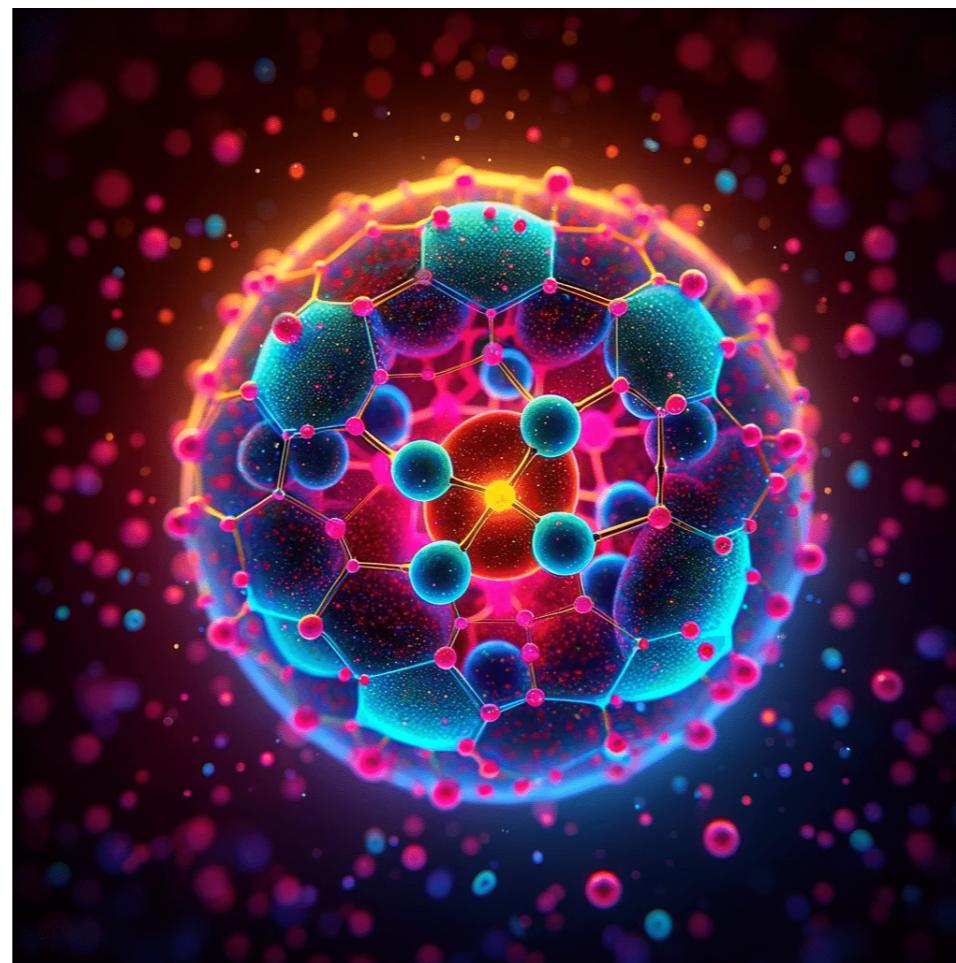


Bounding quantum particles



Wavelike particles

Heisenberg

$$\Delta x \Delta p \geq \frac{\hbar}{2}$$



Sharp momentum
implies entirely
delocalised position
For the particle

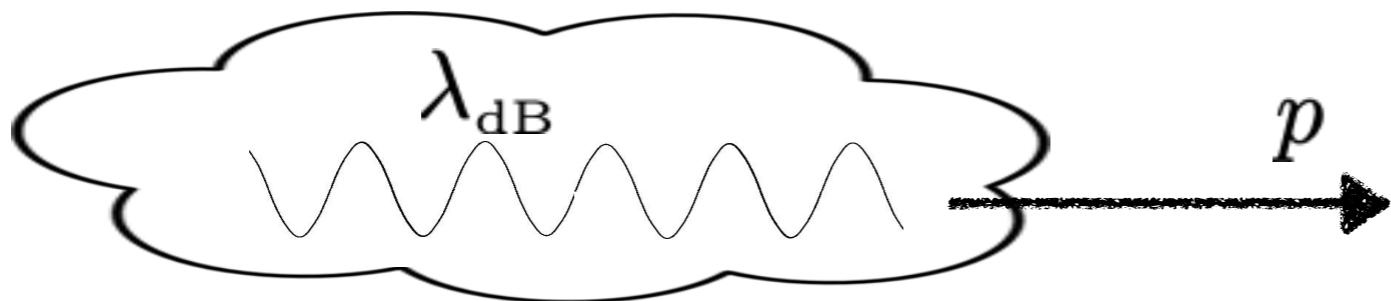
Bohr

$$mvr = n\hbar$$
$$n = 1, 2, 3, 4, \dots$$



Sharp momentum
implies a length scale $\lambda_{dB} = \frac{h}{p}$

de Broglie wavelength



For particle with sharp momentum \mathbf{p} quantum effects begin to dominate at length scale

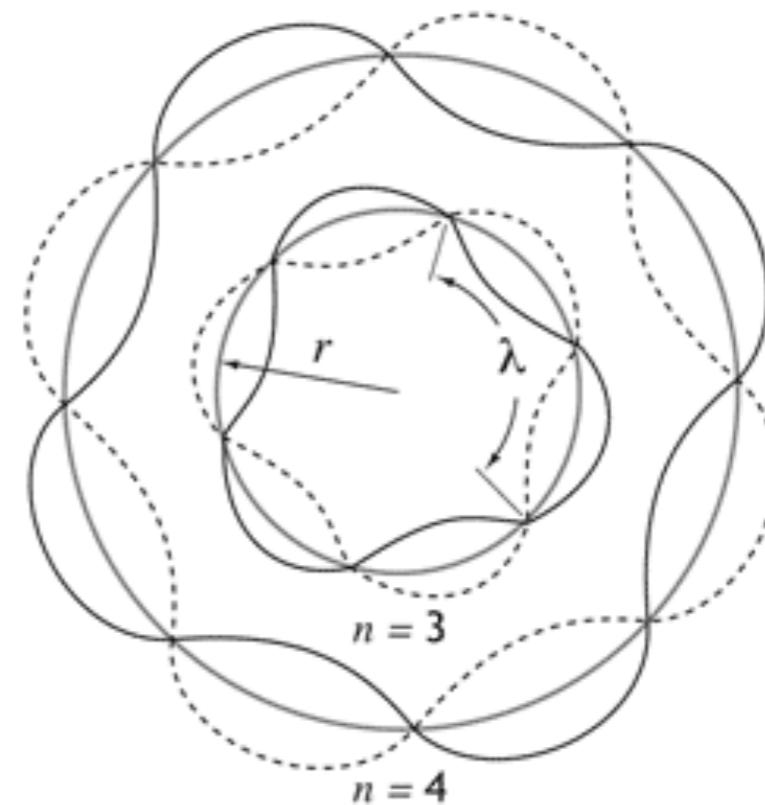
$$\lambda_{dB} = \frac{h}{p}$$

Recall: Bohr's postulate

“Wavelike nature”

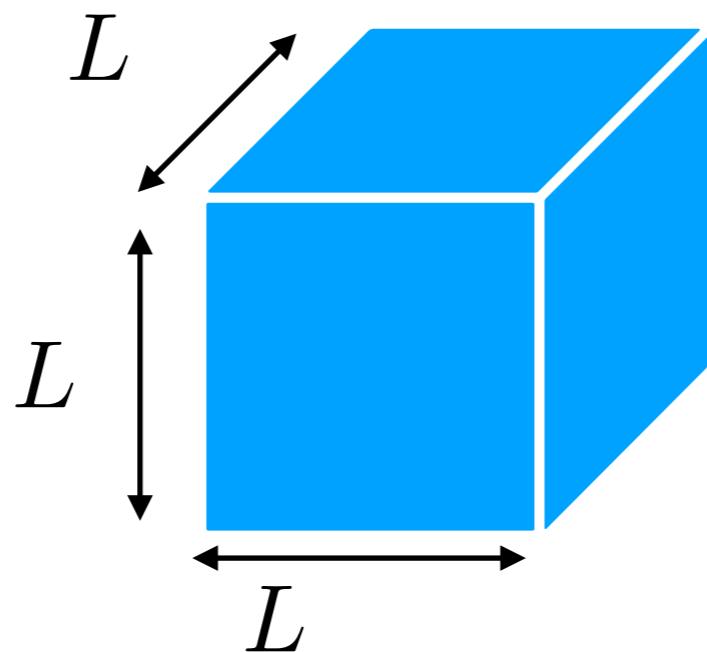
**Define the
de Broglie
Wavelength:**

$$\lambda_{dB} = \frac{h}{p}$$



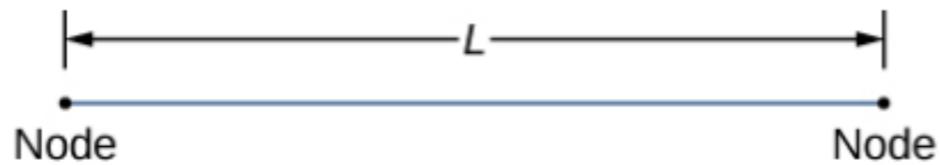
Bohr's postulate can be re-phrased as the assumption that an *integer number of de Broglie wavelengths* loop around the circular orbit!

Particle in a box



$$\lambda_{dB} = \frac{h}{p}$$

- A quantum particle of mass m is in a cubic box of side L .
- **Assume its states of exact momentum have de Broglie wavelengths with nodes at the wall.**
- Compute the kinetic energy of the particle in the box.



$$\lambda_n = \frac{2}{n}L \quad n = 1, 2, 3, \dots$$

$$\lambda_n = \frac{2}{n}L$$

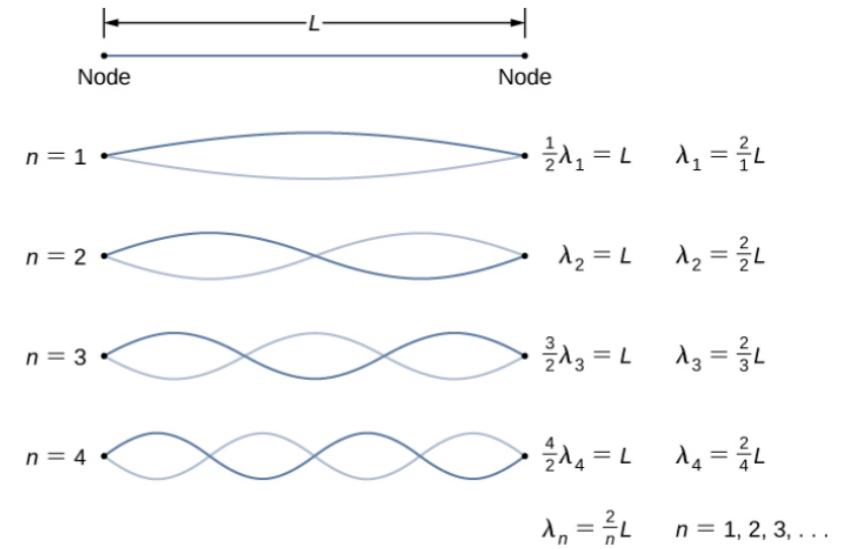
$$\lambda_n = \frac{2}{n}L$$

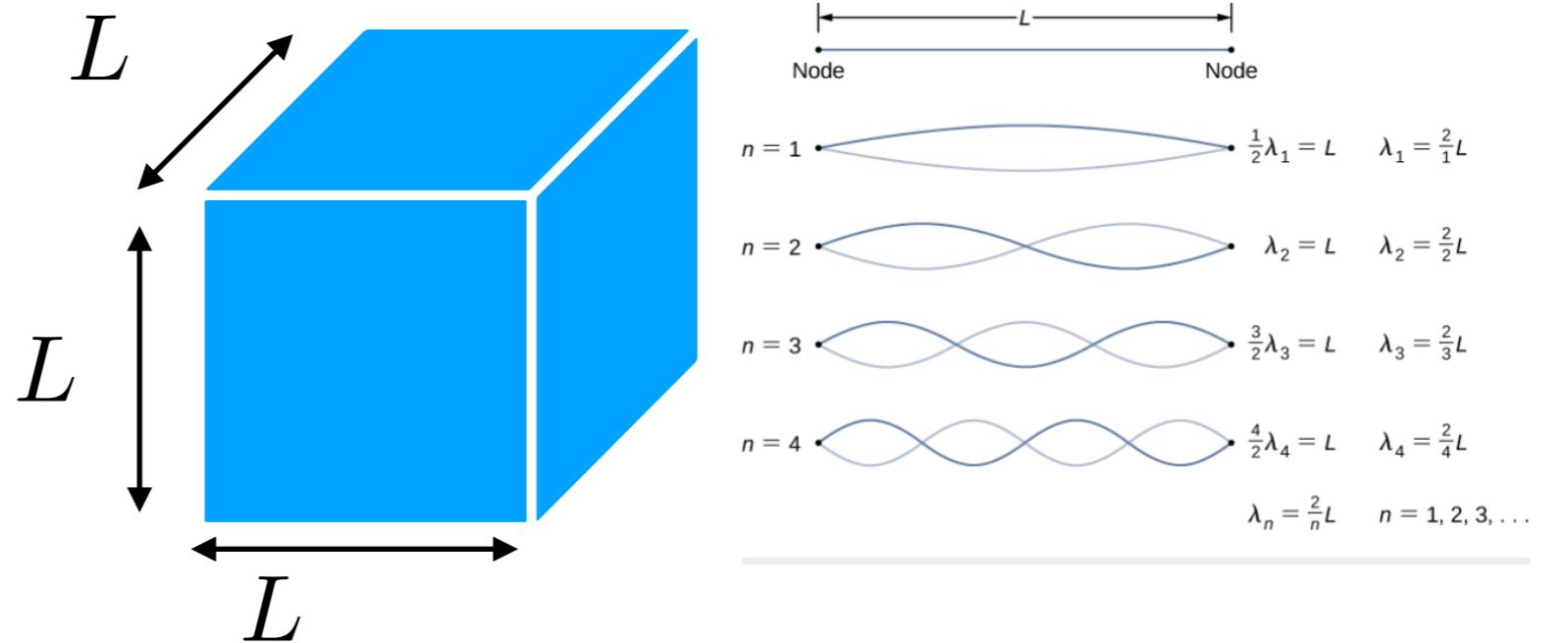
$$\Rightarrow \lambda_n = \frac{h}{p_n} = \frac{2}{n}L$$

$$\Rightarrow p_n = \frac{nh}{2L} \quad n = 1, 2, 3, \dots$$

This is for a 1-d case

For 3-d, we just apply same theory to each dimension





$$\vec{p} = (p_x, p_y, p_z) = \left(\frac{n_x h}{2L}, \frac{n_y h}{2L}, \frac{n_z h}{2L} \right)$$

$$n_x = 1, 2, 3, \dots$$

Quantised momenta in space!

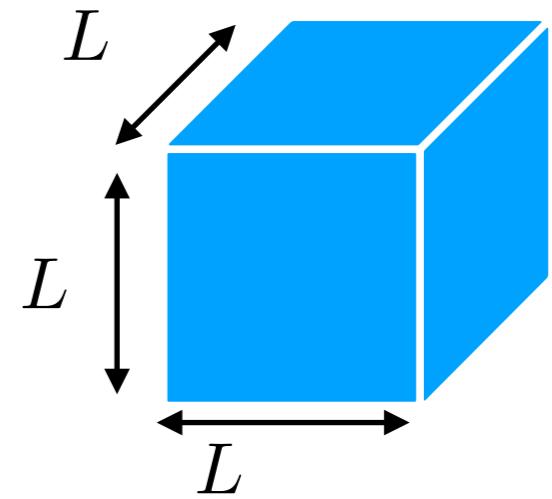
$$n_y = 1, 2, 3, \dots$$

$$n_z = 1, 2, 3, \dots$$

Kinetic energy of particle

$$E = \frac{1}{2}m|\vec{v}|^2$$

$$= \frac{1}{2m}|\vec{p}|^2$$



$$\vec{p} = (p_x, p_y, p_z) = \left(\frac{n_x h}{2L}, \frac{n_y h}{2L}, \frac{n_z h}{2L} \right)$$

Kinetic energy of particle

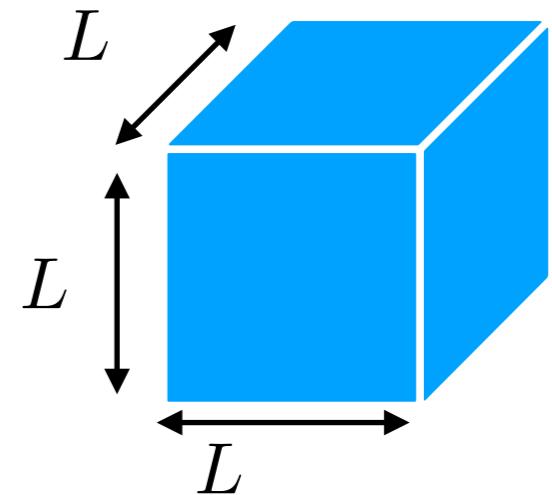
$$E = \frac{1}{2}m|\vec{v}|^2$$

$$= \frac{1}{2m}|\vec{p}|^2$$

$$= \frac{1}{2m}(p_x^2 + p_y^2 + p_z^2)$$

$$= \frac{h^2}{8mL^2}(n_x^2 + n_y^2 + n_z^2)$$

n_x, n_y, n_z positive integers

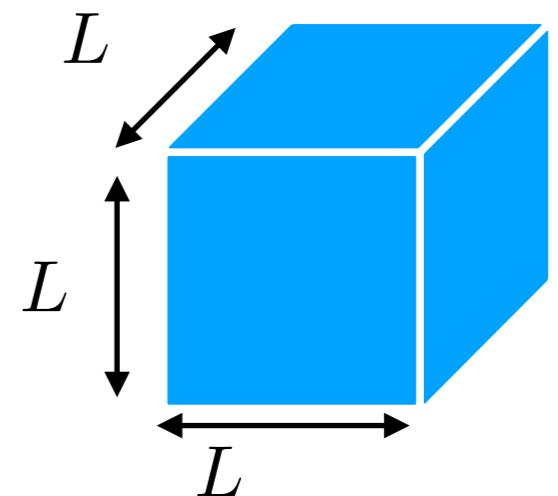


$$\vec{p} = (p_x, p_y, p_z) = \left(\frac{n_x h}{2L}, \frac{n_y h}{2L}, \frac{n_z h}{2L} \right)$$

The ground state?

$$E = \frac{\hbar^2}{8mL^2} (n_x^2 + n_y^2 + n_z^2)$$

What is the lowest energy level?

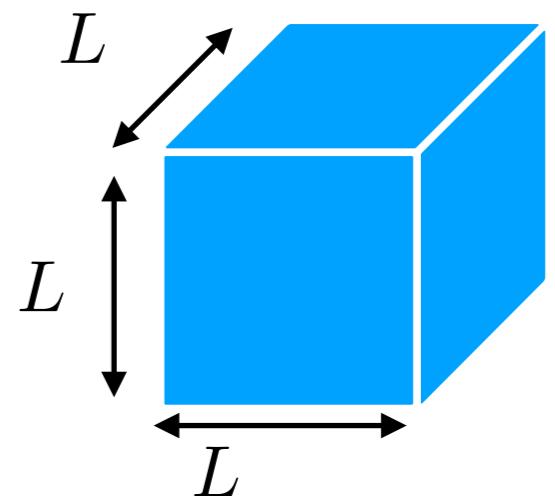


The ground state?

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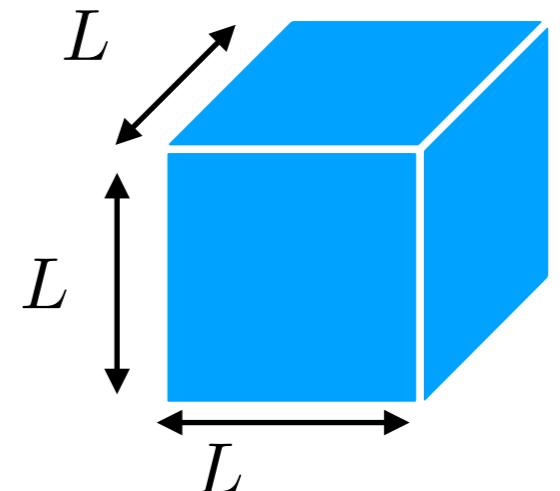
$$n_x = n_y = n_z = 1$$



The ground state?

$$E = \frac{h^2}{8mL^2} (n_x^2 + n_y^2 + n_z^2)$$

What is the lowest energy level?



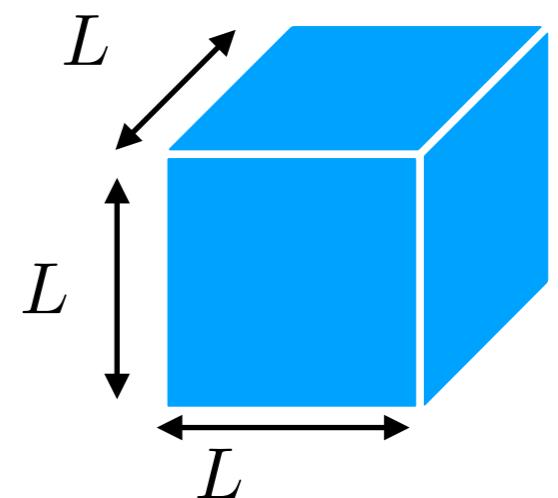
$$n_x = n_y = n_z = 1$$

$$\Rightarrow E = \frac{h^2}{8mL^2} (1^2 + 1^2 + 1^2)$$

$$= \frac{3h^2}{8mL^2}$$

First excited state?

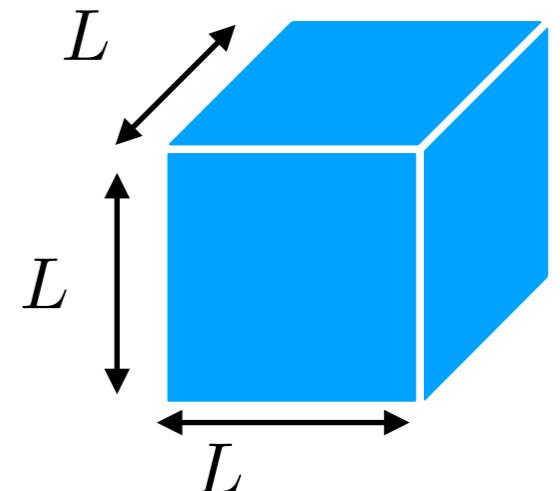
$$E = \frac{h^2}{8mL^2} (n_x^2 + n_y^2 + n_z^2)$$



**What is the first excited level?
(i.e. the one just above the ground state)**

First excited state?

$$E = \frac{h^2}{8mL^2} (n_x^2 + n_y^2 + n_z^2)$$



**What is the first excited level?
(i.e. the one just above the ground state)**

$$(n_x, n_y, n_z) = (2, 1, 1)$$

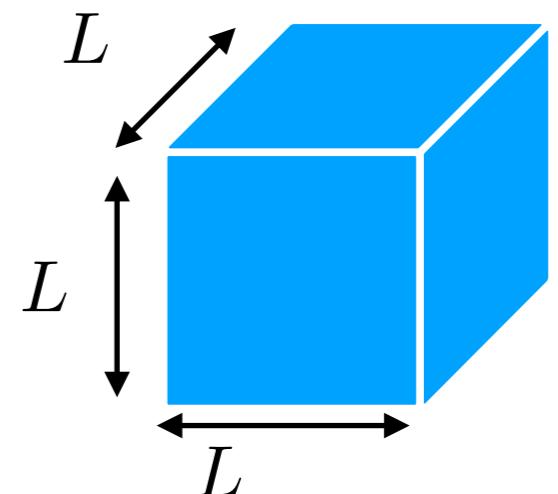
$$\text{or } (n_x, n_y, n_z) = (1, 2, 1)$$

We have three different choices!

$$\text{or } (n_x, n_y, n_z) = (1, 1, 2)$$

First excited state?

$$E = \frac{h^2}{8mL^2} (n_x^2 + n_y^2 + n_z^2)$$



**What is the first excited level?
(i.e. the one just above the ground state)**

$$\Rightarrow E = \frac{h^2}{8mL^2} (2^2 + 1^2 + 1^2)$$

$$= \frac{3h^2}{4mL^2}$$

Degenerate levels

quantum numbers
 (n_x, n_y, n_z)

$(2, 1, 1)$
 $(1, 2, 1)$
 $(1, 1, 2)$

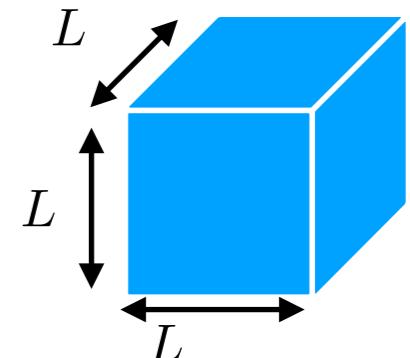
Energy

$$\frac{6h^2}{8mL^2}$$



same energies

$$(1, 1, 1) \rightarrow \frac{3h^2}{8mL^2}$$



$$(n_x, n_y, n_z) = (3, 1, 1)$$

$$\Rightarrow n_x^2 + n_y^2 + n_z^2 = 9 + 1 + 1 = 11 \quad \longleftarrow \quad \textbf{Fourth level}$$

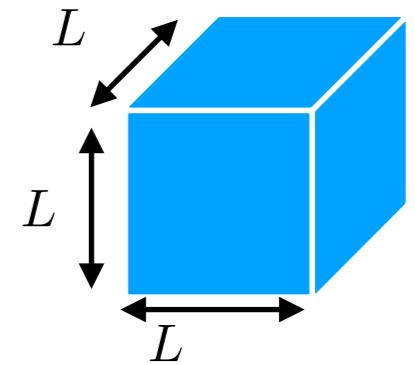
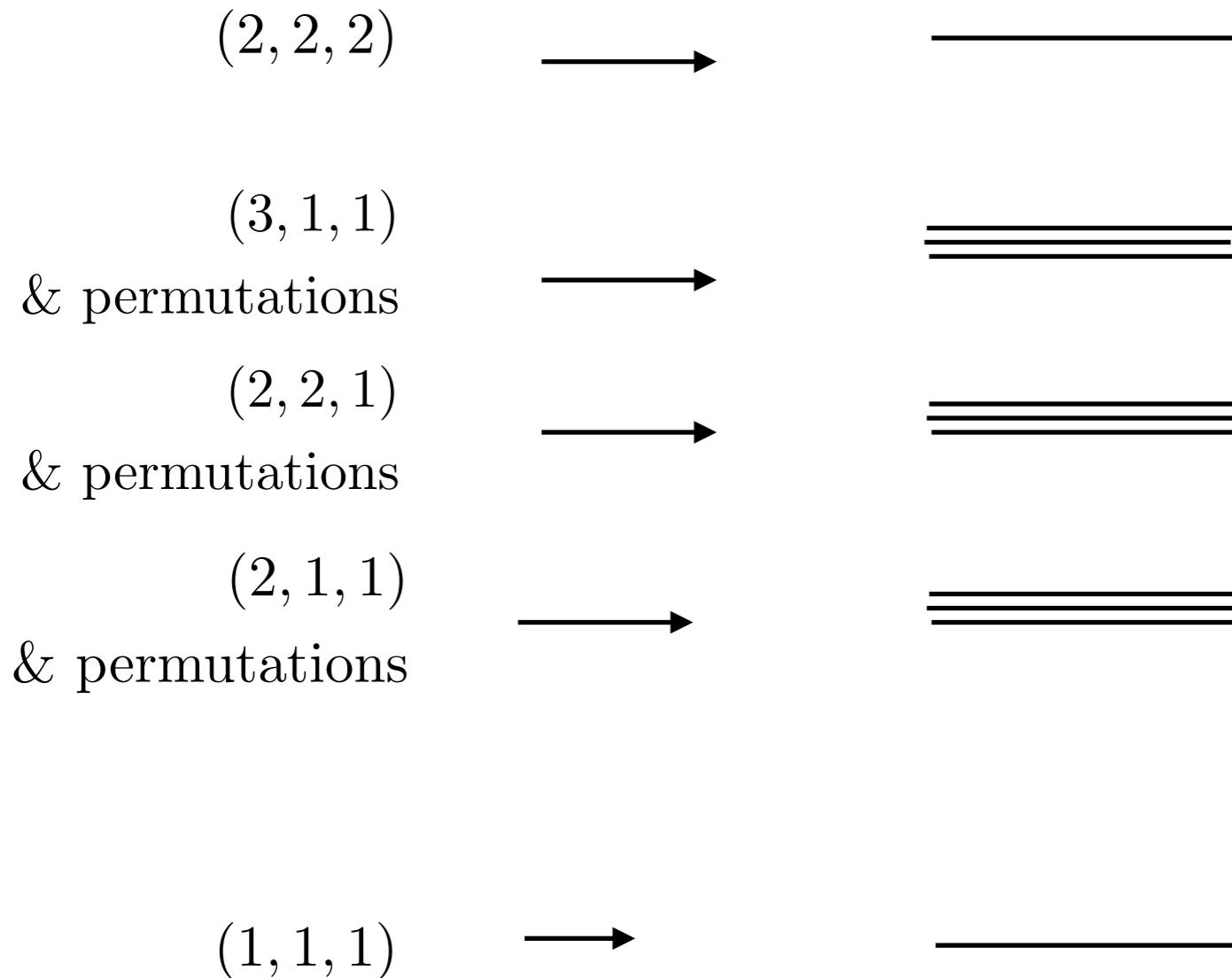
$$(n_x, n_y, n_z) = (2, 2, 1)$$

$$\Rightarrow n_x^2 + n_y^2 + n_z^2 = 4 + 4 + 1 = 9 \quad \longleftarrow \quad \textbf{Third level}$$

$$(n_x, n_y, n_z) = (2, 2, 2)$$

$$\Rightarrow n_x^2 + n_y^2 + n_z^2 = 4 + 4 + 4 = 12 \quad \longleftarrow \quad \textbf{Fifth level}$$

Higher levels?



$$E = \frac{h^2}{8mL^2}(n_x^2 + n_y^2 + n_z^2)$$

Emission spectra?

(2, 2, 2)



(3, 1, 1)

& permutations



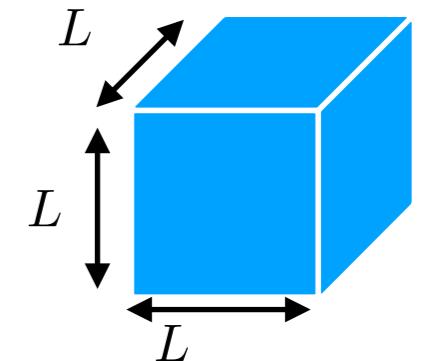
(2, 2, 1)
& permutations



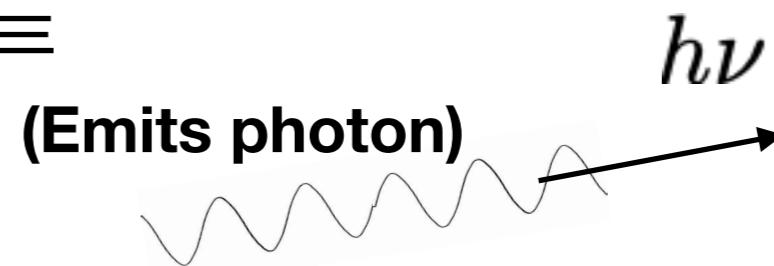
(2, 1, 1)
& permutations



(1, 1, 1)



$$E = \frac{h^2}{8mL^2}(n_x^2 + n_y^2 + n_z^2)$$



Emission spectra?

The particle in the box de-excites from the level with quantum numbers:

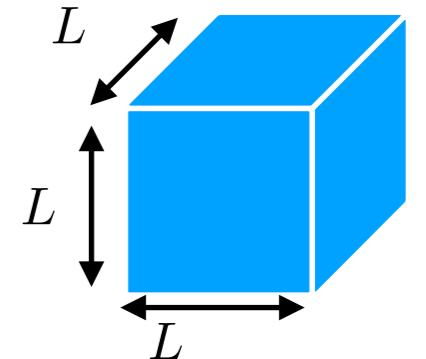
$$(n_x, n_y, n_z)$$

To the level with quantum numbers:

$$(m_x, m_y, m_z)$$

Energy difference:

$$\Delta E = \frac{h^2}{8mL^2}(n_x^2 + n_y^2 + n_z^2) - \frac{h^2}{8mL^2}(m_x^2 + m_y^2 + m_z^2)$$



Emission spectra?

The particle in the box de-excites from the level with quantum numbers:

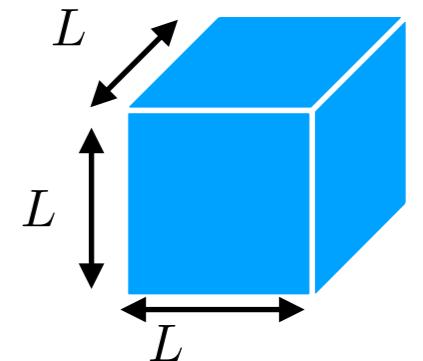
$$(n_x, n_y, n_z)$$

To the level with quantum numbers:

$$(m_x, m_y, m_z)$$

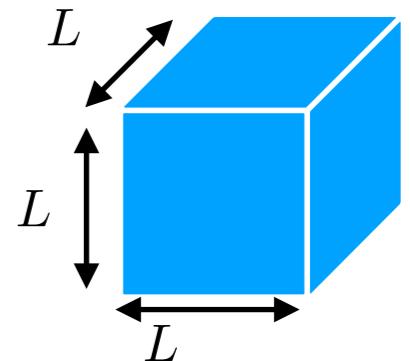
Energy difference:

$$\Rightarrow \Delta E = \frac{h^2}{8mL^2} (n_x^2 - m_x^2 + n_y^2 - m_y^2 + n_z^2 - m_z^2)$$



Emission spectra?

Smallest possible drop in energy?



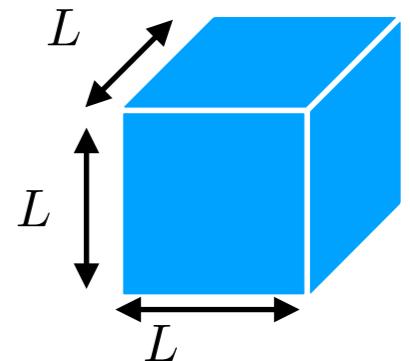
$$\Delta E = \frac{h^2}{8mL^2} (n_x^2 - m_x^2 + n_y^2 - m_y^2 + n_z^2 - m_z^2)$$

$$= \frac{h^2}{8mL^2} (2^2 - 1^2 + n_y^2 - n_y^2 + n_z^2 - n_z^2)$$

$$= \frac{3h^2}{8mL^2}$$

Emission spectra?

Smallest possible drop in energy?



$$\Delta E = \frac{h^2}{8mL^2} (n_x^2 - m_x^2 + n_y^2 - m_y^2 + n_z^2 - m_z^2)$$

$$= \frac{h^2}{8mL^2} (2^2 - 1^2 + n_y^2 - n_y^2 + n_z^2 - n_z^2)$$

$$= \frac{3h^2}{8mL^2}$$

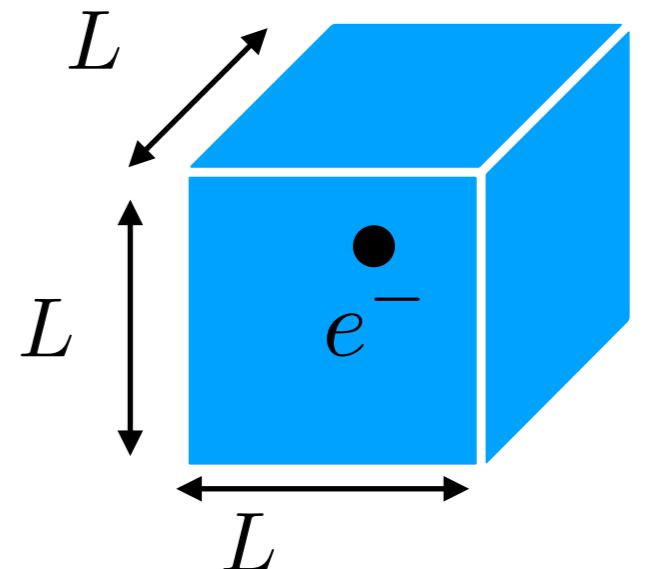
Emitted photon:

$$h\nu = \frac{3h^2}{8mL^2}$$

$$\Rightarrow \nu = \frac{3h}{8mL^2}$$

Electron confined to a region

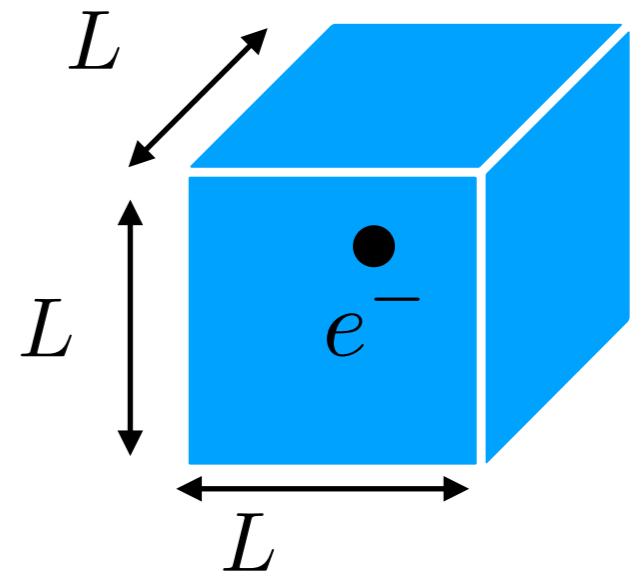
Suppose the particle is an electron. Find the size of box for which the smallest energy drop is in visible range of light.



Electron confined to a region

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$$\nu = \frac{3h}{8m_e L^2}$$

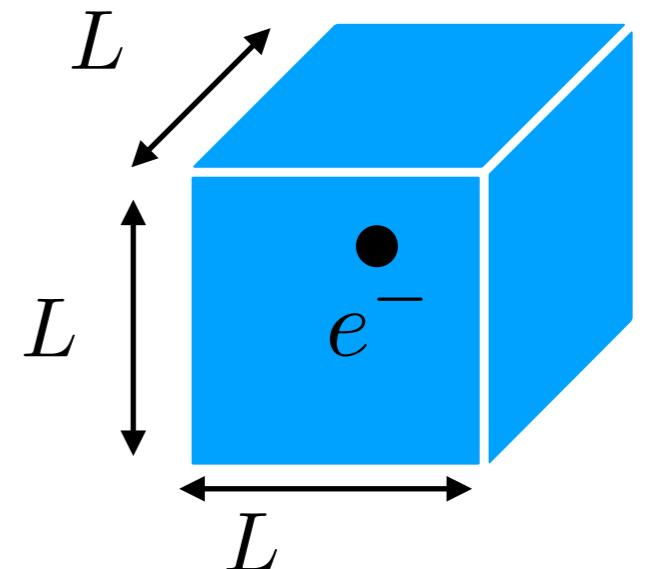


Smallest energylongest wavelength....Red light!

Electron confined to a region

Suppose the particle is an electron. Find the size of box for which the smallest energy drop is in visible range of light.

$$\nu = \frac{3h}{8m_e L^2}$$



Smallest energylongest wavelength....Red light!

$$\lambda_{\text{red}} = 800\text{nm}$$

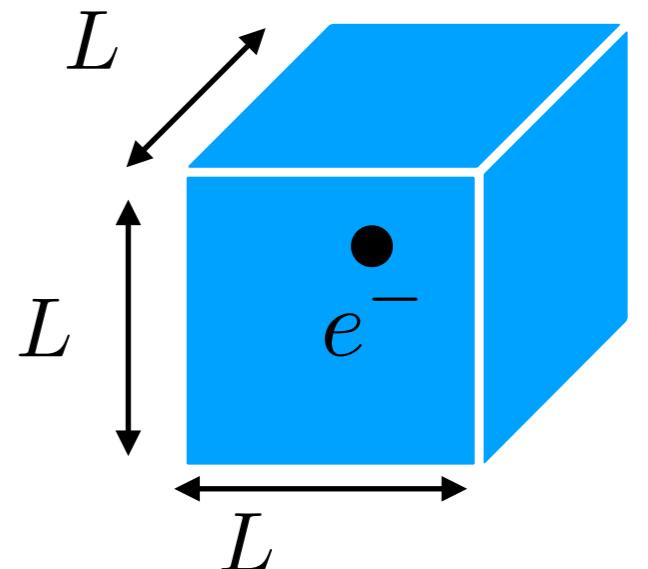
$$\Rightarrow \nu_{\text{red}} = \frac{c}{\lambda_{\text{red}}} = \frac{3 \times 10^8}{800 \times 10^{-9}} = 3.75 \times 10^{14} \text{Hz}$$

Electron confined to a region

Suppose the particle is an electron. Find the size of box for which the smallest energy drop is in visible range of light.

$$\nu = \frac{3h}{8m_e L^2}$$

$$\Rightarrow L^2 = \frac{3h}{8m_e \nu_{\text{red}}}$$



Electron confined to a region

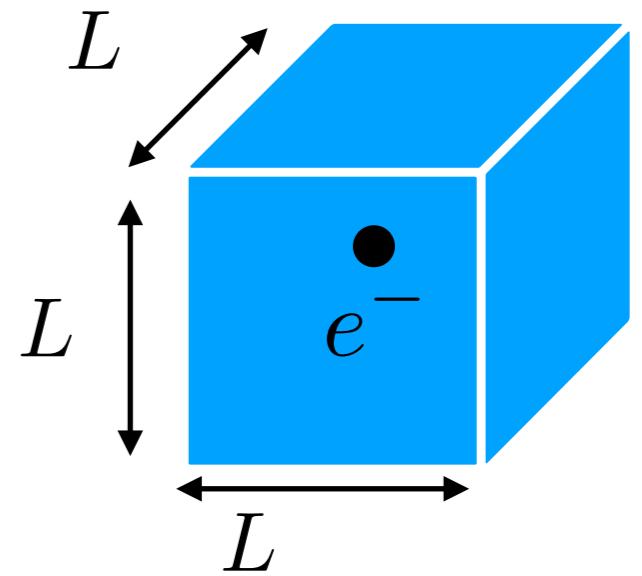
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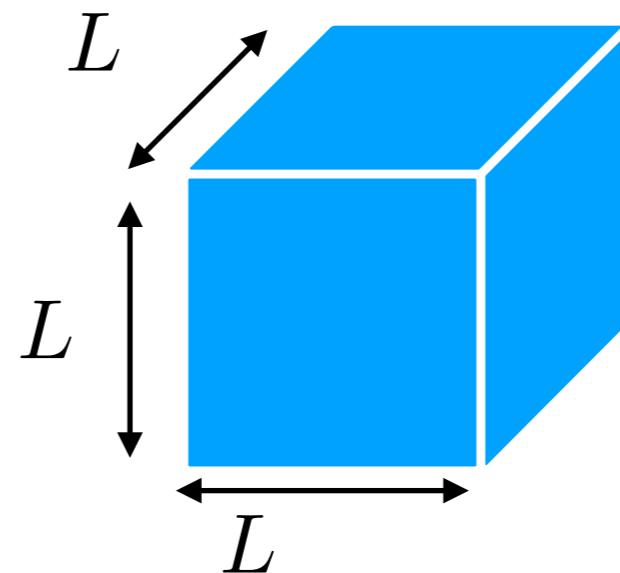
$$\Rightarrow L = \sqrt{\frac{3h}{8m_e \nu_{\text{red}}}} = \sqrt{\frac{3(6.6)(10^{-34})}{8(9.1)(10^{-31})(3.75)(10^{14})}}$$

$$= 8.5 \times 10^{-10} m \quad \text{Scale of an atom again!}$$



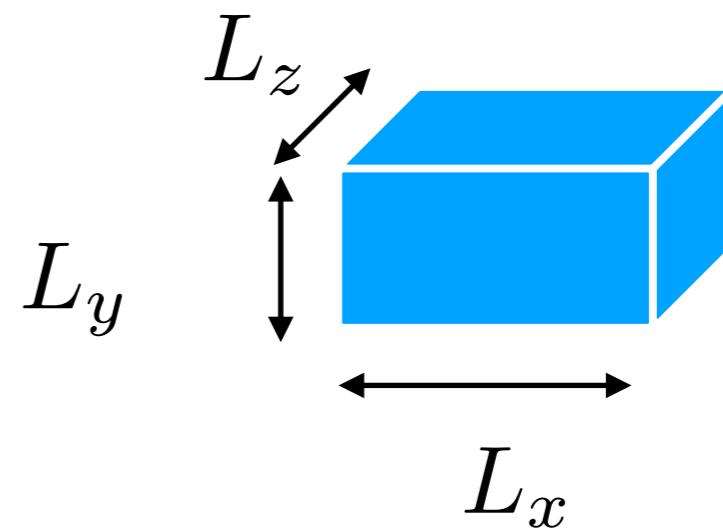
Rectangular boxes

$$E = \frac{h^2}{8mL^2} (n_x^2 + n_y^2 + n_z^2)$$



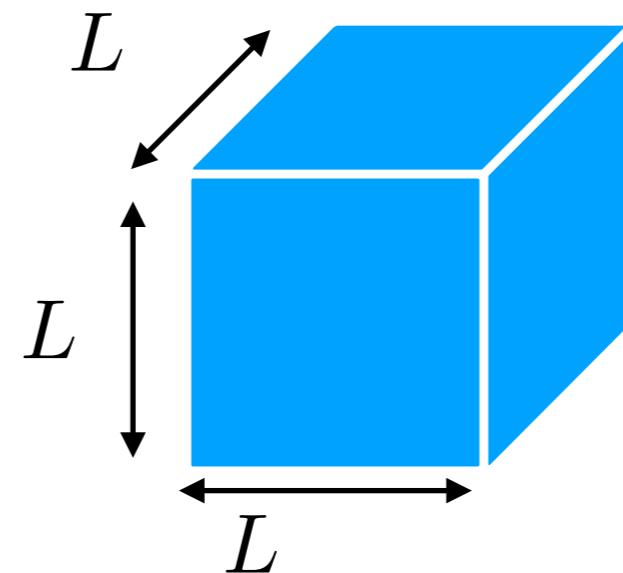
**Conjecture what equation holds for a rectangular box
Of dimensions**

$$L_x \times L_y \times L_z$$



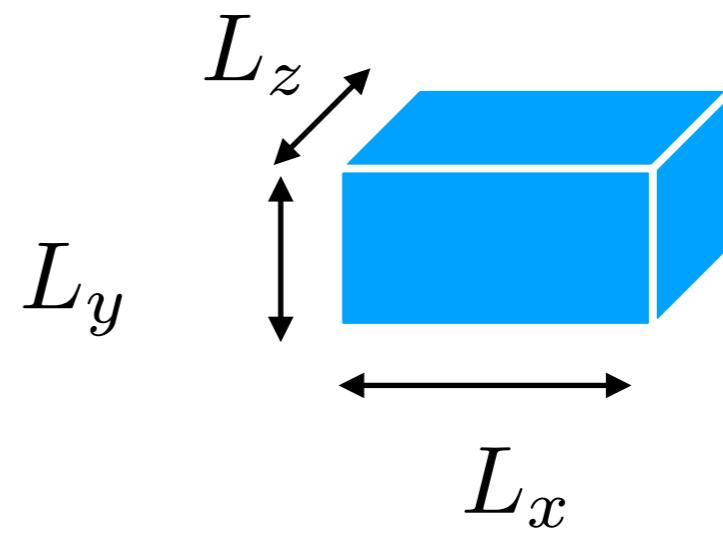
Rectangular boxes

$$E = \frac{h^2}{8mL^2} (n_x^2 + n_y^2 + n_z^2)$$



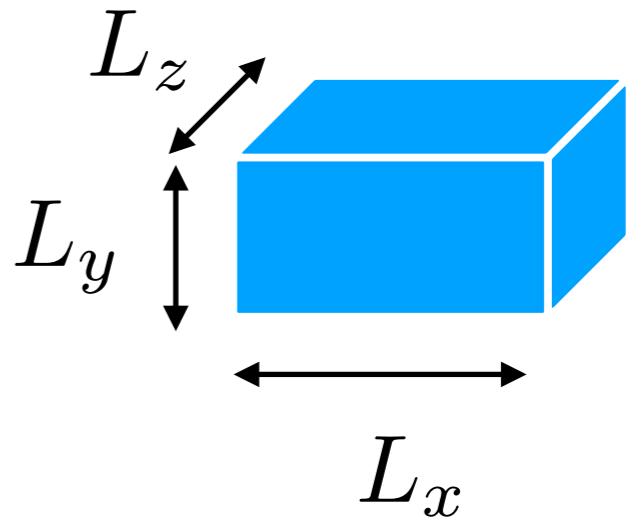
**Conjecture what equation holds for a rectangular box
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$$E = \frac{h^2}{8m} \left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2} \right)$$

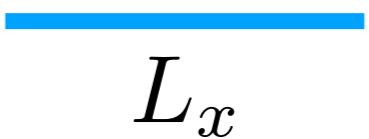
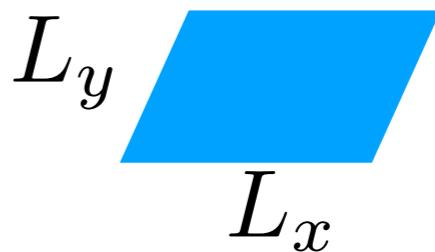


1-d, 2-d boxes

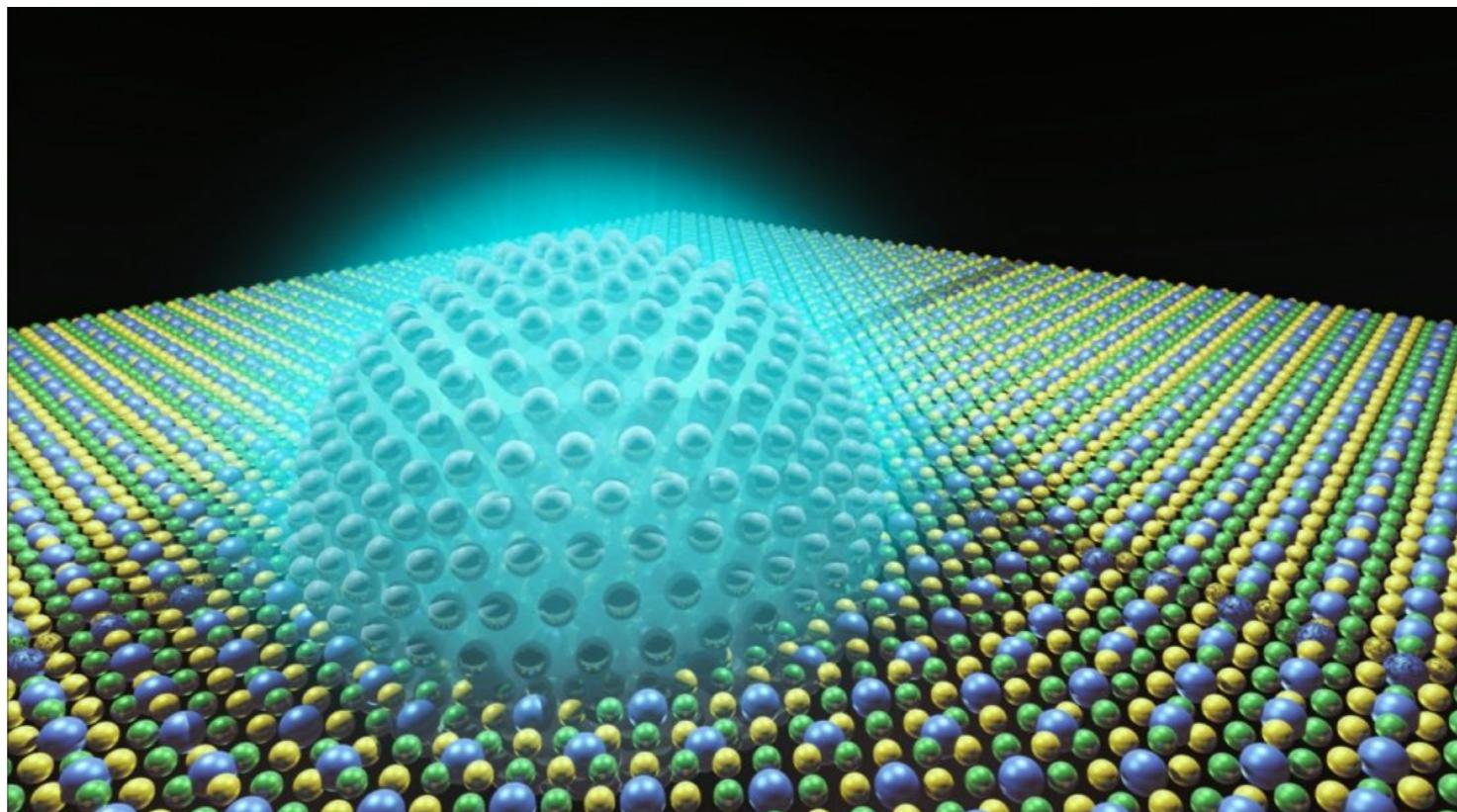
$$E = \frac{h^2}{8m} \left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2} \right)$$



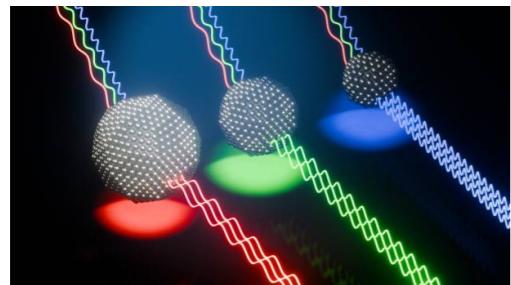
What if we only confine it in 1 direction? Or 2 directions?



Quantum dots



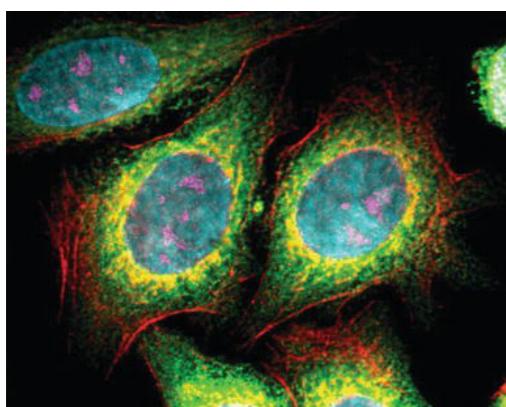
Quantum dots



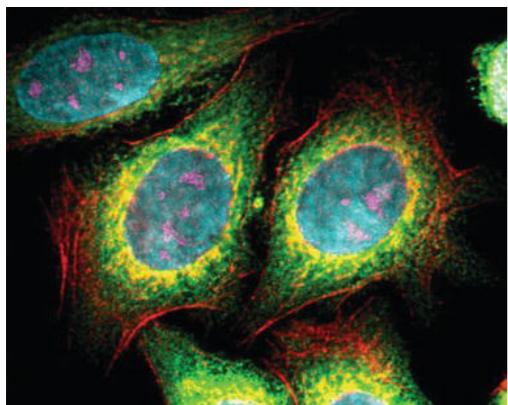
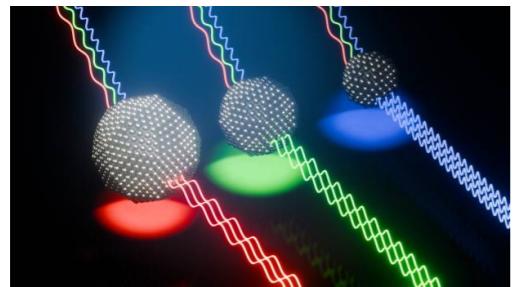
- “Artificial atoms”.
- Key structures in Nano-technologies.
- Used to build solar cells, LED displays, biomedical imaging technologies (fluorescent markers).



- Electrons confined in semi-conducting chunk.
- Tunable optical properties.
- Change size....change properties.

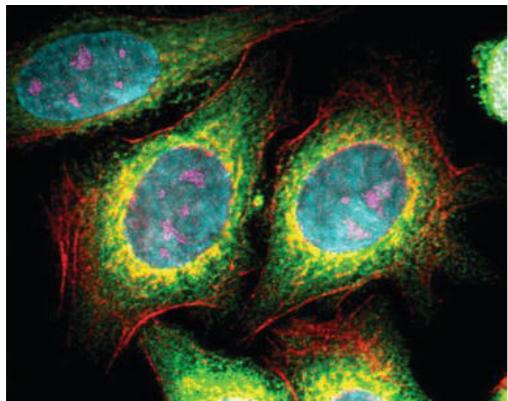
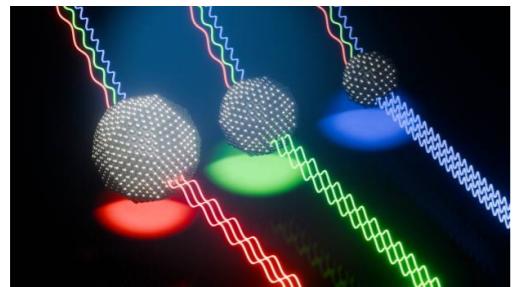


Quantum dots



Example: A quantum dot that de-excites from the first excited state to the ground state emits a photon of wavelength 275nm.
If we wanted to double this wavelength how should we change the size of the quantum dot?

Quantum dots

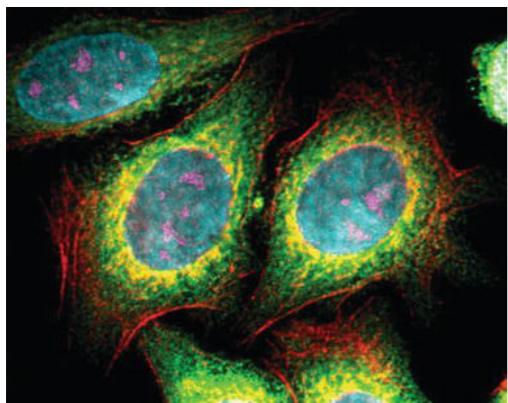
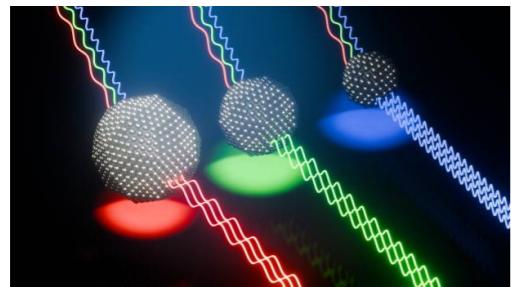


Example: A quantum dot that de-excites from the first excited state to the ground state emits a photon of wavelength 275nm.
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$$E = \frac{h^2}{8mL^2} (n_x^2 + n_y^2 + n_z^2)$$

$$\Delta E = \frac{3h^2}{8mL^2} = h\nu = \frac{hc}{\lambda}$$

Quantum dots

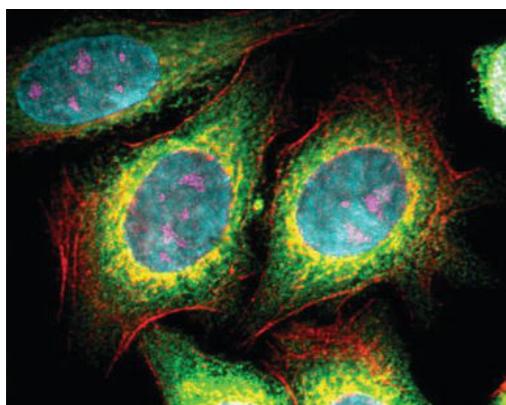
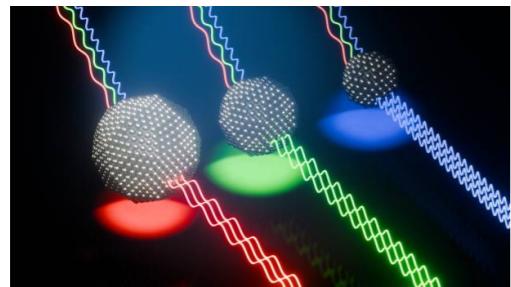


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$$\Delta E = \frac{3h^2}{8mL^2} = h\nu = \frac{hc}{\lambda}$$
$$\Rightarrow \lambda = (\text{constant})L^2$$

Quantum dots



Example: A quantum dot that de-excites from the first excited state to the ground state emits a photon of wavelength 275nm.

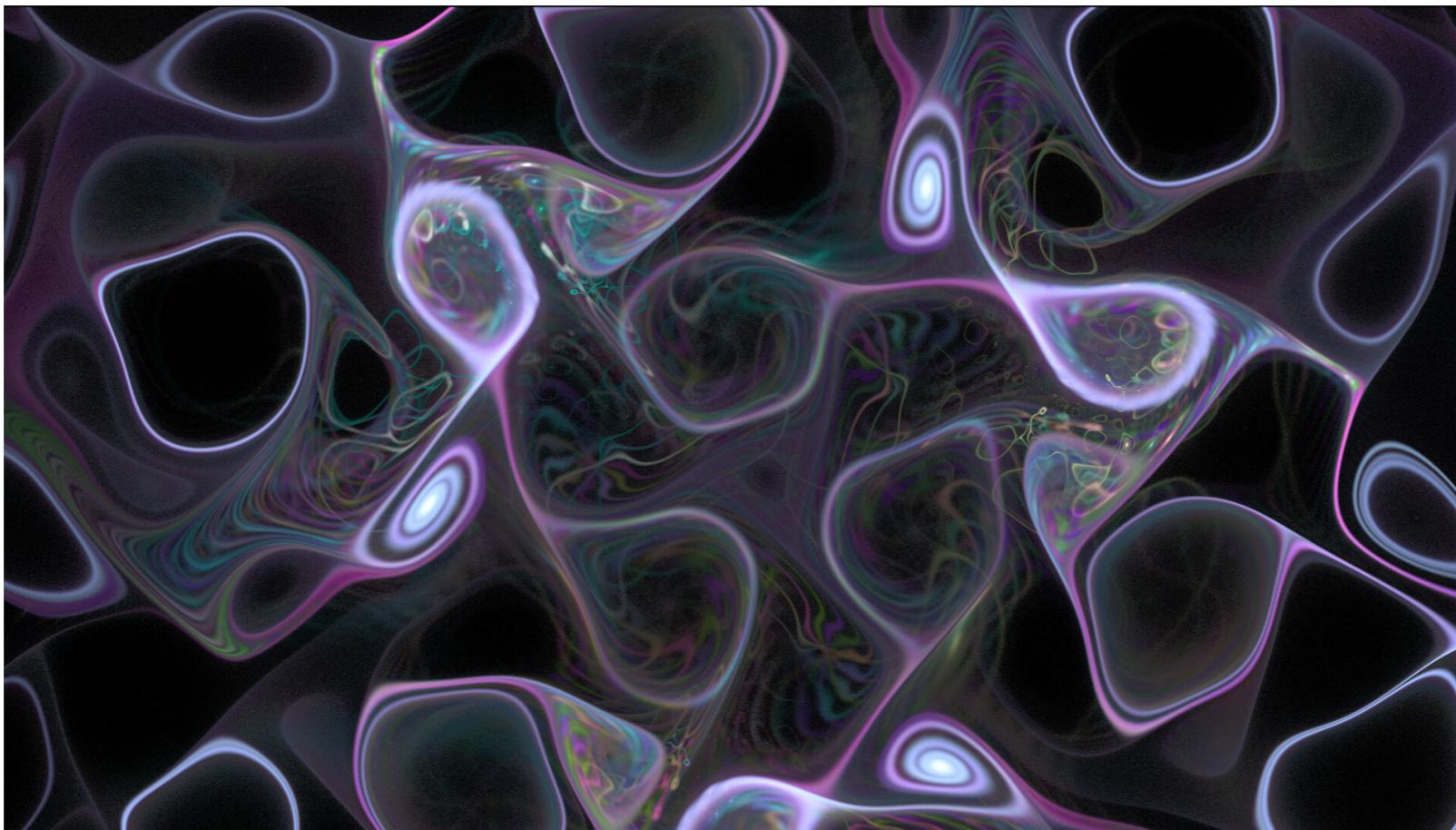
If we wanted to double this wavelength how should we change the size of the quantum dot?

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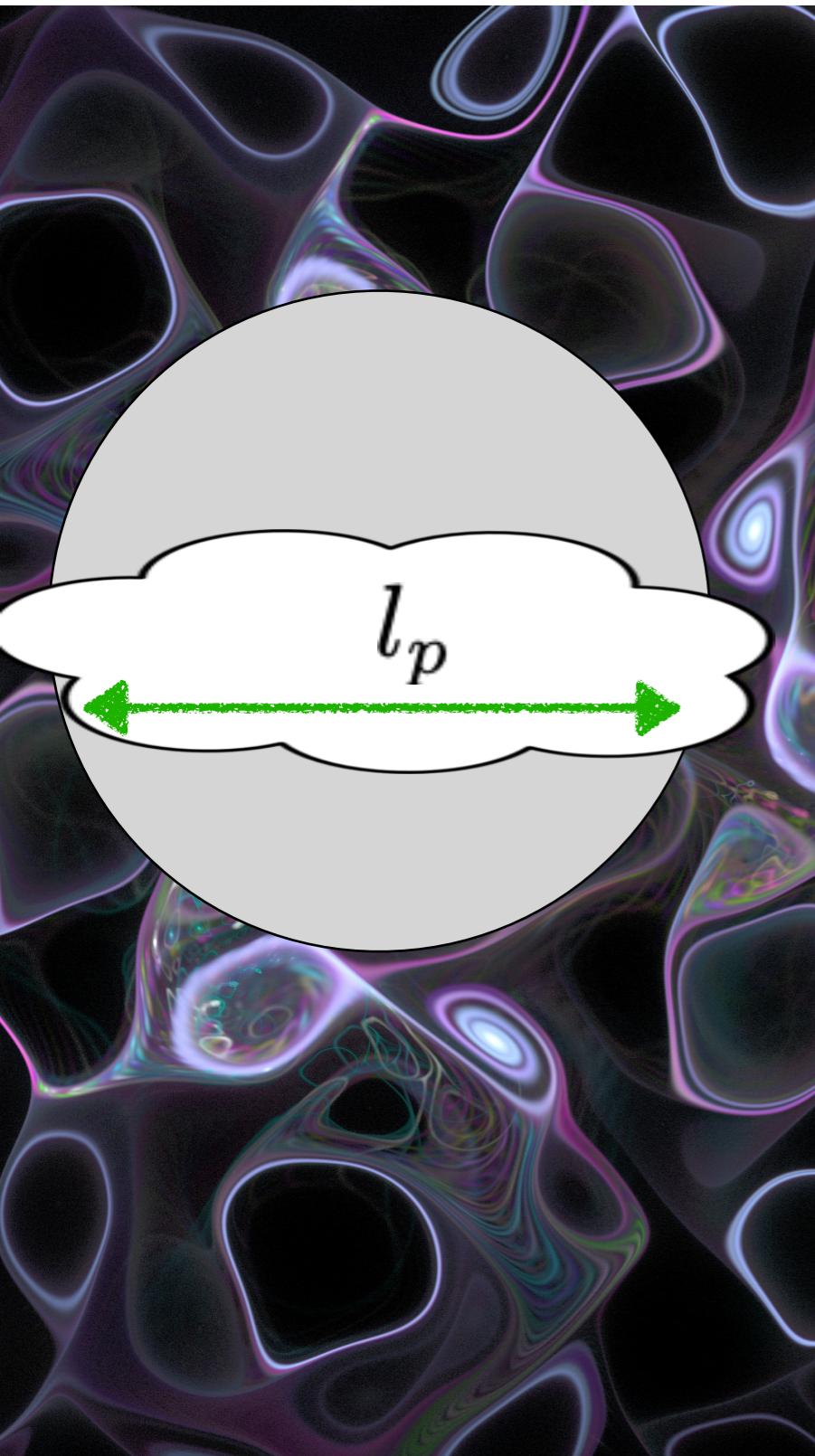
increase L by factor $\sqrt{2}$ to double λ

Exercise: Show that the quantum dot has $L \sim 5\text{nm}$.

Planck Scale Black Holes



Planck-scale black hole.



A Planck mass is confined inside of box of side equal to the Planck length.

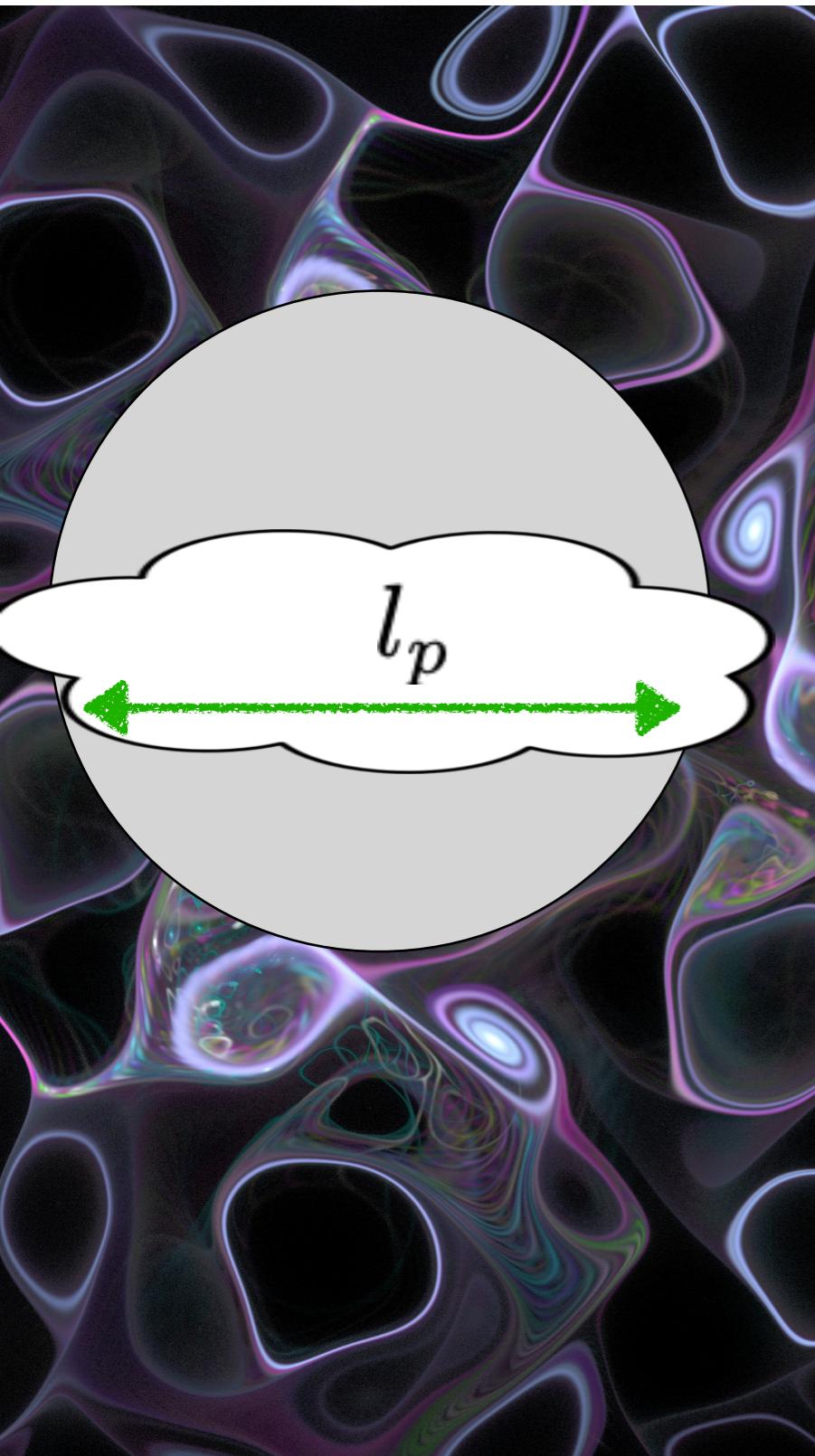
Estimate its ground state energy.

$$l_p = \sqrt{\frac{hG}{c^3}}$$

$$l_p = 1.6 \times 10^{-35} m$$

$$M_p = \sqrt{\frac{hc}{G}} = 2.176 \times 10^{-8} kg$$

Planck-scale black hole.



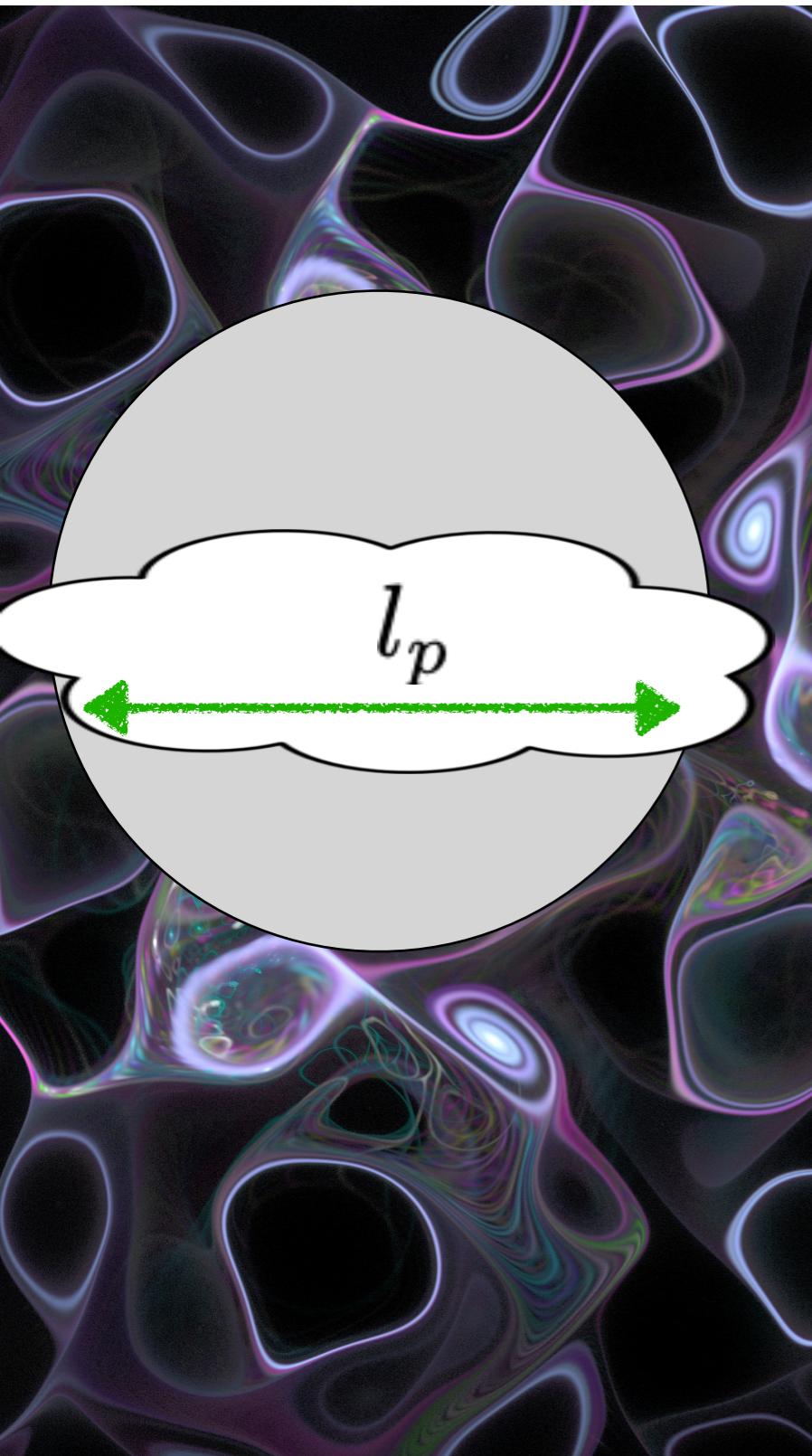
A Planck mass is confined inside of box of side equal to the Planck length.

Estimate its ground state energy.

$$E_{\text{ground}} = \frac{3h^2}{8M_p l_p^2}$$

$$\Rightarrow E_{\text{ground}} = \frac{3h^2}{8 \left(\sqrt{\frac{hc}{G}} \right) \frac{hG}{c^3}}$$

Planck-scale black hole.



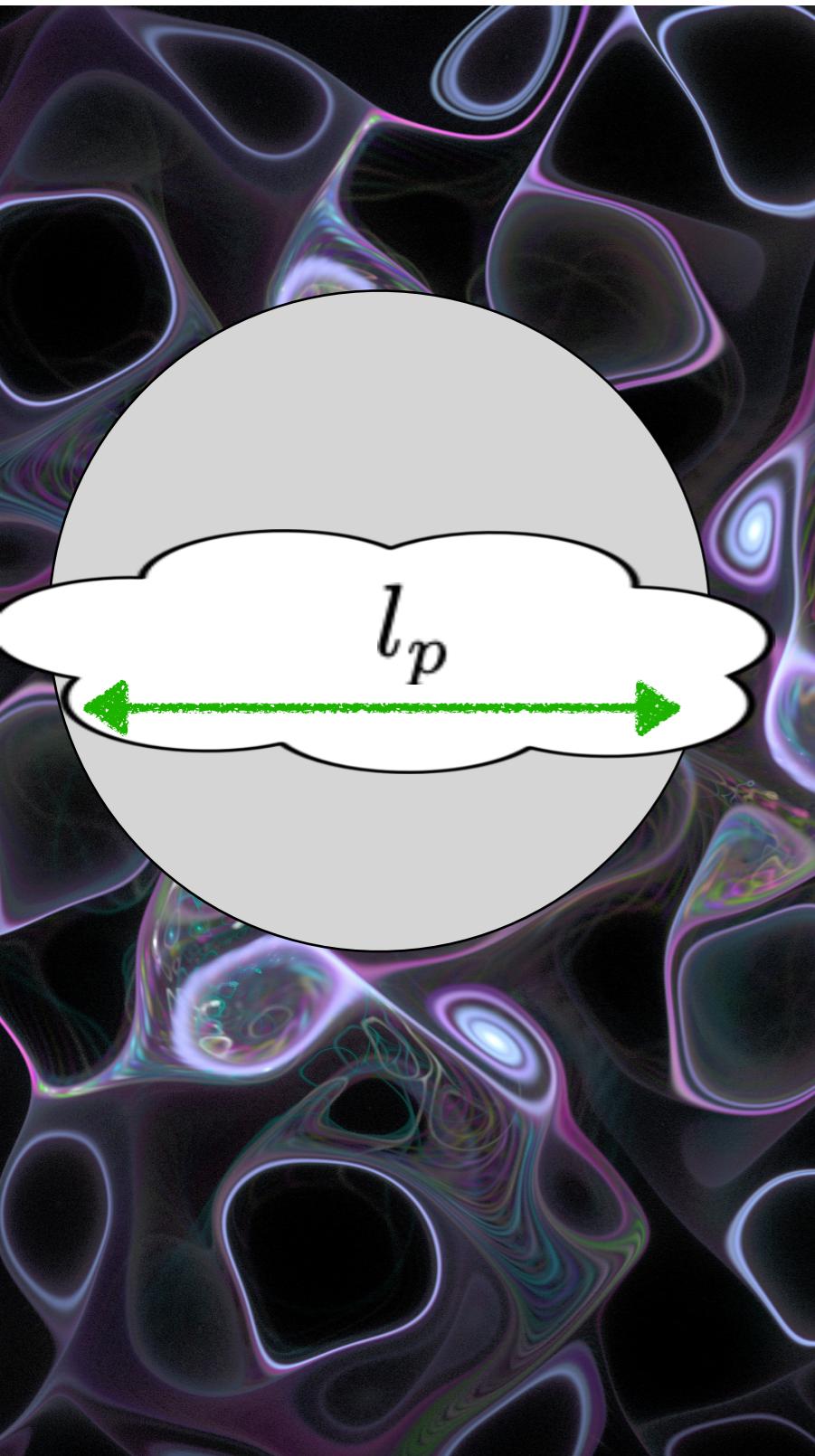
A Planck mass is confined inside of box of side equal to the Planck length.

Estimate its ground state energy.

$$E_{\text{ground}} = \frac{3\hbar^2}{8M_p l_p^2}$$

$$\Rightarrow E_{\text{ground}} = \frac{3hc^3}{8(\sqrt{hc})\sqrt{G}}$$

Planck-scale black hole.



A Planck mass is confined inside of box of side equal to the Planck length.

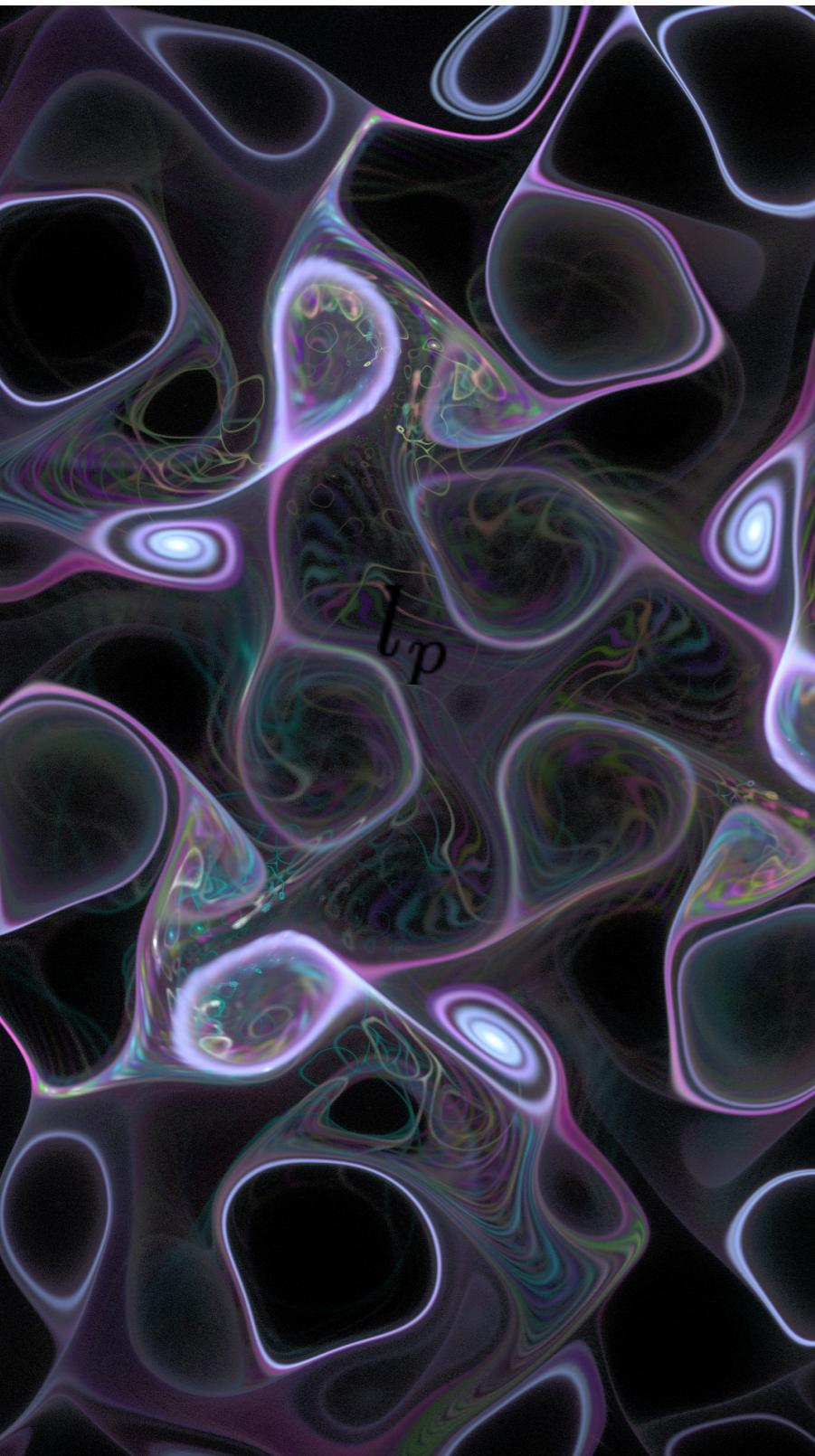
Estimate its ground state energy.

$$E_{\text{ground}} = \frac{3\hbar^2}{8M_p l_p^2}$$

$$\Rightarrow E_{\text{ground}} = \frac{3\sqrt{\hbar}c^{5/2}}{8\sqrt{G}}$$

$$= 1.83 \times 10^9 \text{ Joules}$$

Planck-scale black hole.



$$E_{\text{ground}} = \frac{3\sqrt{hc^{5/2}}}{8\sqrt{G}} \approx M_p c^2$$

- Kinetic energies are at this scale.
- Energy can be converted into mass.
- Mass would be confined to within Schwarzschild radius.
- Energy could “create” more Planck-scale black holes?

Back-of-envelope analysis is **very** simplistic. Much more advanced theory needed!