theta}{r}$$

***gr***

$$\left[ \begin{array}{l} \frac{\cos^2 \theta \cos^2 \phi}{r} + \frac{\sin^2 \phi}{r} \\ \\ + \frac{\sin^2 \theta}{r} + \frac{\cos^2 \theta \sin^2 \phi}{r} + \frac{\cos^2 \phi}{r} \end{array} \right] = \frac{2}{r}$$

$$(f_x)_x = \left( g_r \sin \theta \cos \phi + \left( \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta} \right)_r \right) \sin \theta \cos \phi$$

$$+ \left( g_r \sin \theta \cos \phi + \left( \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta} \right)_\theta \right) \frac{\cos \theta \cos \phi}{r}$$

$$- \left( g_r \sin \theta \cos \phi + \left( \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta} \right)_\phi \right) \frac{\sin \phi}{r \sin \theta}$$

$$(f_y)_y = \left( g_r \sin \theta \sin \phi + \left( \frac{g_\theta}{r} \cos \theta \sin \phi + \frac{g_\phi \cos \phi}{r \sin \theta} \right)_r \right) \sin \theta \sin \phi$$

$$+ \left( g_r \sin \theta \sin \phi + \left( \frac{g_\theta}{r} \cos \theta \sin \phi + \frac{g_\phi \cos \phi}{r \sin \theta} \right)_\theta \right) \frac{\cos \theta \sin \phi}{r}$$

$$+ \left( g_r \sin \theta \sin \phi + \left( \frac{g_\theta}{r} \cos \theta \sin \phi + \frac{g_\phi \cos \phi}{r \sin \theta} \right)_\phi \right) \frac{\cos \phi}{r \sin \theta}$$

$$(f_z)_z = \left( g_r \cos \theta - \frac{g_\theta \sin \theta}{r} \right)_r \cos \theta$$

$$- \left( g_r \cos \theta - \frac{g_\theta \sin \theta}{r} \right)_\theta \frac{\sin \theta}{r}$$

$g_r$  [

$$\begin{aligned} & \frac{\cos^2 \theta \cos^2 \phi}{r} + \frac{\sin^2 \phi}{r} \\ & + \frac{\sin^2 \theta}{r} + \frac{\cos^2 \theta \sin^2 \phi}{r} + \frac{\cos^2 \phi}{r} \end{aligned} ] = \frac{2}{r}$$

$g_\theta$  [

$$\begin{aligned} & -\frac{\sin \theta \cos \theta \cos^2 \phi}{r^2} - \frac{\sin \theta \cos \theta \cos^2 \phi}{r^2} + \frac{\cos \theta \sin^2 \phi}{r^2 \sin \theta} \\ & -\frac{\sin \theta \cos \theta \sin^2 \phi}{r^2} - \frac{\sin \theta \cos \theta \sin^2 \phi}{r^2} + \frac{\cos \theta \cos^2 \phi}{r^2 \sin \theta} \\ & + \frac{\sin \theta \cos \theta}{r^2} + \frac{\sin \theta \cos \theta}{r^2} \end{aligned} ] = \frac{\cos \theta}{r^2 \sin \theta}$$

$$(f_x)_x = \left( g_r \sin \theta \cos \phi + \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta} \right)_r \sin \theta \cos \phi$$

$$+ \left( g_r \sin \theta \cos \phi + \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta} \right)_\theta \frac{\cos \theta \cos \phi}{r}$$

$$- \left( g_r \sin \theta \cos \phi + \frac{g_\theta}{r} \cos \theta \cos \phi - \frac{g_\phi \sin \phi}{r \sin \theta} \right)_\phi \frac{\sin \phi}{r \sin \theta}$$

$$(f_y)_y = \left( g_r \sin \theta \sin \phi + \frac{g_\theta}{r} \cos \theta \sin \phi + \frac{g_\phi \cos \phi}{r \sin \theta} \right)_r \sin \theta \sin \phi$$

$$+ \left( g_r \sin \theta \sin \phi + \frac{g_\theta}{r} \cos \theta \sin \phi + \frac{g_\phi \cos \phi}{r \sin \theta} \right)_\theta \frac{\cos \theta \sin \phi}{r}$$

$$+ \left( g_r \sin \theta \sin \phi + \frac{g_\theta}{r} \cos \theta \sin \phi + \frac{g_\phi \cos \phi}{r \sin \theta} \right)_\phi \frac{\cos \phi}{r \sin \theta}$$

$$(f_z)_z = \left( g_r \cos \theta - \frac{g_\theta \sin \theta}{r} \right)_r \cos \theta$$

$$- \left( g_r \cos \theta - \frac{g_\theta \sin \theta}{r} \right)_\theta \frac{\sin \theta}{r}$$

$g_r$

$$\left[ \begin{aligned} & \frac{\cos^2 \theta \cos^2 \phi}{r} + \frac{\sin^2 \phi}{r} \\ & + \frac{\sin^2 \theta}{r} + \frac{\cos^2 \theta \sin^2 \phi}{r} + \frac{\cos^2 \phi}{r} \end{aligned} \right] = \frac{2}{r}$$

$g_\theta$

$$\left[ \begin{aligned} & -\frac{\sin \theta \cos \theta \cos^2 \phi}{r^2} - \frac{\sin \theta \cos \theta \cos^2 \phi}{r^2} + \frac{\cos \theta \sin^2 \phi}{r^2 \sin \theta} \\ & -\frac{\sin \theta \cos \theta \sin^2 \phi}{r^2} - \frac{\sin \theta \cos \theta \sin^2 \phi}{r^2} + \frac{\cos \theta \cos^2 \phi}{r^2 \sin \theta} \\ & + \frac{\sin \theta \cos \theta}{r^2} + \frac{\sin \theta \cos \theta}{r^2} \end{aligned} \right] = \frac{\cos \theta}{r^2 \sin \theta}$$

$g_\phi$

$$\left[ \begin{aligned} & \frac{\sin \phi \cos \phi}{r^2} + \frac{\cos^2 \theta \sin \phi \cos \phi}{r^2 \sin^2 \theta} + \frac{\sin \phi \cos \phi}{r^2 \sin \theta} \\ & - \frac{\sin \phi \cos \phi}{r^2} - \frac{\cos^2 \theta \sin \phi \cos \phi}{r^2 \sin^2 \theta} - \frac{\sin \phi \cos \phi}{r^2 \sin \theta} \end{aligned} \right] = 0$$

$$g_{rr} \left[ \sin^2 \theta \cos^2 \phi + \sin^2 \theta \sin^2 \phi + \cos^2 \theta \right] = 1$$

$$g_{\theta\theta} \left[ \frac{\cos^2 \theta \cos^2 \phi}{r^2} + \frac{\cos^2 \theta \sin^2 \phi}{r^2} + \frac{\sin^2 \theta}{r^2} \right] = \frac{1}{r^2}$$

$$g_{\phi\phi} \left[ \frac{\sin^2 \phi}{r^2 \sin^2 \theta} + \frac{\cos^2 \phi}{r^2 \sin^2 \theta} \right] = \frac{1}{r^2 \sin^2 \theta}$$

$$g_r \quad \frac{2}{r}$$

$$g_\theta \quad \frac{\cos \theta}{r^2 \sin \theta}$$

$$g_\phi \quad 0$$

$$f_{xx} + f_{yy} + f_{zz}$$

$$= g_{rr} + \frac{2}{r} g_r + \frac{1}{r^2} g_{\theta\theta} + \frac{\cos \theta}{r^2 \sin \theta} g_\theta + \frac{1}{r^2 \sin^2 \theta} g_{\phi\phi}$$

$$\nabla^2 = \frac{1}{r} \frac{\partial^2}{\partial r^2} r + \frac{1}{r^2} \Lambda^2$$

1

**find this**

$$\Lambda^2 = \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta}$$

# Road to spherical harmonics

- 1 Hamiltonian in central field

$$H = -\frac{\hbar^2}{2\mu} \nabla^2 - \frac{Ze^2}{r}$$

- 2 separate r and  $\theta, \phi$

$$\nabla^2 = \frac{1}{r} \frac{\partial^2}{\partial r^2} r + \frac{1}{r^2} \Lambda^2$$

- 3 Laplacian in polar coordinate

$$\Lambda^2 = \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta}$$

- .....
- 4 Legendre differential equation is part of Laplacian

- 5 Rodrigues formula is solution Leibniz rule

- 6 full Laplacian is associated Legendre differential equation

- 7 Derivative of Rodrigues formula is solution

---

→ spherical harmonics

$$g_{rr} [\sin^2 \theta \cos^2 \phi + \sin^2 \theta \sin^2 \phi + \cos^2 \theta] = 1$$

$$g_{\theta\theta} \left[ \frac{\cos^2 \theta \cos^2 \phi}{r^2} + \frac{\cos^2 \theta \sin^2 \phi}{r^2} + \frac{\sin^2 \theta}{r^2} \right] = \frac{1}{r^2}$$

$$g_{\phi\phi} \left[ \frac{\sin^2 \phi}{r^2 \sin^2 \theta} + \frac{\cos^2 \phi}{r^2 \sin^2 \theta} \right] = \frac{1}{r^2 \sin^2 \theta}$$

$g_r$	$\frac{2}{r}$
$g_\theta$	$\frac{\cos \theta}{r^2 \sin \theta}$
$g_\phi$	0

$$f_{xx} + f_{yy} + f_{zz}$$

$$= g_{rr} + \frac{2}{r} g_r + \frac{1}{r^2} g_{\theta\theta} + \frac{\cos \theta}{r^2 \sin \theta} g_\theta + \frac{1}{r^2 \sin^2 \theta} g_{\phi\phi}$$

$$\nabla^2 = \frac{1}{r} \frac{\partial^2}{\partial r^2} r + \frac{1}{r^2} \Lambda^2$$

$$\Lambda^2 = \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta}$$

# Exercise today

1

calculate Legendrian

# Seminar topics

20 minutes

subject	keywords
1 NIRSpec on JWST	MSA
2 iSHELL on IRTF	cross-dispersing spectrograph
3 ELT vs JWST	sensitivity, spatial resolution
4 Adaptive optics	choose from Shack-Hartmann / curvature / pyramid
5 IR detectors	band gap, intrinsic semiconductor
6 Frequency comb	mechanism, objectives
7 Laplacian in polar coordinate	vector analysis
8 2D/3D representation of spherical harmonics	minimum 3 different ways
9 development of quantum mechanics in 1920s	Bohr model, spin